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STATISTICAL HANDBOOK FOR ASSESSING PIG CLASSIFICATION METHODS:

Recommendations from the "EUPIGCLASS" project group

by

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FOREWORD

This publication is one of the outcomes of the Growth Project GRD1-1999-10914 "EUPIGCLASS". This project aimed for standardisation of pig carcass classification in the EU through improved statistical procedures and new technological developments. It was co-ordinated by the Danish Meat Research Institute.

The project was divided into three workpackages. The objective of the workpackage II was to solve the main statistical problems encountered in the application of the EC regulations for pig classification, to anticipate future problems and to form a basis to update the regulations. This statistical handbook was therefore written to provide useful and detailed documentation to people responsible for the national assessment of pig classification methods, both in the present and future EU countries.

At the moment, this outcome of the EUPIGCLASS project has to be considered as a working document that could be used in discussions about changes in the EU regulations for pig classification. Depending these changes (probably decided upon in 2005), an update could be necessary before officially replacing the present version of the "Statistical Handbook for assessing pig classification methods" that was distributed at a EU Pigmeat Management Committee meeting in 2000.

This new version of the handbook offers a considerable improvement over the 2000 version. The main proposal for an adaptation of the EC/2967/85 regulation is to replace the present error criterion "RMSE" by the "RMSEP", that estimates the error of prediction and can be evaluated when Partial Least Squares (PLS) is used. The text is enhanced with many details and examples that will be of use to research workers and/or statisticians involved in pig classification.

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Introduction

By Gérard Daumas

The main objective of this document is to help people dealing with pig classification methods. The past and future extensions of the European Union make harmonisation even more necessary. Previous research concerning the harmonisation of methods for classification of pig carcasses in the Community has achieved to:

- the adoption of a simplified dissection method and therefore a new definition of the lean meat percentage;
- the introduction of a sophisticated statistical method, called double regression, as the "new standard";
- amendments of regulations.

The present regulations are not easily understandable. It is therefore necessary for the new scientists dealing with this matter to obtain some interpretations.

In the past member states have chosen different ways for sampling and for parameters estimation. Anyway, two issues have appeared: the reduction of experimental costs and the management of large sets of highly correlated variables. These difficulties have been solved by more complicated statistical methods but all deriving from classical linear regression which was the initial method in the EC regulation.

To cut the cost of one experimental trial, "double regression" has been first introduced in pig classification by Engel& Walstra (1991). To reduce the costs of testing different instruments Daumas & Dhorne (1997) have introduced "regression with surrogate predictors". These methods fulfill the present EU requirements and estimation of accuracy is available.

In parallel the Danes have first introduced PCR (Principal Component Regression) to test the Danish robot Classification Centre (10-20 variables) and then PLS (Partial Least Squares) to test the Danish robot Autofom (more than 100 variables). These methods are not explicitly authorized by the regulations as the compulsory accuracy criteria is not available. It is therefore impossible to check wether the EU requirements are fulfilled or not.

A short discussion in the Pigmeat Management Committee about the trials reports generally do not permit to judge such unusual and complicated methods applied in the scope of classification methods. It seems therefore useful to describe in detail the new statistical methods used and to show how to check the constraints of the regulations.

The first official version (draft 3.1) of this handbook has been distributed on February 2000 to the member states delegates at a meeting of the Pigmeat Management Committee. Contributions came from statisticians or meat scientists who are national expert for pig classification.

The European research project (EUPIGCLASS) about standardisation of pig classification methods, which involves all the contributors of the first version of the handbook, gives the means for a considerable improvement of the former version. Orienting more towards users, achieving a large consensus, increasing harmonisation between sections, going further into details and illustrating with examples are the main ideas followed for writing up this new version. Nevertheless, a central issue was how to estimate accuracy in PLS and how to harmonise the calculation of this criteria in all the statistical methods.

At the same time, this project was an opportunity to make progress on old problems, sometimes discussed but never resolved, like for instance "representative sample" and "outliers".

This new version of the handbook is an outcome of EUPIGCLASS. It contains in particular some recommendations for changing the EU regulations. As the status of the handbook is a kind of complement to the EU regulations it means that an update will probably be necessary after having taken decisions in Brussels concerning the amendments to the regulations. In the case the discussions late a long time a first update based on the present EU regulations might be useful during the transitional period.

Then, at medium term other updates will depend on the progress in research and technologies.

Basis for classification

A brief history

Pig classification is based on an objective estimation of the lean meat content of the carcass. As this criteria is destructive and very expensive to obtain, it has to be predicted on slaughterline. The EC regulations contain some requirements on how to predict the reference. In order to ensure that the assessment results are comparable, presentation (carcass dressing), weight and lean meat content of the carcass need to be accurately defined. These criteria were defined by the following two regulations :

- Council Regulation (EEC) Nr 3320/84 of 13 November 1984 determining

the Community scale for classification of pig carcasses;

- Commission Regulation (EEC) Nr 2967/85 of 24 October 1985 laying down detailed rules for the application of the Community scale for classification of pig carcasses.

These criteria have evolved leading to amendments of the regulations. Firstly, lean meat content was derived from dissection of all striated muscle tissue from the carcass as far as possible by knife. The carcass was defined by the body of a slaughtered pig, bled and eviscerated, whole or divided down the mid-line, without tongue, bristles, hooves and genital organs. As some other parts were removed on the slaughterlines of some Member States, the carcass was later defined (Commission Regulation 3513/93 of 14 December 1993) also without flare fat, kidneys and diaphragm.

However, full dissection, developed by the Institut für Fleischerzeugung und Vermarktung (in Kulmbach, Germany) and called "the Kulmbach reference method", is laborious and very time consuming (10 to 12 hours per half carcass and person). In practice, several Member States used a national dissection method instead of the Kulmbach reference method, which was a source of biases.

In order to assess the extent of biases and to look for a more simplified dissection method an EC wide trial was conducted in 1990/1991. The results of this trial were reported by Cook and Yates (1992). In this trial, a simplified dissection method based on the dissection of four main parts (ham, loin, shoulder and belly) was tested. Following discussions slight adaptations of the tested method were introduced. After large discussions about how to calculate the new lean meat content from the data of the new EU dissection method, a compromise was found on the definition of this new criterion. The new lean meat content and dissection method are briefly described by Commission Regulation (EEC) Nr 3127/94 of 20 December 1994 (amending 2967/85) and described in detail by Walstra and Merkus (1996). Though these new rules were immediately enforced, 4 years later, in 1998, only 5 Member States had implemented them in their slaughterhouses (Daumas and Dhorne, 1998). This very long transitional period, still not ended in 2003, results in new distorsions between Member States.

One reason for delaying the application of regulations could be the high cost of a dissection trial. Though dissection time was halved, the new EU dissection method is still time consuming (4-5 hours per half carcass and person).

Sources of errors

The present way of calculating the lean meat percentage is well documented (Walstra & Merkus, 1996). The formula involves both joints and tissues weights. The sources of errors come from the carcass dressing, the cutting, the dissection and the weighting:

- *Definition of the carcass*

  Because of the high cost of dissection it was decided to dissect only one side (the left side). But in practice both sides are never identical, especially for splitting difficulties. A specific difficulty concerns the head, which is not split on the slaughterlines in some countries. In this case the head should be split to remove the brain. But this split generally provokes a larger error than dividing by 2 the head weight and then subtracting an inclusive amount for a half brain (for instance 50 g).

  The carcass weight used as the denominator of the lean meat percentage is defined as the sum of all the joints regardless if they have to be dissected. This sum includes 12 joints.

- *Jointing procedure*

  Jointing of the carcass originates from the German DLG-method (Scheper and Scholz, 1985). Extraction of the 4 main joints (ham, loin, shoulder and belly) is a potential source of distorsions because of the lack of very precise anatomical markers. Separation of all 4 joints is more or less problematic, but removing the shoulder is the main difficulty.

- *Dissection procedure*

  Only the 4 main joints are dissected. The dissection involves a complete tissue separation of each joint into muscle, bone and fat. Fat is divided into subcutaneous fat (including skin) and intermuscular fat. Remnants, such as glands, blood vessels and connective tissue loosely adhering to fat, are considered as intermuscular fat. Tendons and fasciae are not separated from the muscles.

  Some small difficulties concern:

  → designation of blood-soaked tissue to muscle or fat,

  → differentiation for some small parts between intermuscular fat and connective tissue (therefore weighed as muscle),

  → delimitation in some areas between subcutaneous fat and intermuscular fat (but without consequence for lean meat percentage).

- *Weighting*

  The present definition of muscle weight includes dissection and evaporation losses. These losses are highly dependent on chilling conditions, temperature, speed and quality of dissection. Moreover in some cases carcasses are not dissected the day following slaughtering.

> At present, the specification only concerns the weighing accuracy. All weights should be recorded at least to the nearest 10 g or to the nearest 5 or 1 g, if possible.

The errors on the reference have been studied in WP1. Splitting and operator effect on jointing seem to be the most important.

Evolutions in the definition of the lean meat content

The lean meat percentage, hereafter denoted LMP, has always been defined as a ratio between a muscle weight (MUS) and a joints weight (JOINTS), expressed in %: Y = 100 x C x MUS / JOINTS

When the full Kulmbach dissection was used all the joints were dissected. So, both MUS and JOINTS concerned the whole left side (C = 1).

When a simplified dissection was introduced, MUS refers to the 4 dissected joints while JOINTS still refers to the whole left. The nature of the ratio has therefore changed because numerator and denominator do not refer to the same piece of meat. Simultaneously, a scaling factor ("cosmetic") was introduced in order to maintain the same mean in the EU (C = 1.3). This is the present definition in 2003.

EUPIGCLASS group recommends now to change the definition towards the % of muscle in the 4 main joints which means that numerator and denominator again will refer to the same piece of meat, but sticking with a simplified dissection. Then, a new scaling factor will be a point of discussion. A new value could be around: C = 0.9 .

These changes on the response variable have an influence on the levels of the residual variance and the prediction error.

Classification instruments

Equipments and variables

When Denmark, Ireland and the United Kingdom joined the Community in 1973, they argued that the measurements which they used - fat and muscle depths taken by probe over the m. longissimus - were better predictors of leanness than the criteria used in the common pig classification scheme of the original six member states - carcass weight, backfat measurements on the splitline and a visual assessment of conformation. Even so, these three countries themselves used different instruments and probing positions.

Later on, the principles of the new EC scheme are agreed. To be accepted a method must use objective measurements and must be shown to be accurate. There is also some consistency in the methods used. Some member states use fat and muscle depths measured at similar points because trials have suggested

that these tend to be good predictors. Several member states also use the same instruments with which to measure the fat and muscle depths, simply because the same instruments are widely available throughout the EU and have been shown to be sufficiently accurate.

In the 80's there was a desire to promote harmonisation of classification methods within the Community, although each Member State had its own authorized methods. This could be achieved by all Member States using similar instruments, measuring at the same sites or using the same equations. Unfortunately the pig populations of Member States differ in their genetic history and there is concern that they may differ in their leanness at the same subcutaneous fat and muscle depths. As expected, the results from the 1990 EC trial suggest there would be a noticeable loss in accuracy if a common prediction equation were imposed upon Member States (Cook & Yates, 1992).

The problem with standardisation of equipment is that it could provide one manufacturer with a monopoly from which it would be difficult to change, and might limit the incentive for developing more accurate or cheaper equipment. At present different Member States use a wide variety of equipment, ranging in price and sophistication, from simple optical probes which are hand operated and based on the periscope principle, to the Danish Autofom, a robotic system capable of automatically measure more than 2000 fat and muscle depths. Most of the equipments can be seen on the website : www.eupigclass.org

The most common probes are based on an optical principle. Although hand operated, fat and muscle depths are automatically recorded. A light source near the top of the probe emits light and a receptor measures the reflection level, which is different for fat and muscle tissues.

Some equipments use ultra-sounds also for measuring fat and muscle depths.

Video-image analysis techniques are still under development. Other measurements are used such as areas of fat and muscle tissues.

In the future one can envisage the use of whole body scanners for example.

Documentation of measuring equipment

The need to consider precision arises from the fact that tests performed on presumably identical materials under presumably identical circumstances do not, in general, yield identical results. This is attributed to unavoidable random errors.

Various factors may contribute to the variability of results from a measurement method, including:

- the operator
- the equipment used
- the calibration of the equipment

- the environment (temperature, humidity, etc.)
- the slaughter process
- the time elapsed between measurements

The use of statistical methods for measuring method validation is described in ISO 5725. The use of the standard is well established in analytical chemistry for instance (Feinberg, 1995). In the meat sector, DMRI have started to use the principles in the documentation of any measuring equipment (Olsen, 1997).

ISO 5725 In addition to a manual, the documentation must include a description of the measuring properties. These are laid down on the basis of experiments which include all facets of the application of the instruments and should include the following aspects:

Accuracy

The accuracy of the method includes trueness and precision. Trueness refers to the agreement between the measuring result and an accepted reference value, and is normally expressed as the bias. The precision refers to the agreement between the measuring results divided into repeatability and reproducibility (see the examples below). The two measures express the lowest and the highest variation of the results and are indicated by the dispersions s_r and s_R. Finally the reliability of the method is relevantly defined as the ratio $s_D^2/(s_D^2 + s_R^2)$ where s_D indicates the natural variation of the characteristic. As a rule-of-thumb the reliability should be at least 80 % .

Robustness

It is essential for the determination of accuracy that the sources of measuring variations are known, and thereby a measure of the robustness of the method towards external factors. The influence of external factors (temperature, light etc.) should be limited by determination of a tolerance field for these factors.

Reference

If the reference of the measuring method is another measuring method it should be described by its precision. As far as possible certified reference materials or measurements from accredited laboratories should be applied as absolute references.

Experiences from Danish tests

Repeatability of an automatic equipment

Repeatability is defined as the closeness of agreement between the results of measurements on identical test material, where the measurements are carried out using the same equipment within short intervals of time.

The repeatability of Autofom has been tested by measuring some carcasses twice. When testing the repeatability of Autofom no formula for calculation of lean meat percentage on the basis of fat and muscle depth had been developed. Therefore, the "C measure", which is the smallest fat depth at the loin in the area of the last rib, was used as an expression of the Autofom measurements. The repeatability standard deviation was estimated at approximately 1 mm, as expected.

Reproducibility of a manual equipment

Normally, reproducibility is defined as the closeness of agreement between the results of measurements on an identical test material, where the measurements are carried out under changing conditions.

Apart from random errors, the operators usually contribute the main part of the variability between measurements obtained under reproducibility conditions. When investigating the UNIFOM equipment the total error variance was estimated at $s^2 \approx 2.4$ units and the contribution from the operators was $s^2_{\text{operator}} \approx 0.2 units$. As a consequence the average difference between two operators will be in the interval $0 \pm 1.96 \sqrt{2 s^2_{\text{operator}}}$ or 0 ± 1.1 units (95% confidence limits).

Overview of the handbook

The first drafts of the statistical handbook were organized according the different statistical methods with the same plan for all chapters: model, estimation, validation. A first introductive chapter dealt with general statistical issues. Each chapter has been written by a national expert of pig classification taking part to the meetings of the Pig Meat Management Committee in Brussels. The description of the statistical methods were quite short and time was missing for introducing examples.

For this new version it has been decided to completely modify the structure. As the main users of this handbook will be the national teams responsible of assessing pig classification methods in their country a structure built from the practical problems as they occur during the time appeared more suited. Given the dissection trial is the central point in such projects the handbook is split into 2 main parts: before the trial and after the trial.

The described statistical methods are the same than in the former versions but notation has been harmonized, material has been thoroughly revised and extended, examples have been added and processed according the different softwares, the references have been updated throughout (Appendix A) and a report-writing section has been included. Furthermore, an attempt of harmonisation of the accuracy criteria has led for choosing the RMSEP. This new edition explains therefore how to calculate it in all cases. For some specific cases formulae

have been put in appendix B. The choice of a prediction error criteria has some influence on sampling. Sampling recommendations have therefore been adapted.

Part 1 deals mainly with sampling and the statistical methods for creating prediction formulae. Sampling is split into two chapters, describing first some general issues and then some specificities linked with the statistical method to be used. For the description of the statistical methods it has been taken into account the number of predictors (few vs. many) which is one of the characteristics of the classification instruments. The model underlying these 2 kind of statistical methods (multiple regression vs. PLS / PCR) is described for each one. Then, estimation and validation are presented. A specific chapter describes 2 methods used for saving experimental cost. Finally, the last chapter gives some recommendations on what could be included in the protocol of the trial.

The second Part deals about what has to be done after the trial, i.e. data processing and reporting. The main chapter consists of estimation and validation in practice. Some examples from pig classification support the different stages of data processing which specificities are given for the main available software. Before that, an introductive chapter deals with the initial examination of data giving in particular some recommendations on how to manage outliers and influent data. The last chapter speaks about report-writing concerning the results of the trial which have to be presented in Brussels for gaining approval of the tested classification methods.

The use of this handbook is quite easy. The reader has just a few questions to answer :

- How many instruments to test: one or several ?
- Are there immediately available or not ?
- Do the instruments measure a few or many variables ?
- If many measurements what is the assumed dimensionality of the data ?
- Am I interested in saving experimental cost ?
- Which software may I use ?

According the answers the experimenter has just to read the concerned sections.

Part I

Before the trial

Chapter 1

Sampling with regard to a pig population

By Gérard Daumas

In Commission Regulation No 3127/94, Article 1, it is stated that a prediction formula should be based on "... a representative sample of the national or regional pig meat production concerned by the assessment method ...".

In statistics, sampling is the selection of individuals from a population of interest. Generally, in pig classification context the population of interest is defined as the national population of slaughterpigs in a certain range of carcass weight.

A "representative sample" is an ambiguous concept. Generally, it is interpreted as a sampling scheme with equal probabilities (uniform random sampling). Nevertheless, it is often more efficient to take units with unequal probabilities or to over-represent some fractions of the population (Tillé, 2001). To estimate accurately a function of interest (here: a regression) one must look for information in a wise way rather than to give the same importance to each unit.

We therefore interpret the EU regulation in the sense of a sample which aims to assure valid and unbiased conclusions about the population.

Some basic knowledge about sampling can be obtained from basic text book, like for instance Cochran (1977).

1.1 A short description of the population of interest

In the framework of EUPIGCLASS project a questionnaire about pig population and classification was sent in 2001 to most of the EU member states and candidate countries. Daumas (2003) reported a compilation of the answers. Below is the information relative to the heterogeneousness of the national populations.

"Subpopulations are an important issue for assessing classification methods. The questionnaire proposed the two main factors known having a significant effect on the prediction of the lean meat proportion, i.e. sex and breed. Only Italy mentioned another kind of subpopulations: heavy pigs (110 - 155 kg) vs. light pigs (70 - 110 kg).

According to sex the slaughterpigs can have three sexual types: females, entire males or castrated males (castrates). If evidently all countries slaughter females (around 50 % of the slaughtering) only three countries slaughter both entire and castrated males in non-negligible proportions. Spain estimates to half and half the proportions of entire and castrated males while Denmark and Bulgaria announce that around 10 % of the males are not castrated. Two countries slaughter only entire males: Great Britain and Ireland, but with a low slaughter weight (71 kg). All the other countries slaughter only castrates.

According to breeds the situation is more confused. In general, slaughterpigs are not pure breeds but crosses between two, three or four breeds. Others are synthetic lines developed by genetic companies. Generally no statistics are available on this matter. The answers are therefore to be considered as experts' estimations at a determined time. Some large countries, like Germany or Great Britain, did not provide any piece of information. Some small countries, like Estonia, may be considered as homogeneous.

All the other countries declared between two and four crossbreds, except the Czech Republic with six. The declared crossbred sum up to more than 90 % of the national slaughtering.

Crosses are mainly performed between the five following breeds : Large White (also called Yorkshire), Landrace, Pietrain, Hampshire and Duroc."

Year 2000	Proportion of sexual types (%)			Proportion of crossbreeds (%)				
	Females	Castrates	Entire males	Breed 1	Breed 2	Breed 3	Breed 4	Total 4 breeds
EU countries								
Austria	50	50		68	32			100
Belgium	54.5	45	0.5	50	20	20	5	95
Denmark	49.3	46.7	4.0	50	30	10	10	100
Finland	50	49	1					
France	51	49		55	25	10	10	100
Germany	50	50						
Ireland	50		50					
Italy	50	50		90	10			100
The Netherlands	50	50		60	25	10	5	100
Spain	50	20	30					
Sweden	47	52	1	75	24	1		100
United Kingd.	49		51					
Candidate c.								
Bulgaria	50	46	4	40	40	10	7	97
Cyprus	50	50		70	10	10	10	100
Czech Repub.	50	50		32	28	13	9	81
Estonia	50	50						
Poland	50	50						
Slovak Repub.	50.5	49.4	0.1	45	30	20	5	100
Slovenia	50	50						

Table 1.1: Proportion of subpopulations (sex and breed) in the European countries

1.2 Sampling frame and some practical considerations

National pig populations are so wide that no sampling frame is available. It is a technical barrier for a random sampling.

As it is not possible to directly select the pigs it is therefore needed to select first intermediary units (either pig farms or slaughterhouses). In practice, as the classification measurements (predictors) are taken on slaughterline, it is often more convenient to select slaughterhouses rather than pig farms. This kind of sampling plan is called a "two-level sampling plan" (Tillé, 2001). At each level any plan may be applied.

1.2.1 Selection on line (last level)

If there is no stratification, a kind of systematic sampling can be performed. A systematic sampling is the selection of every kth element of a sequence. Using this procedure, each element in the population has a known and equal probability of selection. This makes systematic sampling functionally similar to simple random sampling. It is however, much more efficient and much less expensive to do.

The researcher must ensure that the chosen sampling interval does not hide a pattern. Any pattern would threaten randomness. In our case care has to be taken about batches which correspond to pig producers. Batches size is variable. It may be judicious for instance to select no more than one carcass per producer (eventually a maximum of two).

1.2.2 Selection of the slaughterhouses (second level)

In most countries there are several ten slaughterhouses. But because of practical considerations, especially regarding dissection, it would be difficult to select randomly the slaughterhouses. Furthermore, it is generally not an important factor structuring the variability. Slaughter and cooling process are much less important than the origin of the pigs. In all cases the selection of the slaughterhouses has to be reasoned.

If the national population is considered as homogeneous then the slaughterhouses selection has no great influence. Nevertheless, higher is the number of slaughterhouses higher is the sample variability.

In some countries the differences between slaughterhouses mainly come from the different proportions of slaughterpigs genotypes. When these differences are marked and the proportions in the national population are known a stratified sampling (see section 1.1) is suited. Then, higher is the number of slaughterhouses higher is the variability within genotypes. After having chosen a certain number of slaughterhouses and taking into account the proportions of genotypes in each

slaughterhouse it can be deduced the proportions of each genotype in the total sample that has to be taken in each slaughterhouse.

1.2.3 Selection of the regions (first level)

In some other countries where regional differences are marked, due for instance to genotype, feeding, housing, a kind of stratification (see section 1.1) may be performed on regions when statistical data are available. Then, one or more "regionally representative slaughterhouses" have to be selected within regions. We therefore have a "3-level plan" (regions, slaughterhouses, pigs).

1.3 Stratification

Stratification is one of the best ways to introduce auxiliary information in a sampling plan in order to increase the accuracy of parameters. Here, the auxiliary information corresponds to the factor(s) of heterogeneousness (like sex and breed) of the national population.

If a population can be divided into homogeneous subpopulations, a small simple random sampling can be drawn from each, resulting in a sample that is "representative" of the population. The subpopulations are called strata. The sampling design is called stratified random sampling.

In the literature many factors influencing the corporal composition have been reported. Among those having the most important effects on the lean meat percentage itself and on its prediction sex and genotype may be identified in a dissection trial.

Significant differences between sexes were reported for instance in the EU by Cook and Yates (1992), in The Netherlands by Engel and Walstra (1991b, 1993), in France by Daumas et al. (1994) and in Spain by Gispert et al. (1996).

Most EC member states considered their pig population to be genetically heterogeneous, with up to six genetic subpopulations (see section 1.1). Most of the European slaughterpigs come from crosses between three or four breeds. The main difference is generally due to the boar (sire line), which gives more or less lean content in the different selection programmes. High differences are expected for instance between Pietrain and Large White boars. This effect is reduced after crosses with the sow (mother line). Nevertheless, in some countries the genotype may have an important effect. In that case the national population cannot be considered as homogeneous and a stratified random sampling is therefore more efficient than a simple random sampling (i.e., same sample size gives greater precision).

Then two cases have to be considered:

- the stratification factor is not used as predictor in the model,

- the stratification factor is also used as predictor in the model,

The first case could be a good way for managing the genotypes. An optimum allocation (or disproportionate allocation) is the best solution when estimates of the variability are available for each genotype. Each stratum is proportionate to the standard deviation of the distribution of the variable. Larger samples are taken in the strata with the greatest variability to generate the least possible sampling variance. The optimal allocation depends on the function of interest: here a regression. Note that to infer a single equation to population one must re-weight the carcasses within stratum (here: genotype) proportional to share of population.

If no (reliable) information is available on the intra stratum variability then a proportional allocation can be performed. Proportionate allocation uses a sampling fraction in each of the strata that is proportional to that of the total population.

The second case (see also section 2.2.4) could be for instance a way for managing the sex. As sex is known on slaughterline and easy to record then sex can be put in the model of prediction of the lean meat proportion. Following the conclusions of the 1990 EC trial (Cook and Yates, 1992), France decided to introduce separate equations for the sexual types when sex effect is significant (Daumas et al., 1998). In that case it does not matter if sampling is proportionate or disproportionate. Nevertheless, as the standard deviation is higher for castrates than for females it is more efficient to select a higher proportion of castrates (Daumas and Dhorne, 1995).

A very specific case is the Dutch situation where sex was used both in the model and for stratification (Engel and Walstra, 1993). Unlike France, sex is not recorded on slaughterline in The Netherlands. So, they decided to use a non-linear model for predicting the sex through a logistic regression (see Appendix B5). As sex is predicted in this two-stage procedure the gain in accuracy is much lower than for separate formulas. Moreover, if the allocation would have been optimal it would have been necessary to re-weight samples (proportional to share of population) to infer to population.

Chapter 2

Statistical Methods for creating Prediction Formulae

By David Causeur, Gérard Daumas, Bas Engel and Søren Højsgaard.

2.1 Introduction

In pig carcass classification, the LMP of a carcass is predicted from of a set of measurements made on the carcass. These measurements (explanatory variables) can be e.g. ultrasound or, as is the case for the data used in the illustrative worked example, measurements of physical characteristics and thicknesses of fat and meat layer at different locations. In practice, a prediction formula is established by applying statistical methods to training data (data for which not only the explanatory variables but also the true LMP is known from e.g. dissection).

Different statistical methods are currently used in the European Union to assess the prediction formulae. The choice for a particular prediction method depends mostly on the instrument which is used to measure the predictors. These instruments can indeed roughly be classified into two groups: the probes measuring a small number of predictors at few specific locations in the carcass, and other instruments extracting many measurements by a more general scanning of the carcass. In the former case, the explanatory variables are usually highly correlated. Consequently, a classical statistical method such as ordinary least squares (OLS) may be inappropriate for constructing the prediction formula because the predictions can have very large variances. Therefore one often use alternative methods, and two such are partial least squares (PLS) or principal component regression (PCR), see Sundberg (1999) for discussion of this.

2.1.1 OLS or rank reduced methods: a matter of dimensionality

The first issue the user is faced with is naturally the choice between OLS and an alternative method. This problem is generally addressed in the statistical handbooks by somewhat theoretical arguments which claim for instance that PLS has always to be be preferred first because it is known to be at least as good as PCR and second because OLS is nothing more than a particular case of PLS. Also it must be true, we will try in the following to give more insight to the choice of a particular method in the specific context of pigs classification.

First, in this context, the practitioners can observe that the prediction formulae assessed with few predictors, usually less than 5, and those assessed with hundreds of predictors are almost as accurate, or at least that the difference in accuracy is not proportional to the difference between the numbers of predictors that are measured. This shall points out that the amounts of predicting information collected in both cases are not so different. Furthermore, whatever the instrument that is used, it appears in all cases that a small number of axis of predicting information can be identified, or equivalently, that only a small number of latent variables are indirectly measured. This number of latent variables is often referred as the dimensionality of the instrumental predictors.

Usually, the most important latent variable can be seen as the fat content in the carcass. The second latent variable characterizes the amount of lean meat and the third one is related to the physical conformation of the carcass. To be more complete, each of the former latent variables can sometimes be doubled to distinguish between fat or lean contents that could be due either to genetics or to feeding. Finally, as a first approximation and only on the basis of what has already been observed in the past experiments, it can be said that about 6 axis of predicting information can at most be expected to be identified in pig carcass data. Consequently, the use of rank reduced method can actually be recommended when the number of instrumental predictors is very large relative to this dimensionality. In the other situations, it seems to be reasonable to inspect carefully the redundancy of the predicting information and even to compare the predictive ability of OLS and PLS.

2.1.2 An harmonized approach of the assessment of accuracy

Harmoniously assessing the accuracy of the prediction formulae is currently one of the objectives of the EC-regulations that frame pigs classification in the European Union. Although these regulations still contain some ambiguity with respect to their practical applications, they tend to ensure a minimum level of accuracy by restrictions on the sample size and the estimated residual standard deviation. However, they do not yet account for substantial differences between

the prediction methods. As it will be mentioned thereafter, in the case of highly correlated predictors, PLS and PCR often work well in practice being superior to OLS in terms of accuracy of the predictions. This is basically achieved by allowing for bias in the estimation of the regression coefficients in order to reduce its variance. Due to this bias, the estimated residual standard deviation does probably not reflect faithfully the predictive ability of PLS and PCR. Moreover, these methods suffer from other deficiencies. First, they are defined iteratively meaning that precise interpretation is difficult to grasp. Second, the statistical properties are difficult to stipulate. To be specific, it is unclear how to estimate the residual variance and how to estimate variance of the parameter estimators.

The will for harmonization obviously appeals for the choice of a single criterion that first can be computed whatever the prediction method and second, that reflects the predictive ability rather than the precision of estimation. In the following sections, it is advised to choose the Root Mean Squared Error of Prediction, designed by RMSEP, computed by a full cross-validation technique and some arguments motivating this choice are given.

2.2 Statistical Methods

Our purpose here is to give technical hints to actually calculate the prediction formulae. Further details on this kind of issues can be found in many handbooks dedicated to statistical models for prediction, for instance Rao and Toutenburg (1999). These estimation procedures are sometimes presented as if the dimensionality was not part of the estimation issue. However, in most of the practical situations of pigs classification, an important and sensitive work is done on the data either to define a relevant set of predictors before the prediction formula is assessed or to investigate the dimensionality problem. In other words, the dimensionality is actually a meta-parameter, which estimation has to be considered in that section and at least accounted for when the problem of validating the prediction formulae will be addressed. For that reason, first in the case the set of predictors and the dimensionality are assumed to be known, we present the usual procedures that underly the prediction packages generally provided by the softwares. Then the estimation of the dimensionality or the selection of a relevant set of predictors is investigated and specific recommendations are given. Hereafter, the validation problem is considered with respect both to the fitting procedure itself and to the selection step.

2.2.1 The prediction model

It is supposed that the LMP, generically denoted by y, is measured together with the p predictors $\boldsymbol{x} = (x_1, \ldots, x_p)$ on n sampled carcasses. The training data that are used to establish the prediction formula are therefore $D = \{(y_i, \boldsymbol{x}_i), i =$

$1, \ldots, n\}$. Further details about sampling are mentioned in chapter 3. Up to sophistications that could be shown to be relevant in some special cases, the following linear regression model is traditionally assumed:

$$y_i \;=\; \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \varepsilon_i,$$

where $\varepsilon_i \sim N(0, \sigma)$ stands for the residual error, β_0 denotes the offset and $\boldsymbol{\beta} = (\beta_1, \ldots, \beta_p)'$ is the $p-$vector of the slope coefficients.

Therefore, the general expression for the prediction formulae is a linear combination of the instrumental predictors:

$$\hat{y}(\boldsymbol{x}) \;=\; \hat{\beta}_0 + \hat{\beta}_1 x_1 + \ldots + \hat{\beta}_p x_p$$

where $\hat{y}(\boldsymbol{x})$ denotes the predicted LMP for a carcass which values for the instrumental predictors are $\boldsymbol{x}$, $\hat{\beta}_0$ is the estimated offset and $\hat{\beta}_j,\ j = 1, \ldots, p$, are the estimated slope coefficients.

Up to now, call $\hat{\boldsymbol{\beta}} = (\hat{\beta}_1, \ldots, \hat{\beta}_p)'$ the $p-$ vector of the estimated slopes.

2.2.2 Estimation when the dimensionality is assumed to be known

The least-squares criterion

Estimation usually consists in minimizing a criterion that measures the global difference between predicted and observed values. For theoretical reasons that go beyond the scope of our purpose, the least-squares criterion appears to be relevant, at least in some extent:

$$SS(\beta_0, \boldsymbol{\beta}) \;=\; \sum_{i=1}^{n} (y_i - \beta_0 - \beta_1 x_{i1} + \ldots + \beta_p x_{ip})^2.$$

It will be shown in section 8 that alternative criteria can be used especially if outliers are suspected to influence abnormally the estimation procedure.

The OLS solution

Minimization of this criterion can be achieved by equating its derivatives relative to each coefficient: for all $j = 0, 1, \ldots, p$, $\frac{\partial SS}{\partial \beta_j}(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) = 0$. Therefore, $\hat{\beta}_0$ and $\hat{\boldsymbol{\beta}}$ are obtained by solving what is called the system of normal equations:

$$\left\{ \begin{array}{rcrcl}
\frac{\partial SS}{\partial \beta_0}(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) & = & -2\sum_{i=1}^{n}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} + \ldots + \hat{\beta}_p x_{ip}) & = & 0, \\
\frac{\partial SS}{\partial \beta_1}(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) & = & -2\sum_{i=1}^{n} x_{i1}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} + \ldots + \hat{\beta}_p x_{ip}) & = & 0, \\
\frac{\partial SS}{\partial \beta_2}(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) & = & -2\sum_{i=1}^{n} x_{i2}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} + \ldots + \hat{\beta}_p x_{ip}) & = & 0, \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
\frac{\partial SS}{\partial \beta_p}(\hat{\beta}_0, \hat{\boldsymbol{\beta}}) & = & -2\sum_{i=1}^{n} x_{ip}(y_i - \hat{\beta}_0 - \hat{\beta}_1 x_{i1} + \ldots + \hat{\beta}_p x_{ip}) & = & 0.
\end{array} \right.$$

The first equation states that the predicted value for the LMP when the values of the instrumental predictors are the mean values $\bar{x}_j$ is simply the average lean meat $\bar{y}$ or in other words:

$$\hat{\beta}_0 \;=\; \bar{y} - \hat{\beta}_1\bar{x}_1 - \ldots - \hat{\beta}_p\bar{x}_p.$$

Imputing this value of the offset in the p other equations yields:

$$\left\{\begin{array}{rcl} \sum_{i=1}^n (x_{i1}-\bar{x}_1)\Big([y_i-\bar{y}] - \hat{\beta}_1\left[x_{i1}-\bar{x}_1\right] + \ldots + \hat{\beta}_p\left[x_{ip}-\bar{x}_p\right]\Big) &=& 0, \\ \sum_{i=1}^n (x_{i2}-\bar{x}_2)\Big([y_i-\bar{y}] - \hat{\beta}_1\left[x_{i1}-\bar{x}_1\right] + \ldots + \hat{\beta}_p\left[x_{ip}-\bar{x}_p\right]\Big) &=& 0, \\ \vdots & \vdots & \vdots \\ \sum_{i=1}^n (x_{ip}-\bar{x}_p)\Big([y_i-\bar{y}] - \hat{\beta}_1\left[x_{i1}-\bar{x}_1\right] + \ldots + \hat{\beta}_p\left[x_{ip}-\bar{x}_p\right]\Big) &=& 0. \end{array}\right. ,$$

or equivalently, with matrix notations:

$$\mathbf{s}_{xy} - S_{xx}\hat{\boldsymbol{\beta}} \;=\; 0,$$

where $\mathbf{s}_{xy}$ and S_{xx} denote respectively the empirical covariance $p-$vector between y and the predictors and the $p \times p$ empirical variance-covariance of the instrumental predictors.

At that point, it has to be noted that solving this equation is just a matter of regularity of S_{xx}. In the very convenient case where S_{xx} is not ill-conditioned, in other words when exhibiting the inverse matrix S_{xx}^{-1} is not subject to numerical problems, solving the least-squares problem leads to the OLS solution:

$$\hat{\boldsymbol{\beta}}_{OLS} \;=\; S_{xx}^{-1}\mathbf{s}_{xy}.$$

It is well-known that the former OLS estimator has desirable properties such as unbiasedness and an easy-to-compute variance, which makes inference, and especially prediction, easier.

Biased solutions

Ill-conditioned matrices S_{xx} are known to be encountered when the predicting information is redundant, or equivalently when the number of predictors is much higher than the dimensionality. In that case, some methods, called biased regression methods, consist in replacing S_{xx}^{-1} by an approximate version, denoted by G:

$$\hat{\boldsymbol{\beta}}_{BR} \;=\; G\mathbf{s}_{xy}.$$

This modification of the OLS estimator makes the new estimator biased. In that case, the mean squared error MSE is traditionally used to reflect more properly the accuracy of the estimator:

$$\text{MSE} \;=\; \text{bias}^2 + \text{variance}.$$

The most relevant choices for G aim at a compensation of the increase of the bias by a reduction of the variance. Globally, this trade-off between bias and variance can even lead to a better accuracy in terms of mean squared error.

Many techniques can be used to find a satisfactory G matrix and some of them are generally provided by the statistical softwares. Maybe the most intuitive technique is the ridge regression that consists in choosing G in a family of matrices indexed by a single value λ:

$$G \in \mathcal{G}_\lambda = \left\{(S_{xx} + \lambda I_p)^{-1}, \lambda > 0\right\}.$$

In this approach, the trade-off between bias and variance is transposed into a kind of cursor λ that can be moved from zero to introduce bias and simultaneously reduce the variance.

Rank-reduced solutions

Other techniques, sometimes said to be rank-reduced, are getting more and more popular since they directly connect the choice of G with the problem of dimensionality. Two of the most widely spread among these methods are PCR and PLS. The first idea behind these methods is the extraction from the predictors of a small number, say k, of independent new variables $\mathbf{t}_j = (t_{1j}, t_{2j}, \ldots, t_{nj})'$ defined as linear combinations of the centered instrumental predictors:

$$t_{ij} = w_{1j}(x_{i1} - \bar{x}_1) + w_{2j}(x_{i2} - \bar{x}_2) + w_{pj}(x_{ip} - \bar{x}_{ip}),$$

where $\mathbf{w}_j = (w_{1j}, w_{2j}, \ldots, w_{pj})'$ is called the jth vector of loadings. To bridge the gap with the introductory words on dimensionality, the extracted components make it concrete the latent variables and therefore k can be interpreted as the dimensionality. For brevity, call X the $n \times p$ matrix of the centered values of the instrumental predictors, T the $n \times k$ matrix of the components values and W the $p \times k$ matrix of loadings, then:

$$T = XW.$$

In both cases of PCR and PLS, the extraction of the components can be presented from an algorithmic point of view as an iterative procedure. In the case of PCR, this extraction procedure is simply a Principal Component Analysis of the instrumental predictors: initially, $\mathbf{t}_1$ is the component with maximal variance, then $\mathbf{t}_2$ is chosen as the component with maximal variance among those with null covariance with $\mathbf{t}_1$, and so on until the kth component. In the case of PLS, the strategy differs only by the criterion which is optimized at each step: the variance is indeed replaced by the squared covariance with the response. This difference is often used as an argument to underline the superiority of PLS relative to PCR in a context of prediction: extraction of the PLS components is indeed oriented

towards prediction whereas extraction of the PCR components does not rely on the values of the response at all.

Once the components are extracted, the second phase consists in predicting the response by OLS as if the predictors were the components. The $n-$vector of fitted values of the response by the rank-reduced methods is therefore obtained as follows:

$$\begin{aligned} \hat{y} &= T(T'T)^{-1}T'Y, \\ &= X \underbrace{W(W'S_{xx}W)^{-1}W's_{xY}}_{\hat{\boldsymbol{\beta}}_{RR}}. \end{aligned}$$

Therefore, in the case of rank-reduced methods, the vector of estimated slope coefficients is given by:

$$\hat{\boldsymbol{\beta}}_{RR} = W(W'S_{xx}W)^{-1}W's_{xY}.$$

Equivalently, the generic expression for the G matrix figuring an approximation of S_{xx}^{-1} is expressed as follows:

$$G = W(W'S_{xx}W)^{-1}W'.$$

The algorithms providing the matrices of loadings in the case of PLS and PCR have been described above. In the particular case of PCR, this algorithm yields in some sense the best approximation of S_{xx} by a matrix G^{-1} with rank k.

Now, in the case of PLS, Helland (1998) showed that the iterative algorithm consists finally in choosing the most relevant G, leading to the smallest MSE, in the following set of matrices:

$$G \in \mathcal{G}_{k,\boldsymbol{\alpha}} = \left\{\alpha_0 I_p + \alpha_1 S_{xx} + \ldots + \alpha_k S_{xx}^k,\ \boldsymbol{\alpha} = (\alpha_0, \alpha_1, \ldots, \alpha_k)'.\right\},$$

which also makes the PLS estimator optimal in some sense.

Although the problem of dimensionality may be considered by some practitioners as an additional trouble specific to rank-reduced methods, it must be noted that this problem is of course only masked while using OLS. It is indeed very tempting to build regression models with all the present predictors to improve the fit but it must be kept in mind that this conservative behavior damages the predictive ability of the prediction formula. This issue is addressed in the next section and recommendations are given to estimate properly the dimension meta-parameter.

2.2.3 Estimation of the dimensionality

It can of course be imagined that estimating the dimension parameter is not strictly speaking a statistical issue. For instance, it can be decided before the

regression experiment that, say three, pre-chosen instrumental predictors will be sufficient to predict the LMP. In that case, provided that this choice is relevant, it can be considered that the dimensionality equals the number of predictors and OLS can simply be performed in the old-fashioned way to derive the prediction formula. Suppose now that hundreds of instrumental predictors are collected by a general scanning of the carcass, but that a prior reliable knowledge available on these instrumental predictors makes it relevant to consider that only, say three, latent variables are measured. In that case as well, setting the dimension parameter to three is also possible without further statistical developments.

However, due to an uncertainty about the redundancy in the predicting information that is collected, a statistical procedure is sometimes needed to chose for a proper value for the dimension parameter. Note that the redundancy analysis can at first be approached by widely spread exploratory data tools, such as Principal Components Analysis (PCA), that enable a simplified reading of a large correlation matrix. However, these tools do not generally allow for a rigorous analysis of the redundancy within the instrumental predictors in our context of prediction since they do not enable a proper display of the partial dependencies between the response and some predictors conditionally on others. Therefore, we recommend an exhaustive comparison of the predictive abilities that can be obtained for each value of the dimension parameter. Note that this strategy supposes that a validation criterion that quantifies the predictive ability of a prediction method is previously defined: this issue is discussed below in section 2.3 and the Root Mean Squared Error of Prediction (RMSEP) is recommended as a validation criterion.

This kind of exhaustive comparison is generally proposed by most of the statistical softwares. Concerning rank-reduced methods, it consists in calculating the validation criterion RMSEP(k) for reasonable choices of the dimension parameter (usually in the context of pigs classification, $k \leq 10$). In the case of OLS, the computations can turn out to be cumbersome since obtaining the predictive ability for a given dimension k consists first in calculating the validation criterion for all the subsets of k predictors before keeping the best one, namely:

$$\text{RMSEP}(k) \quad = \quad \min \left\{ \text{RMSEP}(X_{i_1}, X_{i_2}, \ldots, X_{i_k}),\ 1 \leq i_1 \leq i_2 \leq \ldots \leq i_k \leq p \right\}.$$

As it has already been mentioned before, it is sometimes very tempting to consider that the best value for the dimension parameter corresponds to the minimum value for the RMSEP:

$$\hat{k} \quad = \quad \arg\min_k \text{RMSEP}(k).$$

However, this objective strategy often leads to an over-estimation of the dimension. In fact, it is highly recommended to inspect more carefully the successive differences $\Delta(k) = \text{RMSEP}(k) - \text{RMSEP}(k-1)$: as soon as a difference $\Delta(k_0)$ can be considered as small relative to the successive differences observed previously, it can indicate that k_0 is a good candidate for the dimension.

The estimation procedures presented before are illustrated by the analysis of a real data set in section 9.2.

2.2.4 Regression with structuring factors

As already mentioned in chapter 1 about sampling, most of the European countries are not homogeneous and have several sub-populations. This means that a factor structures the variability of the population. If this factor is unknown on the slaughterline (like genotype for instance) we recommend a suited sampling: stratified sampling (see 1.2 for details), but if this factor can easily be known on the slaughterline (like sex for instance) we recommend to introduce this factor in the model.

This model was implemented in the French slaughterhouses in 1997 using a sex indicator (female vs. castrated male) (Daumas et al, 1998). It is also approved in Italy for "heavy pigs" vs. "light pigs" (two sub-populations differing not only by the carcass weight but also by production area, breed, ...).

Obviously, as for any model, the coefficients have to be significant. The more the sub-populations differ in the relation between carcass measurements and lean meat percentage the more a factorial model will increase the accuracy.

In all cases, member states that decide to address subpopulations, should confirm to the requirement that prediction should be at least as accurate as prediction by an approved standard method applied to a sample of 120 pigs.

To be more specific, suppose that two subpopulations are considered that markedly differ in the relation between carcass measurements and lean meat percentage. In that case it is likely that two separate formulae, each based for instance on 60 animals, conform the minimal requirement of a total of 120 carcasses, would be an improvement over a method that employs random or proportional sampling with respect to subpopulations and ignores subpopulations in the subsequent statistical calculations. When differences are very large, it is not unlikely that even for three subpopulations, separate formulae based on for instance 40 carcasses per subpopulation, again resulting in the minimal total of 120, would offer an improvement. However, when many subpopulations are considered, and the differences are moderate to small, attention to sub populations, for a total sample size of 120, may actually reduce the accuracy for prediction compared with the aforementioned standard method as mentioned in the regulations. In that case the method of prediction would not be approved. Possible remedies are either to choose for the standard approach in combination with random or proportional sampling or to increase the total sample size to such an extent that indicators of subpopulation member ship become more valuable for prediction.

2.3 Validation

2.3.1 MSE - The mean squared error

In regression based on ordinary least squares, the variance is estimated by

$$MSE = \hat{\sigma}^2 = \frac{1}{N-(p+1)} \sum_{i:\text{ training carcasses}} (y_i - \hat{y}(x_i))^2.$$

There are problems with regarding MSE as a measure of predictive performance:

1. The residual error variance σ^2 can be regarded as an *internal* measure of how well the linear model fits to the training data. The residual error variance σ^2 is not in itself a measure of how well the model performs in prediction new carcasses, i.e. it is not a good *external* measure of the predictive abilities of the model.

   (It is well known, that the estimate MSE can be made arbitrarily small by just making the model very complex by adding more predictor variables).

2. Finally, MSE is not a well–defined quantity for some statistical methods – the problem being: What is p in $\frac{1}{N-(p+1)}$? (In PLS/PCR, p is often taken to be the number of latent variables, and although this seems plausible in practice, this lacks theoretical justification)

2.3.2 $MSEP$ – Using external data

An alternative could be to take a new (randomly selected) set of "validation" carcasses D_v and measure y and $x_1, \ldots, x_p$ on these too. Then one could look at Squared Error of Prediction

$$SEP = \sum_{\text{validation carcasses}} (y_i - \hat{y}(x_i))^2$$

– or more conveniently, the average SEP:

$$MSEP = \frac{1}{N} SEP$$

An advantage of $MSEP$ is that it is a realistic quantity, in the sense that it resembles what one would meet in practice. (Provided that the validation carcasses resemble the population in which the prediction formula will be used.) Generally $MSEP > MSE$ because it is more difficult to predict the future than the past! Yet, this approach is in practice not feasible: It is in practice too expensive to dissect two sets of carcasses.

2.3.3 Approximating $MSEP$ by cross–validation

An alternative to having an external validation data set D_v as discussed above is to use cross–validation methods: Here we suggest the use of leave–one–out cross validation, as it is easy to implement in practice:

This works as follows: For each carcass i

1. Delete the ith carcass from the training set:

2. Estimate $\beta_0, \beta_1, \ldots, \beta_p$ from the remaining observations

3. Predict y for the ith carcass and calculate

$$SEP_{-i} = (y_i - \hat{y}_{-i}(x_i))^2$$

where $y_{-1}(x)$ is the predictor obtained when the ith carcass is excluded from the data set before estimating the regression parameters.

Next, calculate the PREdiction Sum of Squares $PRESS = \sum_i SEP_{-i}$ and the average PRESS $APRESS = \frac{1}{N} PRESS$.

How much difference does it make in practice?

The question is now: How similar are APRESS and MSEP in practice? To provide some insight to this question we consider the Danish carcass classification data, see Section 9.2.

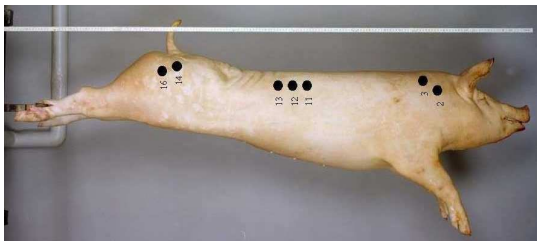


Figure 2.1: Location of fat depth measurements for Danish carcasses

For simplicity we only consider the fat measurements at the 7 "dots" in Figure 2.1 for 300 carcasses.

As statistical method for constructing the prediction we consider Principal Component Regression (PCR) with 1...7 components. Note that PCR with 7 components corresponds to multiple linear regression.

Design of study

The study was made as follows: Split data in two:

- $N = 120$, $N = 60$ and $N = 30$ training carcasses
- $M = 150$ validation carcasses

Then we calculate $RMSE = \sqrt{\frac{1}{N}SE}$, (an internal measure of precision), $RMSEP = \sqrt{\frac{1}{M}SEP}$, (the "truth"), and $RAPRESS = \sqrt{\frac{1}{N}PRESS}$ (a cross-validation quantity, which should be close to the "truth")

Results

For $N = 120$ training carcasses we find the results in Table 2.1. Differences between RAPRESS and RMSEP (the "truth") are smaller than 7 %.

Table 2.1: Results when $N = 120$

	RMSE	RMSEP	RAPRESS	RAPRESS/RMSEP
1 LV's	2.18	2.20	2.23	1.01
2 LV's	2.18	2.22	2.24	1.01
3 LV's	2.17	2.22	2.25	1.01
4 LV's	2.09	2.24	2.22	0.99
5 LV's	2.08	2.15	2.23	1.04
6 LV's	2.08	2.12	2.25	1.06
7 LV's	2.08	2.12	2.26	1.07

For $N = 60$ training carcasses we find the results in Table 2.2. Differences between RAPRESS and RMSEP (the "truth") are smaller than 5 %.

Table 2.2: Results when $N = 60$

	RMSE	RMSEP	RAPRESS	RAPRESS/RMSEP
1 LV's	2.14	2.27	2.20	0.97
2 LV's	2.09	2.26	2.17	0.96
3 LV's	2.04	2.26	2.15	0.95
4 LV's	2.03	2.29	2.22	0.97
5 LV's	1.96	2.27	2.18	0.96
6 LV's	1.96	2.16	2.19	1.02
7 LV's	1.96	2.15	2.25	1.05

For $N = 30$ training carcasses we find the results in Table 2.2. Differences between RAPRESS and RMSEP (the "truth") are smaller than 20 % (and this large number appears only for the model with 7 latent variables, i.e. for a classical multiple linear regression).

Table 2.3: Results when $N = 60$

	RMSE	RMSEP	RAPRESS	RAPRESS/RMSEP
1 LV's	2.33	2.65	2.53	0.95
2 LV's	2.18	2.64	2.46	0.93
3 LV's	2.18	2.58	2.46	0.95
4 LV's	2.14	2.52	2.68	1.07
5 LV's	2.13	2.51	2.75	1.09
6 LV's	1.96	2.52	2.60	1.03
7 LV's	1.95	2.26	2.72	1.20

2.3.4 Summary

If the data is a random sample from the population, then $MSEP$ can be quite well approximated using simple leave–one–out cross validation.

Chapter 3

Sampling: selection on variables

By Bas Engel

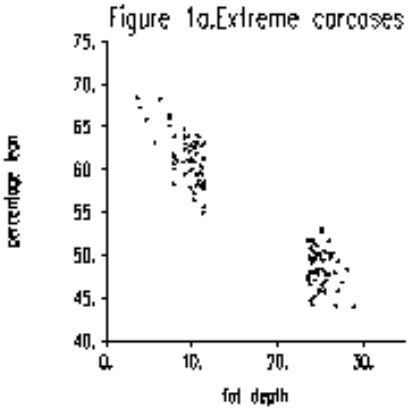
3.1 The nature of the sample

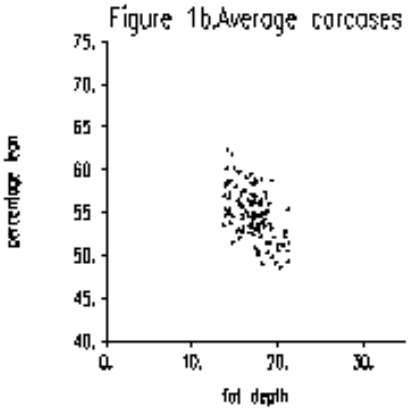
In Commission Regulation No 3127/94, Article 1, it is stated that a prediction formula should be based on "...a representative sample of the national or regional pig meat production concerned by the assessment method ...".

To be considered representative, samples do not need to be chosen completely at random. In fact, because we focus on the variation in y given the value of x in LR, statistical theory allows us to select the carcasses on the basis of x. This can be profitable, because selection of carcasses with more extreme fat or muscle depth measurements will improve the accuracy of the estimated values $\hat{\beta}_0$ and $\hat{\beta}_1$ for constant β_0 and coefficient β_1 and thus improve the accuracy of prediction. This is illustrated in Figure 1, where the standard errors of the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$ are considerably smaller for selection of carcasses with extreme x-values compared to selection of carcasses with moderate x-values. Consequently, carcasses for dissection are often not selected randomly but according to a sampling scheme that favors a larger percentage of more extreme instrumental measurements. Of course carcass values should not be too extreme, in other to avoid selection of carcasses of abnormal animals. Also, in practise sampling scheme (a) in Figure 1 is usually supplemented with carcasses with moderate x-values as well, otherwise departures from linearity can hardly be detected. Curvature may lead to poor predictions for moderate x-values.

A common sampling scheme in carcass classification is the 40-20-40 % scheme. Suppose that μ_x and σ_x are the mean and standard deviation for x in the population. In the 40-20-40 % scheme, 40 % of the sample is selected such that values of x are below $\mu_x - \sigma_x$, 40 % is above $\mu_x + \sigma_x$ and 20 % is in between.

Carcasses may be selected on the basis of an "old" prediction formula, when that formula is based on the same or similar instrumental carcass measurements.





Thus, carcasses may for instance be selected on the basis of a linear combination of fat and muscle depth. With respect to the carcass measurements, carcasses represent points in the plane with fat and muscle depth along the horizontal and vertical axes. Selection with an old formula will tend to produce a cluster of carcasses with low fat depth and high muscle depth, a cluster with high fat depth and low muscle depth and a cluster with intermediate values for both fat and muscle depth. Roughly the carcasses will be along a line from the upper left-hand corner to the lower right-hand corner, with emphasis on the upper left and lower right-hand corners of the muscle and fat depth plane. Such a configuration of carcasses that tends to be concentrated on a lower dimensional sub space (the plane has dimension 2, while the line is a subset of dimension 1) is rather vulnerable with respect to outliers and departures from linearity (Dhorne, 2000). Therefore, such a selection procedure, although intuitively appealing, is not to be recommended.

Problems may occur when some of the selection variables are not intended to be included among the prediction variables. It may happen, for example, that carcass weight is included as a selection variable, but not as a prediction variable.

This is a common phenomenon among many past proposals. Such a sampling procedure is not covered by standard LR theory. For standard theory to apply, all selection variables have to be included as prediction variables as well. Such a potentially faulty combination of selection and LR may have direct consequences for authorization of a carcass measurement instrument (Engel et al., 2003). We will return to this particular problem later on.

3.2 The size of the sample

In ordinary linear regression, intercept β_0 and slope β_1 are estimated by the method of least squares, i.e. estimates $\hat{beta}_0$ and $\hat{\beta}_1$ minimize the sum of squared deviations:

$$\sum_{i=1}^{n}(y_i - \beta_0 - \beta_1 x_i)^2$$

Denoting the minimum value by RSS (residual sum of squares), an estimate for the variance σ^2 is:

$$s^2 \;=\; RSS/d.$$

The degrees of freedom d in the numerator are equal to the sample size n reduced by the number p of unknowns to be estimated in the formula:

$$d \;=\; n - p.$$

For example, with one prediction variable x, we have two unknowns β_0 and β_1, so $p = 2$ and for a sample of $n = 120$ we have $d = 120 - 2 = 118$ degrees of freedom. Somewhat confusingly both the (unknown) population standard error σ and its estimate s are often referred to as the residual standard deviation (RSD).

The accuracy of estimators $\hat{\beta}_0$ and $\hat{\beta}_1$ is reflected by their associated standard errors. Each of these standard errors is a multiple of σ^2, say $c_0\sigma^2/\sqrt{n}$ and $c_0\sigma^2/\sqrt{n}$. Constants c_0 and c_1 depend on the configuration of x-values. Roughly: the more widely separated the values of x, the smaller these constants will be. With increasing sample size, the standard errors decrease with order $1/\sqrt{n}$.

The minimum required sample size for LR in the EC regulations is fixed in Article 1 of Commission Regulation No 3127/97 at $n = 120$. Each procedure proposed should be as accurate as LR based on a sample of $n = 120$ carcasses. An example of an alternative procedure to LR that we mentioned before is double-regression (DR). DR is based on a double-sampling procedure. Carcasses are dissected by a relatively quick and cheap national dissection method and only part of these carcasses are also dissected by the more time consuming and expensive EC-reference method. The two dissection procedures may be applied to the same

or to different carcass halves of the same carcass. DR is specifically mentioned in Article 1 of Commission Regulation No 3127/97. The number of carcasses n which are (also) dissected according to the EC reference method should at least equal 50. The total number of carcasses N, all dissected by the quick national method, should be high enough such that the precision is at least as high as LR for 120 EC-reference dissections. In Engel & Walstra (1991a) it is shown how large the sample sizes N and N should be for DR to be as precise as LR for 120 EC-reference dissections. Engel & Walstra (1991a) present accurate large sample results that avoid complete distributional assumptions. More accurate small sample results, assuming normality, are presented in Causeur and Dhorne (1998).

3.3 The accuracy of the prediction formula

The accuracy of prediction depends on the accuracy of estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, but also on the size of the error components ε. The accuracy of $\hat{\beta}_0$ and $\hat{\beta}_1$, as follows from the discussion so far, depends on the sample size and on the configuration of x-values. The size of the error terms ε is quantified by the residual variance σ^2. It is important to realize that the selection of carcasses does affect the accuracy of $\hat{\beta}_0$ and $\hat{\beta}_1$, but not the accuracy of s^2 as an estimator for σ^2. The accuracy of s^2 is measured by its standard error. Under a linear regression model this standard error is equal to $\sigma^2\sqrt{2/d}$, where d is the degrees of freedom. Since $d = n-p$ and n is at least 120 and with LR p will be relatively small, say smaller than 6, roughly the standard error of s^2 decreases with order $1/\sqrt{n}$. By choosing larger samples and appropriate configurations of x-values, we can make sure that $\hat{\beta}_0 + \hat{\beta}_1 * x$ is as close to $\beta_0 + \beta_1 * x$ as we want it to be. In fact with a sample size of 120 the difference between a random sample and a sample of selected carcasses is fairly small (Engel et al., 2003; Font I Furnols,2002). However, we cannot reduce the contribution to the prediction error of the error terms ε, as quantified by the residual variance σ^2. The size of σ^2 depends on the measurement instrument and the pig population. Unless some of the instrumental measurements that were initially not used, perhaps for practical reasons, are added to the equation later on, there is no possibility to reduce σ^2. Similar comments can be made with respect to a cost saving method such as DR, where we estimate the same coefficients β_0 and β_1 as in ordinary LR, but in a more efficient way. Hence, with DR we can attain a high accuracy for the estimates $\hat{\beta}_0$ and $\hat{\beta}_1$, but we have to deal with the same residual variance σ^2 as in LR. This implies that σ is the crucial quantity for authorization of an instrument. It is therefore very important to form a correct impression of the size of σ. When, due to an inept sampling procedure, s does not offer an accurate impression of σ, this can have unfortunate consequences for authorization. This may happen when some of the variables that are included for selection are not included in the prediction formula. For details

we refer to Engel et al. (2003).

Chapter 4

Cost saving/precision increasing methods

By David Causeur, Gérard Daumas, Thierry Dhorne and Bas Engel

In the previous chapters, some aspects of the interactions between the statistical recommendations that are expected from this handbook and the requirements laid down by the EC-regulations have been dealt with. Some of these requirements (EC, 1994a and 1994b) are aiming to ensure a minimum level of accuracy by restrictions on the methodology used to establish the prediction formula. Roughly speaking, unreliability of the prediction formulæ is expected to be avoided or at least reduced by a minimum sample size (currently 120 reference dissections) and a maximum limit for a validation criterion (currently 2.5 for the Residual Standard Deviation). As the reference dissections are heavily time-consuming, an indirect consequence of the EC-requirements is the need for expensive regression experiments. This chapter is devoted to the presentation of statistical methods that can be used to face that problem of experimental costs, or equivalently to save experimental units in the framework of the EC-requirements.

Some countries have chosen indeed to adopt new statistical methodologies which account for both the experimental cost and the EC-requirements in the definition of the sampling scheme. Basically, these new methods consist in replacing reference dissection by cheaper approximated versions for some of the sampled carcasses. Section 4.1 is devoted to a further investigation of the practical advantages of such a novelty.

As it is explained in details by Engel and Walstra (1991a and 1991b) or Causeur and Dhorne (1998), the subsequent sampling scheme involves two samples: a first one for which reference dissections and approximate reference dissections are performed together with measurements of the predictors and a second one where only cheaper dissections are performed. Table 4.1 displays the general form of the two-phase sampling schemes. Minimum costs strategies are then obtained by relevant choices of the sample sizes. More detailed explanations are

given in section 4.2.

The need for frequent new calculations or updates of the prediction formulae have motivated new strategies. For instance, up to the EC regulations, each time a new instrument is candidate for authorization, a new trial has to be conducted, involving new reference dissections. In the French context, it has been decided to derive once for all a prediction formula of the lean meat percentage on the basis of predictors, that are supposed to be sophisticated enough to be considered as better than any other predictors used in the slaughter-line. Each time an update of the prediction formula is needed, the only trial that is conducted consists in common measurements of the instrumental predictors and the sophisticated predictors introduced in the first experiment. Table 4.1 illustrates the type of sampling scheme we are dealing with in such a context. Further details on the construction of optimal sampling scheme are given in section 4.3. On a methodological point of view, this two-phase approach leads to a combination of two regression equations. The proper statistical framework in which such a combination is possible is presented in Causeur and Dhorne (2003).

At this point, it can be noted that multivariate and/or multi-sample refinements of these statistical methods can lead to further improvements. The resulting sampling strategies can be found in Causeur (2003). Finally, validation issues are dealt with in section 4.4 and illustrations by worked examples are postponed in section 9.3.

4.1 The practical interest in these methods

4.1.1 Reducing dissection cost

Direct measurement of carcass composition involves carcass dissection. This dissection largely destroys the financial value of the carcass and also requires expensive laboratory facilities and staff. The minimum sample size imposed by the EU regulation, actually 120 pigs, involves sizeable total costs.

This minimum is the same for all the EU countries, whatever the pig slaughtering is less than 1 million per year or more than 20 millions per year. In order to take into account the heterogeneousness of this slaughtering, especially in the large producing countries, this minimum may be too low. A sample size of at least 200 is probably more realistic for ensuring a certain representativeness. In such a case the interest for saving experimental costs is still more acute.

Furthermore, such dissection trials have periodically to be performed because:

- The approved equations are old and the pig sector has some doubts about their validity,
- The nature of the pig production has changed (different proportions of breeds or sexes,),

Design for double-regression

Sampling item	Lean meat %	Approximate Lean meat %	Instrumental predictors
1	×	×	×
2	×	×	×
⋮	⋮	⋮	⋮
n	×	×	×
n+1	?	×	×
	?	⋮	⋮
⋮	?	⋮	⋮
	?	⋮	⋮
	?	⋮	⋮
N	?	×	×

Design for updates without new reference dissections

Sampling item	Lean meat %	Sophisticated predictors	Instrumental predictors
1	×	×	?
2	×	×	?
⋮	⋮	⋮	⋮
n	×	×	?
n+1	?	×	×
	?	⋮	⋮
⋮	?	⋮	⋮
	?	⋮	⋮
	?	⋮	⋮
N	?	×	×

Table 4.1: Two-phase sampling scheme for updates without new reference dissections. Missing values are figured by ?, observed values by ×.

- A new classification instrument has to be tested,
- The EU definition of the LMP has changed.

There is evidence that the relationship between fat and muscle depths change over time as well as between Member States. These changes suggest that more frequent monitoring of the equations is necessary to ensure their continuing accuracy (Cook & Yates, 1992). Nevertheless, the expensive dissection procedure discourages both the updating of the equations and the development of cheaper or more accurate measuring techniques.

So, the authors of the report on research concerning the harmonisation of methods for classification of pig carcases in the Community recommended to reduce the cost by the use of sample joint dissection and double regression. As a consequence of this research double regression was introduced as the new standard of the statistical technique in the EU regulations in 1993-1994.

Since then, several Member States have used this method for assessing their classification methods. Works have been made for searching for the best concomitant variable(s) and for optimizing the sample sizes. One of the best solution used until now consists in removing the subcutaneous fat of ham, loin and shoulder and to build several concomitant variables from these weights. The major constraint is the minimum sub-sample size of 50 imposed by the EU regulation in order to ensure a certain representativeness. Using efficient concomitant variables the total sample size may be around 180. Such a design permits to cut the experimental costs by 30% compared with 120 carcasses dissected according the EU reference. Furthermore, the increase of 50 % of the sample size (180 vs. 120) improves the representativeness.

This method may also be used as a mean for increasing the accuracy for a fixed cost. Nevertheless, this case is less frequent in practice.

The statistical aspects of this method, called "double regression", are developed in §5.2.

4.1.2 Testing several instruments

Several companies sell different classification instruments. They differ in their technology, price, size, accuracy, All the slaughterhouses have not the same needs. So, most of the Member States are interested in testing several instruments.

Nevertheless, the present EU regulation specifies that the assessment of a classification method is based on a sample of at least 120 carcases (or 50 in the sub-sample if double regression). Using the same sample for all the instruments is attractive. Unfortunately, it is difficult to manage a lot of equipments at the same time. Moreover, most of the present instruments are invasive, which deters the tissues. It means that a second instrument cannot measure the same variable as a first one. Sure, another location could be used for the second instrument.

By the way on one hand, the companies often recommend the same location and on the other hand, different locations for the instruments may decrease the comparability of classification data of the pig producers.

So, some Member States have chosen to test only one instrument. This situation has the main disadvantage to introduce a monopoly. Other Member States have preferred to test a few equipments using "surrogate locations". Generally, these are either the same location but on the right side or another location at 1 cm around the first hole. The former does not correspond to the real conditions of use. As the equipments are manufactured for right-handlers one can expect a significant effect between measurements on right and left sides. The latter introduces also an error because the depths are not homogeneous, especially between 2 ribs. Furthermore, nobody until now has estimated these kinds of error and taken into account when assessing the prediction equations. Such practices cannot therefore be recommended.

A Member State has preferred to perform a separate trial for 2 instruments. Experimental cost was therefore double.

France & Germany have introduced in the 80' a strategy eliminating all these disadvantages. This strategy was based in a two-stage procedure based on the use of a reference instrument, more accurate than the to be tested instruments. This has made possible to approve several instruments on a time period of some years having only performed one dissection trial. Nevertheless, this procedure has 2 disadvantages: obliging all the instruments to measure at the same location(s) and eventually modifying the instruments software after the calibration against the reference instrument.

For these reasons France has deepened its strategy introducing now a reference method instead of a reference instrument. The difference is that each instrument may have its own measuring locations. For applying such a strategy new statistical developments were needed. The statistical aspects of this method, called "surrogate predictor regression", are developed in §5.3.

Thanks to this great improvement France has got the official approval of 3 methods using different predictors, has calibrated several old methods and has developed different classification control methods. Some of the methods were not available at the dissection period which was the initial motivation to develop such a procedure.

In a 5 years time around 10 equations have been assessed. This represents a colossal saving cost and time compared to a dissection trial for each method. With only 2 equipments to be tested the cost is nearly divided by 2 because the cost of the 2nd stage (instruments calibration) is negligible compared to this of the 1st stage (dissection trial). The gain is therefore much more important than using double regression. Furthermore, surrogate predictor regression can be combined with double regression in order to reduce even more the costs.

4.2 Double regression

4.2.1 Introduction

Double regression (from now on referred to as DR) is a potentially useful method when a surrogate for the EC reference percentage (Walstra and Merkus, 1995) is available. With DR we can either considerably reduce the cost of dissection or increase the precision of predictions without further experimental cost compared to linear regression (from now on referred to as LR). The surrogate percentage may take the form of a quick rough and ready national dissection method. The reduction in cost (or increase in precision) is realized by reducing the number of relatively expensive EC reference dissections and adding a larger number of national dissections in a double sampling scheme. The national method must be considerably cheaper than the EC reference method. Also, in addition to the instrumental carcass measurements, the percentage obtained by the national dissection method should have considerable predictive power for the EC reference percentage. Otherwise there will be little to gain with DR compared with LR.

In technical statistical terms the national lean meat percentage is a concomitant variable. DR has been generalized to the case of several concomitant variables by Causeur and Dhorne (1998). In principle, any set of variables that is closely connected to the EC reference percentage and is not intended to be included as prediction variables in the prediction formula, are a set of candidate concomitant variables in DR. Here, attention will be restricted to the case of one concomitant variable only. For illustrative purposes we will assume that the concomitant variable is the lean meat percentage obtained by a simplified, faster and cheaper national dissection method. When several candidate concomitant variables are available, the most promising variable or a summary variable may be used in DR. DR with several concomitant variables may offer a markedly larger reduction in experimental cost compared with DR with one of the concomitant variables only (Causeur and Dhorne, 1998). In Causeur and Dhorne (1998) the lean meat percentage of the ham offers a reduction in cost of 25%. The lean meat percentages of the loin should and filet each offer a reduction of less than 5 %. However, all four concomitant variables together offer a reduction of 38 %. Some notation before we proceed:

Y = EC reference lean meat percentage;

Y^* = faster and cheaper dissection method, e.g. a national method;

x_1, x_2, ... = instrumental carcass measurements, e.g. a fat and muscle depth measurement.

The predictive power for the EC reference percentage of the national percentage Y^*, in addition to the instrumental measurements x_1, x_2, ... is measured by the partial correlation between Y and Y^* given x_1, x_2, ... This partial correlation

must be sufficiently large, otherwise DR will offer no marked advantage over LR. Details will be discussed below.

The double sample consists of N carcasses that are dissected by the cheap national method. From the N carcasses a typically much smaller subset of n carcasses are also dissected according to the EC reference method. Practical implementation may consist of, say, n carcass halves being dissected first by the national method and then further dissected by the EC reference method, while an additional $(N - n)$ carcasses are dissected by the national method only. If further dissection from national to EC reference percentage is a problem, and carcass halves are dissected, n out of the N other halves of the carcasses may be dissected by the EC reference method. For example, N right carcass halves may be dissected by the cheap national method, while n out of the N available left carcass halves are dissected by the EC reference method. Some details about selection of carcasses and required sample sizes n and N will be provided below.

We will introduce DR with data from a dissection experiment carried out in 1986 in The Netherlands to derive a prediction formula for the EC lean meat percentage with the Henessy Grading Probe (HGP). This was the first application of DR and predates the amendment of the EC regulations with respect to use of DR. The instrumental measurements with the HGP were a back fat measurement (x_1) and a muscle thickness (x_2), both measured at the third to fourth from last rib position 6 cm from the dorsal mid line (Walstra, 1986). The surrogate percentages Y^* were obtained by the IVO standard method (Walstra, 1980). This is a quick incomplete dissection method that takes about 45 minutes per carcass half.

4.2.2 Sampling

$N = 200$ right carcass halves were dissected according to the IVO standard method (Walstra, 1980). A sub sample of $n = 20$ of these carcasses halves were further dissected according to the EC reference method. Please note that according to the regulations, at present a minimum sub sample size of $n = 50$ carcasses is required for the EC reference dissections in DR.

Carcasses were selected on the basis of HGP back fat thickness (x_1). At the time it was decided to mimic a random sample. Five back fat classes were chosen. The numbers of dissected carcasses in these classes were chosen proportional to the numbers in the population. An alternative sampling procedure would have been the 40-20-40 % sampling scheme that is popular in pig carcass classification experiments and mentioned elsewhere in the handbook. Carcasses were selected from 5 slaughterhouses and 40 carcasses were selected from each slaughterhouse. In order to reduce batch effects, every 10th carcass in the slaughterline was measured. The same team dissected all carcass halves. Twenty carcasses were dissected at a time and two of them were further dissected by the EC reference method. Further details may be found in Walstra (1986) and Engel & Walstra

(1991a).

4.2.3 Calculations

This section is based on Engel and Walstra (1991a, b). The calculations are in three steps. First of all we establish a regression formula for the total sample of size $N = 200$ with the IVO standard percentage Y^* as the dependent variable and the HGP fat and muscle depth measurements x_1 and x_2 as the explanatory variables.

$$\hat{Y}^* = 65.64 - 0.6762x_1 + 0.0903x_2,\ RSD_1 = 1.79,\ N = 200. \quad (4.1)$$

RSD1 is the estimated value of the residual standard deviation (the root from the mean sum of squares for residual). Second, we establish a regression formula for the EC reference lean meat percentage Y with fat and muscle depth x_1 and x_2 and the IVO standard lean meat percentage Y^* as explanatory variables. This regression is based on the sub sample of $n = 20$ carcasses only.

$$\hat{Y} = -12.3 - 0.0564x_1 + 0.0711x_2 + 1.079Y^*,\ RSD_2 = 0.833,\ n = 20 \quad (4.2)$$

In the third and last step we construct the final prediction formula for the EC reference lean meat percentage. We replace Y^* in (4.2) by the right hand side of (4.1):

$$\hat{Y} = -12.3 - 0.0564x_1 + 0.0711x_2 + 1.079\,(65.64 - 0.6762x_1 + 0.0903x_2)\,.$$

This yields

$$\hat{Y} = 58.52 - 0.786x_1 + 0.168x_2,\ n = 20 \text{ and } N = 200. \quad (4.3)$$

In Engel and Walstra (1991b) it is shown how simple approximations to the standard errors for the estimated constant and coefficients can be obtained from the output of the two regression equations. These approximate standard errors are based on large sample results. Simulations show that these approximations are adequate. Exact results are also available (Causeur and Dhorne, 1998).

As a suitable substitute for the RMSE we calculate an estimate for the residual standard deviation (RSD) of the final prediction formula (4.3):

$$RSD^2 = RSD_2^2 + \hat{\gamma}^2 RSD_1^2. \quad (4.4)$$

The coefficient $\hat{\gamma}$ in expression (4.4) is the coefficient for the surrogate percentage in (4.2). So, in this example $\hat{\gamma} = 1.079$. Furthermore, $RSD1$ and $RSD2$ are the residual standard deviations in regressions (4.1) (total sample) and (4.2) (sub sample). In this example $RSD1 = 1.79$ and $RSD2 = 0.833$. For the final formula this yields:

$$RSD = \sqrt{(0.833)^2 + (1.079)^2(1.79)^2} = 2.10.$$

An estimator with smaller order of bias than the maximum likelihood estimator (4.4) is presented in Causeur and Dhorne (1998).

It is important to realize that DR offers an estimation procedure in combination with a double sampling scheme for the same constant and coefficients and residual standard deviation that are estimated by LR. Hence, DR is no remedy for measurement instruments where the value of σ is too high! The value of σ depends on the pig population, the instrument and the measurements used, and is for LR and DR the same.

There is the temptation in DR to leave the fat and muscle depth measurements out of regression (4.2). In that case, when the relationship between the EC reference and the national lean meat percentage has already been established in the past, no further EC reference dissections would be needed to authorize a new instrument. It would be enough to collect instrumental measurements and perform national dissections only. However, when the instrumental measurements add significantly to regression (2), such an approach may produce poor estimates for the constant and coefficients in the final regression formula and the true RSD may be considerably underestimated. For details we refer to Engel and Walstra (1991b) and Engel (1987).

4.2.4 Required sample sizes n and N

In order to calculate the required sample sizes, we need to evaluate the partial correlation between the EC reference and the national lean meat percentage, given the instrumental carcass measurements. This partial correlation measures correlation between the EC and national lean meat percentages that is not already explained through the instrumental carcass measurements. It is a measure of the contribution of Y^* to regression (4.2) in addition to the instrumental measurements, e.g. the HGP fat and muscle depth in the example.

The partial correlation, say ρ, can be estimated as follows:

$$\hat{\rho} \;=\; \hat{\gamma}\frac{RSD_1}{RSD}.$$

In the example: $\hat{\rho} = 1.079 * 1.79/2.10 = 0.92$. Suppose that we want DR to be as accurate as LR with a sample size of m EC reference dissections. In that case the total cost of LR would be

$$Cost_{LR} = C * m.$$

Here, C is the cost of dissection of a carcass (half) by the EC reference method. It is assumed that the additional cost of the instrumental carcass measurements is negligible. The following sample sizes are required:

$$n \;=\; m\left\{1-(1-f)\hat{\rho}^2\right\} \text{ and } N = \frac{n}{f},$$

where

$$f \;=\; minimumof\sqrt{\frac{c}{C-c}\frac{1-\hat{\rho}^2}{\hat{\rho}^2}} \text{ and } 1.$$

Here, c is the cost of dissection of a carcass (half) by the national method. These sample sizes are based on large sample approximations. Details may be found in Engel & Walstra (1991a,b). In the derivation it is assumed that carcasses are either selected at random or on the basis of the instrumental measurements. The carcasses for the sub sample are assumed to be selected according to the same sampling scheme as the total sample. For instance, suppose that the total sample is based on selection with three back fat classes, where boundary values are equal to mean back fat plus or minus one standard deviation. Let the numbers in the classes be $0.4{*}N$, $0.2{*}N$ and $0.4{*}N$ for lean, average and fat pigs respectively. Then a fraction n / N of the carcasses in each class are randomly chosen to obtain the sub sample. In practise, carcasses for the sub sample could be selected on the basis of Y^* as well, in that case DR can be expected to be even more accurate. Hence, the calculations yield somewhat liberal sample sizes. Since the value of ρ will not be very well known, it will often be a "guesstimate" close to the lowest value still considered likely. Consequently, some liberality in the sample sizes is not a point of grave concern.

For example, suppose that $m = 120$ (the minimum required sample size for LR according to the EC regulations). Let $C/c = 5$ and $\hat{\rho} = 0.9$. Then:

$$\begin{aligned} f &= \sqrt{\frac{1}{5-1}\frac{1-(0.9)^2}{(0.9)^2}} = 0.2422, \\ n &= 120\left\{1-(1-0.2422)(0.9)^2\right\} = 46.3, \\ N &= 46.3/0.2422 = 191.3. \end{aligned}$$

Suppose that we take $n = 50$ and $N = 200$. The cost for DR with further dissection from national to EC reference lean meat percentage is:

$$Cost_{DR} \;=\; 50 * C + (200-50) * c = C * (50 + 150 * 0.2) = C * 80$$

.

So, in this example cost by DR are reduced by $(Cost_{LR} - Cost_{DR})/Cost_{LR} * 100 = \{(120-80)/120\} * 100 = 33\%$ relative to LR.

4.3 Two-phase updates based on reference predictors

For convenience, we present the statistical framework in the case of only one instrumental predictor x, say a fat depth and only one reference predictor z, say an

approximated lean meat percentage obtained by a partial dissection. Moreover, y will denote the response, say the lean meat percentage obtained by a reference dissection.

In what follows, preliminaries concerning the regression models are first discussed. Then we show how minimum cost strategies are achieved under the restrictions laid down by the EC-regulations.

4.3.1 Creating the prediction formula

Our aim is to derive the prediction formula of y by the instrumental predictor x on the basis of the following linear regression model:

$$y = \beta_0 + \beta_1 x + \varepsilon,$$

where $\varepsilon \sim N(0, \sigma)$ stands for the residual error, β_0 denotes the offset and β_1 is the slope coefficient. However, y and x are never measured on a common sample. Therefore, the prediction formula is achieved through two auxiliary regression models. First, call reference model the following one:

$$y = \gamma_{r,0} + \gamma_{r,1} z + \varepsilon_r,$$

where $\varepsilon_r \sim N(0, \sigma_r)$ stands for the residual error, $\gamma_{0,r}$ denotes the offset and $\gamma_{1,r}$ is the slope coefficient.

Similarly, call scaling model the following one:

$$z = \gamma_{s,0} + \gamma_{s,1} x + \varepsilon_s,$$

where $\varepsilon_s \sim N(0, \sigma_s)$ stands for the residual error, $\gamma_{0,s}$ denotes the offset and $\gamma_{1,s}$ is the slope coefficient.

The regression experiments which are conducted to estimate the coefficients of the auxiliary models are usually not simultaneous: first, $\gamma_{0,r}$ and $\gamma_{1,r}$ are estimated on a sample of size n_r, and then, for instance when an instrument is candidate for authorization, $\gamma_{0,s}$ and $\gamma_{1,s}$ are estimated on another sample of size n_s.

Although it appears as very intuitive to combine transitively the auxiliary regression equations to obtain a prediction formula for y by x, it is recalled by Engel and Walstra (1991) that this is generally misleading. To combine properly the regression equations, the reference model must indeed include x among its predictors. However, provided z is a better predictor of y than x, in the sense that (z, x) is as good a predictor as z, Causeur and Dhorne (2003) have shown that a transitive combination of the regression equations was appropriate. Therefore, the prediction formula can be derived as follows:

$$\begin{aligned} \hat{y} &= \hat{\gamma}_{0,r} + \hat{\gamma}_{1,r} \hat{z}, \\ &= \hat{\gamma}_{0,r} + \hat{\gamma}_{1,r} \left(\hat{\gamma}_{0,s} + \hat{\gamma}_{1,s} x \right), \\ &= \underbrace{\hat{\gamma}_{0,r} + \hat{\gamma}_{1,r} \hat{\gamma}_{0,s}}_{\hat{\beta}_0} + \underbrace{\hat{\gamma}_{1,r} \hat{\gamma}_{1,s}}_{\hat{\beta}_1} x. \end{aligned}$$

The previous formula only gives the proper way of combining regression coefficients estimated on two separate samples. Causeur and Dhorne (2003) give the equivalent formulæ in the more frequent case of many x variables and many z variables and the standard deviations in the special case the auxiliary regression equations are fitted by OLS. These standard deviations are the main support to provide minimum costs strategies.

As it is discussed in chapter 2, the estimation of the auxiliary regression coefficients can be performed using OLS, PLS, PCR or any other relevant method.

4.3.2 Minimum costs sampling scheme

A regression experiment is first conducted in order to have common measurements of the response and the reference predictors. Let c_{yz} denote the experimental cost per sampled carcass in this regression experiment, usually the time needed to obtain the measurements. When a prediction formula has to be assessed on the basis of instrumental predictors, a scaling experiment is performed, which consists in common measurements of the reference and the instrumental predictors. Call c_{zx} the experimental cost per sampled carcass in this scaling experiment. The overall experimental cost which is engaged for assessing the prediction formula is therefore:

$$c \quad = \quad n_r c_{yz} + n_s c_{zx}.$$

According to the EC-requirements, the statistical method which is used to fit the regression model has to be at least as accurate as the usual least-squares method on a sample of $n = 120$ carcasses. This kind of requirements obviously appeal for the definition of a criterion which aim is to compare the efficiencies of a two-phase procedure and the usual least-squares method. Provided OLS is used to fit the auxiliary regression models, Causeur and Dhorne (2003) have proposed a relative efficiency criterion that can be considered as the ratio of the variances of the estimators of the regression coefficients. For instance, if we focus on the slope coefficient b, this relative efficiency criterion turns out to be:

$$RE(b; n, n_r, n_s) \quad = \quad \frac{n}{n_r}\left(\frac{n_r}{n_s}\rho^2_{yz.x} + (1-\rho^2_{yz.x})(1+\rho^2_{zx})\right),$$

where $\rho^2_{yz.x} = 1 - \sigma^2_r/\sigma^2$ is the squared partial correlation coefficient between y and z conditionally on x and ρ^2_{zx} is the squared correlation coefficient between z and x.

Provided prior values of $\rho^2_{yz.x}$ and ρ^2_{zx} are available, the 120 carcasses-equivalent EC-requirement is therefore transposed in the following equation:

$$RE(b; 120, n_r, n_s) \quad = \quad 1.$$

In the French context of pigs classification, the only remaining unknown of this equation is the sample size n_s since n_r has been chosen previously.

4.4 Validation issues

Many aspects of the validation of prediction formulæ have already been discussed in chapter 2. Among the recommendations that have emerged from the discussions, the use of the RMSEP have been proposed as a validation criterion. Therefore, in the present situation of double-sampling, validation will also be considered according to this choice.

First, note that, on the basis of the techniques that are mentioned in section 2, it is clear that auxiliary RMSEP can be calculated. Call RMSEP_y the RMSEP related to the auxiliary model including y and RMSEP_z the RMSEP related to the auxiliary model including only z. It can be shown, at least approximately if the sample sizes are large enough, that the global RMSEP used to validate the prediction formula estimated by a double-sampling method can be deduced from the following combination:

$$RMSEP^2 \;=\; RMSEP_y^2 + \hat{\gamma}^2 RMSEP_z^2,$$

where γ stands for the slope coefficient of z in the auxiliary model including y. In the preceding equation, not only the auxiliary RMSEP can be calculated whatever the estimation procedure is used to fit the auxiliary models but also the estimated slope coefficient $\hat{\gamma}$.

Chapter 5

Reporting to the Commission. Protocol for the trial

By Gérard Daumas

The present EU regulation lays out:
"Part one of the protocol should give a detailed description of the dissection trial and include in particular:

1. the trial period and time schedule for the whole authorization procedure,
2. the number and location of the abattoirs,
3. the description of the pig population concerned by the assessment method,
4. a presentation of the statistical methods used in relation to the sampling method chosen,
5. the description of the national quick method,
6. the exact presentation of the carcasses to be used."

These items have not been specifically discussed. Nevertheless, one can look for the following items at the corresponding sections:

- Item 2: see section 1.2.2.
- Item 3: see section 1.1.
- Item 4: see chapters 2 and 4.

Part II

During and after the trial

Chapter 6

Some general comments on the management of the trial

By Gérard Daumas

During the trial a certain number of problems can occur which could affect the quality of the results. In general, decisions have to be taken very quickly because of practical constraints. It is therefore very important that the bench scientist would be aware of all the issues, inclusive the statistical issues, in order to get an acceptable compromise.

Some of the main problems occurring in classification experiments are as follows:

- staff unavailability,
- abattoir unavailability,
- missing pigs in some categories for selection,
- instrument failure,
- changes in some environmental parameters,
- changes in work quality,
- wrong measurements,
- mixture of joints between carcasses,
- mixture of tissues between joints,
- mixture of tissues between carcasses.

These problems can be split into 2 categories according their consequences:

- selection of the pigs,
- data reliability.

Selection of the pigs

If there is a selection on factors (sex, breed,) it can be difficult sometimes to find the needed category. This can lead to proportions different as initially planned, affecting therefore the representativeness of the sample and introducing an overall bias.

Afterwards, this bias can be removed by a re-weighting of the observations at the estimation stage. Nevertheless, it is important to avoid such changes in the proportions, especially for the small categories.

When there is an over-sampling at the extremes of predictor(s) some days it can be very difficult to find the right pigs. The risk is all the more high since over-sampling intensity is high, the number of concerned predictors is high, the daily number of selected carcasses is high and the slaughtering is low. This may lead to accept some pigs with some defects, especially an uncorrect splitline. In order to avoid a lower data reliability it is preferable to decrease the over-sampling intensity. Indeed, the latter has only an effect on the estimators variance ; moreover, this effect is relatively small in the current designs for dissection trials.

Data reliability

Concerning the lean meat proportion (LMP)

The lean meat proportion may be affected by a lot of events for 2 reasons:

- it is not a direct measurement but a calculated variable from a lot of variables,
- the measurement of all these variables is spread over several hours.

As the LMP is very expensive, temptation is high to conserve a carcass with a wrong measurement. These wrong measurements may affect either joint weights or tissue weights. It is therefore very important to check the data at each stage. After jointing a first check consists in calculating the jointing losses before starting dissection. In case of too high losses each joint can be weighted again. The same holds for the dissection of the 4 joints. After dissection of a joint the dissection losses have to be calculated before throwing the different tissues in a tank where there are mixed with the tissues of other joints and other carcasses.

Some errors are more difficult to detect when they come from a (more or less) continuous change. For instance, the laborious dissection work can have a poorer quality in the afternoon or at the end of the week. This can be avoided

by the planning of a reasonable time schedule and by a supervising of the dissection team. Some changes in the environmental conditions, like for instance the temperature, may affect losses and the hardness of the work. It is therefore recommended to write down some environmental parameters, some carcass characteristics and in general all kind of events which could help to explain some doubtful data observed during the data processing.

Concerning the predictors

The statistical methods used until now in the pig classification context assume there is no error on the independent variables. In fact, this is not the case with the actual classification instruments.

Most of these instruments measure fat and muscle depths, muscle depth being more difficult to measure accurately. Moreover, these errors are not independent, because there is a common limit between fat and muscle tissues. Furthermore, some errors, especially on muscle depth, may be very high (5 or 10 mm).

But it is not always easy to immediately detect such errors. It means that this problem can be solved with the outliers management (see chapter 7).

The most dramatic incident is the failure of the tested instrument. Replacing equipment has to be foreseen.

Chapter 7

Departures from the model (lack-of-fit)

By Bas Engel

Although the average of the estimated error terms $\hat{\varepsilon}_i$ is always 0 for LR, lack of fit may be detected by plotting the individual estimates $\hat{\varepsilon}_i$ (referred to as residuals) against the predictions $\hat{y}_i$ (often referred to as fitted values). According to standard theory fitted values and residuals are uncorrelated for LR and nearly so for non-linear regression. This implies that in the aforementioned residual plot, there should be no obvious pattern, when the regression model fits the dissection data well. If there is a pattern, this may indicate some serious departure from the model assumptions. For instance, an increase of the absolute residuals with an increase of the fitted values, suggests that the residual variance is not constant. A simple remedy may be to replace observations y by log-transformed observations $log(y)$. However, this is not always an appropriate remedy, either because heterogeneity of variances may remain, or because a LR model may no longer apply after transformation. In that case the use of non-linear regression or the use of a variance function may be considered. A curve in the residual plot may indicate the need for a quadratic term x^2 in the model. So far, there is no evidence supplied for marked variance heterogeneity or curvi-linearity.

Since y and $\hat{y}$ are strongly correlated, it is generally a better idea to supply a plot of residuals $\hat{e}$ against $\hat{y}$, rather than a plot of y against $\hat{y}$. Unfortunately, the last plot has been a regular feature in many proposals so far.

Departures from normality may be apparent from a so-called probability plot of the residuals. Residuals are ordered in increasing size and plotted against their expected values under normality. Departures from a straight line, usually in the form of a sigmoid curve, indicate non-normality. These plots tend to be more informative than formal tests of significance. Non-normality is generally considered to be a less serious problem than heterogeneity of variances or apparent lack of additional predictors such as quadratic terms x^2 in the formula.

Chapter 8

Managing outliers

By Thierry Dhorne

8.1 Aim

The elaboration of "good" models for pig classification is achieved by two statistical means:

- specifying and using models with good theoretical properties,
- adjusting the models in the best way in the best way.

Both are the major aims of the present handbook.

The last (and not the less) point is to get good datas to adjust the model. Many things are suggested by meat scientists to obtain good datas and we will concentrate here on the specific aspect of assessing in some way the quality of the data obtained in a trial in order to get reliable prediction formulas.

It is important to make a difference between what is acceptable (for instance with respect to the regulation) and what is reliable.

The aim now is then to deal with the management of both observations that:

- have a great influence on the assessment of the formula and/or
- are badly predicted by the TVM prediction formula.

8.2 The issue

As mentioned above, the problem is that quality is more or less subjective and that two scientists could consider as different the same situation.

We will then concentrate here on the way to detect problems and leave the decision of interpreting the problems to meat scientists.

Let us then mention clearly the issues: what can be thought of a formula equation in some countries where one carcass, or five or twenty-five out of a hundred is (are) really badly predicted ? Suppose that the formula for the fair carcasses has a standard-error of let say 2, and that the bad carcasses are predicted at random, let say with a standard-error of 3.5, to be compared with the 2.5 of the regulation. In the three cases (if it is assumed that the mean is known), we have:

1. 1 % bad predictions: $\sqrt{99.2^2 + 1.3.5^2} = 2.02$
2. 5 % bad predictions: $\sqrt{95.2^2 + 5.3.5^2} = 2.10$
3. 25 % bad predictions: $\sqrt{75.2^2 + 25.3.5^2} = 2.46$

and everything is all-right.

Furthermore, what can be thought of a formula established on a set of a hundred carcasses and where the deletion of one, three, nine carcasses in the sample could change the equation in a sensible way for the millions of pigs classified every year.

The objective of this part is to evaluate the importance of these two issues and to give some solutions to them.

8.3 Definitions

Though the statistical vocabulary is not completely established in this field some main key-words are important.

First the topic concerned is usually defined by *robustness*. This topic deals with the capacity of the predictors to resist to practical factors that could decrease the reliability of the model essentially because they invalidate assumptions made by the statistician to choose it.

Due to the fact that prediction equations are always obtained explicitly or implicitly through the minimization of a criterion of discrepancy between the real observed values and the predicted values, it is clear that these errors in the data can generate two different negative effects:

- some observations far from the others "attracts" the model through the minimization,
- some observations show a great discrepancy between the predicted and observed values.

The first type of observations is usually refered as *influential observations* (or *leverage points*), the second type as *outliers*.

As mentioned above these two aspects are independent in the sense that the four situations can be encountered, namely: standard observation (neither influential nor outlying), outlier not influential, influential observation not outlying, influential outlier.

8.4 Statistical solutions

8.4.1 Graphical studies

It is probably the easiest way to deal with the problem as suggested by very impressive but specific graphics proposed here and there. This approach suggests nevertheless problems of two kinds:

- first the subjectivity of the observer and then of the procedure,
- the difficulty to generalize this approach when the model is more complex (multivariate) and when many data sets are involved.

There was then a need to develop more technical methods to solve this problem.

8.4.2 Residuals analysis

Residuals analysis has been widely used for years in the treatment of regression data. Unfortunately this analysis is not suited to evaluate influential observations which has been shown above to be different with the outlier problems. Moreover the analysis is made after classical least squares adjustment. This strategy is somewhat paradoxical because the aim is to avoid influence of some points while the initial estimation may be widely influenced by these points in an undetectable way.

This points out that one single observation can pollute the other ones and attract to itself the regression line and leads to the interest of studying the individual influence of each point on the assessment of the regression.

8.4.3 Influence analysis

As defined previously, the influence of a single observation can be roughly defined as the discrepancy between the prediction formulae obtained on the one hand with the whole dataset and on the other hand without this observation. Statistical procedures in influence analysis are mainly based on two formal interpretations of the former definition of influence:

- individual influence can first be defined as the impact of a single observation on the prediction procedure: this approach is consistent with the detection of influential observations,
- influence analysis can also consist in measuring the consequence of the deletion of a single observation on the estimated parameters of the model: both outliers and influential observations can be pointed out throughout this approach.

8.4.4 Robust estimation

The naturel extension of influence analysis would be to try to study the influence of couples of points, then triplets and so on, to avoid the joint effect of multiple influential observations. The limit should be the number of errors of any kind that can be made in getting the data.

This aspect has led to the notion of breakdown point corresponding to the percentage of contaminated data sufficient to "break" the "real" regression line. It is easy to appreciate intuitively this notion in the easier case of the estimation of the location parameter of a data set.

Let us examine a univariate series of values and consider the departure of some points to plus or minus infinity. It is obvious that in the case of the mean, one single observation can pull it to plus of minus infinity, whereas the median can be seen to resist up to nearly 50 % of the observations contaminated. It is then said that the mean has a O % breakpoint while the median has a 50 % breakpoint.

In the field of multiple regression it has been a challenge for years to investigate the existence of robust regression procedures that could improve the catastrophic break point of the usual least squares estimator.

The main ideas at the basis of such investigations are the following:

1. Though the problem seems to be quite easy for a location parameter (median versus mean), it is not so obvious that a generalization holds for regression parameters. It is known that not even a generalization of the median is easily available for a two dimensional location parameter.

2. Furthermore even if this goal can be achieved, the example of the median shows that protection against influential points has a cost at least in term of variance of estimators.

3. The idea that an exhaustive procedure that could identify every subset of influential points conveys the impression that any robust procedure should lead to complex numberings and therefore to computer intensive procedures.

8.5 Robust estimation

The idea of robust estimation focused on the field of regression is then really appealing. Indeed, where the classical procedures make an adjustment and then examine the influential points with the risk that they are hidden by themselves, a robust procedure would give an adjustment free of influential points which would then be implicitly identified. Furthermore it could enable the examination of outliers in a safe way.

The point is now to define such procedures.

8.5.1 Criteria

Two generations of criteria have been proposed in the literature to achieve the former goals. One deals with influential functions of the observations, the other with general robust criterions.

Influence fonctions The classical least squares estimator is known to minimize the quantity:

$$\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} e_i^2.$$

Global criterion One of the most significant result in robustness was worked by Rousseuw and Leroy (1987). It is also a very sensitive approach for non statisticians and therefore it can easily be understood.

The idea is simply to consider the former criterion:

$$\sum_{i=1}^{n}(Y_i - \hat{Y}_i)^2 = \sum_{i=1}^{n} e_i^2,$$

as its equivalent:

$$1/n \sum_{i=1}^{n} e_i^2,$$

the mean of the squares of the residuals, and then replace the mean by a more robust quantity. Two variants have been proposed by Rousseuw and Leroy (1987):

- the median of squares:

$$med_i e_i^2,$$

- the trimmed mean of squares:

$$\sum_{i=1}^{h} e_{(i)}^2,$$

  where $e_{(i)}^2$ means the ascendant ordering of the residuals and $n/2 \leq h \leq n$.

Both variants are subject to minimization with respect to the regression parameters, leading to so-called:

1. least median of squares estimator: LMS,

2. least trimmed squares estimator (the fraction of trim being h/n): LTS.

8.5.2 Efficiency

The efficiency of such procedures has been studied theoretically. The LTS estimator has been shown to be more efficient than the LMS estimator and to be as efficient (up to a constant) as the classical LS estimator.

It can therefore be recommended to use the LTS estimator even with a high level of protection i.e. 50 %.

8.5.3 Algorithm

As suspected before, the global minimum of such a quantity as trimmed squares of the residual is not so easy to reach. Indeed iterative methods must be used but nevertheless two points should be pointed out:

1. there exists generally many local minima to the objective function,
2. there exists no obvious initial value for an iterative method, and in particular, least squares solution is generally a bad initial value leading to a local minimum.

Fortunately, many softwares implementation are now available and consequent improvements have been made. Such procedures are indeed available in S/R or SAS systems.

8.5.4 Protocol

In practice, what is to be down ?

- First accept that a part of the data may be spoiled or what is equivalent accept to leave out part of the data in order to have more confidence on the prediction formula.

  The percentage suggested is about 5 % (former studies of the homologation reports gives an interval of 3 to 7 %). A more precise study could be to let the percentage vary from say 2 to 10 % in order to get a best appreciation of the real percentage.

- Then use least trimmed squares procedures to adjust regression (or equivalent other method: for PLS minimal volume estimation can be used) and identify influent data by decreasing order of influence.

- Status then on these data (are they considered as acceptable or not ?), some arguments should be given here and specially reference to information obtained during the trial.

- Perform the classical (without outliers and influential observations) on the restricted set of data.

- Calculate the required criterion (RMSEP) with the suspicious data considered in the calculation.

Chapter 9

Estimation and validation in practice. Examples

By David Causeur, Bas Engel, Maria Font i Furnols and Søren Højsgaard

9.1 Available software

It would be too ambitious to pretend proposing a comprehensive list of the solutions to actually run rank-reduced methods for many softwares have been edited since the first one in the mid-1980s. This pioneering software, called LVPLS, was for a long time the only solution for practitioners. The current version runs in DOS and is freely distributed by Mc Ardle J. (1987). We are only intending here to list some packages that can be used to establish prediction formulæwith rank-reduced methods. Furthermore, we have chosen to focus on PLS packages since OLS functions are usually included in all the statistical softwares and also since PCR functions are most of the times delivered in the PLS packages.

Some widely spread statistical softwares such as SAS or Splus propose their own PLS packages. For instance, the SAS system version 6.11 includes an experimental PROC PLS and version 8 has the definitive one. Online documentation (in Adobe PDF format) is available by Tobias R.D. (1997a, 1997b). At the same time, public domain PLS procedures were also developed, initially for the non-commercial version of Splus called R (that can be downloaded at http://cran.r-project.org/). The idea behind R is clearly to propose a free copy of the Splus programming environment. However, note that in the last ten years, Splus have improved its commercial attractiveness by adopting a Windows-like aspect which makes it possible to run some usual data analysis through toolbars and dialog boxes instead of the programming environment. The PLS package is currently not running through toolbars but only in the programming environment. This package was based on Denham (1995) and can be downloaded freely (the free

download at http://cran.r-project.org/src/contrib/Devel/ includes minimal documentation). A port of a Denham (1995)s S/S-Plus implementation is available in the Carnegie-Mellon S archive (http://lib.stat.cmu.edu/S/), which also includes Fortran and Matlab implementations of the algorithm.

Finally, it must be noted that GENSTAT 5 (details about this software can be found at http://www.nag.co.uk/stats/TT_soft.asp) implements PLS and also that some other commercial software especially dedicated to PLS analysis are until recently available. Most of the times, they enable a more detailed examination of the prediction properties. Their working environment is quite easy to discover since all the analysis are available by toolbars, whereas SAS or R/Splus appeals for a prior knowledge of the programming environment. As an example, The Unscrambler from Camo Inc (www.camo.no) implements PLS, including jackknife-based significance testing.

9.2 A worked example

9.2.1 Description of data

The ideas and models discussed below have been evaluated on a small dataset consisting of measurements on 344 carcasses delivered to three Danish abattoirs. At two abattoirs, 150 normal carcasses were measured. At the third abattoir additionally 44 large carcasses were measured. The distribution of the carcasses among the three slaughterhouses and in different weight groups is shown in Table 9.1 together with the average LMP.

Table 9.1: Distribution of carcasses among the three slaughterhouses and in different weight groups and the average LMP.

Abattoir	(60,70]	(70,75]	(75,80]	(80,90]	(90,105]	LMP
1	35	54	43	18	0	59.2
2	35	48	41	26	0	59.7
3	0	0	0	17	27	58.7

Fat and meat depth was measured on several locations together with slaughter weight, length and other physical characteristics. The locations of the measurements are shown in Figure 9.1.

9.2.2 Doing it in R/Splus

Preliminaries: general issues on R and Splus

Most of the commands that are used in the programming environment can roughly be described by the following generic command:

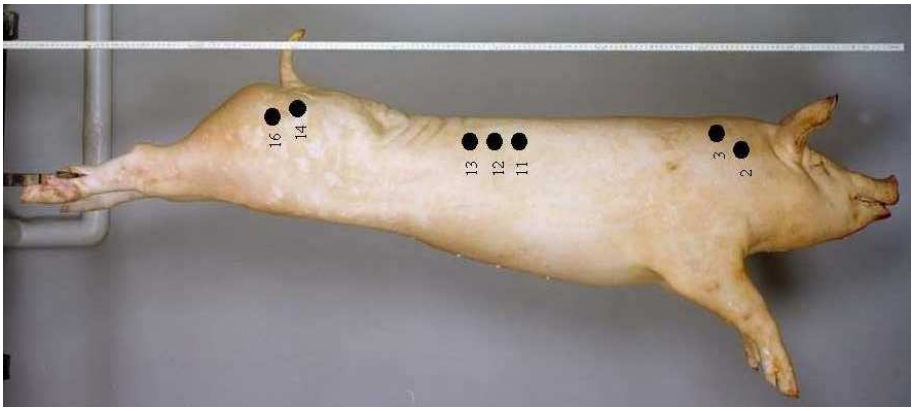


Figure 9.1: Locations of the measurements of the 344 pig carcasses in the study.

```
> result <- func(arg1,arg2,...)}
```

where `>` is the usual prompt, `result` stand for the R/Splus object that contains the values resulting from the application of the function `func` with the arguments `arg1, arg2, ...` .`<-` is used to direct the results into the object `result`.

To edit the results, just type `result` in the commands window or, in the case the function delivers many results, each partial result can be edited by the commands `result$part1, result$part2, ....`

Importing the data

Data files coming from almost any other software dedicated to the management or the statistical analysis of databases can be imported into Splus very easily, thanks to toolbars and dialog boxes. If data are imported by the commands window, they are supposed to be in a `text` file. For instance, call `EUdata.txt` the file containing the dataset, the following commands will create a R/Splus version of this dataset:

```
> EUdata <- read.table("EUdata.txt",header=TRUE)
```

where `header` is an optional boolean argument that must be set to `TRUE` when the first line of the data file contains the names of the variables. Some basic functions can be used to check the success of the importing procedure. For instance, the function `dim` gives the numbers of rows and columns of `EUdata`:

```
> dim(EUdata)
[1] 344  25
```

Another useful example that edits the names of the variables in the data set:

```
> names(EUdata)
 [1] "P.weight" "SEX"      "P.length" "P.forb"   "P.skam"   "F02"
 [7] "F03"      "F11"      "M11"      "F12"      "M12"      "F13"
[13] "M13"      "F14"      "F16"      "LMP96"    "SL.house" "A"
[19] "B"        "C"        "D"        "E"        "F"        "G"
[25] "H"
```

It will be helpful for the following calculations to create two separate objects from the data set: one is called `X` and contains the values of the instrumental predictors and the other one is called `Y` and contains the response values:

```
X <- EUdata[ ,c(1,3:15)]
Y <- EUdata[ ,16]
```

In the former commands, 14 variables have been collected in `X`: the first column of `EUdata` and the 3rd to 15th columns, whereas `Y` corresponds to the 16th column.

Analysis of the redundancy

It has been mentioned above that some classical tools of exploratory data analysis can be very useful to exhibit some kind of structure in the dependencies between the variables. Principal Component Analysis can for instance be used to re-organize the variables in order to point out poorly correlated blocks of variables with high intra-block correlations. In the present situation, the re-organization is rather intuitive since the instrumental predictors can be divided into three natural groups: meat (`M11, M12, M13`) or fat (`F02, F03, F11, F12, F13, F14, F16`) layers and physical characteristics (`P.weight P.length P.forb P.skam`).

Simple commands are available in R and Splus to re-organize the instrumental predictors to make more obvious the natural groups of variables:

```
neworder <- c(5,6,7,9,11,13,14,8,10,12,1,2,3,4)
X <- X[ ,neworder]
```

where `neworder` contains the vector of permuted column indices that enables a better exposition of the predictors. Up to now, the previous `X` matrix is replaced by its re-organized version. The needed correlations can be calculated:

```
> round(cor(X,Y),2)
         [,1]
    F02 -0.59
    F03 -0.55
    F11 -0.75
    F12 -0.74
    F13 -0.70
    F14 -0.76
    F16 -0.73
    M11  0.26
    M12  0.23
    M13  0.31
P.weight -0.09
P.length -0.05
  P.forb -0.01
  P.skam -0.09
> round(cor(X),2)
          F02  F03   F11   F12  F13  F14  F16  M11  M12   M13 P.w  P.l  P.f  P.s
     F02 1.00 0.76  0.61  0.62 0.63 0.60 0.64 0.11 0.14  0.06 0.45 0.20 0.16 0.16
     F03 0.76 1.00  0.61  0.61 0.63 0.59 0.61 0.15 0.19  0.08 0.48 0.27 0.24 0.19
     F11 0.61 0.61  1.00  0.84 0.82 0.74 0.77 0.04 0.08 -0.03 0.28 0.04 0.04 0.02
     F12 0.62 0.61  0.84  1.00 0.83 0.77 0.77 0.04 0.01 -0.03 0.33 0.07 0.10 0.06
     F13 0.63 0.63  0.82  0.83 1.00 0.75 0.77 0.13 0.11  0.02 0.40 0.14 0.16 0.09
     F14 0.60 0.59  0.74  0.77 0.75 1.00 0.86 0.03 0.05  0.02 0.27 0.05 0.05 0.00
     F16 0.64 0.61  0.77  0.77 0.77 0.86 1.00 0.07 0.07  0.05 0.38 0.14 0.15 0.09
     M11 0.11 0.15  0.04  0.04 0.13 0.03 0.07 1.00 0.87  0.86 0.56 0.26 0.36 0.16
     M12 0.14 0.19  0.08  0.01 0.11 0.05 0.07 0.87 1.00  0.90 0.47 0.18 0.27 0.09
     M13 0.06 0.08 -0.03 -0.03 0.02 0.02 0.05 0.86 0.90  1.00 0.48 0.20 0.28 0.10
P.weight 0.45 0.48  0.28  0.33 0.40 0.27 0.38 0.56 0.47  0.48 1.00 0.71 0.75 0.52
P.length 0.20 0.27  0.04  0.07 0.14 0.05 0.14 0.26 0.18  0.20 0.71 1.00 0.90 0.83
  P.forb 0.16 0.24  0.04  0.10 0.16 0.05 0.15 0.36 0.27  0.28 0.75 0.90 1.00 0.75
  P.skam 0.16 0.19  0.02  0.06 0.09 0.00 0.09 0.16 0.09  0.10 0.52 0.83 0.75 1.00
```

where `round(...,2)` is an editing function that prints numbers in a rounded version with 2 digits.

Note that intra-block correlations are around 0.7 for fat layers, 0.9 for meat layers and 0.7 for physical characteristics, whereas inter-block correlations are rather low as expected. As usually observed in the pigs classification data, the LMP is highly correlated with the fat layers, poorly correlated with the meat layers and almost non-correlated with the physical characteristics.

Running OLS

First, let us edit a short report of the OLS fit with all the instrumental predictors in the regression model:

```
> EUdata.ols <- lsfit(X,Y)
> ls.print(EUdata.ols)
Residual Standard Error = 1.6477,  Multiple R-Square = 0.7987
N = 344,  F-statistic = 93.2198 on 14 and 329 df, p-value = 0

              coef std.err   t.stat p.value
Intercept  82.7738  3.6912  22.4249  0.0000
      F02  -0.2116  0.0645  -3.2787  0.0012
```

```
      F03  -0.0525  0.0507  -1.0362  0.3009
      F11  -0.2359  0.0590  -3.9965  0.0001
      F12  -0.1606  0.0668  -2.4050  0.0167
      F13  -0.0858  0.0695  -1.2347  0.2178
      F14  -0.3382  0.0608  -5.5602  0.0000
      F16  -0.1315  0.0536  -2.4550  0.0146
      M11   0.0367  0.0373   0.9842  0.3257
      M12   0.0089  0.0342   0.2612  0.7941
      M13   0.0933  0.0373   2.5010  0.0129
 P.weight   0.1301  0.0247   5.2743  0.0000
 P.length  -0.0326  0.0438  -0.7458  0.4563
   P.forb  -0.0649  0.0496  -1.3093  0.1913
   P.skam  -0.1811  0.0848  -2.1358  0.0334
```

It clearly appears in the former report that some kind of redundancy in the instrumental predictors could be avoided by selecting a subset of relevant predictors. Some native functions are dedicated to such a selection in R and Splus provided the validation criterion is either the Mallows C_p, the R^2 or its adjusted version. However, these functions are not easy to adapt to the validation criterion recommended in section 2.3. Therefore, we have created our own new functions that first calculate the RMSEP criterion by a full cross-validation method and then rank the subset of predictors relative to their predictive ability. These functions are provided in appendix B. First, let us calculate the RMSEP obtained by OLS with all the predictors:

```
> rmsep.ols(X, Y)
[1] 1.6928
```

Now, let us investigate in all the possible subsets of predictors to look for the best ones:

```
> bestones <- bestrmsep.ols(X, Y)
> bestones$labels
$"1":
[1] "F14"
$"2":
[1] "F14" "M13"
$"3":
[1] "F11" "F14" "M13"
$"4":
[1] "F11"    "F14"    "M13"    "P.skam"
$"5":
[1] "F02"    "F11"    "F14"    "M13"    "P.skam"
...
> round(bestones$minrmsep,2):
```

```
   1    2    3    4    5    6    7    8    9   10   11   ...
2.36 2.04 1.82 1.78 1.76 1.72 1.70 1.69 1.68 1.68 1.68   ...
```

Visualizing the trace of the minimal RMSEP for subsets of equal number of predictors is possible by the following commands:

```
> plot(1:14,bestones$minrmsep,type="b",pch=3,
xlab="Number of predictors",ylab="RMSEP",
main="Best subsets of predictors")
> text(1:4,bestones$minrmsep[1:4],bestones$labels[1:4])
```

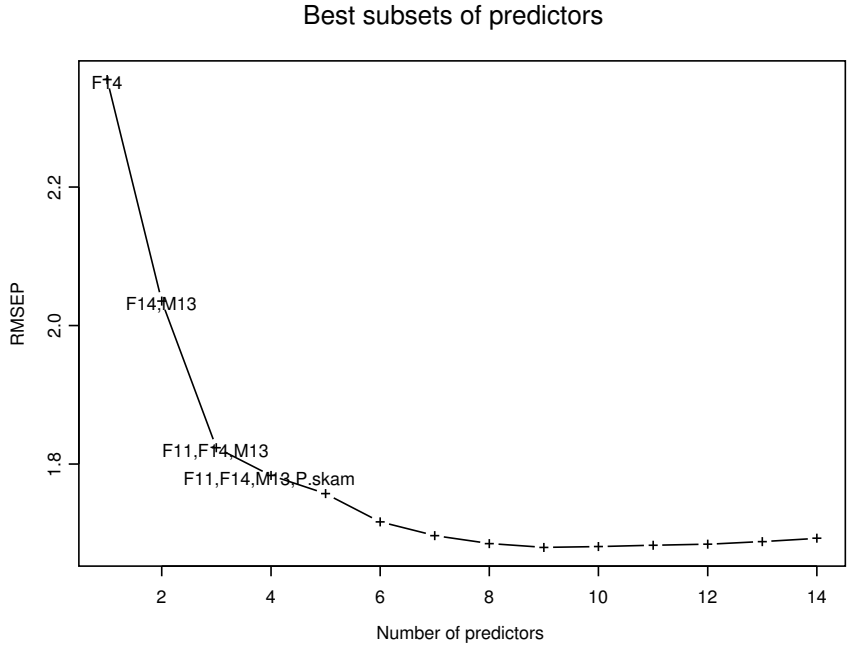


Figure 9.2: Trace graph to select the best subset of instrumental predictors

The graph produced by the previous command is displayed in figure 9.2. With respect to this graph, we would personally recommend to consider that 4 predictors have to be kept in the chosen model, since the gain resulting from adding some other predictors is not so important. According to this choice, the calculations point out the subset containing F11, F14, M13 and P.skam as the best one with a RMSEP equal to 1.78.

Let us edit a short report of the OLS fit with only these 4 predictors in the regression model:

```
> best.ols <- lsfit(X[, bestones$subsets[[4]]], as.numeric(Y))
```

```
> ls.print(best.ols)
Residual Standard Error = 1.7668,  Multiple R-Square = 0.7615
N = 344,  F-statistic = 270.5294 on 4 and 339 df, p-value = 0

              coef std.err   t.stat p.value
Intercept  74.5122  2.5803  28.8778       0
      F11  -0.4002  0.0425  -9.4191       0
      F14  -0.5606  0.0459 -12.2196       0
      M13   0.1802  0.0149  12.0640       0
   P.skam  -0.2057  0.0494  -4.1658       0
```

Running PLS

The PLS package based on Denham (1994) is used here. First, let us chose the proper number of latent variables.

```
> LMPpls <- pls(X,Y,validation="CV",grpsize=1)
> LMPpls$validat$RMS
             [,1]
 1 LV's 1.989200
 2 LV's 1.838436
 3 LV's 1.758272
 4 LV's 1.678250
 5 LV's 1.706633
 6 LV's 1.693239
 7 LV's 1.693916
 8 LV's 1.691238
 9 LV's 1.692060
10 LV's 1.693143
11 LV's 1.692832
12 LV's 1.692802
13 LV's 1.692800
14 LV's 1.692800
```

The previous results gives the RMSEP calculated by the leave-one-out method for every possible number of PLS components. Visualizing the trace of the minimal RMSEP for different number of PLS components is possible by the following command:

```
> plot(1:14,LMPpls$validat$RMS,type="b",pch=3,
xlab="Number of latent variables",ylab="RMSEP")
```

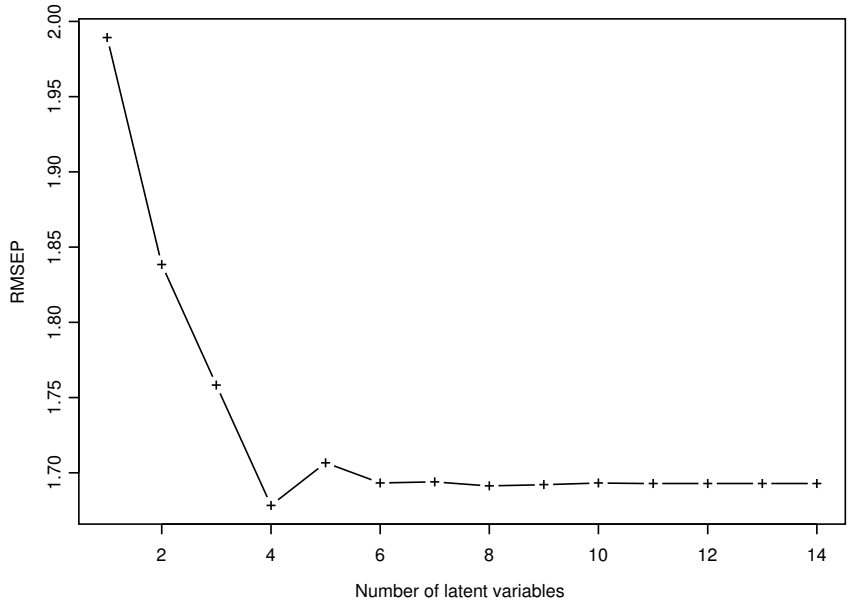


Figure 9.3: Trace graph to select the best number of PLS components

The graph produced by the previous command is displayed in figure 9.3. With respect to this graph, it can be recommended to consider that 4 latent variables have to be kept in the final model. According to this choice, the calculations gives a RMSEP equal to 1.68.

The estimated slope coefficients of the prediction formula are obtained by the following command:

```
> round(LMPpls$training$B[,  , 4], 3)
[1] -0.112 -0.108 -0.216 -0.170 -0.141 -0.231 -0.212  0.062
[9]  0.002  0.079  0.139 -0.085 -0.044 -0.063
```

Running PCR

The PCR functions that are used here are also provided in the PLS package based on Denham (1994). First, let us chose the proper number of latent variables.

```
> LMPpcr <- pcr(X,Y,validation="CV",grpsize=1)
> LMPpcr$validat$RMS
            [,1]
 1 LV's 3.609532
 2 LV's 2.965700
```

```
 3 LV's 1.898612
 4 LV's 1.672098
 5 LV's 1.677329
 6 LV's 1.681840
 7 LV's 1.685620
 8 LV's 1.691075
 9 LV's 1.696127
10 LV's 1.703245
11 LV's 1.695460
12 LV's 1.684851
13 LV's 1.690075
14 LV's 1.692800
```

Visualizing the trace of the minimal RMSEP for different number of PCR components is possible by the following command:

```
> plot(1:14,LMPpcr$validat$RMS,type="b",pch=3,
xlab="Number of latent variables",ylab="RMSEP")
```

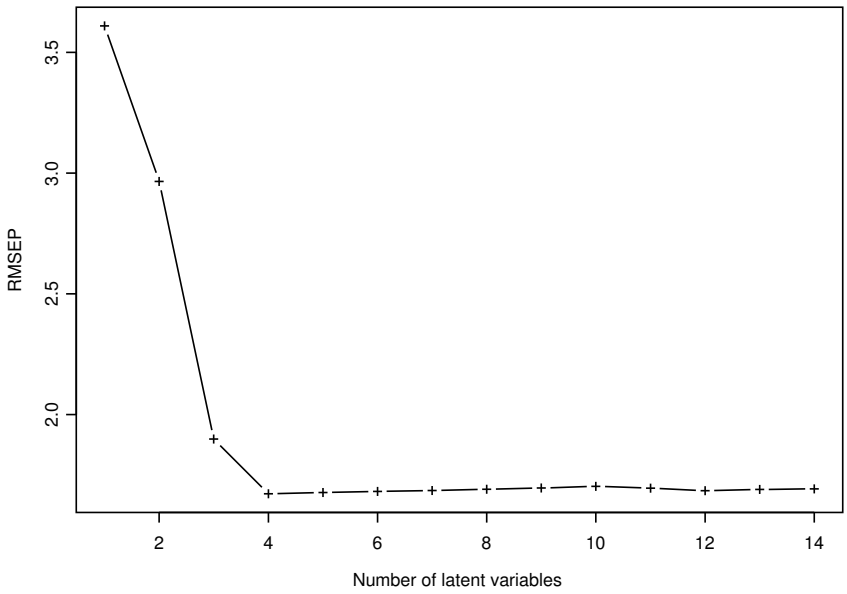


Figure 9.4: Trace graph to select the best number of PCR components

As it was mentioned in chapter 2, the computation of the PCR components do not directly intend to provide the best predictions. This results in the fact that

the PCR prediction model with one or two components are obviously worse than those created with PLS. However, if 4 components are finally kept in the PCR model, as suggested by figure 9.4 the predictive ability of the resulting model, with RMSEP=1.67, is close to the PLS solution.

The estimated slope coefficients of the prediction formula are obtained by the following command:

```
> round(LMPpcr$training$B[,  , 4], 3)
[1]  0.130 -0.089 -0.036 -0.040 -0.086 -0.123 -0.213  0.086
[9] -0.167 -0.005 -0.150  0.070 -0.205 -0.230
```

The near-equivalence between the predictive abilities of OLS, PLS and PCR in the present case is illustrated by the graphs produced by the following commands and displayed in figures 9.5, 9.6, 9.7:

```
> plot(Y,Y-best.ols$residuals,xlab="Observed",
ylab="Predicted",main="OLS",xlim=c(45,70),ylim=c(45,70))
> plot(Y,LMPpcr$training$Ypred[,,4],xlab="Observed",
ylab="Predicted",main="PCR",xlim=c(45,70),ylim=c(45,70))
> plot(Y,LMPpls$training$Ypred[,,4],xlab="Observed",
ylab="Predicted",main="PLS",xlim=c(45,70),ylim=c(45,70))
```

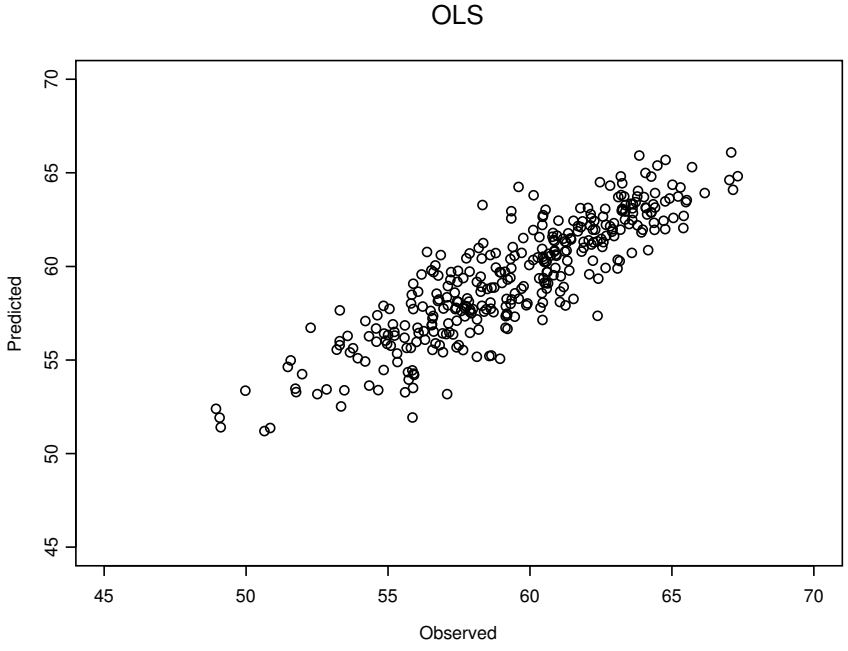


Figure 9.5: Observed LMP vs. Predicted values

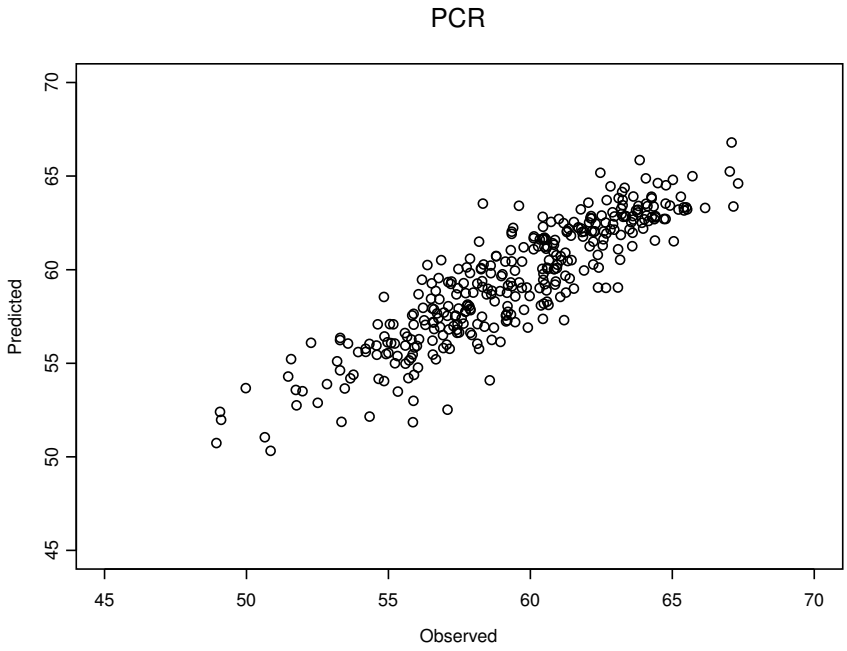


Figure 9.6: Observed LMP vs. Predicted values

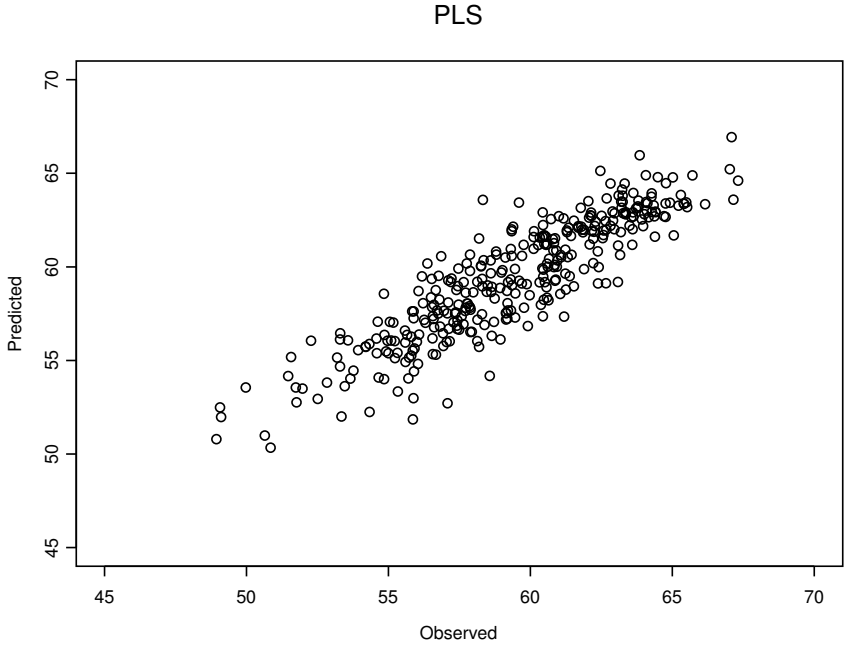


Figure 9.7: Observed LMP vs. Predicted values

9.2.3 Doing it in SAS

By Maria Font i Furnols

A. Multiple regression

A procedure used to do multiple regression is `PROC REG`. Suppose the SAS data set is `ptrain` (located in the temporary library work). To regress LMP (lmp) against the different carcass measurements the following instructions are needed:

```
proc reg data=ptrain;
   model lmp=P_WEIGHT P_LENGTH P_SHOULDER P_PELVIC
             F02 F03 F11 M11 F12 M12 F13 M13 F14 F16;
run;
```

The SAS output is the following:

The REG Procedure
Model: MODEL1
Dependent Variable: LMP

.....

Parameter Estimates

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	82.77382	3.69116	22.42	<.0001
P_WEIGHT	1	0.13012	0.02467	5.27	<.0001
P_LENGTH	1	-0.03264	0.04376	-0.75	0.4563
P_shoulder	1	-0.06490	0.04957	-1.31	0.1913
P_pelvic	1	-0.18112	0.08480	-2.14	0.0334
F02	1	-0.21163	0.06455	-3.28	0.0012
F03	1	-0.05250	0.05066	-1.04	0.3009
F11	1	-0.23591	0.05903	-4.00	<.0001
M11	1	0.03667	0.03726	0.98	0.3257
F12	1	-0.16058	0.06677	-2.40	0.0167
M12	1	0.00895	0.03424	0.26	0.7941
F13	1	-0.08583	0.06952	-1.23	0.2178
M13	1	0.09329	0.03730	2.50	0.0129
F14	1	-0.33818	0.06082	-5.56	<.0001
F16	1	-0.13148	0.05356	-2.46	0.0146

The equation obtained is the following:

lmp= 82.77382 + 0.13012·P_WEIGHT .... - 0.13148·F16

A.a. Methods to select the model. The variables to be included in the model can be selected in order to keep those that have a higher influence and to drop those less important. SAS has the option of different methods to look at it. This can be added as an option after the model and can be, among others the following:

```
/selection=stepwise
/selection=rsquare
/selection=cp   (Mallow's Cp statistic)
```

The option `none` is the default and uses the full model. No one of these models selects for the best RMSEP.

A.b. Calculation of the RMSEP. After the model statement it can be added the option `/PRESS` that let us to have this value in the outset dataset:

```
proc reg data=ptrain outest=value;
model lmp=P_WEIGHT P_LENGTH P_SHOULD P_PELVIC F02 F03 F11 M11 F12
M12 F13 M13 F14 F16 / PRESS;
run;
HER
```

The PRESS obtained was: 985.757. To obtain the RMSEP it is necessary to do:

$$\text{RMSEP} = \sqrt{\frac{\text{PRESS}}{n}}$$

or to run the following:

```
data rmsep;
set value;
RMSEP=SQRT(_PRESS_/344);                /*adapt the n in each case*/
proc print; VAR _press_ RMSEP;
run;
```

So, the RMSEP is 1.69280.

B. Partial least squares regression

In SAS version 8, PLS can be made using the `PLS` procedure. A system of macros can be used with PROC PLS to produce high-resolution plots for the model. These macros can be find in the file `plsplot` (plsplot, 2003) that can be obtained in the following address: `http://ftp.sas.com/techsup/download/stat/.` In the file `plsplote` (plsplote, 2003) in the same web site, and in the SAS v. 8 Manual (included in the SAS program) an example of `PROC PLS` statement can be found. Below, PLS with the example data.

B.a. How to start with PLS Again assume that data are in the SAS data set `ptrain` in the temporary work directory in SAS. The PLS procedure for the `ptrain` data is the following:

```
proc pls data=ptrain outmodel=est1 method=PLS;
   model lmp= P_WEIGHT P_LENGTH P_SHOULD P_PELVIC F02 F03 F11 M11 F12
              M12 F13 M13 F14 F16;
   output out=outpls predicted = yhat1
                     yresidual = yres1
                     xresidual = xres1-xres127
                     xscore    = xscr
                     yscore    = yscr
```

```
                        stdy=stdy  stdx=stdx h=h
                        press=press t2=t2 xqres=xqres yqres=yqres;
run;
```

In the `proc pls` procedure the number of factors to be extracted can be specified (`lv` or `nfac` option). If not specified `pls` extracts as many factors as input factors. After the outmodel option, the name for a data set to contain information about the fit model has to be written (for instance: `est1`).

By default, PLS is performed with responses and predictors that are centered and scaled before fitting. If `noscale` is added after `proc pls` the scaling is not performed, as well as the centering if `nocenter` is added.

If the

```
METHOD (method=factor-extraction-method)
```

option is not specified, by default PLS is the factor extraction method. Of course it can also be specified `method=pls`.

If the `output out` option is included (optional), the predictions, residuals, scores and other information can be found in the out data set (named `outpls` in the example). These values can be used later on to detect data irregularities.

The table displayed from this PLS procedure is the following:

The PLS Procedure

Percent Variation Accounted for
by Partial Least Squares Factors

Number of Extracted Factors	Model Effects		Dependent Variables	
	Current	Total	Current	Total
1	37.8501	37.8501	71.5594	71.5594
2	28.2036	66.0536	5.1801	76.7395
3	13.6456	79.6992	1.3162	78.0557
4	5.5932	85.2924	1.4023	79.4580
5	3.5230	88.8154	0.2825	79.7405
6	1.6259	90.4413	0.1205	79.8610
7	2.1442	92.5855	0.0045	79.8654
8	1.4419	94.0274	0.0008	79.8663
9	1.3820	95.4094	0.0001	79.8663
10	1.1314	96.5408	0.0000	79.8663
11	0.8361	97.3769	0.0000	79.8663
12	0.7891	98.1660	0.0000	79.8663
13	0.9231	99.0891	0.0000	79.8663
14	0.9109	100.0000	0.0000	79.8663

In this results it is obtained how much predictor and response variation is explained by each PLS component. It can be seen that the percentage of variation in the dependent variable does not change a lot after the first factors. Next step is to select the number of extracted factors by cross-validation.

B.b. Selection of the number of factors: cross-validation, press statistic. In order to validate the model and choose the number of PLS components some forms of cross-validation can be used. Cross-validation is a validation

method where some samples are kept out of the calibration and used for prediction. This is repeated until all samples have been kept out once and the overall capability of the model can be measured. There are several different types of cross-validation that can be done: block, split, random, test set and one. The recommended is the one-at-a time or leave-one-out cross validation, which is the cross validation SAS performs by default. However, it also can be specified after the option `cv`, as `cv=one`.

After the cross-validation the number of extracted factors can be determined as the one that present the minimum root mean PRESS.

Sometimes models with fewer factors have PRESS statistics that are only marginally larger than the absolute minimum. Although cross-validation helps in selecting the number or PLS components, it should not be used blindly, because sometimes it can overfit the data, which means it fits the observations used in the modelling well but will predict new observations poorly.

`Proc pls` has the option (`cvtest`) to apply van der Voet's test in order to test whether this difference is significant. By default `cvtest` uses Hotelling's T^2 statistic as a test statistic for the model comparison. If `stat=PRESS` is written in parentheses after this option, PRESS statistic is used. The default cut-off probability to consider significant difference is 0.1, but it can be changed (option `pval=n` in parenthesis after cvtest option).

An example of `proc pls` that uses one-at-a-time cross-validation is showed bellow. In that example Hotelling's T^2 test (a) or PRESS test (b) is performed in order to know the number of extracted factors. Both can be done and results can be compared.

```
(a) proc pls data=ptrain outmodel=est1 method=pls cv=one cvtest;
(b) proc pls data=ptrain outmodel=est1 method=pls cv=one cvtest(stat=PRESS);
```

The results are the following:

```
(a) Cross Validation for the Number of Extracted Factors
```

Number of Extracted Factors	Root Mean PRESS	T**2	Prob > T**2
0	1.002915	90.55304	<.0001
1	0.539445	18.51642	<.0001
2	0.490167	4.537484	0.0280
3	0.4792	1.535283	0.2290
4	0.46998	0.009844	0.9180
5	0.469683	0	1.0000
6	0.470811	0.354835	0.5580
7	0.470861	0.3668	0.5490
8	0.471032	0.467607	0.4850
9	0.471233	0.620087	0.4180
10	0.471354	0.717061	0.3900
11	0.471387	0.74558	0.3860
12	0.471388	0.746142	0.3850
13	0.471388	0.746366	0.3850
14	0.471388	0.746383	0.3850

```
Minimum root mean PRESS                      0.4697
Minimizing number of factors                      5
Smallest number of factors with p > 0.1           3

(b) Cross Validation for the Number of Extracted Factors

          Number of        Root
          Extracted        Mean    Prob >
            Factors       PRESS     PRESS

                  0    1.002915    <.0001
                  1    0.539445    <.0001
                  2    0.490167    0.0130
                  3      0.4792    0.1050
                  4     0.46998    0.4800
                  5    0.469683    1.0000
                  6    0.470811    0.2850
                  7    0.470861    0.2800
                  8    0.471032    0.2490
                  9    0.471233    0.2190
                 10    0.471354    0.2050
                 11    0.471387    0.1990
                 12    0.471388    0.1990
                 13    0.471388    0.1990
                 14    0.471388    0.1990


Minimum root mean PRESS                      0.4697
Minimizing number of factors                      5
Smallest number of factors with p > 0.1           3
```

In both cases the number of extracted factors is 3, so we obtain the following percentage of variance accounted for :

```
Number of Extracted        Model Effects        Dependent Variables
  Factors     Current       Total     Current       Total

        1     37.8501     37.8501     71.5594     71.5594
        2     28.2036     66.0536      5.1801     76.7395
        3     13.6456     79.6992      1.3162     78.0557
```

B.c. Detection of irregularities in the data: possible outliers. By means of the plots and other variables obtained using the SAS macros cited above, some outliers can be selected. First of all, the file `plsplot`, which includes the macros, has to be run, in order to have them in the temporal library "works". Before preparing the following plots some parameters have to be defined:

```
%global xvars yvars predname resname xscrname yscrname num_x num_y lv;
%let xvars= P_WEIGHT P_LENGTH P_SHOULD P_PELVIC F02 F03 F11 M11 F12 M12 F13 M13 F14 F16;
  %let yvars= lmp;
  %let ypred=yhat1;       Predicted values for responses
  %let yres=yres1;        Residuals for responses
  %let predname=yhat;
  %let resname=res;
  %let xscrname=xscr;     Names of scores in output data set
  %let yscrname=yscr;
  %let num_y=1;           Number of variables in the data set
  %let num_x=14;
  %let lv=3;              Number of extracted factors
```

as well as the n:

```
data ptrain;
set ptrain;
n=_N_;
run;
```

Plot X-score vs. Y-score. PLS algorithms choose successive orthogonal factors that maximize the covariance between each X-score and the corresponding Y-score. For a good PLS model, the first few factors show a high correlation between the X- and Y-scores. The correlation usually decreases from one factor to the next.

The relationship between X-scores and Y-scores is a summary of the relationship between X and Y along a specific model component. This relationship can be visualized calling the following macro:

```
%plot_scr(outpls);
```

Figure 9.8 plots X-score vs. Y-score for the first extracted factor. The same plot but for the second and third extracted factors are also obtained (results not showed). X- and Y-scores are highly correlated for the first extracted factor but somewhat less correlation for the second component, and much more less correlation for the third. For the first factor, observation 187 is the one with less correlation between scores, but this is not extreme in the other plots.

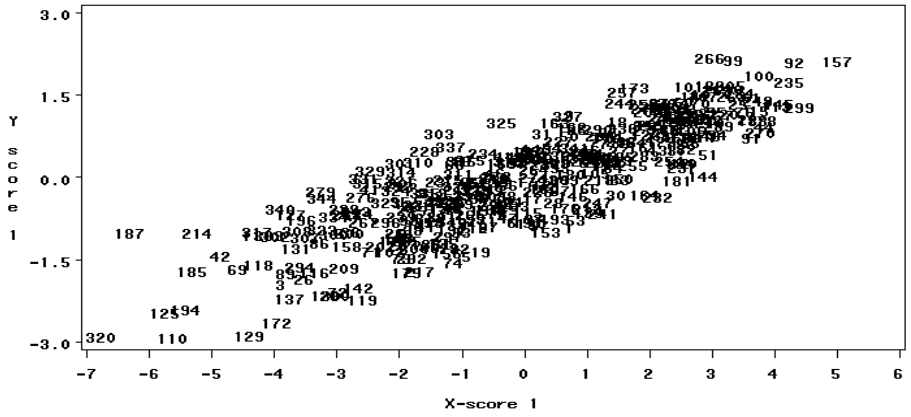


Figure 9.8: X-scores vs. Y-scores for the first extracted factor

Plot X-scores against each other. To check for irregularities in the predictors, such as outliers or distinct groupings, we should plot the X-scores against each other. It can be done using the following statement to call the macro.

```
%plotxscr(outpls,max_lv=3);
```

The plot of the first and second X-scores is shown in Figure 9.9. This plot appears to show most of the observations close together, with a few being more spread out with larger negative X-scores for component 1. There are not any distinct grouping patterns in the plot, which would indicate some kind of sub-populations.

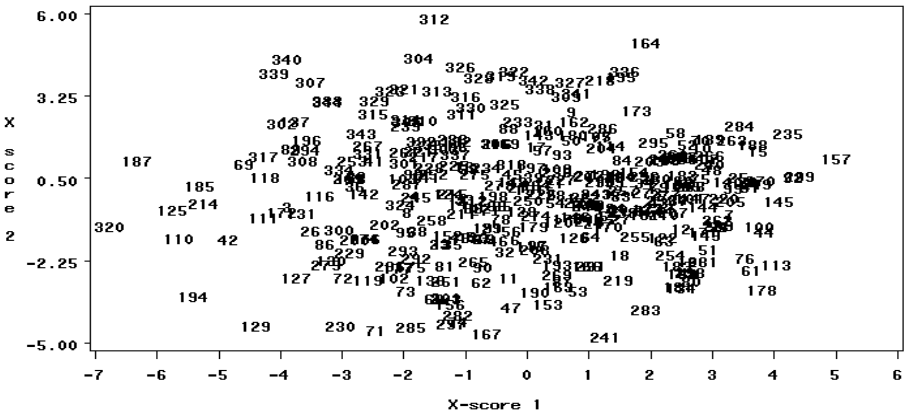


Figure 9.9: First and second X-scores.

Residual plots and normal quantile plots. These plots help in detecting outliers that might be harming the fit; also help in detecting non-linearities or lack of fit, non-normality, autocorrelations, and heteroscedasticity, all of which can cause various problems in constructing confidence and tolerance bounds for predictions. The ideal residual plot presents the residuals randomly distributed, free from systematic trends. In an ideal normal plot, the points fall on a straight line. It is possible to produce the plots of residuals versus predicted values and the normal quantile plot of the residuals calling the following macros respectively.

```
%res_plot(outpls);
%nor_plot(outpls);
```

Figure 9.10 shows the residuals versus the predicted lean meat percentage values. This plot shows nothing unusual.

The normal quantile plot of lean meat percentage residuals (Figure 9.11) shows a distribution in which some observations are more extreme at the lower and higher end.

Euclidean Distances. Another way to check for outliers is to look at the Euclidean distance from each point to the PLS model in both, X and Y. No point should be dramatically farther from the model than the rest. If there is a

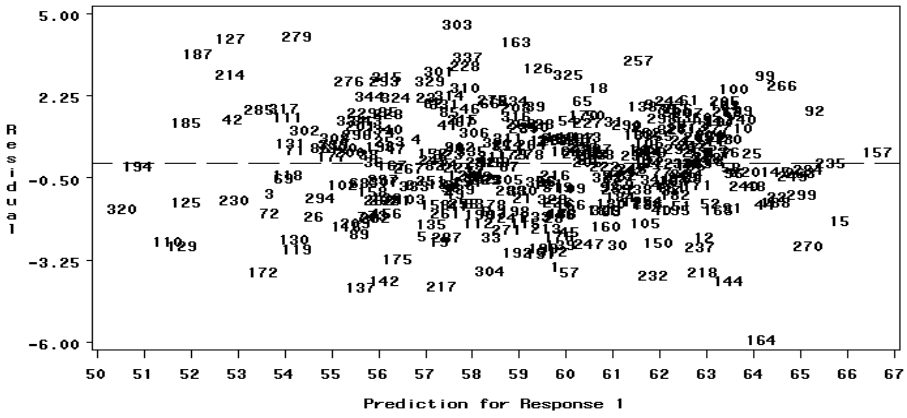


Figure 9.10: Residuals versus predicted lean meat percentage values.

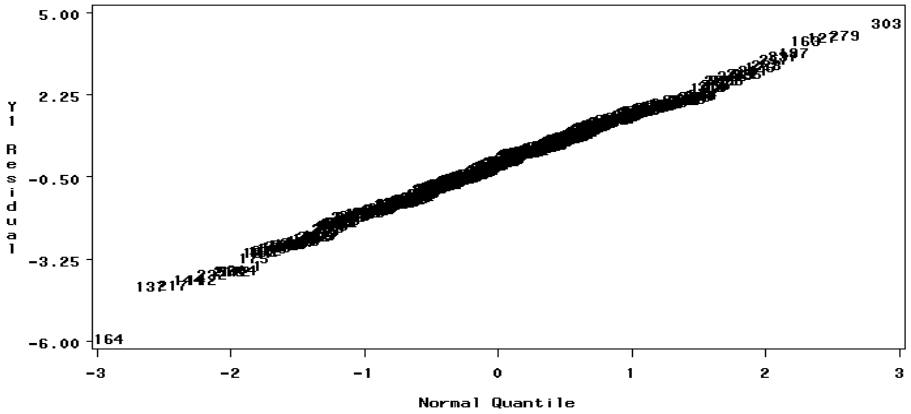


Figure 9.11: Normal quantile plot of lean meat percentage residuals.

group of points that are all farther from the model than the rest, maybe they have something in common and should be analyzed separately. The next statement computes and plots these distances to the model:

```
%get_dmod(outpls,dsdmod=distmd,qresname=qres,id=n);

proc gplot data=distmd;
    plot dmodx*n;
    plot dmody*n;
    symbol1 i=needless v=dot;
    symbol2 i=needless v=dot;
run;
```

The plots for the Euclidean distances for x-variable is reproduced in Figure 9.12 (results not showed for the y-variable).

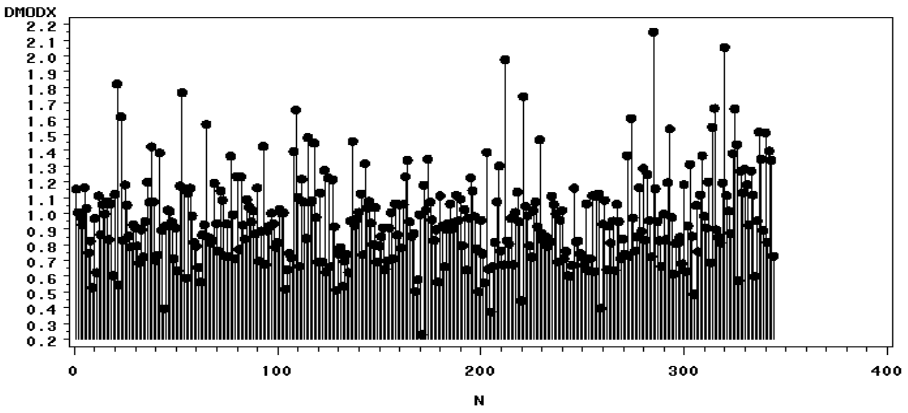


Figure 9.12: Euclidean distances from the X-variables to the model.

With the plot it is difficult to identify the samples, so, if it is necessary to identify some samples in order to remove them, it would be good to output the value of these distances. It can be done with the following statement:

```
proc print data=distmd; run;
```

In the first plot some samples are higher than the others (212,320 and 285), but not dramatically higher. In the second one (not showed), sample 164 is the highest.

It is always difficult to decide if any sample is an outlier. SAS do not give any criteria to select them. If we look at the plot (Figure 9.12) only sample 164 (only in the first one) is far from the others.

It is necessary to check the raw data in order to know if there were a problem in it. In that case it would be a good exercise to consider sample 164 as an outlier, drop down this sample and repeat the PLS analysis in order to look at the new results.

Nevertheless in this example we are going to let this observation in the data set.

B.d. Selection of the explanatory variables. Plots of the weights give the direction toward which each PLS factor projects. They show which predictors are most represented in each factor. Those predictors with small weights are less important than those with large weights (in absolute value).

Plot X-weights and X-loadings. The X-weights W represent the correlation between the X-variables and the Y-scores. The Y-loadings represent the correlation between the lmp (Y-variable) and the X-scores. The X-loadings represent how much the X-variable contributes to a specific model component. The X-loadings and X-weights are usually very similar to each other. To produce the X-weights plots, first a macro that compute the weights for each PLS component has to be called and then, the macro that plots the X-weights. So, the following statements:

```
%get_wts(est1,dsxwts=xwts);
%plot_wt(xwts,max_lv=3);
```

It is also possible to plot the X-loadings, with the following statement, but the results are similar to those obtained for the X-weights and they are not presented.

```
%getxload(est1,dsxload=xloads);
%pltxload(xloads,max_lv=3);
```

One of the results of these macros is plot in Figure 9.13 (previously arranged) (the plot of the X-weights for the 2nd and 3rd X-scores are not presented).

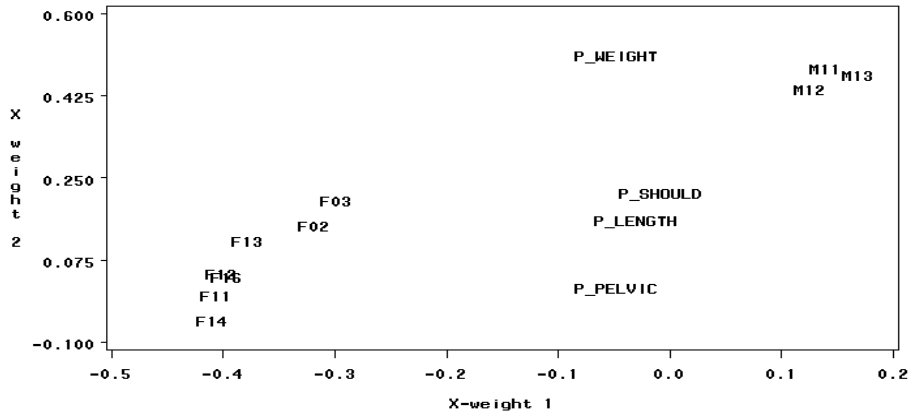


Figure 9.13: First and second X-weights.

The plot of the X-weights shows three clusters of variables. One of them composed by the different fat thickness measurements (F), the other for the muscle thickness measurements (M) and the last one for the physical characteristics (P). The weight of the carcass is not clearly defined in any of these clusters. Physical variables are situated nearly zero for the first factor. So, they add little to the model fit (first axis) however they had some importance in the second or third factors. The plot helps in the visualization of the weight of the variables but it would be better to have a more subjective method to decide which variables

should be drop out of the model. SAS User's Guide (included in the SAS program) suggests another method to determine if any factor has to be removed, using the regression coefficients and the variable importance for the prediction, explained in the next point.

Regression coefficients (B) and variable importance for the projection (VIP). In order to determine which factors to eliminate from the analysis, SAS proposes to look at the regression coefficients in the B (PLS) matrix and at the Variable Importance for the Projection (VIP) of each factor. The regression coefficients represent the importance each factor has in the prediction of the lean meat percentage. The VIP represents the value of each autofom variable in fitting the PLS model for both predictors and responses.

The following statement obtains B coefficients and VIP values and produces a list of them:

```
%get_bpls(est1,dsout=bpls);
%get_vip(est1,dsvip=vip_data);
data eva1; merge bpls vip_data; run;
proc print data=eva1; run;
```

Following SAS User's Guide instructions, if a predictor has a relatively small coefficient (in absolute value) and a small value of VIP (Wold, (1994), cited by SAS User's Guide considers less than 0.8 to be "small"), then it is a prime candidate for deletion.

The results are the following (marked with two asterisks variables with low values of B1 and VIP and with one asterisk variables with only low levels of VIP):

Obs	X_VAR	B1	VIP	
1	P_WEIGHT	0.08619	0.52406	**
2	P_LENGTH	-0.03503	0.28177	**
3	P_SHOULD	-0.01391	0.28278	**
4	P_PELVIC	-0.08579	0.35822	**
5	F02	-0.09529	1.12025	
6	F03	-0.07165	1.06235	
7	F11	-0.16942	1.41771	
8	M11	0.12408	0.66437	*
9	F12	-0.14545	1.40113	
10	M12	0.10257	0.60322	*
11	F13	-0.12098	1.32585	
12	M13	0.13524	0.73518	*
13	F14	-0.19579	1.43623	
14	F16	-0.15902	1.38373	

The physical variables are those with low VIP value (¡0.8) and the lowest coefficient values. This result suggest that they can be kept out of the model and are in accordance with Figure 9.13. Nevertheless these variables are important for the 2nd or 3rd components (plot not showed), so they will be kept in the model. In case to keep them out of the model, the PLS has to be repeated for the reduced model.

B.e. Regression equation. In the point **B.d**, the regression coefficients were found. However, these coefficients are the parameters estimates for centered and scaled data. It is necessary to make a transformation of the matrices in order to obtain the parameter estimates of the raw data, so, the data obtained directly from the KC and the physical measurements.

In SAS version 8.0, there is an option that gives you these coefficients directly. This option does not exist in version 6.1. In order to obtain these coefficients `/solution` has to be added after the model, as is showed below.

```
proc pls data=ptrain outmodel=est1 method=PLS lv=3;
   model lmp= P_WEIGHT P_LENGTH P_SHOULDER P_PELVIC
              F02 F03 F11 M11 F12 M12 F13 M13 F14 F16
              /solution;
run;
```

In version 8 it is also possible to obtain the details of the fitted model for each successive factor (option `details` in the `proc pls` statement). The equation obtained has the following estimated parameters:

```
Intercept       74.75168808
P_WEIGHT         0.03880723
P_LENGTH        -0.02133746
P_SHOULD        -0.01079795
P_PELVIC        -0.15875736
F02             -0.14454850
F03             -0.08501179
F11             -0.18064572
F12             -0.17497353
F13             -0.15735502
F14             -0.22559589
F16             -0.15410603
M11              0.07759910
M12              0.05118159
M13              0.07544520
```

The centered and scaled parameters are

```
Intercept      0.0000000000
P_WEIGHT       0.0861931107
P_LENGTH       -.0350321806
P_SHOULD       -.0139076643
P_PELVIC       -.0857945001
F02            -.0952859962
F03            -.0716460553
F11            -.1694195692
F12            -.1454493558
F13            -.1209773093
F14            -.1957865229
F16            -.1590170073
M11            0.1240823100
M12            0.1025652907
M13            0.1352409513
```

with a minimum root mean PRESS of 0.4792.

B.f. RMSEP SAS calculates the PRESS dividing by $n-1$. It implies that the root mean PRESS (RMPRESS) has not exactly the same result as RMSEP calculated as explained before in this handbook. However this can be calculated by means of the following operations:

1. Calculate the PRESS from the Root mean RMPRESS given by SAS as:

$$\text{PRESS} = n(\text{RMPRESS})^2$$

2. Change the divisor of the PRESS (calculated by $n-1$) and obtain the new PRESS calculated dividing by n (say NPRESS):

$$\text{NPRESS} = \frac{n-1}{n}\text{PRESS}$$

3. Find the RMSEP as the root mean of the new PRESS

$$RMSEP = \sqrt{\frac{\text{NPRESS}}{n}}.$$

Otherwise, the macro provided in appendix B can be used.

After running the macro it is necessary to call it and the following statement have to be done in our case:

```
%rmsepls(ptrain,sel_lv=3);
```

The result obtained is the following

```
rmsep

1.72085
```

B.g. Prediction for the remaining observations. In order to make predictions for another set of data (say test) the last equation can be used. It is also possible to obtain the predicted values directly from SAS, appending the test set to the training set with missing values for the responses and specifying the p or predicted option in the output statement. After that it is possible to check the predictions based on the model against their actual values in order to check the validity of the model.

To analyse the results and to check if there is a pattern between the set used to obtain the model (`ptrain` set) and the predicted values (test set) it is possible to represent again the Euclidean distances. Also, to study these predictions, the plot of the predicted lean meat % with respect to the lean meat percentage can help. In that case, it would help if the samples from the set `ptrain` used for calibration are plotted with a symbol, say `'c'`, and samples from the set `ptest` used for validation can be plotted with another symbol, say `'v'`.

C. Principal component regression.

The way to do the PCR in SAS is the same as the PLS but specifying the method. The program to do it, centering and scaling previously, and to find the number of extracted factors would be the following:

```
proc pls data=ptrain method=pcr outmodel=est1 cv=one cvtest; model
lmp=P_WEIGHT P_LENGTH P_SHOULDER P_PELVIC F02 F03 F11 M11 F12 M12
F13 M13 F14 F16;
      output out=outpls predicted = yhat1
                        yresidual = yres1
                        xresidual = xres1-xres127
                        xscore    = xscr
                        yscore    = yscr
                        stdy=stdy  stdx=stdx h=h
                        press=press t2=t2 xqres=xqres yqres=yqres;
run;
```

The result with the example data was:

```
                    The PLS Procedure

    Cross Validation for the Number of Extracted Factors

        Number of        Root
        Extracted        Mean                Prob >
          Factors       PRESS        T**2      T**2

                0    1.002915    90.97538    <.0001
                1    0.775435    64.70637    <.0001
                2     0.53262    16.94419    <.0001
                3    0.497499     7.80227    0.0060
                4    0.493226    6.455032    0.0140
                5    0.489598    5.552566    0.0160
                6    0.471513    0.361837    0.5620
                7    0.472875      0.7236    0.4060
                8    0.473043    0.802246    0.3820
                9    0.475135    1.738072    0.1940
               10     0.47027    0.334039    0.5780
               11    0.471133    0.825394    0.3550
               12    0.468286           0    1.0000
               13     0.46984    27.47782    <.0001
               14    0.471388    46.51094    <.0001


    Minimum root mean PRESS                      0.4683
    Minimizing number of factors                    12
    Smallest number of factors with p > 0.1          6


                    The PLS Procedure

  Percent Variation Accounted for by Principal Components

 Number of
 Extracted        Model Effects        Dependent Variables
   Factors     Current       Total     Current       Total

         1     41.6880     41.6880     40.7726     40.7726
         2     25.7537     67.4417     31.3812     72.1538
         3     14.9702     82.4119      3.7603     75.9141
         4      4.6045     87.0164      0.5603     76.4744
         5      2.6327     89.6491      0.5125     76.9869
         6      2.3022     91.9513      1.7806     78.7675
```

It can be seen than in that case the number of extracted factors are 6, as well as if PRESS statistic was used as a criteria (results not showed).

In PCR the same plots and tests as PLS can be done to detect irregularities in the data, select the regression parameters and obtain the regression equation.

The regression equation obtained with PCR method, with 6 extracted factors, has the following parameters:

	LMP
Intercept	74.66894502
P_WEIGHT	0.06860239
P_LENGTH	-0.00604778
P_shoulder	0.04828023
P_pelvic	-0.35064071
F02	-0.13894244
F03	-0.06848733
F11	-0.18899734
M11	0.07811813
F12	-0.17066883
M12	0.03462094
F13	-0.13945642
M13	0.04466358
F14	-0.25906075
F16	-0.18755636

If we would like centered and scaled parameters the coefficients are:

Intercept	0.0000000000
P_WEIGHT	0.1523698811
P_LENGTH	-.0099293343
P_SHOULD	0.0621845389
P_PELVIC	-.1894907076
F02	-.0915904913
F03	-.0577196069
F11	-.1772521841
F12	-.1418710080
F13	-.1072165445
F14	-.2248294677
F16	-.1935333174
M11	0.1249122430
M12	0.0693785849
M13	0.0800626705

with a minimum root mean PRESS of 0.471513.

RMSEP can be calculated as explained for the PLS or running the macro `rmsepcr` provided in appendix B:

```
%rmsepcr(ptrain,sel_lv=6);
```

The result obtained is the following

rmsep
1.69325

9.3 Implementing cost saving methods

9.3.1 Double regression

Below a GenStat (2000) program and output are presented that illustrate the use of double regression (DR). A SAS procedure is also available by Daumas (1994).

The data are fictional and obtained by simulation. In the example a total sample size of $N = 200$ and a sub sample size of $n = 50$ are chosen. The samples are random. Apart from minor details that are typical for options and parameters in GenStat, the program is largely self-explanatory and transcription to another statistical language is straightforward. The standard errors of estimates and approximate degrees of freedom are calculated by the approximations presented in Engel and Walstra (1991a). Somewhat more complicated expressions for the standard errors, that are exact under normality assumptions, are presented by Causeur and Dhorne (1998).

For simplicity the example comprises only one prediction variable, e.g. a fat depth measurement. An informal derivation of the standard errors is sketched below. Extension to the case of several prediction variables is straightforward. We will derive the standard error of the coefficient B of x in the final prediction formula. The two regressions that are combined in DR are:

$$Y_* \;=\; a + bx + \delta \;\; and \;\; Y = \alpha + \beta x + \gamma Y_* + \varepsilon,$$

where δ and ε denote the error terms. The regression of interest is:

$$Y \;=\; A + Bx + e,$$

where e is the error term. The expression for B is:

$$B \;=\; \beta + \gamma b.$$

The estimate for B is derived by substitution of the estimated values of b, g and b as derived from the two regressions that are combined in DR. Suppose that we denote these estimates, indicated by a hat, by a sum of the true parameter value and a random term:

$$\begin{aligned} \hat{\beta} &= \beta + \varepsilon_\beta, \\ \hat{\gamma} &= \gamma + \varepsilon_\gamma, \\ \hat{b} &= b + \varepsilon_b. \end{aligned}$$

These expressions are substituted in the expression for B. All products of e's are assumed to be negligible compared with the linear terms and omitted. Thus, we get the following approximation:

$$\begin{aligned} \hat{B} &= (\beta + \varepsilon_\beta) + (\gamma + \varepsilon_\gamma)(b + \varepsilon_b), \\ &\approx \beta + \gamma b + \varepsilon_\beta + \gamma\varepsilon_b + b\varepsilon_\gamma, \\ &\approx B + \varepsilon_\beta + \gamma\varepsilon_b + b\varepsilon_\gamma. \end{aligned}$$

The variance of the expression on the right hand side is:

$$Var(\hat{B}) \;=\; Var(\hat{\beta}) + \gamma^2 Var(\hat{b}) + b^2 Var(\hat{\gamma}) + 2bCov(\hat{\beta}, \hat{\gamma}).$$

Estimators for constants and coefficients from the two separate regressions in DR are uncorrelated, e.g. $Cov(\varepsilon_\beta, \varepsilon_b) = Cov(\hat{\beta}, \hat{b}) = 0$. Estimated values for the variances and covariances can be obtained from the regression output of the separate regressions. Taking the square root we get the estimated value for the standard error of $\hat{B}$. In the program, variances and covariances are saved in matrices and the expressions for the standard errors are derived by matrix manipulation. The covariance matrices of the two regressions are placed in a block diagonal matrix (called "W" in the program). This matrix is pre multiplied by a matrix (called "work" in the program), and post multiplied by the transpose of that same matrix. The last matrix ("work") takes care that the relevant variance and covariance terms get the proper coefficients. Of course it is also possible to extract the relevant terms and program the expressions for the se's directly, without use of matrix manipulation.

In appendix B, the GenStat program is reproduced. Comments in the program are between quotes ("") and highlighted (). The annotated output, including the data, follows immediately afterwards.

9.3.2 Surrogate predictor regression

Preliminaries

As far as we know, the double-sampling methods that are presented in chapter 4 are not currently implemented in any software. Therefore, the illustrations we propose are based on home made programs that only work (when they work) in the R/Splus programming environment. These functions are given in appendix B.

The illustrative example is based data extracted from the data set introduced in section 9.2.1. In this example, the response variable remains the lean meat percentage and instrumental predictors are a fat layer (F03) and a meat layer (M11). Our aim is to derive a prediction formula but it is asked to the reader to forget for a while that the whole data set contains common measurements of the response and the instrumental predictors.

Suppose that a first prediction equation of the lean meat percentage by 4 reference predictors is available thanks to an experiment involving n_r =50 carcasses (for our purpose, these carcasses will be the first 50 carcasses in the data set). These reference predictors are supposed to be fat layers (F02, F11 and F14) a meat layer (M13). It is rather clear here that the reference predictors forms a complete set of predictors in the sense that the instrumental predictors have no additional predictive ability once the reference predictors are observed. As it was mentioned in section 4.3, this property makes is valid the use of the present method.

`Yr` and `Zr` will denote the matrix containing respectively the values of the response and the reference predictors on the reference sample:

```
Yr <- Y[1:50]
Zr <- X[1:50,c("F02","F11","F14","M13")]
```

According to the previous examination of the dimensionality of the instrumental predictors in section 9.2, PLS with 2 components is used here to establish the reference prediction formula. The slope coefficients are given by:

```
> ref.pls <- pls(Zr, Yr)
> sloperef <- ref.pls$training$B[,  , 2]
> offsetref <- mean(Yr) - sum(sloperef * apply(Zr, 2, mean))
> coefref <- c(offsetref, sloperef)
> round(coefref, 2)
[1]  65.63  -0.25  -0.41  -0.45   0.18
```

Deriving a prediction formula for the lean meat percentage by the instrumental predictors will now be achieved through a new experiment consisting only in common measurements of the reference predictors and the instrumental predictors. The first question that has to be addressed is the sample size in this scaling experiment.

Sampling scheme

Some inputs are of course needed to find a sampling scheme that can ensure that the EC-requirements are satisfied. More precisely, some prior information on the variance-covariance of the instrumental and reference predictors is needed. This information can either be obtained by some knowledge from past experiments or from a few scaling experiments. Here, it is chosen to get informations through 50 scaling experiments (say the carcasses numbered 51 to 100 in the data set):

```
> Zs <- X[51:100, c("F02", "F11", "F14", "M13")]
> Xs <- X[51:100, c("F03", "M11")]
> varzx <- var(cbind(Zs, Xs))
```

Up to now, the R/Splus object `varzx` contains the variances and covariances of both the reference and the instrumental predictors.

Finally, an estimation of the residual standard deviation of the reference prediction equation is necessary. Although the use of PLS does not enable a proper calculation, it will be supposed that the reference residual standard deviation equals about 1.7.

The function `optisamp.spr` have been written to find the minimum sample size for the scaling experiment that will provide estimators as efficient as those

that would have been obtained from OLS on a sample of 120 units. The arguments of this function are the target sample size `n` ($n = 120$ according to the EC-requirements), the reference sample size `nr` (here $n_r = 50$), the variance-covariance `sigmazx` of both the reference and the instrumental predictors, the reference residual standard deviation `rsdref` and the slope coefficients in the reference prediction equation `sloperef`:

```
> optisamp.spr(n = 120, nr = 50, sigmazx = varzx, rsdref = 1.7,
sloperef = ref.pls$training$B[,  , 2])
[1] 222
```

It is therefore suggested to run 172 new scaling experiments. It will be supposed that the scaling sample contains the carcasses numbered 51 to 272:

```
Zs <- as.matrix(X[51:272,c("F02","F11","F14","M13")])
Xs <-  as.matrix(X[51:272,c("F03","M11")])
```

Suppose just for the illustrative purpose that the cost for a single reference dissection is 100 and that the cost for a scaling experiment is only 20. The global cost for such an experiment then equals `50*100+222*20=9440`, or equivalently a reduction of approximately 22 % relative to the required 120 reference dissections.

Creating the prediction formula

The home made function `spr`, which arguments are the measurements of the instrumental predictors `Xs` and the reference predictors `Zs` on the scaling sample and the coefficients `coefref` of the reference prediction equation, can be used to derive the prediction formula of the lean meat percentage by the instrumental predictors:

```
> spr(Xs, Zs, coefref)
           [,1]
     60.1831859
F03  -0.7232963
M11   0.1984338
```

Although it does not validate the present method at all, it can be argued that the estimated coefficients would not have been very different if OLS could have been performed on the whole data set:

```
> ls.print(lsfit(X[, c("F03", "M11")], Y))
Residual Standard Error = 2.7348,  Multiple R-Square = 0.4251
N = 344,  F-statistic = 126.0704 on 2 and 341 df, p-value = 0
```

```
             coef std.err   t.stat p.value
Intercept  59.6111  1.4674  40.6245       0
      F03  -0.7188  0.0493 -14.5796       0
      M11   0.2197  0.0260   8.4548       0
```

Validation

First, let us derive the RMSEP for the reference prediction equation:

```
> rmsep.ref <- pls(Zr, Yr, validation = "CV",
grpsize = 1)$training$RMS[2, 1]
> rmsep.ref
   2 LV's
 1.902015
```

Now the home made function `rmsep.spr` gives the RMSEP for the prediction formula:

```
 > rmsep.spr(Xs, Zs, sloperef = ref.pls$training$B[,  , 2],
 rmsepref = rmsep.ref)
[1] 2.997035
```

At both phase of the sampling scheme, full cross-validation have been used to derive the RMSEPs. According to the content of section 4.3, the resulting RMSEP is obtained by a combination of the intermediate RMSEPs derived on the reference sample and the scaling sample.

Chapter 10

Prospects

By Bas Engel

10.1 Non-linear regression

In classical non-linear regression, it is assumed that

$$y_i = f(x_i; a, b, c) + \varepsilon_i,$$

where $f(x; a, b, c)$ is a function of prediction variable x and some unknown coefficients, say a, b and c, which have to be estimated from the data. The mutually independent error terms ε_i are assumed to have equal variance σ^2. Function f is assumed to be non-linear in at least one of the variables a, b or c. Obviously, LR, where $f(x; a, b) = a + b * x$, is a special case, without non-linear coefficients.

Estimation of a, b and c proceeds analogous to LR by the method of least squares. Estimates A, B and C minimise the sum of squares:

$$\sum_{i=1}^{n} [y_i - f(x_i; a, b, c)]^2 .$$

The minimum value offers an estimate for σ^2:

$$s^2 = \sum_{i=1}^{n} [y_i - f(x_i; A, B, C)]^2 / d.$$

Again, d are the degrees of freedom and equal to the sample size n reduced by the number p of unknowns to be estimated in the formula: $d = n - p$. With coefficients a, b and c: $p = 3$.

Minimisation of the sum of squares is more complicated than in LR and usually involves some iterative numerical procedure. Least squares estimates A, B and C will be biased estimators for a, b and c. Likewise, s^2 will be a biased

estimator for σ^2. Statistical inference in a non-linear models is mostly based on large sample theory, even under assumption of normality of error terms ε_i few exact small sample results are available for statistical inference. There is no guarantee that the large sample approximations will yield proper results for small sample sizes. For a sample size of $n = 120$, estimators may be expected to be well behaved, e.g. they will be nearly unbiased and they will offer a reasonable impression of a, b, c and σ^2. By way of an RMSE, the estimated residual standard error s may be evaluated. When inclusion of non-linear terms markedly improves results obtained by LR, it seems reasonable to extend the minimum sample size of 120 carcasses for LR to classical non-linear regression as well. There is quite some literature devoted to non-linear regression; we just mention Gallant (1975, 1987). There is ample software in most of the larger statistical packages. The approach of Engel & Walstra (1993) is actually based on a very specific non-linear model. For this particular problem a combination of least squares and non-linear regression, i.e. logistic regression, was used.

10.2 Variance functions

Variance functions have not been used yet in carcass grading. Therefore we will only supply a few, rather technical, details. When the variance of the error terms is not constant, quite often because it increases with the mean, a logarithmic transformation may stabilise the variance. After logarithmic transformation, a non-linear model may be more appropriate. Note that either with a linear or a non-linear model, after transformation, s^2 is not a proper substitute for the RMSE anymore, because it refers to observations $\log(y)$ and not to the original observations y. Assuming normality after transformation, the original observations are following a lognormal distribution with the following relationship between the residual variance $Var(y_i)$ and the mean $E(y_i)$ (Mood et al., 1974, p117):

$$Var(y_i) \;=\; \left\{\exp(\sigma^2) - 1\right\} E(y_i)^2.$$

$E(y_i)$ will either look like (linear model after transformation):

$$\exp(a + bx_i + \sigma^2/2)$$

or (non-linear model after transformation):

$$\exp\left[f(x_i; a, b, c) + \sigma^2/2\right].$$

Note that back-transformation includes the term $\sigma^2/2$ in the exponential.

Alternatively, we may employ a so called generalized linear model (GLM) (McCullagh and Nelder, 1989), specifying a logarithmic link function and a variance function of the form:

$$Var(y_i) \;=\; \phi E(y_i)^2.$$

Under the assumption of normality of $\log(y)$ we have $\phi = \exp(\sigma^2) - 1$, and estimation may be performed by least squares on the log-transformed data. Alternatively, an estimation procedure called maximum quasi-likelihood (Nelder and Wedderburn, 1972; McCullagh and Nelder, 1989) may be applied to the original data. Maximum quasi-likelihood avoids the need for further distributional assumptions, e.g. no assumption of a (log) normal distribution is needed. Maximum quasi-likelihood is a natural extension of the method of least squares for variables y where the variance is a multiple of a known function of the mean (McCullagh, 1983). Standard software for GLMs may be employed to derive maximum quasi-likelihood estimates.

Note that it may sometimes be appealing to apply a transformation to obtain a linear model. For instance when the theoretical mean is equal to:

$$E(y_i) \quad = \quad b \exp(-cx_i),$$

it follows that

$$\log\left[E(y_i)\right] \quad = \quad \log(b) - cx_i.$$

The latter expression is linear in $\log(b)$ and c. Obviously, when the variance was constant before transformation, it will not be constant after transformation. In that case, a GLM with a logarithmic link function and a constant variance function could be employed. This is a special case of the classical non-linear regression model with all the non-linearity concentrated in the logarithmic link function.

Both for least squares after log-transformation and maximum quasi-likelihood with a (quadratic) variance function, it is not immediately apparent what a suitable substitute for the RMSE should be. The problem is that the RMSE will depend on the prediction variable x through the mean $E(y)$. Evaluation of the maximum RMSE over a suitable range of x-values seems to be an acceptable approach.

Chapter 11

Reporting to the Commission - results of the trial

By Gérard Daumas

The present EU regulation lays out:
"Part two of the protocol should give a detailed description of the results of the dissection trial and include in particular:

1. a presentation of the statistical methods used in relation to the sampling method chosen,
2. the equation which will be introduced or amended,
3. a numerical and a graphic description of the results,
4. a description of the new apparatus,
5. the weight limit of the pigs for which the new method may be used and any other limitation in relation to the practical use of the method."

These items have not been specifically discussed. Nevertheless, one can look for the following items at the corresponding sections:

- Item 1: see chapters 2 and 4.
- Item 3: see chapters 8 and 9.

Appendix A

References

Causeur, D. (2003) Optimal sampling from concomitant variables for regression problems. *J. Stat. Plan. and Inf.* To appear.
Causeur, D. and Dhorne, T. (1998) Finite sample properties of a multivariate extension of double regression. *Biometrics* **54** 1591-1601.
Causeur, D. and Dhorne, T. (2003) Linear Regression Models under Conditional Independence Restrictions. *Scand. J. Statist* 30, 637 - 650.
Cochran, W.G. (1977). Sampling Techniques. 3rd edition, New York: Wiley.
Cook, G.L. and Yates, C.M. (1992). A report to the Commission of the European Communities on Research concerning the harmonization of methods for grading pig carcasses in the Community.
Daumas, G (1994). La double régression sous SAS. *Lettre d'information SAS ACTA*, 23.
Daumas, G. (2003). A description of the European slaughterpig populations and their classification. *EUPIGCLASS report*, 42 p.
Daumas, G., Causeur, D., Dhorne, T., Schollhammer, E. (1998). The new pig carcass grading methods in France. *Proceedings 44th ICoMST*, Barcelona (Spain), C-64, 948-949.
Daumas, G. and Dhorne, T. (1995). French protocol for updating of pig carcasses classification methods in 1996 - 1st part - *EC Working document.*
Daumas, G. and Dhorne, T. (1997). The lean meat content of pig carcasses: determination and estimation. *French Swine Research Days*, 29, 171-180.
Daumas, G. and Dhorne, T. (1998). Pig carcass grading in European Union. *Proceedings of 44th ICoMST*, Barcelona, Spain. C-63, 946-947.
Daumas, G., Dhorne, T., Gispert, M. (1994). Accounting for the sex effect on prediction of pig carcass lean meat percentage in the Community. *Proc. 40th ICoMST*, La Haye (The Netherlands), S III. 11, 9 pp.
Denham, M.C. (1995) Implementing Partial Least Squares. *Statistics and Computing* 5, 191-202.
Dhorne, T.J. (2000). Contribution to EUPIGCLASS workshop, Lelystad, The Netherlands.

Draper, N.R., Smith, H. (1981). Applied regression analysis. 2nd edition. New York: John Wiley.
Engel, B. (1987). Increasing precision or reducing expense in regression experiments by using information from a concomitant variable. *GLW research report LWA-87-1,* Wageningen, The Netherlands.
Engel, B. and Walstra, P. (1991a) Increasing precision or reducing expense in regression experiments by using information from a concomitant variable. *Biometrics* **47** 1011-1023.
Engel, B and Walstra, P. (1991b) A simple method to increase precision or reduce expense in regression experiments to predict the proportion of lean meat of carcasses. *Animal production* **53** 353-359.
Engel, B., Walstra, P. (1993). Accounting for subpopulations in prediction of the proportion of lean meat of pig carcasses. *Animal Production* 57: 147-152.
Engel, B., Buist, W.G., Walstra, P., Olsen, E., Daumas, G. (2003a). Accuracy of prediction of percentage lean meat and authorization of carcass measurement instruments: adverse effects of incorrect sampling of carcasses in pig classification. *Animal Science* 76: 199-209.
Engel, B., Buist, W.G., Font I Furnols, M., Lambooij, E. (2003b). Subpopulations and accuracy of prediction in pig carcass classification. *Animal Science*, in press.
European Community (1994a) *EC regulation No. 3127/94, amending regulation (EC) No 2967/85 laying down detailed rules for the application of the community scale for grading pig carcasses.*
European Community (1994b) *Commission Decision amendment to the decision authorizing methods for grading pig carcasses in Spain (94/337/EEC).*
Feinberg, M. (1995). Basics of interlaboratory studies: the trends in the new ISO 5725 standard edition. *Trends in analytical chemistry*, vol. 14, no.9, Paris.
Font i Furnols, M. (2002). Contribution to EUPIGCLASS meeting, Gent, Belgium.
Gallant, A.R. (1975). Nonlinear regression. *The American Statistician* 29: 73-81.
Gallant, A.R. (1987). Nonlinear Statistical Models. New York: John Wiley.
Gispert, M., Dhorne, T., Diestre A., Daumas, G., (1996). Efecto del sexo en la predicción del contenido en magro de la canal porcina en España, Francia y Países Bajos. *Invest. Agr. : Prod. Sanid. Anim.* Vol. **11** (1), 1996.
Helland, I.S. (1998) Model reduction for prediction in regression models. *Scand. J. Statist* 27, 1-20.
ISO 5725 (1994). Accuracy (trueness and precision) of measurement methods and results.
Mc Ardle, J. (1987). LVPLS Ver. 1.8. Downloadable freely at ftp://kiptron.psyc.virginia.edu/pub/lvpls.
McCullagh, P., Nelder, J.A. (1989), Generalized linear models. 2nd edition. London: Chapman and Hall.

McCullagh, P. (1991), Quasi-likelihood and estimating functions. *Ch. 11 of: Statistical theory and modelling.* In honour of Sir David Cox, FRS. Edited by: D.V.Hinkley, N. Reid and E.J.Snell. London: Chapman and Hall.

Mood, A.M., Graybill, F.A. and Boes, D.C. (1963). Introduction to the theory of statistics. 3rd edition. Tokyo: McGraw-Hill.

Montgomery, D.C., Peck, E.A. (1992). Introduction to linear regression analysis. 2nd edition. New York: John Wiley.

Naes, T., Irgens, C., Martens, H. (1986). Comparison of linear statistical methods for calibration of NIR instruments. *Applied Statistics* 35: 195-206.

Nelder, J.A., Wedderburn, R.W.M. (1972). Generalized linear models. *Journal of the Royal Statistical Society A* 135: 370-384.

Olsen, E.V. (1997). Accuracy of industrial methods for meat quality measurements. *Congress Proceedings, 43rd ICOMST.*

Plsplot (2003). Consulted in http://ftp.sas.com/techsup/download/stat/ in July 2003.

Plsplote (2003). Consulted in http://ftp.sas.com/techsup/download/stat/ in July 2003.

Rao, C.R. and Toutenburg, H. (1999) Linear Models : Least Squares and Alternatives. *2nd Edition. Springer Verlag Ed.*

Rousseuw, P. and Leroy, A. (1987) Robust Regression and Outlier Detection. *John Wiley & and sons eds.*

Scheper J. and Scholz W. (1985). DLG-Schnittführung für die Zerlegung der Schlachtkörper von Rind, Kalb, Schwein und Schaf. *Arbeitsunterlagen DLG.*

Sundberg, R. (1999) Multivariate calibrationdirect and indirect regression methodology (with discussion). *Scand. J. Statist* 26, 161-207.

Tillé, Y. (2001). Théorie des sondages : échantillonnage et estimation en populations finies. Paris. Dunod. 284 p.

Tobias, R.D. (1997a) An Introduction to Partial Least Squares Regression. (http://ftp.sas.com/techsup/download/technote/ts509.pdf) TS-509, SAS Institute Inc., Cary, N.C.
(see also http://support.sas.com/techsup/faq/stat_ proc/plsproc.html)

Tobias, R.D. (1997b) Examples Using the PLS Procedure.
(http://support.sas.com/rnd/app/papers/plsex.pdf)
SAS Institute Inc., Cary, N.C.

Walstra, P. (1980). Growth and carcass composition from birth to maturity in relation to feeding level and sex in Dutch Landrace pigs. *PhD-thesis.* Mededelingen, Landbouwhogeschool Wageningen, 80-4.

Walstra, P. (1986). Assessment of the regression formula for estimation of the lean percentage by HGP-measurements in The Netherlands. *EC-working paper*, Brussels, VI/4849/86.

Walstra, P., Merkus, G.S.M. (1995). Procedure for assessment of the lean meat percentage as a consequence of the new EC reference dissection method in pig carcass classification. Unpublished document ID-Lelystad, The Netherlands.

Walstra, P. and Merkus, G.S.M. (1996). Procedure for assessment of the lean meat percentage as a consequence of the new EU reference dissection method in pig carcass classification. *Report ID-DLO 96.014*, March, 22 pp.

Appendix B

Technical details

B.1 SAS Macros for PLS and PCR

```
/definition of the data/
%global xvars yvars ;
%let xvars= P_WEIGHT P_LENGTH P_SHOULDER P_PELVIC F02 F03 F11 M11 F12 M12 F13 M13 F14 F16;
    %let yvars=lmp;

/macro to calculate the different RMSEP with leave one out/
Variables required to be defined: dades=name of the data set
(without missing values)

%macro rmsep(dades);
data regre;  set &dades(keep= &xvars &yvars );
 call symput('num_x',_N_);run;
%do i=1 %to &num_x;
data regres; set regre; if  _N_=&i then &yvars=.; proc reg
noprint; model &yvars=&xvars/p; output out=tt&i
        p=yhat;
run;
%end;
%do i=1 %to &num_x;
data rr&i; merge tt&i &dades; if _N_=&i;
ysqu=(&yvars-yhat)*(&yvars-yhat); run; data kk&i; set rr&i
(keep=ysqu); run;
%end;
%do i=1 %to 1;
data mitja&i; set kk&i; run;
%end;
%do i=2 %to &num_x;
data mitja&i;
%let j=%eval(&i-1);
set kk&i mitja&j; run;
%end;
%do i=&num_x %to &num_x;
proc means data=mitja&i noprint; output out=mitjana; run;
%end;
data result; set mitjana; if _STAT_='MEAN' ; rmsep=(YSQU)**0.5;
proc print noobs; var rmsep; run;
%mend rmsep;


/definition of the variables/
%global xvars yvars ypred;
  %let xvars= P_WEIGHT P_LENGTH P_SHOULD P_PELVIC F02 F03 F11 M11 F12 M12 F13 M13 F14 F16;
  %let yvars= lmp;
```

```
  %let predicted=yhat1;

/macro to calculate RMSEP for PLS/ Variables required to be
defined:
    dades= name of the data set and should not contain missing values
    sel_lv= number of factors to take into consideration

%macro rmsepls(dades,sel_lv=&lv);
data pls1;  set &dades(keep= &xvars &yvars );
 call symput('num_x',_N_);run;
%do i=1 %to &num_x;
data pls2; set pls1; if  _N_=&i then &yvars=.; proc pls method=pls
lv=&sel_lv noprint ; model &yvars=&xvars; output out=tt&i
predicted=yhat1 ; run;
%end;
%do i=1 %to &num_x;
data rr&i; merge tt&i &dades ; if _N_=&i;
ysqu=(&yvars-yhat1)*(&yvars-yhat1); run; data kk&i; set rr&i
(keep=ysqu); run;
%end;
%do i=1 %to 1;
data mitja&i; set kk&i; run;
%end;
%do i=2 %to &num_x;
data mitja&i;
%let j=%eval(&i-1);
set kk&i mitja&j; run;
%end;
%do i=&num_x %to &num_x;
proc means data=mitja&i noprint; output out=mitjana; run;
%end;
data result; set mitjana; if _STAT_='MEAN' ; rmsep=(YSQU)**0.5;
proc print noobs; var rmsep; run;
%mend rmsepls;

/definition of the variables/
%global xvars yvars ypred;
  %let xvars= P_WEIGHT P_LENGTH P_SHOULD P_PELVIC F02 F03 F11 M11 F12 M12 F13 M13 F14 F16;
  %let yvars= lmp;
  %let predicted=yhat1;

/macro to calculate RMSEP for PCR/ Variables required to be
defined:
    dades= name of the data set and should not contain missing values
    sel_lv= number of factors to take into consideration

%macro rmsepcr(dades,sel_lv=&lv);
data pcr1;  set &dades(keep= &xvars &yvars );
 call symput('num_x',_N_);run;
%do i=1 %to &num_x;
data pcr2; set pcr1; if  _N_=&i then &yvars=.; proc pls method=pcr
lv=&sel_lv  noprint ; model &yvars=&xvars; output out=tt&i
predicted=yhat1 ; run;
%end;
%do i=1 %to &num_x;
data rr&i; merge tt&i &dades ; if _N_=&i;
ysqu=(&yvars-yhat1)*(&yvars-yhat1); run; data kk&i; set rr&i
(keep=ysqu); run;
%end;
%do i=1 %to 1;
data mitja&i; set kk&i; run;
%end;
%do i=2 %to &num_x;
data mitja&i;
%let j=%eval(&i-1);
```

```
set kk&i mitja&j; run;
%end;
%do i=&num_x %to &num_x;
proc means data=mitja&i noprint; output out=mitjana; run;
%end;
data result; set mitjana; if _STAT_='MEAN' ; rmsep=(YSQU)**0.5;
proc print noobs; var rmsep; run;
%mend rmsepcr;
```

B.2 Genstat program for double-regression

The program

```
"
Example of double-regression (DR) with simulated data.
Program in GenStat (2000). The Guide to genStat. VSNInt.Oxford.
Based on Engel & Walstra (1991a,b).

Notation:

y     = EC reference lean meat percentage
ystar = lean meat percentage obtained by a national method
x     = prediction variable, e.g. a fat depth measurement

a, b, v1 are the constant, coefficient and squared rsd in the regression
of ystar on x

alpha, beta, gamma, v2 are the constant, coefficients and squared rsd in
the regression of y on x and ystar

A, B, RSD are the constant, coefficient and rsd of the final
prediction formula

rho is the partial correlation between y and ystar conditional upon x

Estimated values are denoted by ahat, bhat, etc. except estimated values
for v1, v2 and trueRSD that are denoted RSD1, RSD2 and RSD.

Here, sample sizes are N = 200 (total sample) and n = 50 (sub sample).
"

scal start,v1,v2,a,b,alpha,beta,gamma

"true parameter values (fictional)"

calc a       = 70
calc b       = -0.4
calc alpha   = -12.0
calc beta    = -0.1
calc gamma   = 1.1
calc v1      = 3.2
calc v2      = 0.7
calc trueRSD = sqrt( v2 + gamma*gamma*v1)
calc truerho = gamma* sqrt(v1) / trueRSD
calc trueA   = alpha+gamma*a calc trueB   = beta  +gamma*b

"generation of data"

"subset indicates sub sample membership"
"here all samples are random"

vari[nval=200] ystar,x,y
```

```
vari[nval=200] subset;val=!(50(1), 150(0))
vari[nval=200] tel; val=!(1...200)

calc start   = urand(347883)
calc  e      =urand(0;200)
calc  x      = ned(e) * sqrt(12.5) + 16.4

calc del     = urand(0;200)
calc del     = ned(del)*sqrt(v1)
calc ystar  = a + b * x + del

calc eps = urand(0;200)
calc eps = ned(eps)*sqrt(v2)
calc y     = alpha  + beta * x + gamma * ystar + eps
calc y     = y / subset

prin tel, x, ystar, y; f=4(8); d=0, 3(2)

"first regression, ystar on x"

model ystar
fit x
rkeep ystar; estimates=coef1;vcov=cov1;deviance=SS1;df=df1

"second regression, y on x and ystar"

model y
fit x + ystar
rkeep y; estimates=coef2;vcov=cov2;deviance=SS2;df=df2

"combination of regressions"

calc ahat     = coef1$[1]
calc bhat     = coef1$[2]
calc alphahat = coef2$[1]
calc betahat  = coef2$[2]
calc gammahat = coef2$[3]
calc RSD1     = sqrt(SS1/df1)
calc RSD2     = sqrt(SS2/df2)

calc A        = alphahat + gammahat * a
calc B        = betahat   + gammahat * b
calc RSD      = sqrt(RSD2*RSD2+RSD1*RSD1*gammahat*gammahat)
calc rhohat   = gammahat*RSD1/RSD

"standard errors of estimates"

matrix[rows=2;col=5] work; val=!(gammahat,0,1,0,a,0,gammahat,0,1,b)
symmetricmatrix [rows=2] COVAR
diag[rows=2] se
matrix[rows=5;col=5] W
matrix[rows=2;col=2] c1
matrix[rows=3;col=3] c2
calc c1 = cov1
calc c2 = cov2
calc W  = 0
equate[newf=!((2,-3)2, (-2,3)3)] !P(c1,c2); W
calc COVAR = prod(work;rtprod(W;work))
calc se    = COVAR
calc se    = sqrt(se)
calc seA   = se$[1] calc seB   = se$[2]

"calculation of approximate degrees of freedom"

calc df = RSD**4
```

```
calc df=df/((RSD2**4)/47+(gammahat**4)*(RSD1**4)/(198)+2*(RSD1**4)*gammahat*gammahat*cov2$[3;3])

"true and estimated parameters, se's, approximate degrees of freedom"

prin trueA, A, seA, trueB, B, seB, trueRSD, RSD, df,truerho,rhohat; f=8(8); d= 9(2)

"estimated efficiency relative to linear regression (LR) with 120 dissected carcasses"

calc Efficiency = (50/120)/(1-0.75*rhohat*rhohat)

"sample size of LR with equal efficiency"

calc nLR = 50/(1-0.75*rhohat*rhohat)

print Efficiency; d=2
print nLR;d=2

stop
```

The output

The first part of the output reproduces the program and is omitted. We start by reproducing the data.

```
67  prin tel, x, ystar, y; f=4(8); d=0, 3(2)

     tel       x   ystar       y
       1   17.23   62.14   55.55
       2   21.93   59.90   50.58
       3   12.54   66.55   60.14
       4   20.29   63.16   55.93
       .........................
       .........................
      45   13.47   67.09   59.80
      46   18.72   64.89   57.48
      47   15.09   63.02   56.35
      48    6.73   66.17   61.53
      49   17.56   60.10   52.87
      50   15.45   61.06   54.24
      51    7.74   66.63       *
      52   21.66   60.20       *
      53   13.15   63.55       *
      54   13.80   66.00       *
       .........................
       .........................
     195   12.47   65.71       *
     196   20.97   60.16       *
     197   12.40   62.30       *
     198   13.86   62.52       *
     199   20.98   62.56       *
     200   11.16   64.58       *

  68
  69  "first regression, ystar on x"
  70
  71  model ystar
  72  fit x

72.....................................................................
```

```
***** Regression Analysis *****

 Response variate: ystar
     Fitted terms: Constant, x


*** Summary of analysis ***

              d.f.         s.s.         m.s.      v.r.
Regression       1        331.8      331.842    108.83
Residual       198        603.7        3.049
Total          199        935.6        4.701

Percentage variance accounted for 35.1
Standard error of observations is estimated to be 1.75
* MESSAGE: The following units have high leverage:
         Unit     Response    Leverage
           28        61.15       0.035
           39        67.39       0.037
           48        66.17       0.048
           51        66.63       0.040
          124        64.34       0.032
          128        65.28       0.029


*** Estimates of parameters ***

                  estimate         s.e.    t(198)
Constant            70.010        0.626    111.86
x                  -0.3872       0.0371    -10.43

  73  rkeep ystar; estimates=coef1;vcov=cov1;deviance=SS1;df=df1
  74
  75  "second regression, y on x and ystar"
  76
  77  model y
  78  fit x + ystar

78.....................................................................


***** Regression Analysis *****

 Response variate: y
     Fitted terms: Constant + x + ystar


*** Summary of analysis ***

              d.f.         s.s.         m.s.      v.r.
Regression       2       453.54     226.7688    275.74
Residual        47        38.65       0.8224
Total           49       492.19      10.0447

Percentage variance accounted for 91.8
Standard error of observations is estimated to be 0.907
* MESSAGE: The following units have large standardized residuals:
         Unit     Response    Residual
           28       55.584        2.81
* MESSAGE: The following units have high leverage:
         Unit     Response    Leverage
           14       48.547       0.160
           48       61.534       0.163
```

```
*** Estimates of parameters ***

                             estimate         s.e.     t(47)
Constant                       -16.55         4.65     -3.56
x                             -0.0545       0.0436     -1.25
ystar                          1.1627       0.0656     17.73

  79  rkeep y; estimates=coef2;vcov=cov2;deviance=SS2;df=df2
  80
  81  "combination of regressions"
  82
  83  calc ahat     = coef1$[1]
  84  calc bhat     = coef1$[2]
  85  calc alphahat = coef2$[1]
  86  calc betahat  = coef2$[2]
  87  calc gammahat = coef2$[3]
  88  calc RSD1     = sqrt(SS1/df1)
  89  calc RSD2     = sqrt(SS2/df2)
  90
  91  calc A        = alphahat + gammahat * a
  92  calc B        = betahat   + gammahat * b
  93  calc RSD      = sqrt(RSD2*RSD2+RSD1*RSD1*gammahat*gammahat)
  94  calc rhohat   = gammahat*RSD1/RSD
  95
  96  "standard errors of estimates"
  97
  98  matrix[rows=2;col=5] work; val=!(gammahat,0,1,0,a,0,gammahat,0,1,b)
  99  symmetricmatrix [rows=2] COVAR
 100  diag[rows=2] se
 101  matrix[rows=5;col=5] W
 102  matrix[rows=2;col=2] c1
 103  matrix[rows=3;col=3] c2
 104  calc c1 = cov1
 105  calc c2 = cov2
 106  calc W  = 0
 107  equate[newf=!((2,-3)2, (-2,3)3)] !P(c1,c2); W
 108  calc COVAR = prod(work;rtprod(W;work))
 109  calc se    = COVAR
 110  calc se    = sqrt(se)
 111  calc seA   = se$[1]
 112  calc seB   = se$[2]
 113
 114  "calculation of approximate degrees of freedom"
 115
 116  calc df = RSD**4
 117 calc df = df/((RSD2**4)/47+(gammahat**4)*(RSD1**4)/
 118                       (198)+2*(RSD1**4)*gammahat*gammahat*cov2$[3;3])
 118
 119  "true and estimated parameters, se's, approximate degrees of freedom"
 120
 121  prin trueA,A,seA,trueB,B,seB,trueRSD,RSD,df,truerho,rhohat; f=8(8); d= 9(2)


  trueA      A    seA  trueB      B    seB trueRSD     RSD      df truerho   rhohat
  65.00  64.84   0.93  -0.54  -0.52   0.06    2.14    2.22  117.39    0.92     0.91



 122
 123 "estimated efficiency relative to linear regression (LR)
 124                                              with 120 dissected  carcasses"
 124
 125  calc Efficiency = (50/120)/(1-0.75*rhohat*rhohat)
 126
 127  "sample size of LR with equal efficiency"
```

```
 128
 129  calc nLR = 50/(1-0.75*rhohat*rhohat)
 130
 131  prin Efficiency; d=2


  Efficiency
        1.11


 132  prin nLR;d=2

         nLR
      133.42

 133
 134  stop
```

B.3 Programs in R/Splus to select the best subset of predictors according to the RMSEP

```
fact <- function(k) gamma(k+1)

binom <- function(n,p) round(fact(n)/(fact(p)*fact(n-p)))

suivant <- function(s,nbvar) {
    k <- length(s)
    if (k==0) res <- as.list(1:nbvar)
    if (k==nbvar) res <- NULL
    if ((k!=0)&(k!=nbvar)&(s[k]==nbvar)) res <- NULL
    if ((k!=0)&(k!=nbvar)&(s[k]!=nbvar)) res <- as.list(
        as.data.frame(t(cbind(matrix(rep(s,nbvar-s[k]),nrow=nbvar-s[k],ncol=k,byrow=T),
        (s[k]+1):nbvar))))
}

stadesuivant <- function(s,nbvar) {
    k <- length(s[[1]])
    res <- NULL
    for (j in 1:length(s))
    if (nbvar-s[[j]][k]>0) res <- rbind(res,cbind(matrix(rep(s[[j]],nbvar-s[[j]][k]),
    nrow=nbvar-s[[j]][k],ncol=k,byrow=T),(s[[j]][k]+1):nbvar))
   as.list(as.data.frame(t(res)))
}

arrangements <- function(nbvar) {
    res <- vector("list",2^(nbvar)-1)
    stade <- as.list(1:nbvar)
    res[1:nbvar] <- stade
    long <- nbvar
    for (i in 2:nbvar) {
        li <- binom(nbvar,i)
        stade <- stadesuivant(stade,nbvar)
        res[(long+1):(long+li)] <- stade
        long <- long+li
    }
    res
}

rmsep.ols <- function(X,Y) {
```

```
    res <- lsfit(X,Y)$res
    sqrt(mean(res^2/(1-hat(X))^2))
}

rmsepsub.ols <- function(subset,predictors,response) {
    rmsep.ols(predictors[,subset],response)
}

bestrmsep.ols <- function(X,Y) {
    nbvar <- ncol(X)
    arr <- arrangements(nbvar)
    rmsep.all <- unlist(lapply(arr,rmsep.sub,predictors=X,response=Y))
    arr.length <- as.factor(unlist(lapply(arr,length)))
    bests <- tapply(rmsep.all,arr.length,order)
    subsets <- vector("list",length=nbvar)
    labels <- vector("list",length=nbvar)
    minrmsep <- tapply(rmsep.all,arr.length,min)
    for (i in 1:nbvar) {
        subsets[i] <- arr[arr.length==as.character(i)][unlist(bests[i])[1]]
        labels[[i]] <- dimnames(X)[[2]][unlist(subsets[i])]
    }
    names(subsets) <- 1:nbvar
    names(labels) <- 1:nbvar
    list(subsets=subsets,labels=unlist(lapply(labels,paste,collapse=",")),
    minrmsep=minrmsep)
}
```

B.4 Programs in R/Splus for double-sampling schemes

```
optisamp.spr <- function(n,nr,sigmazx,rsdref,sloperef) {
    if (is.vector(sloperef))
    sloperef <- matrix(sloperef, ncol=1)
    nbz <- nrow(sloperef)
    nbx <- nrow(sigmazx)-nbz
    sigmaz <- sigmazx[1:nbz,1:nbz]
    sigmax <- sigmazx[(nbz+1):(nbz+nbx),(nbz+1):(nbz+nbx)]
    covzx <- sigmazx[(nbz+1):(nbz+nbx),1:nbz]
    sigmaz.x <- sigmaz-t(covzx)%*%solve(sigmax)%*%covzx
    tau <- max(eigen(covzx%*%ginverse(sigmaz)%*%t(covzx)%*%ginverse(sigmax),sym=T)$values)
    rsd <- sqrt(rsdref^2+t(sloperef)%*%sigmaz.x%*%sloperef)
    rho <- sqrt(1-(rsdref/rsd)^2)
    h <- nr/n
    f <- (h-(1-rho^2)*tau)/rho^2
    as.integer(round(nr/f)+1)
}

spr <- function(Xs,Zs,coefref) {
    solve(t(cbind(1,Xs))%*%cbind(1,Xs))%*%t(cbind(1,Xs))%*%cbind(1,Zs)%*%coefref
}

msep.ols <- function(X,Z) {
    if (is.vector(Z)) Z <- matrix(Z,ncol=1)
    res <- matrix(lsfit(X,Z)$res,nrow=nrow(Z),ncol=ncol(Z))
    wghts <- matrix(rep(1/(1-hat(X)),ncol(res)),nrow=nrow(res),ncol=ncol(res))
    wres <- res*wghts
    (t(wres)%*%wres)/nrow(res) }
```

B.5 Logistic regression for dealing with sub-populations

By Bas Engel

We will consider an example with two sub-populations, where sampling scheme III consists of one separate sub-sample for each sub-population that is considered. Generalization to several sub-samples is straightforward.

In 1990, throughout the EC, a dissection trial was carried out as a first step towards harmonisation of methods for pig classification in the EC. The proposal for the trial (EC, 1989a) specifically mentioned a possible interest in differences between sub populations. In The Netherlands at that time there was an interest in differences between gilts and castrated males. Separate samples were taken for the two sexes in accordance with the sampling proposal for this EC-trial, thus ensuring sufficient accuracy for a comparison between these two sub-populations. The instrumental carcass measurements were a fat and muscle depth measured by the Henessy grading probe (HGP) (Walstra, 1986).

Separate formulas for gilts and castrated males were calculated and found to be significantly (P ¡ 0.05), although not markedly, different. Due to practical limitations, it was not possible to use separate prediction formulas for the sexes in slaughterhouses in The Netherlands. Therefore, the different formulae for the sexes had to be combined into one overall formula. Since castrates are generally fatter than gilts, obviously the overall formula should be closer to the formula for gilts for small fat measurements, while for large fat measurements it should be closer to the formula for castrates. Consequently, in combining the two formulas, the sexes should get different weights that depend on the carcass measurements.

To evaluate expressions for these weights, extra information was needed about the proportions of gilts and castrated males in the pig population, in relation to the prediction variables as collected with the HGP. To that end an additional large sample of 134158 carcasses was collected from data registered in Dutch slaughterhouses. For all these carcasses gender and HGP measurements were available. No additional dissections were needed.

As was observed before, ignoring the sexes in the regression calculations would not be a statistically sound approach. Due to the sampling scheme, in the total sample, which is a combination of the sub samples for the two sub-populations, gilts are over-represented for the fat carcasses, while castrates are over-represented for the lean carcasses.

Suppose that for a particular pair of observed values for backfat and muscle thickness there are K carcasses in the underlying population with these same carcass measurements. Suppose that k of these carcasses correspond to gilts and $(K-k)$ carcasses to castrates. Let $p = k/K$ and $1-p = (K-k)/K$ be the corresponding proportions of gilts and castrates in the population. The overall mean lean meat proportion m of the K carcasses in the population would be the best prediction for the carcass on the basis of the HGP values observed. When m_g and m_c are the means corresponding to the k gilts and $(K-k)$ castrates respectively:

$$m \quad = \quad pm_g + (1-p)m_c$$

The predictions from the separate formulas for gilts and castrates, say $\hat{y}_g$ and $\hat{y}_c$, are estimates for the means m_g and m_c and a natural choice for the overall prediction $\hat{y}$ is:

$$\hat{y} \quad = \quad p\hat{y}_g + (1-p)\hat{y}_c$$

The proportions p and $(1-p)$ depend on the observed fat and muscle depth. For small fat measurements, p will approach 1 and $(1-p)$ will approach 0 and the prediction $\hat{y}$ will be close to the prediction $\hat{y}_g$ for a gilt. For large fat measurements, p will approach 0 and $(1-p)$ will approach 1, and the prediction will be close to the prediction $\hat{y}_c$ for a castrate.

So, the weights employed to combine the separate predictions for the sexes are not constant! They are estimates for the proportions of gilts and castrates in the population, and depend on the observes instrumental measurements. In Engel and Walstra (1993) it is shown how expressions for these weights can be obtained from the additional sample where both sex and objective carcass measurements are known. In Engel et al. (2003b) the performance of the Engel & Walstra approach is compared with the use of LR ignoring the sexes. The Engel & Walstra approach is clearly superior, but the gain depends on the size of the differences between the populations.

For the evaluation of a suitable substitute for the RMSE we refer to the calculations in Engel and Walstra (1993) for the 1990 EC-harmonisation trial. There are additional details about the model and the construction of the overall prediction formula in Engel et al. (2003b).

In Engel et al. (2003b) the potential improvement of the use of separate prediction formulae for sub-populations is investigated in a simulation study. This simulation study is based on practical data from The Netherlands and Spain. The study shows that a marked bias may occur between sub populations. This bias can be eliminated, and prediction accuracy can be substantially increased, when separate formulae per sub population are used. It is likely that such improvements will have a commercial interest for producers that specialize in certain sub populations. When the technology for implants improves in the near future, sub populations will be recognizable automatically in the slaughter-line and the use of different prediction formulae will become practically feasible. Additional details are provided in Engel et al. (2003b).