Application of spectral analysis to feed and food quality monitoring

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SPECTRAL ANALYSIS:

Raman Spectroscopy

Mid Infrared Spectroscopy (FT-IR)

Near Infrared Spectroscopy (NIRS)

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Near Infrared Spectroscopy (NIRS)

Instrumentation

Chemometrics & Calibration

Applications

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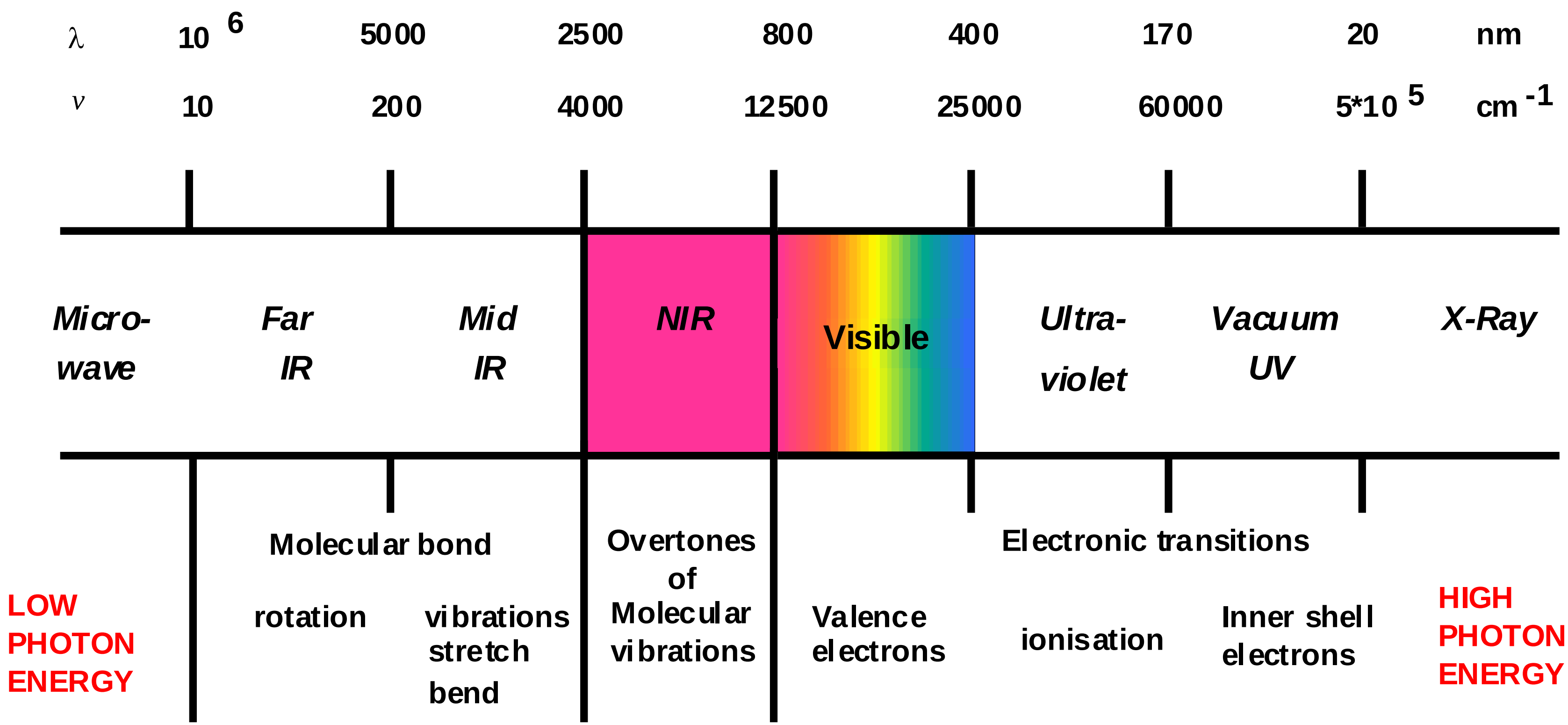
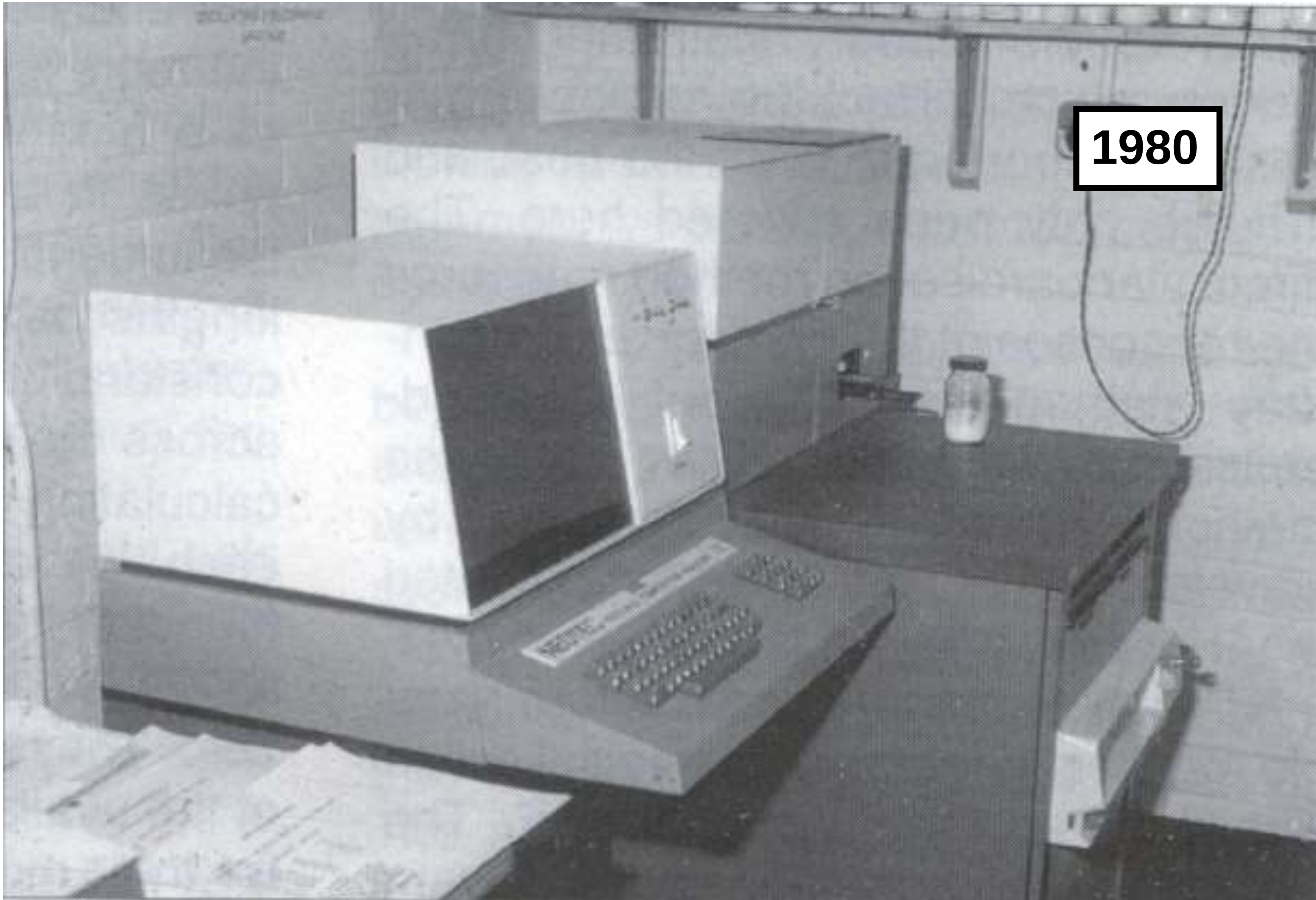
The Electromagnetic Spectrum



$\lambda\nu = c = 3 \times 10^{8}\ m\ s^{-1}$ $E_{photon} = h\nu$ $h = 6.6 \times 10^{-34} Js$



The first commercial monochromator instrument, the Neotec 6350.

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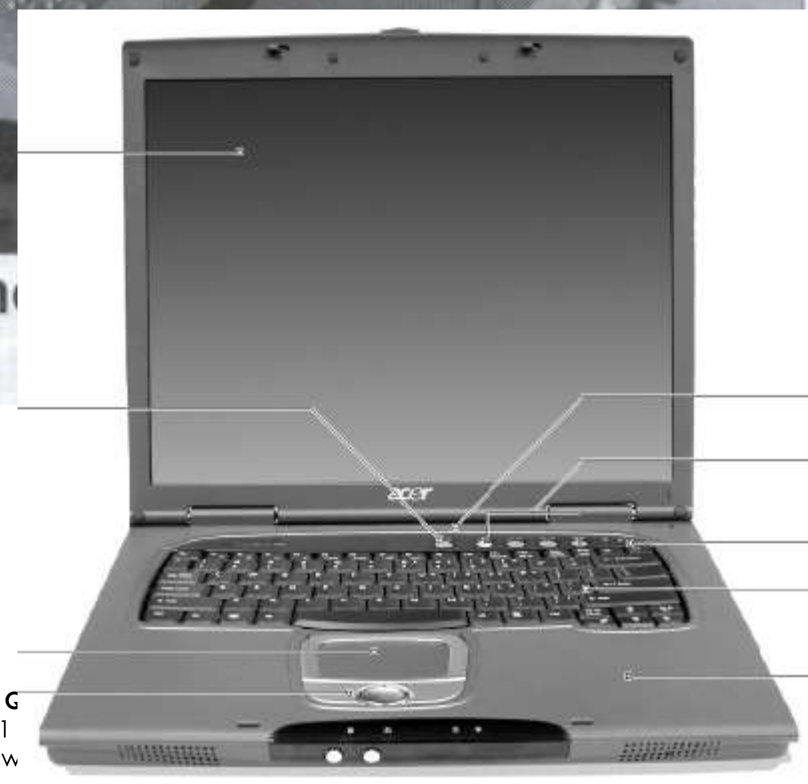

rtement G
- 32 (0)81
tp://cra.w

INSTRUMENT IMPROVEMENTS:

-Sources
-Optical components
-Detectors
-Electronics (communication)

Sample presentation:

- large cups
- slurries
- liquids
- on-line (belts, pipes, …)
  - fibre optics
  - remote scanning

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INSTRUMENTATION TRENDS:

miniaturization → portable

imaging

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The questions are:

How long does it last to complete a calibration?

How many samples are needed to obtain a robust model?

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NIR EQUATION STABILITY OVER TIME

Product: WHOLE PLANT MAIZE SILAGE

Constituents:

PROTEIN	CRUDE FIBER	STARCH	OMD
(1600)	(1700)	(1950)	(2400)

	90	91	92	93	94	95
Model 1	Calib	Validation				
Model 2	Calibration		Validation			
Model 3	Calibration			Validation		
Model 4	Calibration				Validation	
Model 5	Calibration					Valid

Validation is <u>INDEPENDENT</u>

Dardenne *et al.*,NIR News vol.7 N°5 (1996)

STARCH

Mod	N	Min	Max	SEC	R^2C	SecV	R^2V	Tpls
90	198	2	48	1.26	.99	1.69	.98	8
91	245	2	48	1.37	.98	1.70	.97	9
92	522	2	53	1.37	.98	1.62	.98	13
93	709	2	53	1.59	.98	1.74	.97	10
94	1125	2	53	1.61	.98	1.74	.97	11

Model	Val	N	SEP	%H>3
90	91-95	1779	2.80	22
91	92-95	1733	2.47	21
92	93-95	1448	2.41	13
93	94-95	1259	2.31	11
94	95	831	1.89	10

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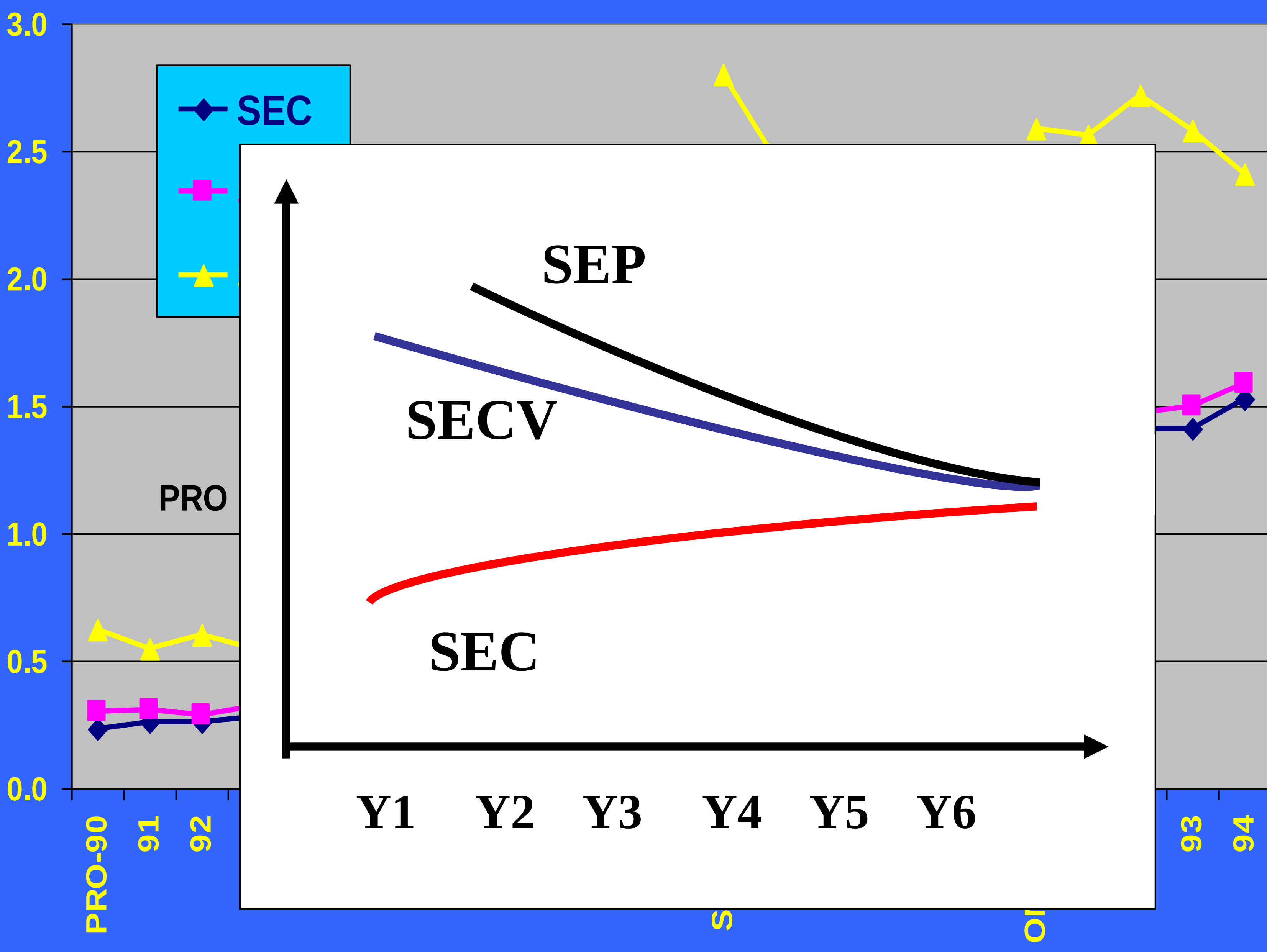
NIR EQUATION STABILITY OVER TIME



In NIR models

ADD NEW INFORMATION (new samples) & RECALIBRATE:

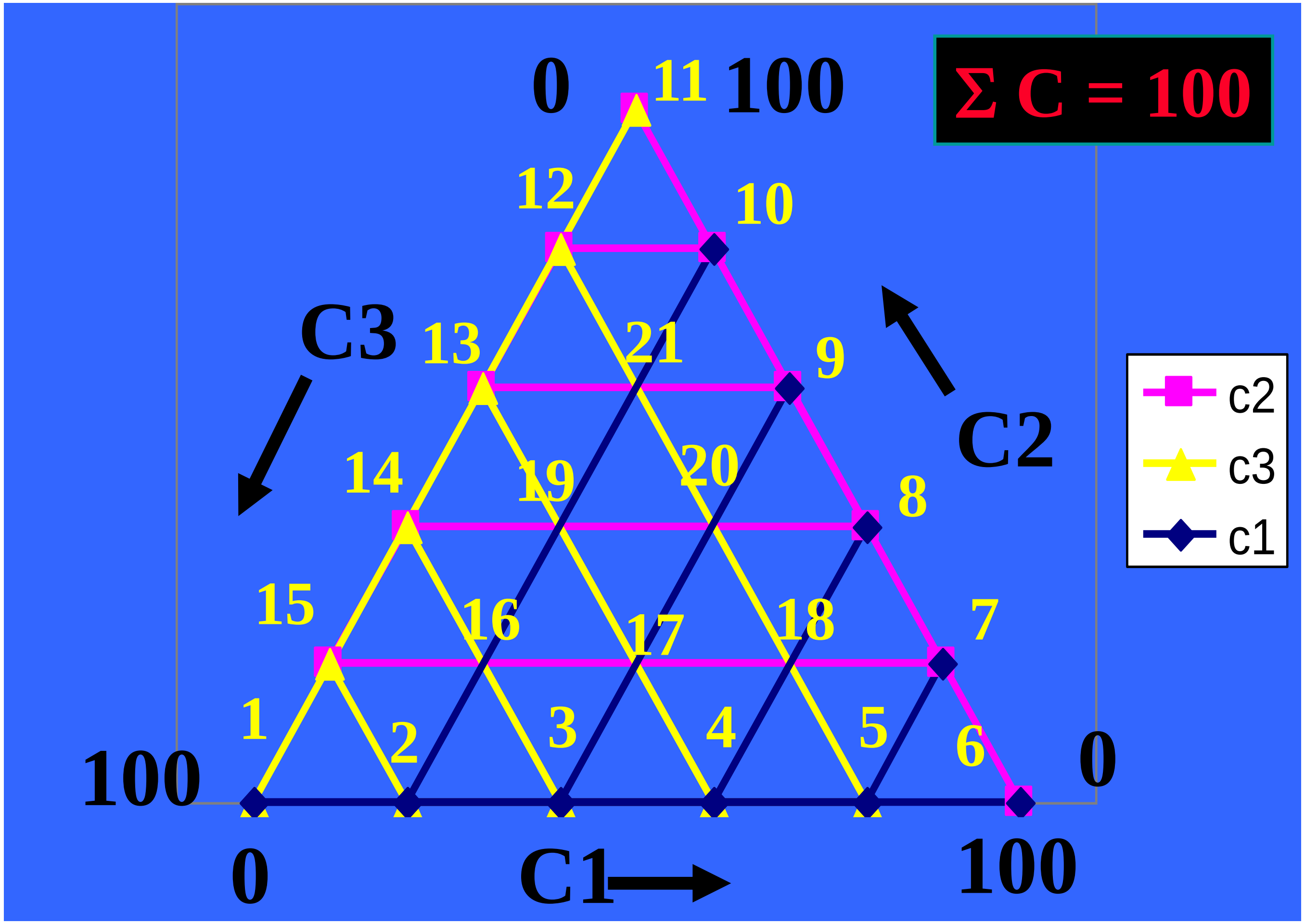
1) While SECV # SEC

2) While SEP # SECV

Shenk & al., Agriculture Handbook, N°643

3 Constituents : 2 dimensions

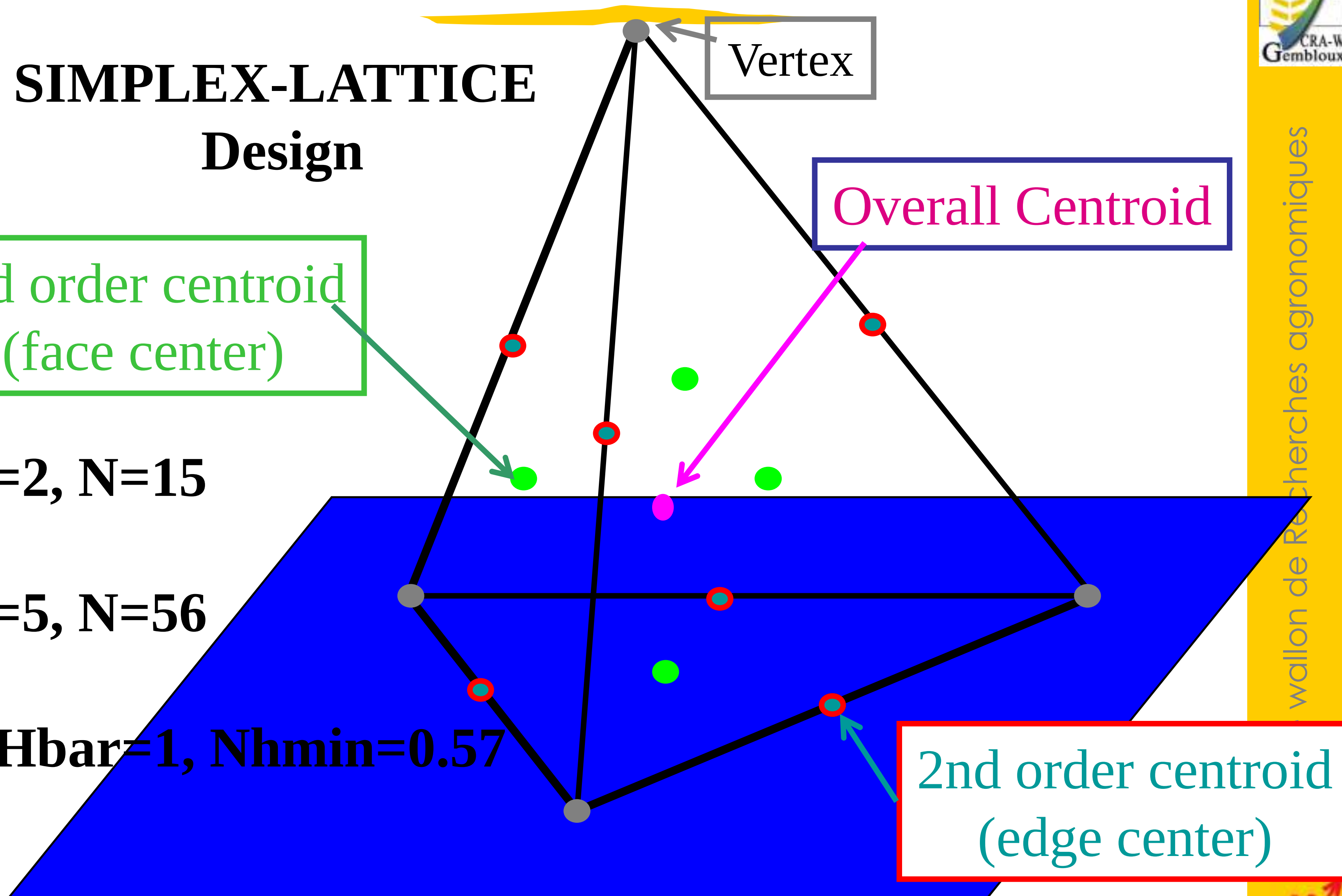
N=21



GHbar=1, NHmin=0.60

4 Constituents : 3 dimensions

SIMPLEX-LATTICE Design



R=2, N=15

R=5, N=56

GHbar=1, Nhmin=0.57

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p **Constituents :**

***p*-1 dimensions**

Ranges /5 → r=5

$$Nspl = C_{r+p-1}^{p-1}$$

$$C_{r+p-1}^{p-1} = \frac{(r+p-1)!}{r!(p-1)!}$$

GHbar=1, NHmin=0.57

Const.	Dim.	Nspl
3	2	21
4	3	56
5	4	126
6	5	252
7	6	462
8	7	792
9	8	1287
10	9	2002
11	10	3003
13	12	6108
15	14	11628
:	:	:
25	24	118755

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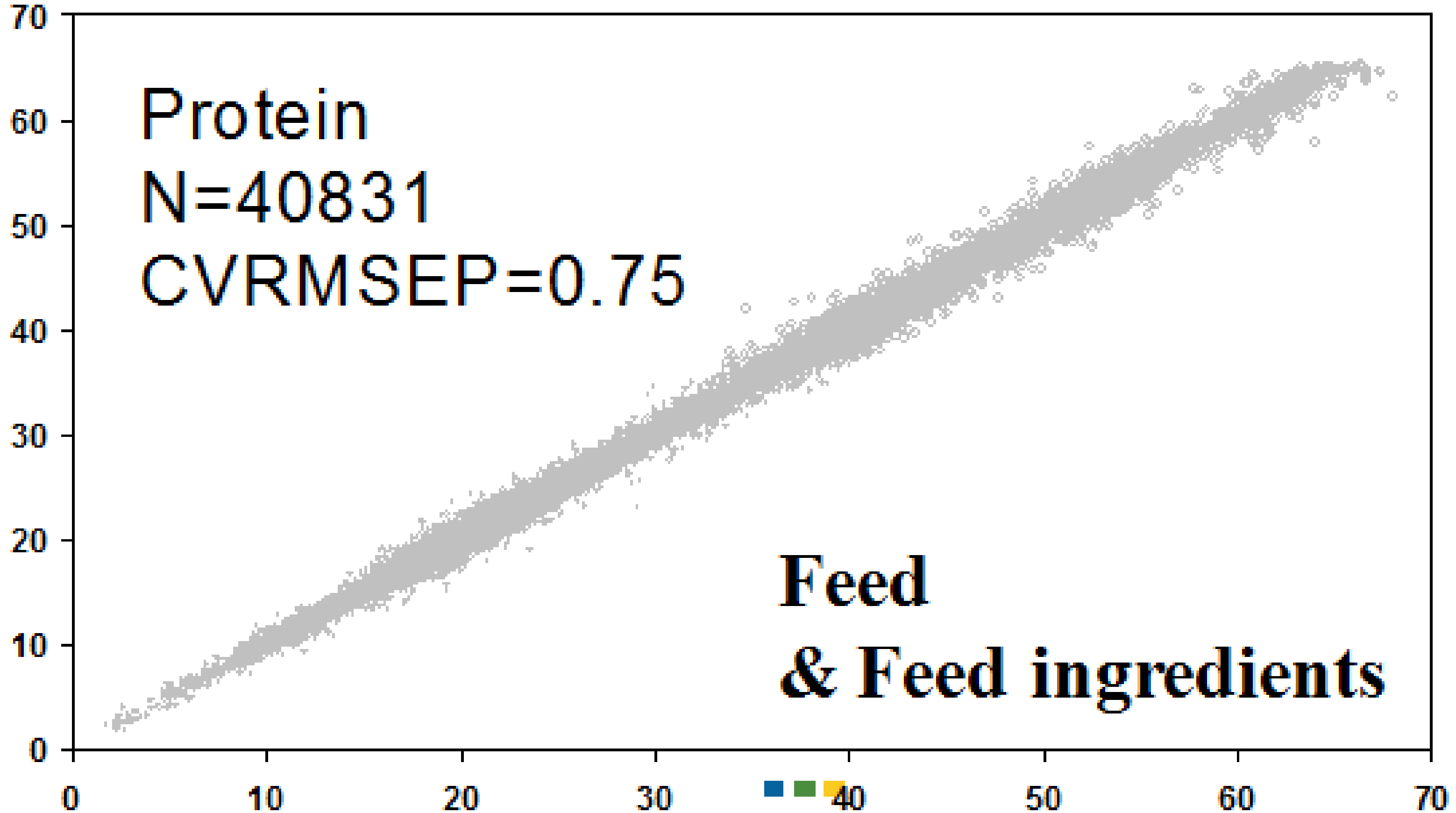
Merging data base: CRA-W & Central Laboratories, UK

Example : PROTEIN
N=40831 by LOCAL WinISI III®
Neighbours samples = 250, Factors ignored=3,
Max factors=33, SNVD 1,4,4 1100-2498/12



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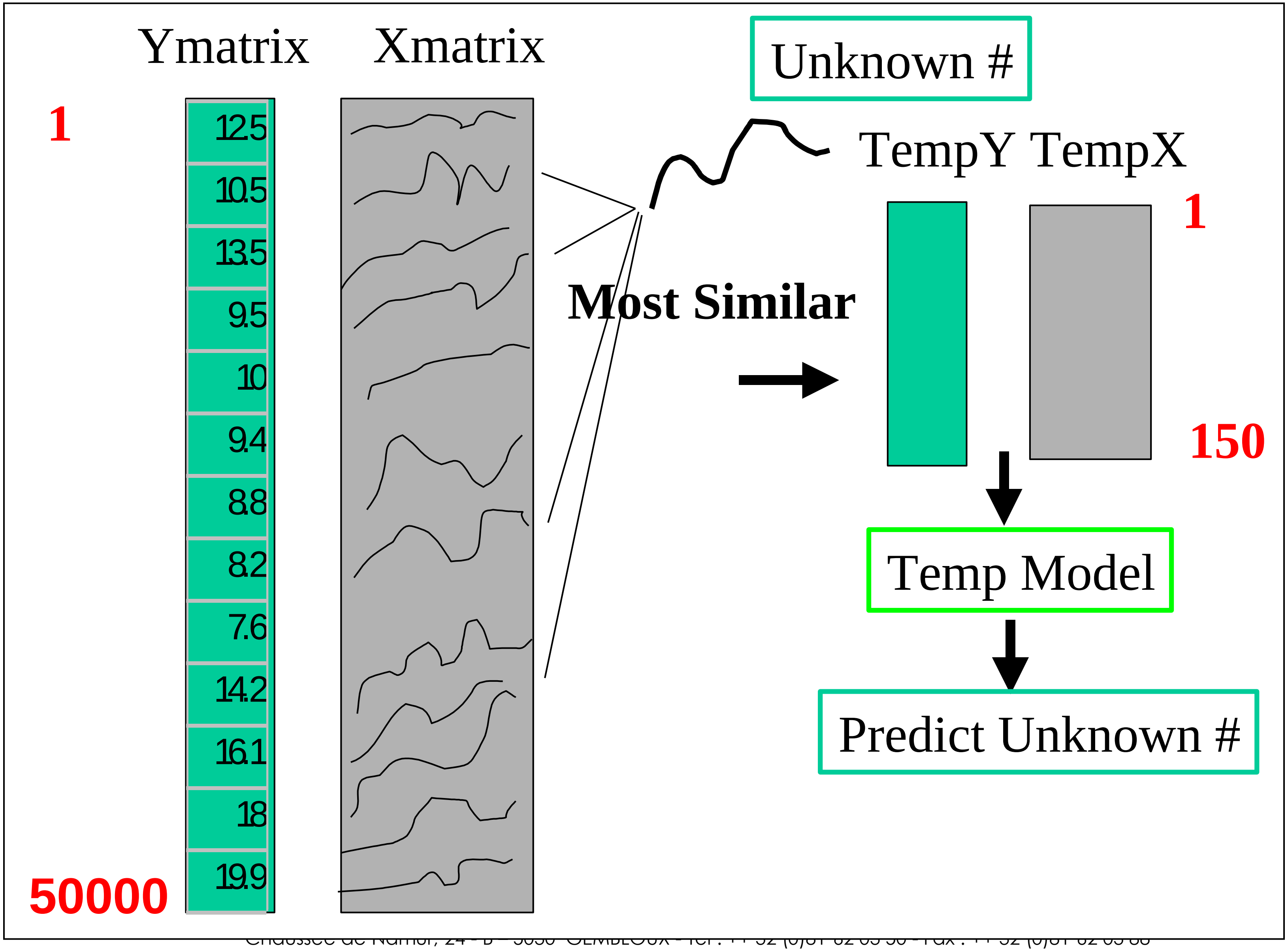
LOCAL concept, Dr. J. Schenk, Infrasoft International LLC



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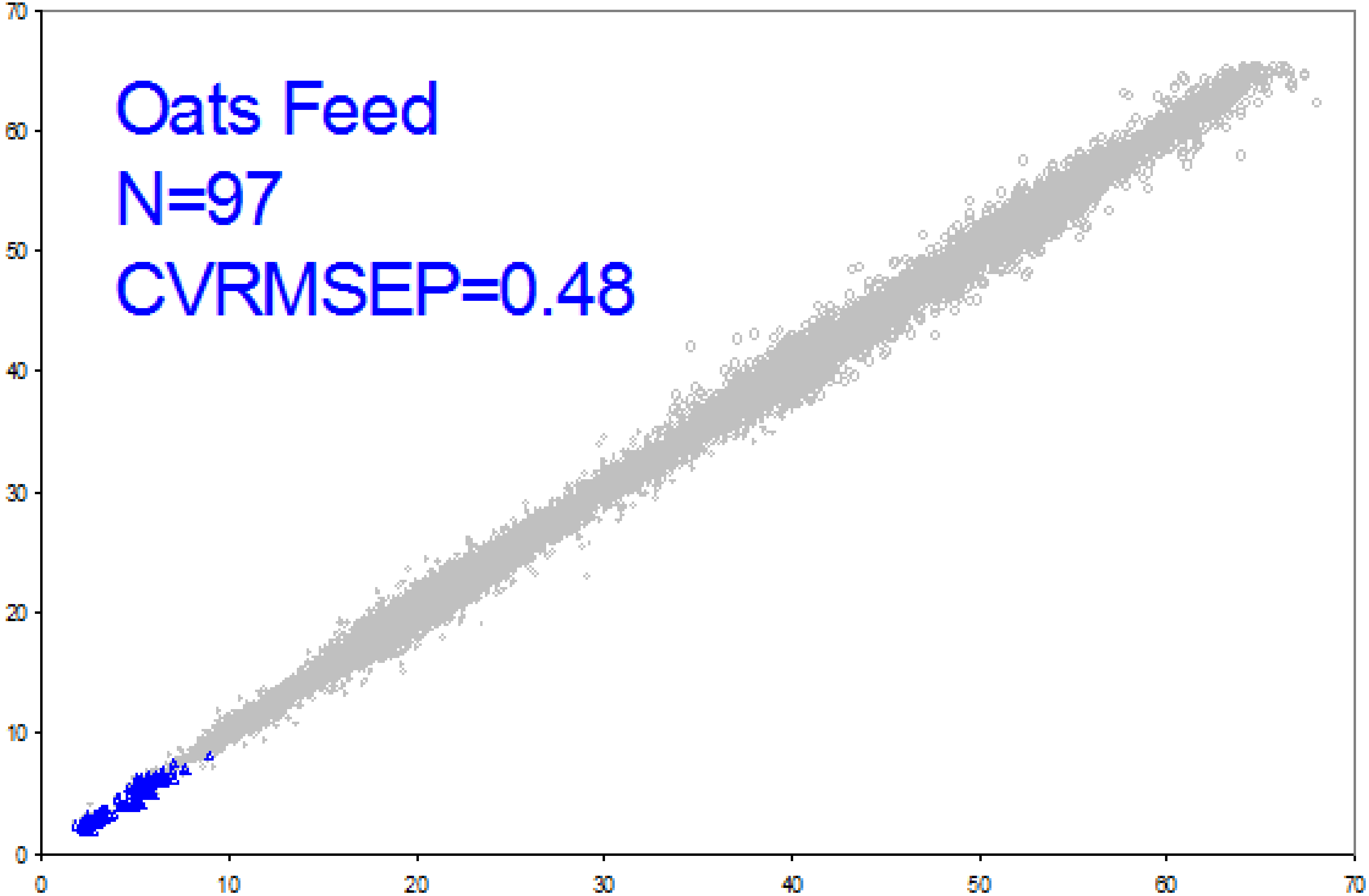
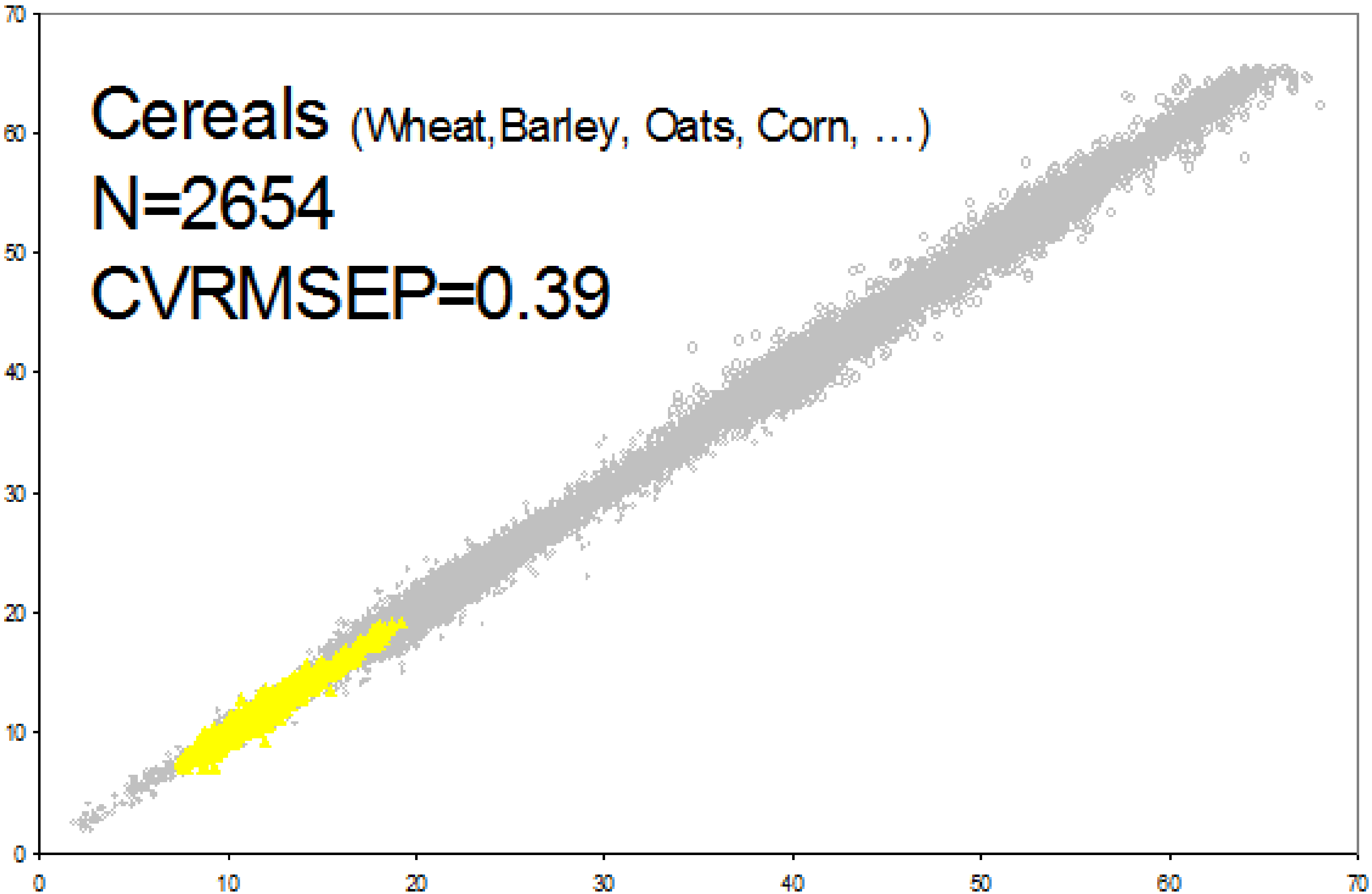


Oats Feed
N=97
CVRMSEP=0.48
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70



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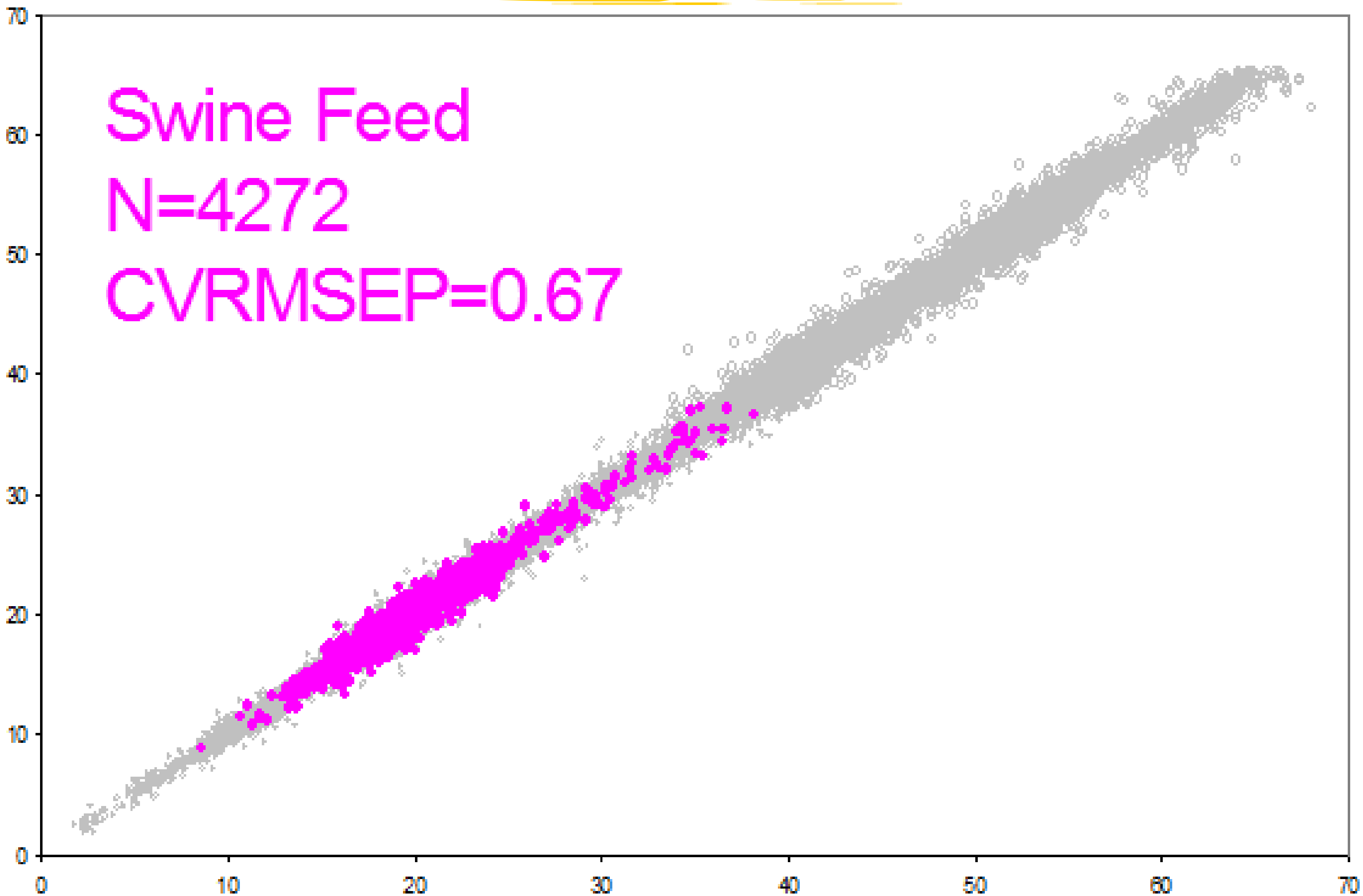

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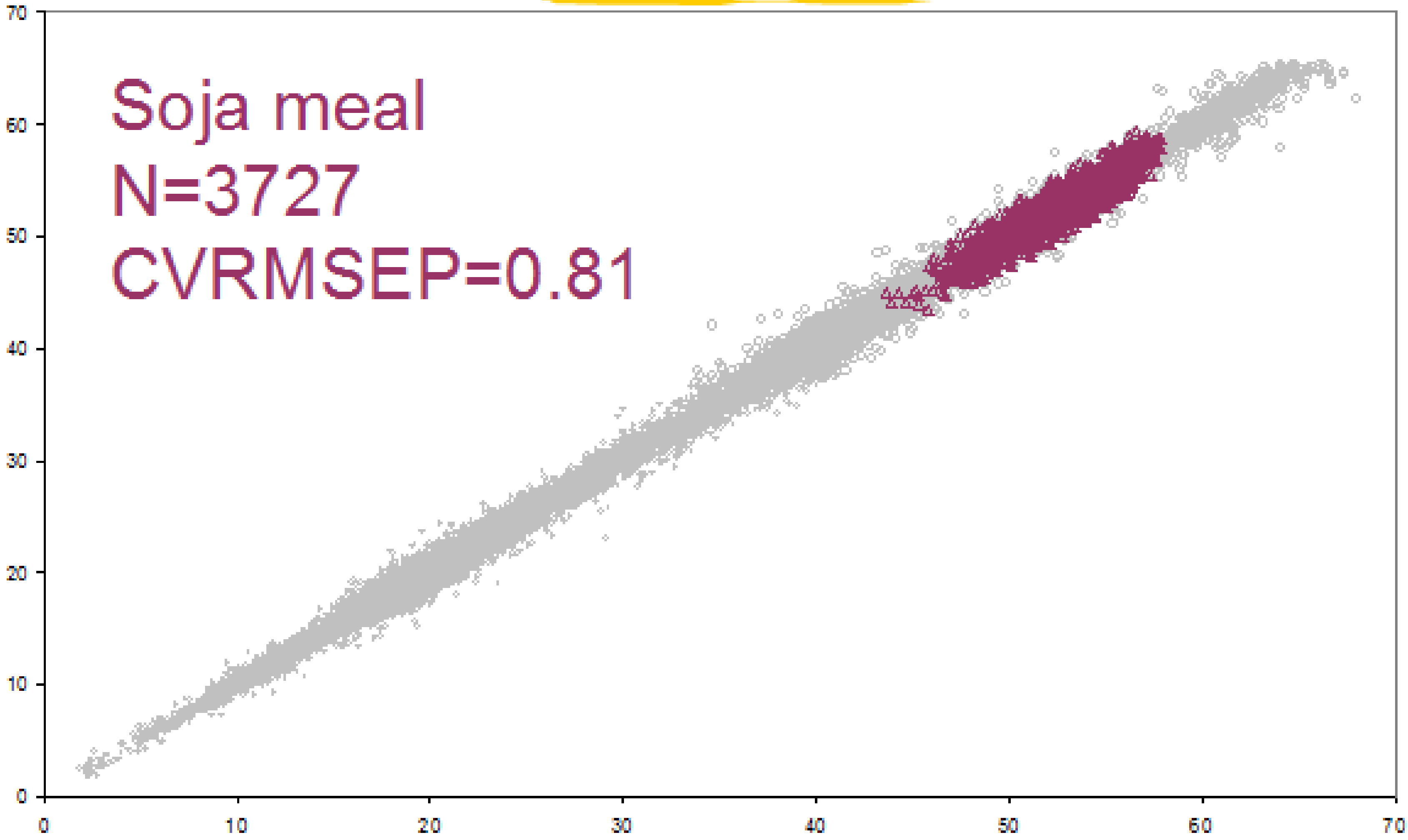

Soja meal
N=3727
CVRMSEP=0.81
70
60
50
40
30
20
10
0
0
10
20
30
40
50
60
70

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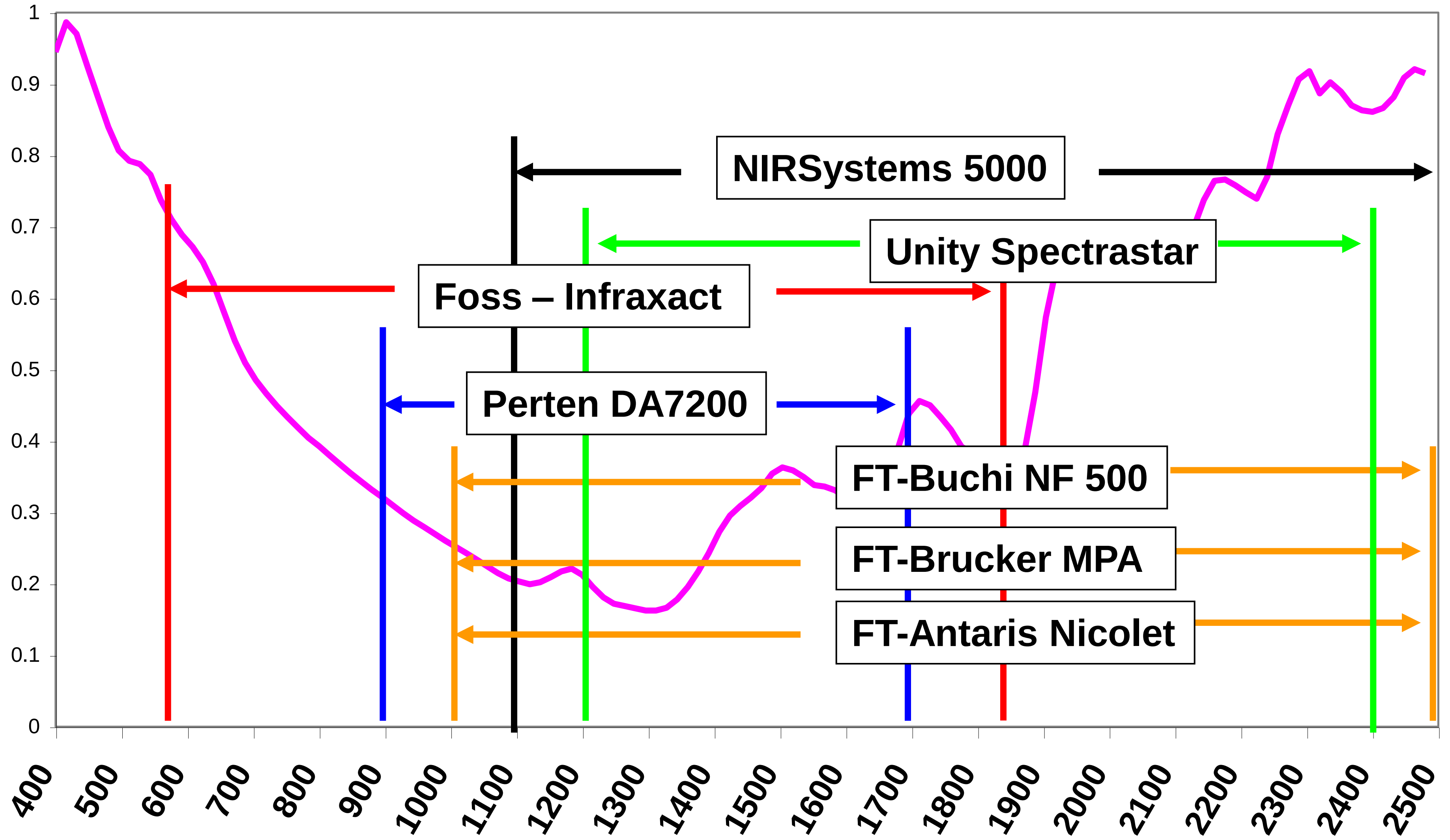
2005


Unity
APPAREIL EN PRET POUR ESSAI
SpectraStar
2400


Thermo

INSTRUMENTS POWERED BY INGOT®

http://www.central-labs.co.uk/



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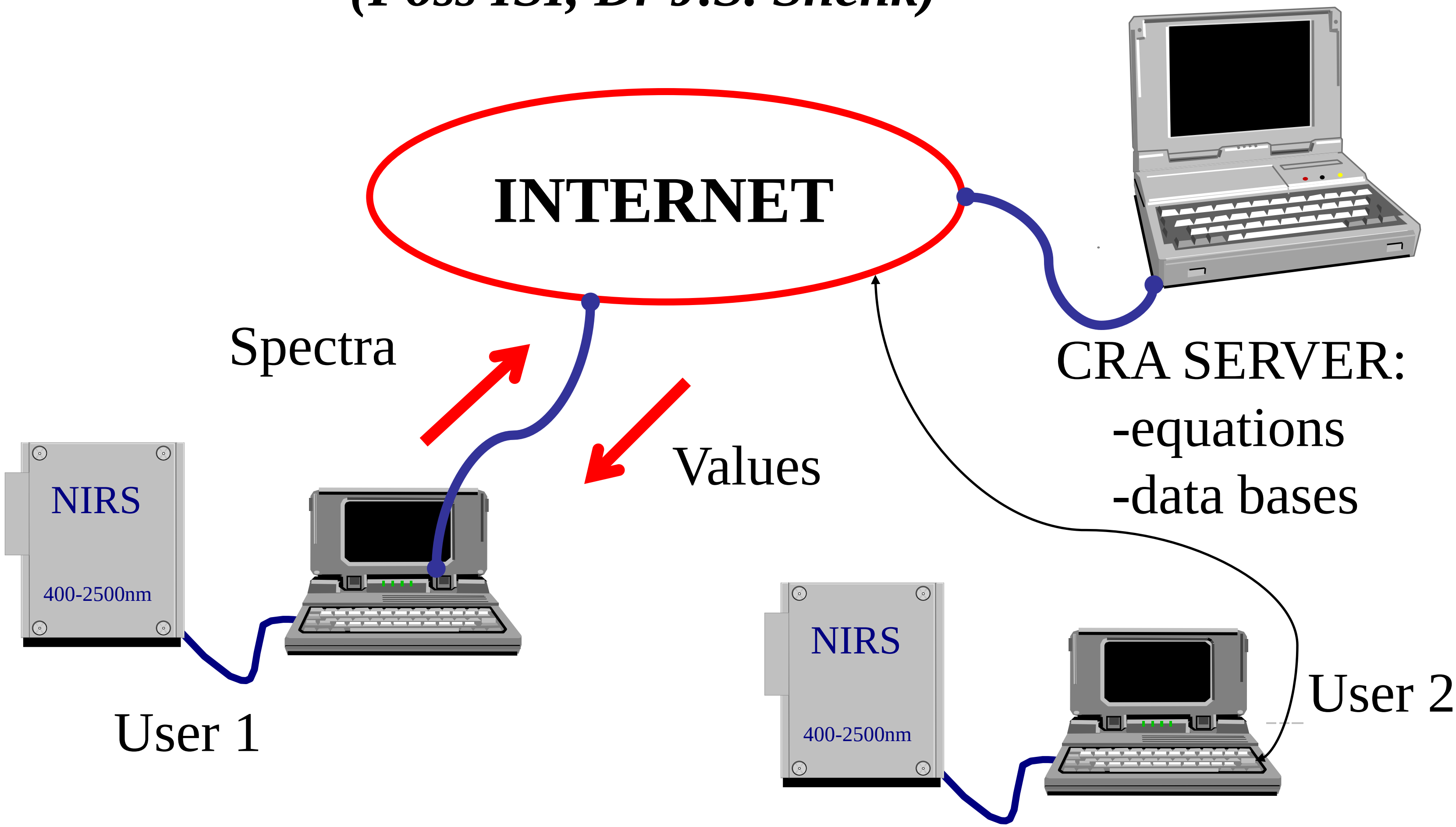
•Networks of instruments   (2000)

RINA® : ***Remote Instrument Near Analysis***
(Foss ISI, Dr J.S. Shenk)



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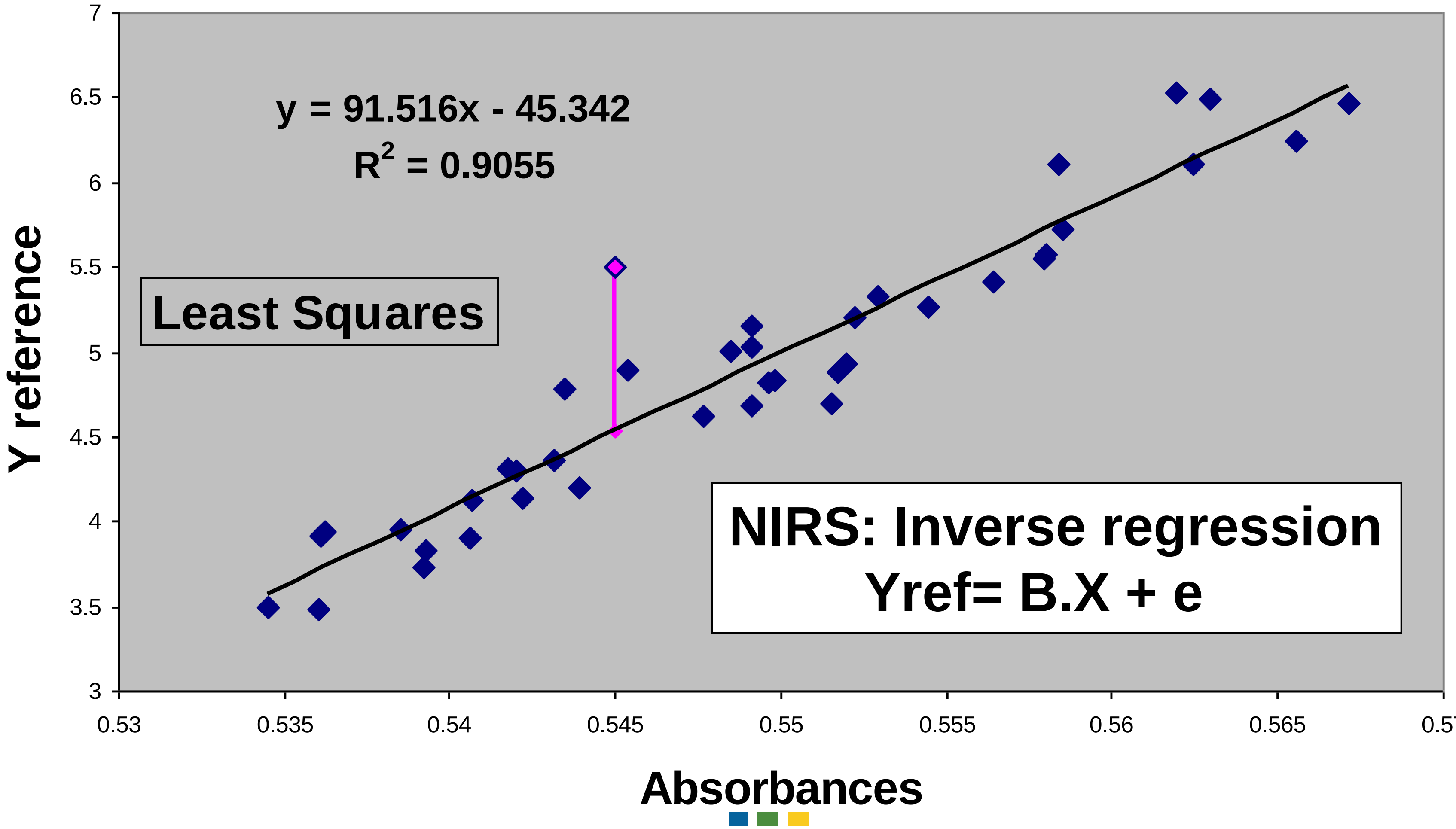
Chemometrics : uncertainty

CALIBRATION



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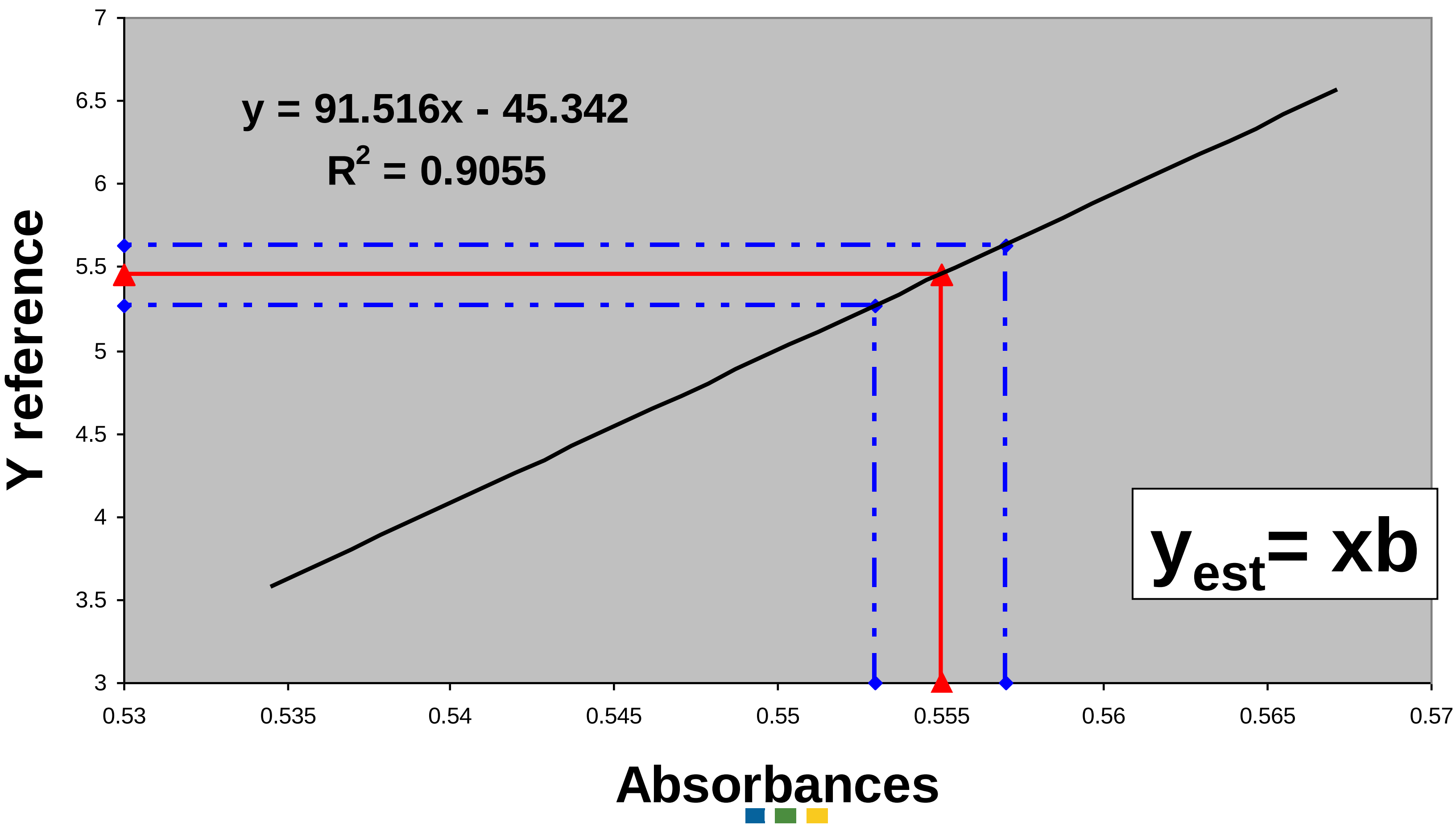
Chemometrics : uncertainty

PREDICTION



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Chemometrics

Uncertainty

of the NIR analyses

$$s(\hat{y}_i - y_i) = \left[(1+h_i).SEC^2 - S_{ref}^2\right]^{1/2}$$

Faber and Bro, *Chemom., Intell. Lab. Syst.* 61, 133 (2002)
Fernandez Pierna & *al., Chemom., Intell. Lab. Syst.* 65,281 (2003)

$$SEP_{actual}^2 = SEP_{observed}^2 - SEL_{ref}^2$$

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Near Infrared Spectroscopy (NIRS)

Instrumentation

Chemometrics & Calibration

Applications

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APPLICATIONS developed at CRA-W

- Fertilizers
- Soils
- Seeds & Phyto-sanitary Protection
- Crop monitoring (N)
- Precision Agriculture
- Nutritive value (feed & forages)
- Technology (flour, baking quality,…)
- Authentication (olive oil, meat, honey,…)
- Fruits
- Transformed Products (meat, dairy, juices,…)
- Bio-fermentation monitoring

•NUTRITIVE VALUE OF FEED

CHEMICAL COMPOSITION & DIGESTIBILITY

- **Moisture – DM**
- **Ashes – OM**
  + P, Ca, K, Mg
- **Fat**
  + FA profile
- **Proteins (N)**
  + AA profile
- **Fibres**
  (cellulose, NDF,ADF,ADL)
- **Starch**
  + amylose - amylopectin
- **Total Sugar**
  + sugar profile
- **OMD**
  in vivo, *in vitro*, enzymatic

Feed Ingredients

Cereals & by-products
Wheat bran
Soyameal
Sugarbeet pulp
Animal protein (MBM)
……

Complete feed

Cattle
Swine
Poultry
Pet food

•<u>FRUITS</u>

Collaborations: Unité de Techno. des IAA, FUSAGx

Dpt Biotechnologie et Phyto. et ressources génétiques

Diode array – apple sorting

Static Mode :

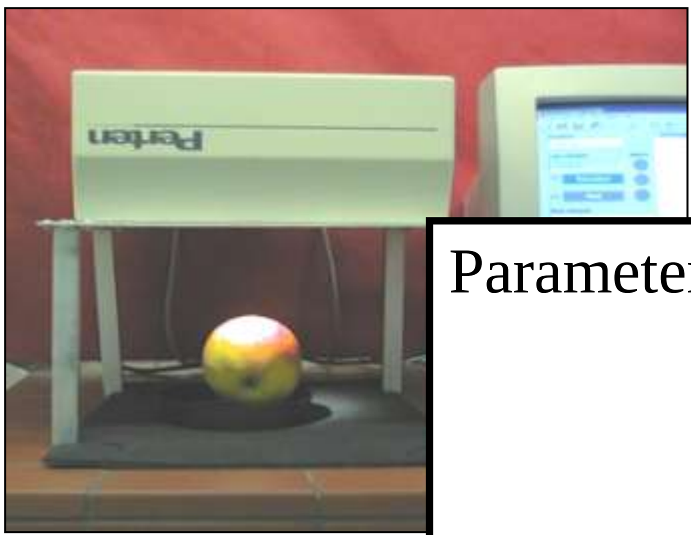
Scan : 1 sec

4 scans / apple

Dynamic Mode

1 scan / apple : 0.3 sec

3 apple / sec



Parameters: Brix
Acidity
pH
Firmness

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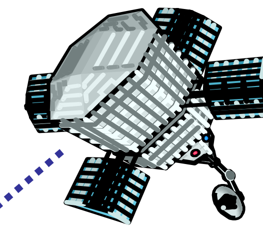

Precision agriculture

Precision agriculture

Breeding companies: *Pioneer, Limagrain, KWS, Syngenta, Monsanto, RAGT, Caussade, Euralis, R2N, Maisadour, NPZ, DLF and Euro-Grass*

1 site : 10000 plots

Oven drying : time consuming, energy cost, …

DM SEP ~ 1.0 - 1.3 %

+ Protein, Starch, OMD, …

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Forage Harvester at CRA-W

CRA-W Gembloux

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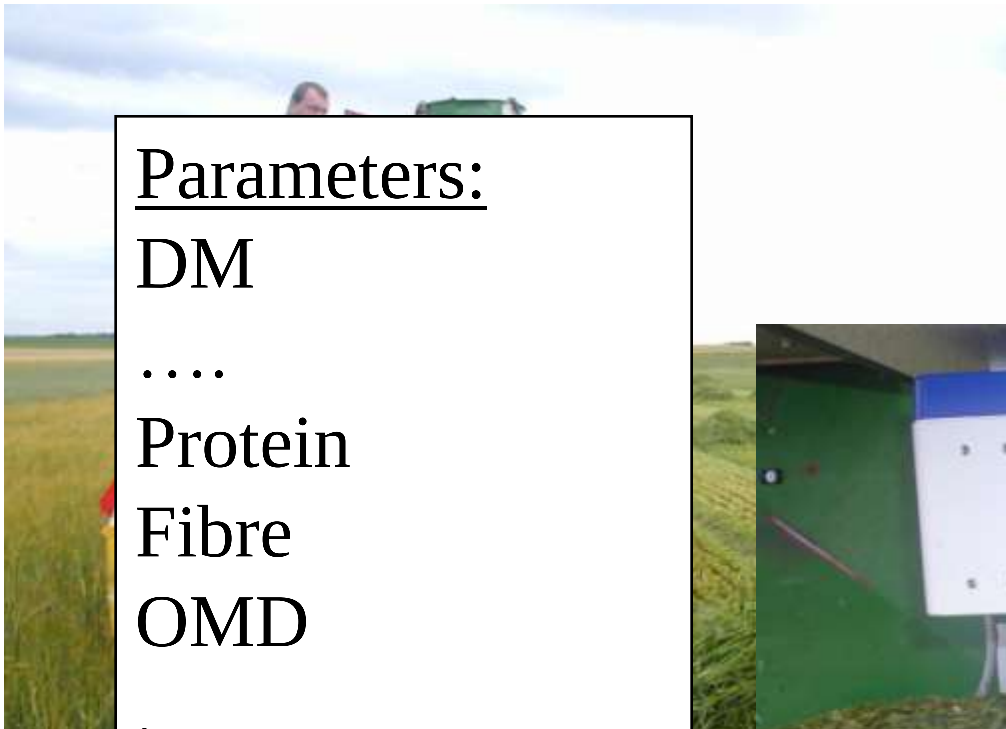
RÉGION WALLONNE

•Embedded SPECTROMETER – Precision agriculture

Collaboration Dpt Production Végétale CRA-W

DM forage yield & quality



Parameters:

DM

….

Protein

Fibre

OMD

.

.

Next: Feb 2007
FAL, Germany
Christian Paul

2nd International Conference on "Embedded Near Infrared Spectroscopy"

CRAW - Gembloux – Belgium 18th and 19th November

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Applications & Instrumentations

Low cost spectrometer – farm level

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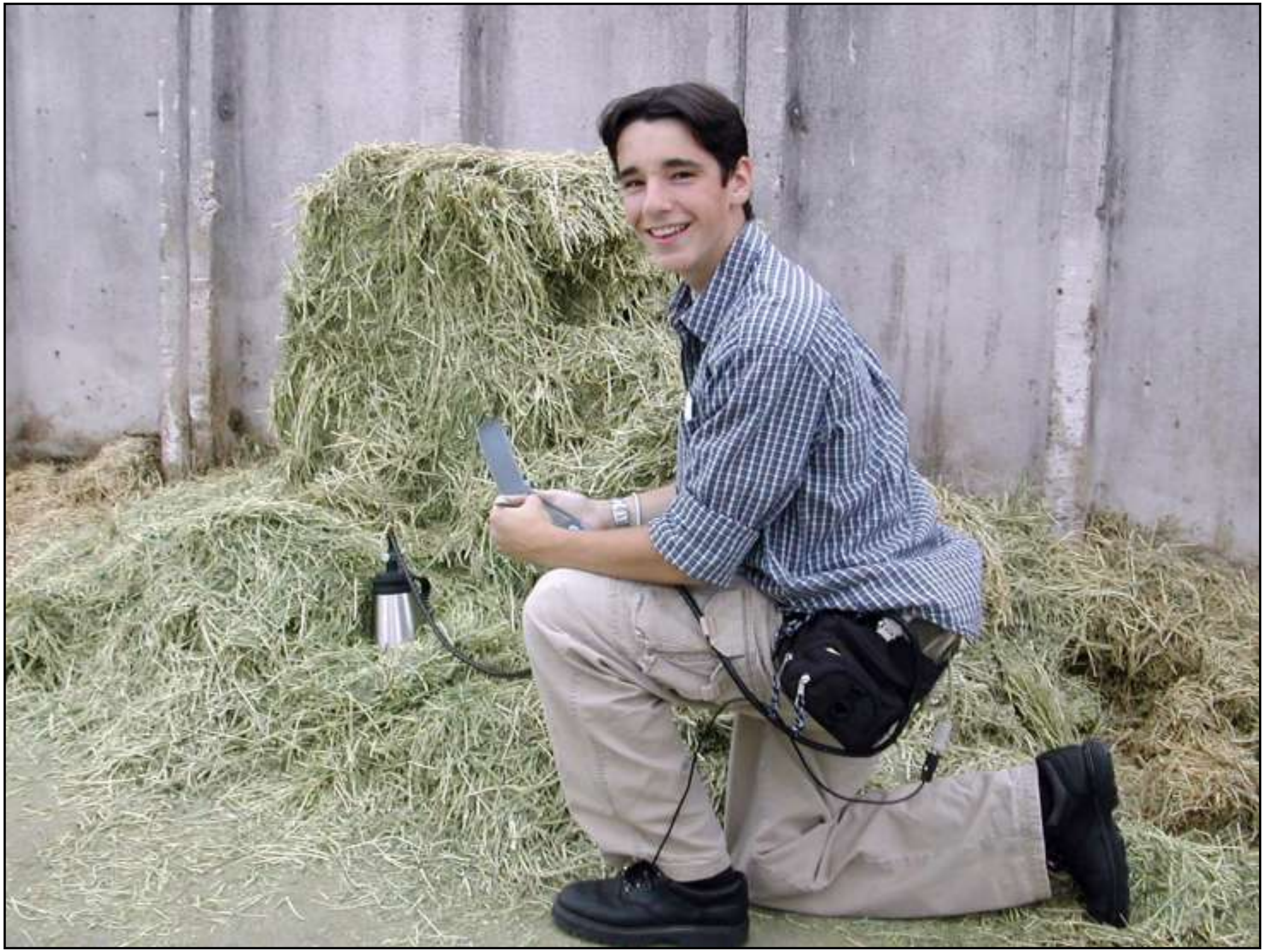

Courtesy of Dr John Schenk

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Mobile TURF

Are you tired of wasting valuable time and money shipping turfgrass samples to a lab for analysis and then having to wait for results?

What if you were able to get the results you needed ***FAST*** – in the time it took you to walk across your golf course green.

It's possible with Mobile Turf, the newest turfgrass analyzer in the industry. On the cutting edge of technology, Mobile Turf allows the golf course superintendent or sports turf manager to **measure the essential nutrients in turfgrass (N, P, K, Ca, Mg, and micronutrients) plus moisture,** quickly and easily.

HOW IT WORKS:

Mobile Turf is a portable, lightweight instrument that uses the visible and near-infrared (NIR) spectrum of light to analyze the turfgrass it contacts.

The operator simply pulls the instrument over the turf that he wishes to analyze and the results are ***INSTANTLY*** recorded in the hand-held PDA.

ADVANTAGES:

Because of all the capabilities of Mobile Turf, the advantages are numerous.

- **Fast results**/No waiting
  Results when you need them.
- **More accurate results** because it actually measures the nutrients in the ***living plant.***
- **More convenient**
  Allows you to take measurements in the field. Measure specific areas or average results across an area.
- **Portable/Hand-Held/Lightweight**
  Weighs less than 5 lbs.
- **Easy to Use and Operate**
  No complicated system to learn.
- **Allows you to fine tune your fertility management**
  Eliminates guesswork and the possibility of over or under-fertilizing.
- **Helps with irrigation water management** because it measures the moisture content of the turfgrass.
- **Reduces pesticide costs**
  because healthy turf is less susceptible to disease.
- Finally Mobile Turf **gives you peace of mind, confidence, and assurance** that you are growing quality turf, tournament turf.
- Best of all, Mobile Turf is **affordable** and will quickly pay for itself.

Figure # 1. NIR Hand-held Analyzer is taking readings for Brix, pH, TA in vineyard without removing it from vine

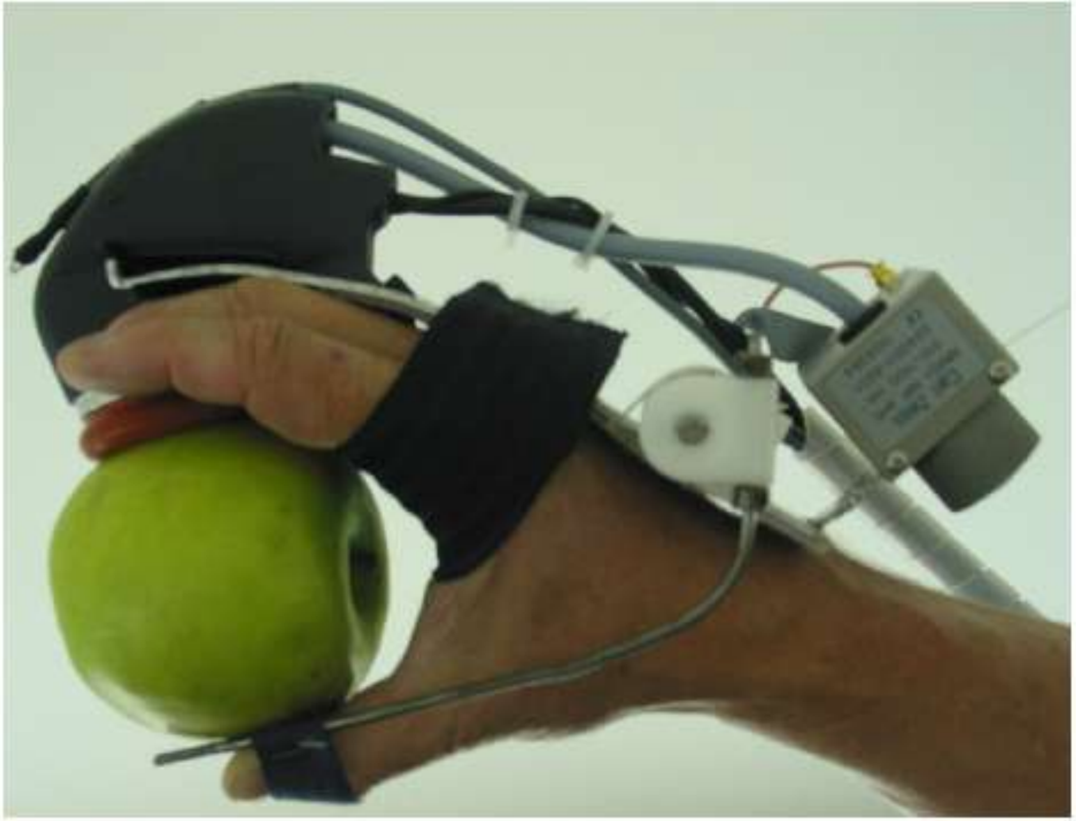
Brimrose Corporation, USA

Gant instrumenté pour mesurer la qualité des fruits

GLOVE

Projet Européen PL 97- 3399 (1998 - 2001)

Partenaires : (Belgique) ; APOFRUIT (Italie); Institut für Agrartechnick Bornim e. V. (Allemagne) VERHAERT (Belgique); Katholieke Universiteit Leuven - sous la coordination du CEMAGREF - UR Giqual



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Hyperspectral imaging and support vector machines for the trace back of compound feeds

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[1]Walloon Agricultural Research Centre (CRA-W), Quality of Agricultural Products Department, Chaussée de Namur n°24, 5030 Gembloux, Belgium
[2]Scientific collaborator F.N.R.S. Statistics and Informatics Department, University of Agronomical Sciences, Avenue de la Faculté 8, 5030 Gembloux, Belgium

3 methods:

1. Classical Microscopy

2. NIR:

2.1 Classical "Macro" NIRS

2.2 NIR & Microscopy (NIRM)

3. PCR *(Polymerase Chain Reaction)*

Agricultural Research Centre of Gembloux (CRAGx, Belgium)
Dr P. Dardenne, Dr V. Baeten, Ir Ph. Vermeulen, Dr. R. Oger, Dr G. Berben
- Management
- PCR method
- NIR Microscopy method
- Data Base Development
- Graphical Query Module Development
- Web Site Creation

State Official Laboratory (ROLT, Belgium)

CRA Gembloux

Gembloux Agricult…
Prof D. Portetelle
- PCR method

des sciences agronomiques

10 Partners

… of Agricultural Products (RIKILT, The Netherlands)
Dr J. de Jong, Dr L. van Raamsdonck, Dr. H. Aarts
- Classical microscopy method
- PCR method
- NIR Spectroscopy method
- Expert system development

Scottish Agricultural C…
Dr I. Murray
- NIR Spectroscopy metho…

…therlands)

Laboratory of the Autonomous G…
Dr J. Bosch
- Classical micros…
- NIR Spectrosco…

…M, UE)

Materials and Measurements

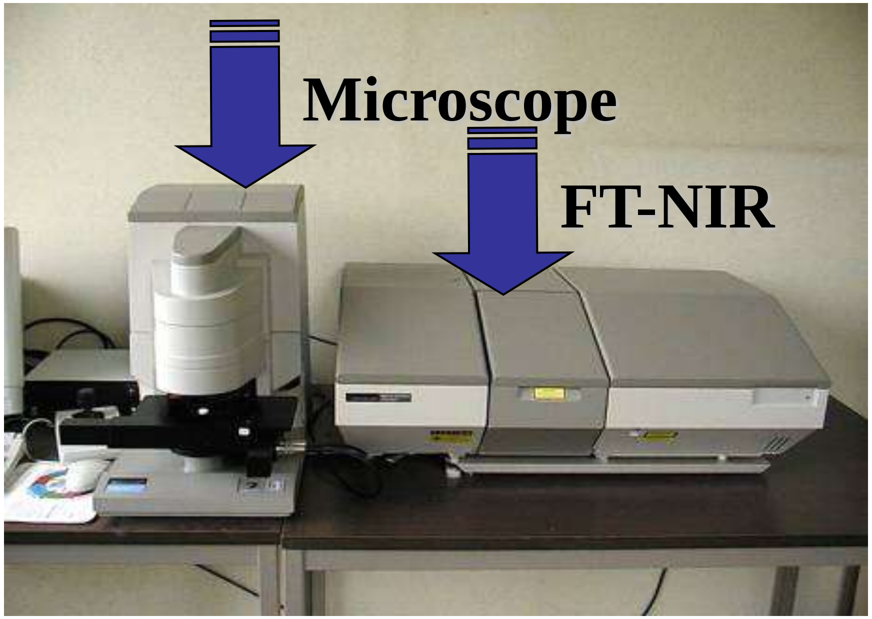
School of Agriculture and Forestry E…

- NIR Spectroscopy method

Web site : http://stratfeed.cra.wallonie.be

Instrument : microscope coupled to a FT-NIR

NIR microscope (NIRM)



Sample particles

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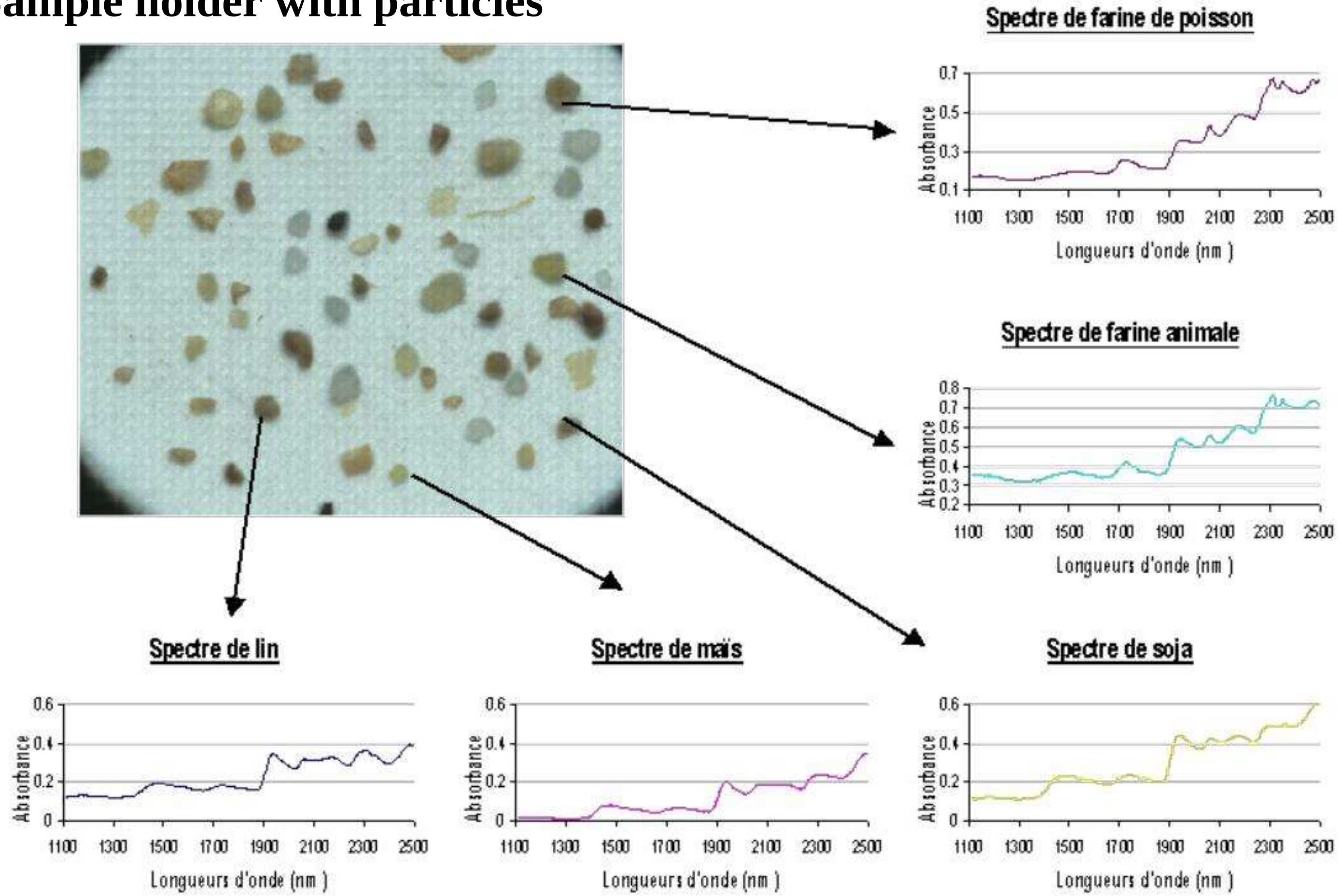
One spectrum / particle

Sample holder with particles



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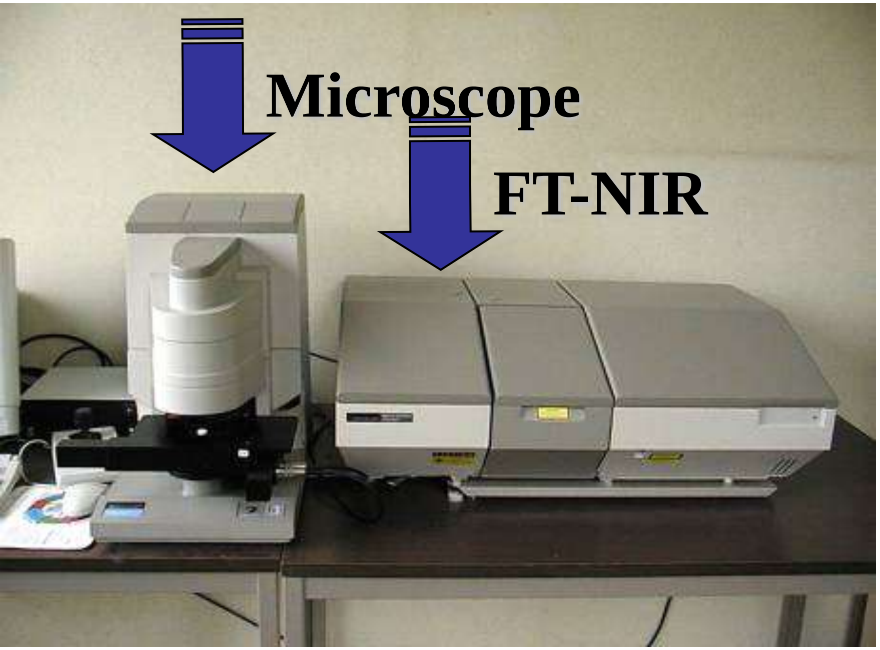
NIR microscopy (NIRM)



Good results but too slow : spectrum acquisition time particle by particle

At 0.5% contamination, 600 particles must be analyzed to get at least 1 with P=.95

At 0.1% , 3000 particles

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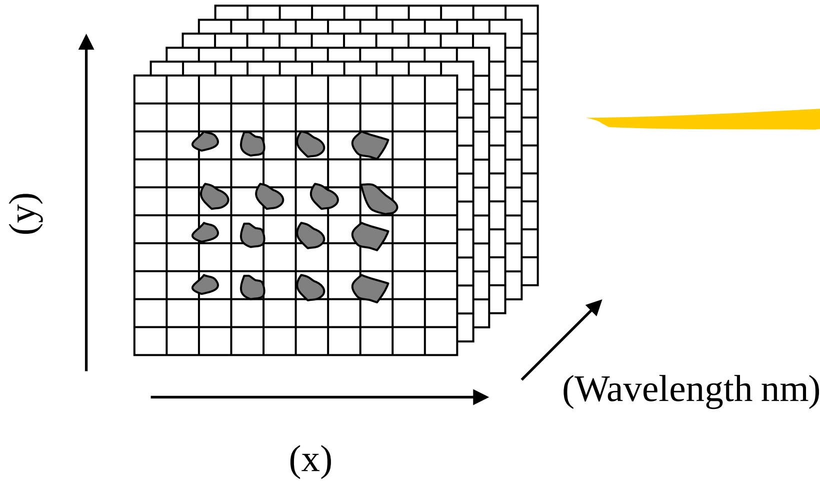
NIR Camera

Matrix NIR,
Spectral Dimensions, Inc.



- Camera InGaAs

- 900 - 1700 / 10 nm

- 240 x 320 pixels

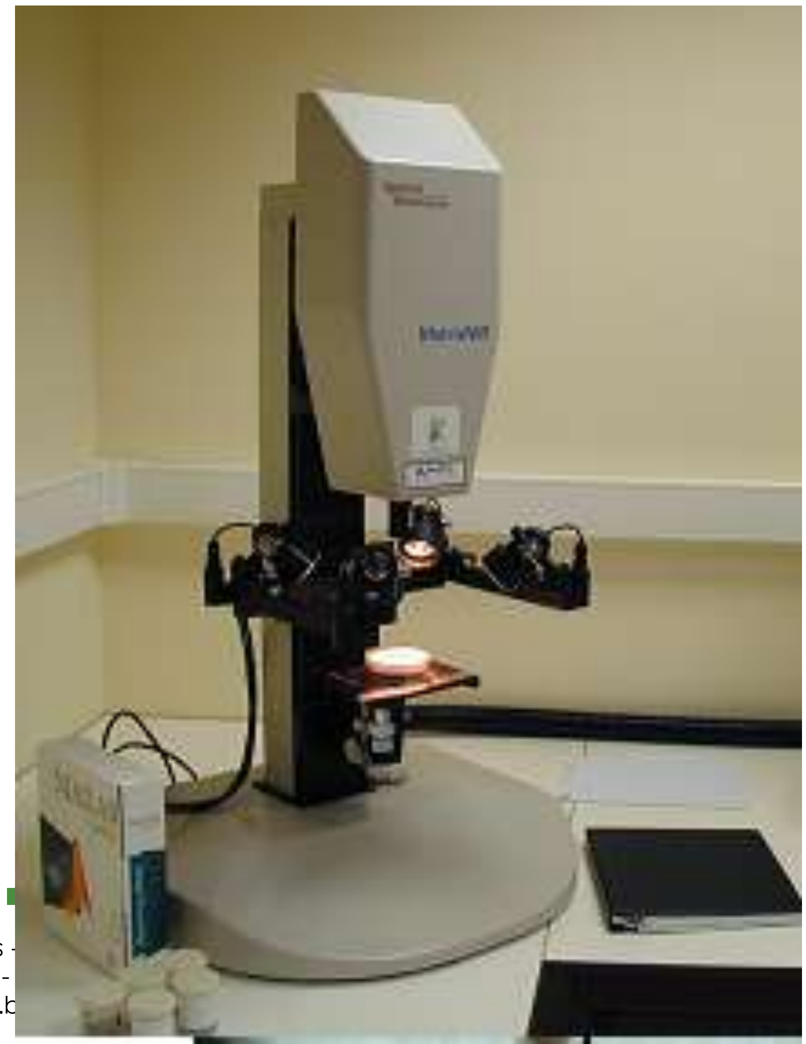
- Each pixel: 70 µm*70 µm

- Analyzed surface : 5 cm²

- 76 800 spectra   24 MB

- 300 - 350 particles

- Analysis time : +/- 5 min



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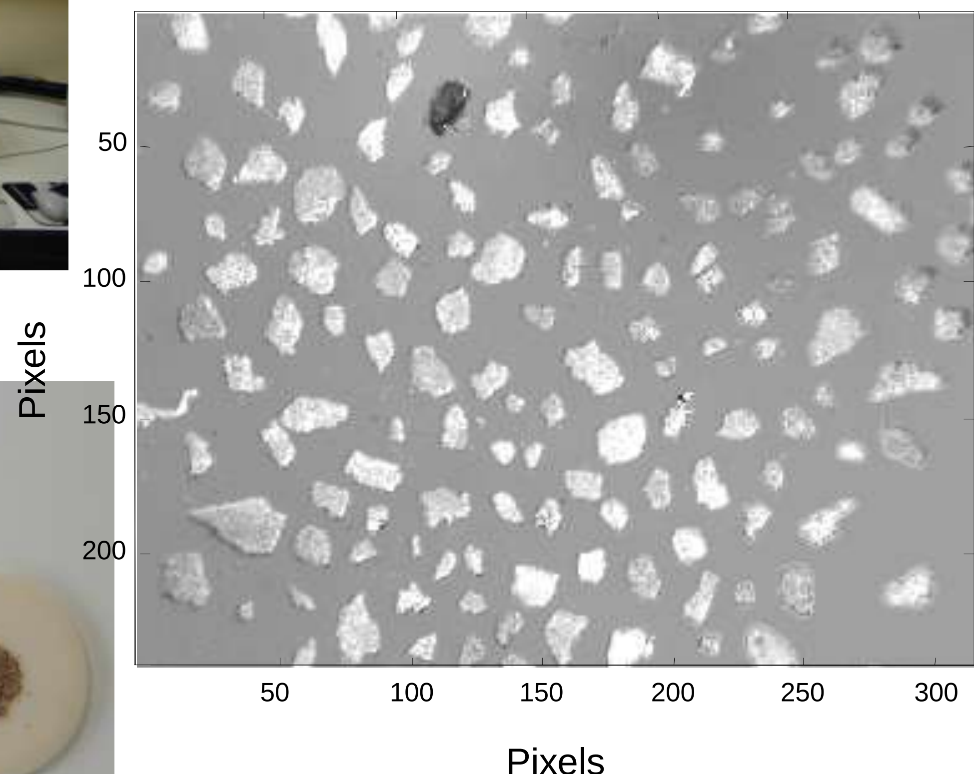
NIR Camera

Matrix NIR,
Spectral Dimensions, Inc.



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Learning data base

2233 animal particles:

- **meat & bone meal**
- **fish meal**
- **poultry meal**

3288 plant particles:

- **cereals (wheat, oats, barley, corn, ..)**
- **protein sources** *(rapeseed meal, peas, soya meal,…)*
- **tropical by-products** *(peanuts, cocoa, coconut, manioc, palm kernel)*
- **other vegetal meals** *(sugar beet by-products, bakery by-products, chicory, lucern, potatoes by-products,..*

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DISCRIMINATION METHODS :

- PLS

- LDA & QDA

- ANN

- SVM

***J. Near Infrared Spectrosc.* 12, 93–100 (2004)**
Least-squares support vector machines for chemometrics: an introduction and evaluation
R.P. Cogdill and P. Dardenne

Support Vector Machines, V.N. Vapnik

(The Nature of Statistical Learning Theory, Springer-Verlag, New York, 1995)

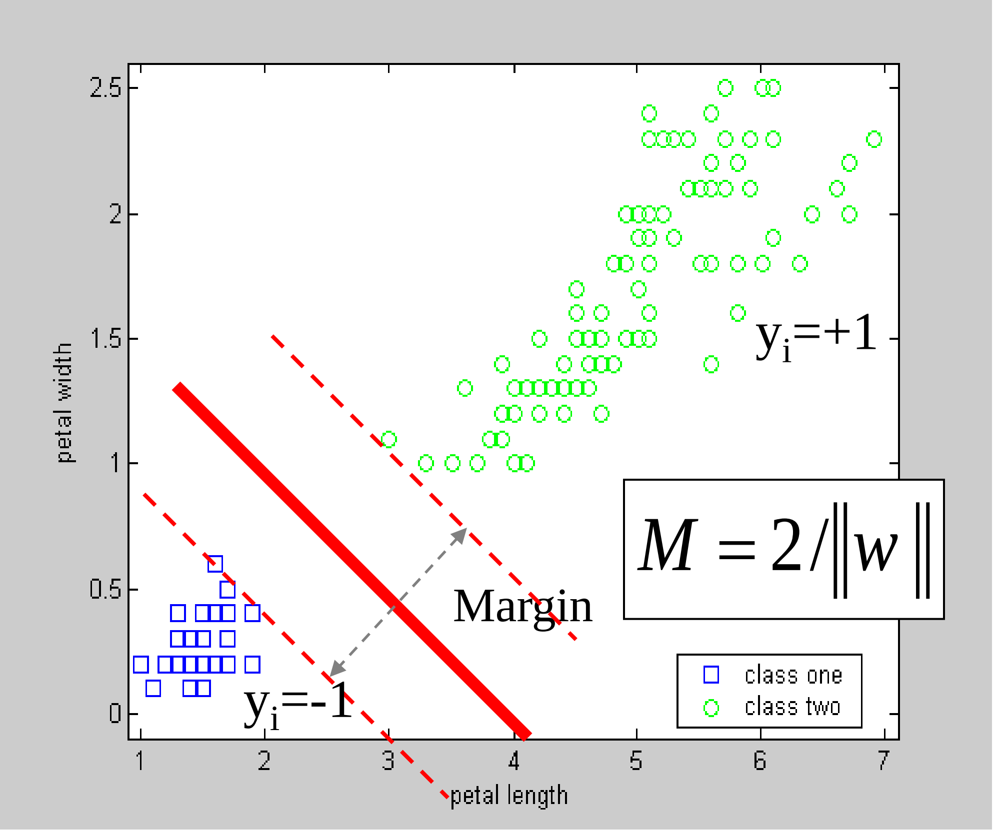
J. Chemometrics 2004; 18: 341–349

Combination of support vector machines (SVM) and near-infrared (NIR) imaging spectroscopy for the detection of meat and bone meal (MBM) in compound feeds.

J.A.Fernandez Pierna[1],V.Baeten[1],A.Michotte Renier[1],R.P.Cogdill[2] and P.Dardenne[1]*

SVM (Support Vector Machine)

The linearly separable case



$$f(x) = w' \cdot x + b$$

Classifier that maximises the margin → Optimal sparating hyperplane → good generalization is expected

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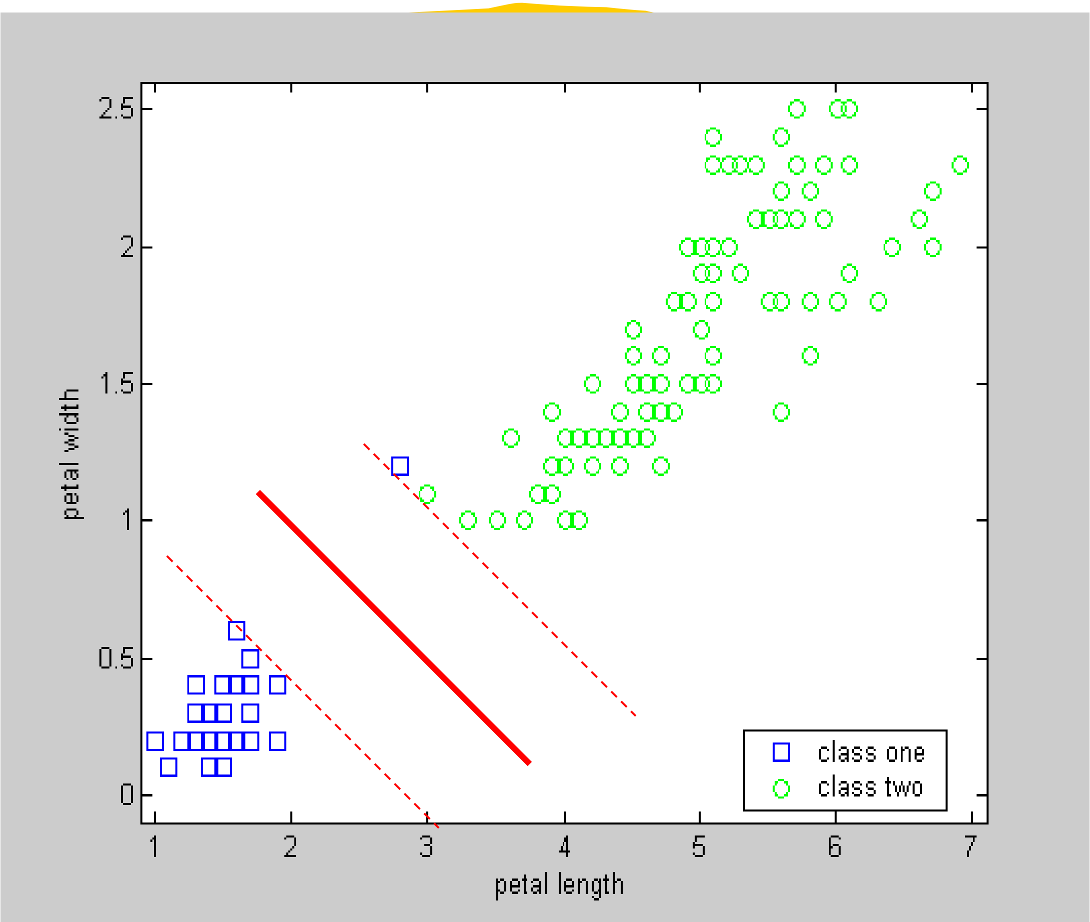
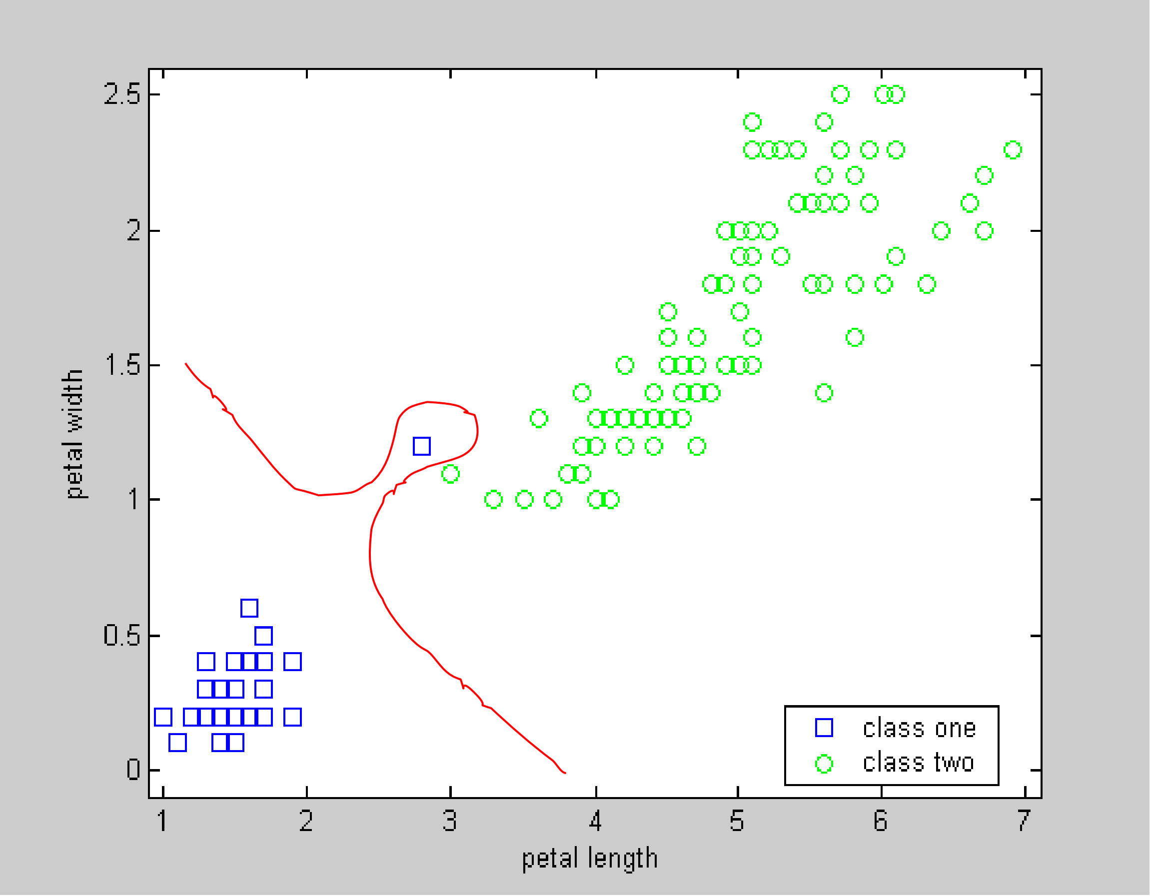
The non linearly separable case



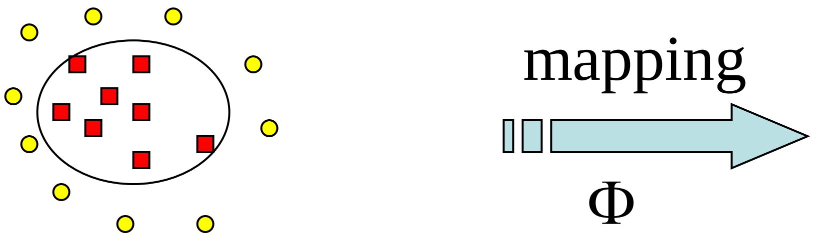
Linear separation → more prediction errors, but better generalization

The non linearly separable case



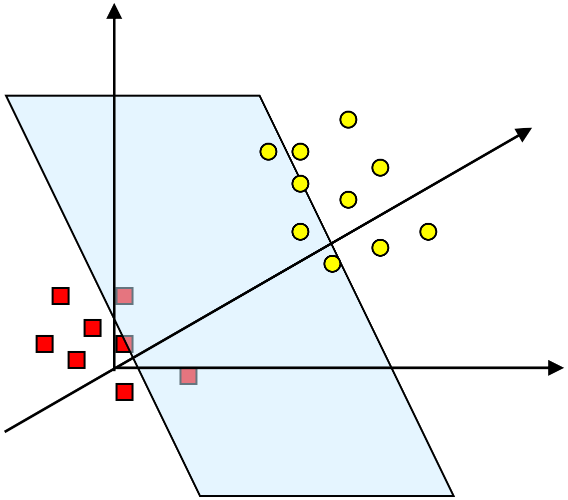
Non linear separation → less prediction errors, but poorer generalization

The non linearly separable case: Linearisation in a higher dimensional space



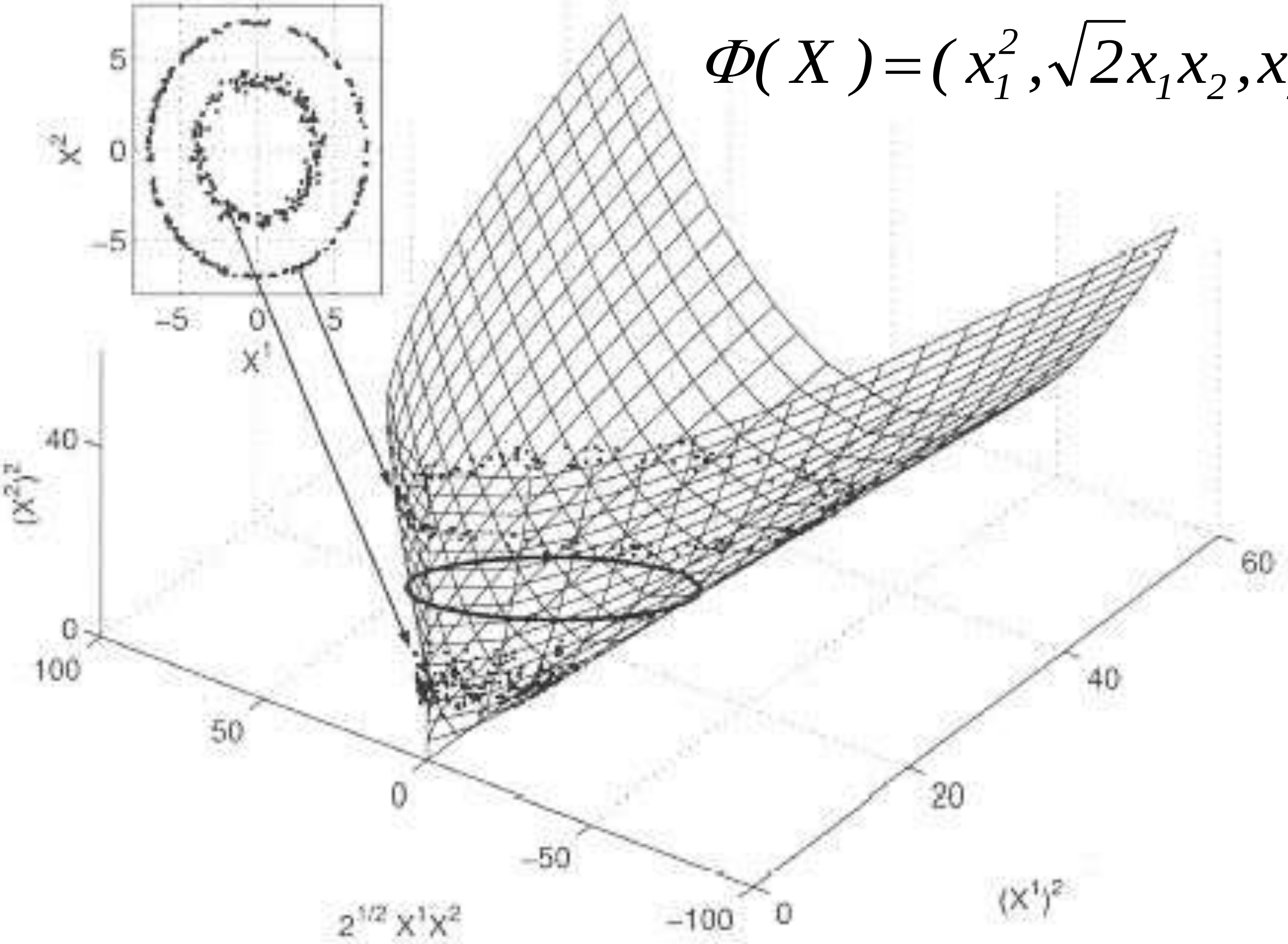
$$\Phi : \Re^d \rightarrow \Re^D \quad (D >> d)$$

$$x \rightarrow \Phi(x)$$



Separating hyperplane with maximal margin

$$\Phi(X) = (x_1^2, \sqrt{2}x_1x_2, x_2^2)$$



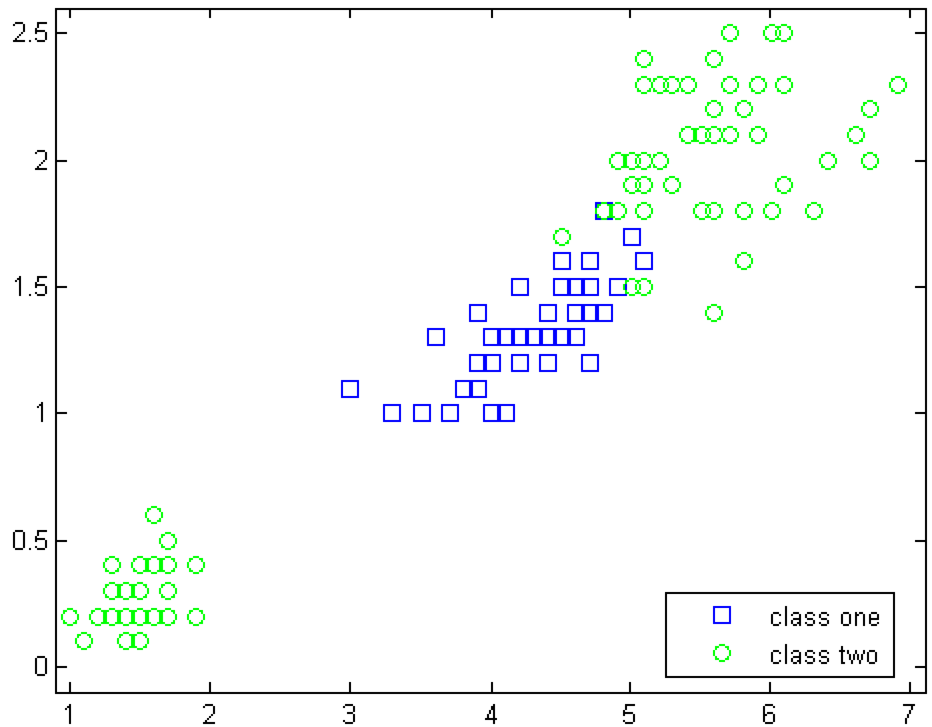
Source: Belousov et al.

Mapping is done with Kernels

Linear	$K(x_i, x_j) = x_i x_j$
Polynomial	$K(x_i, x_j) = (x_i x_j + c)^n$
Gaussian Radial Basis Function	$K(x_i, x_j) = \exp\left(-\frac{\lVert x_i - x_j \rVert^2}{2\sigma^2}\right)$
Sigmoid Function	$K(x_i, x_j) = tanh((a(x_i x_j) - b))$

RBF:
- Simple
- Large ability to model data of arbitrary complexity
- Computationally easy
- Only one parameter sigma to be optimized

Fisher's Iris data set



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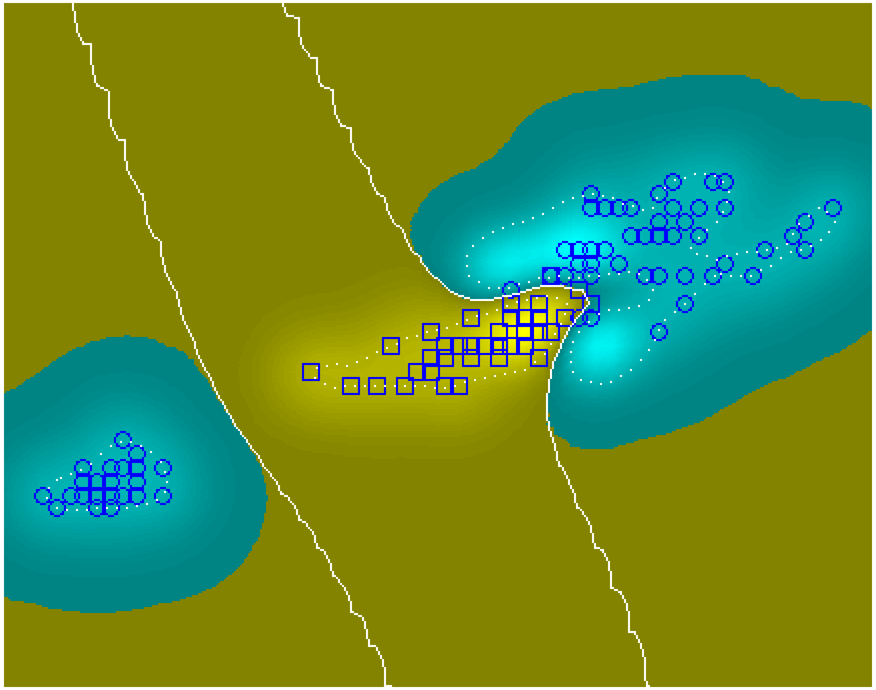
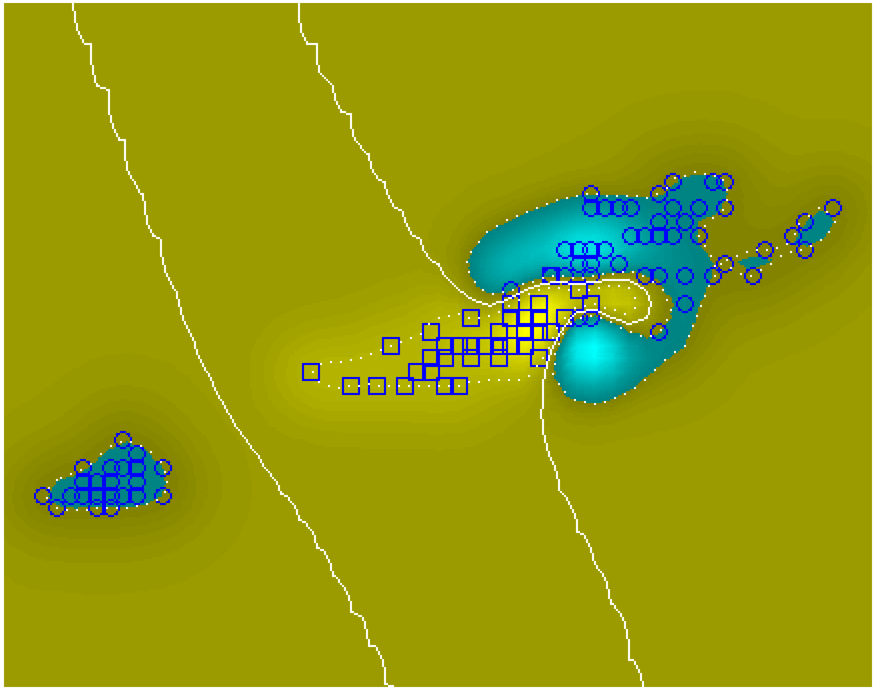
SVM & RBF Gaussian Kernel C=10 / σ = 0.25



RBF Gaussian Kernel C=100 / σ = 0.25



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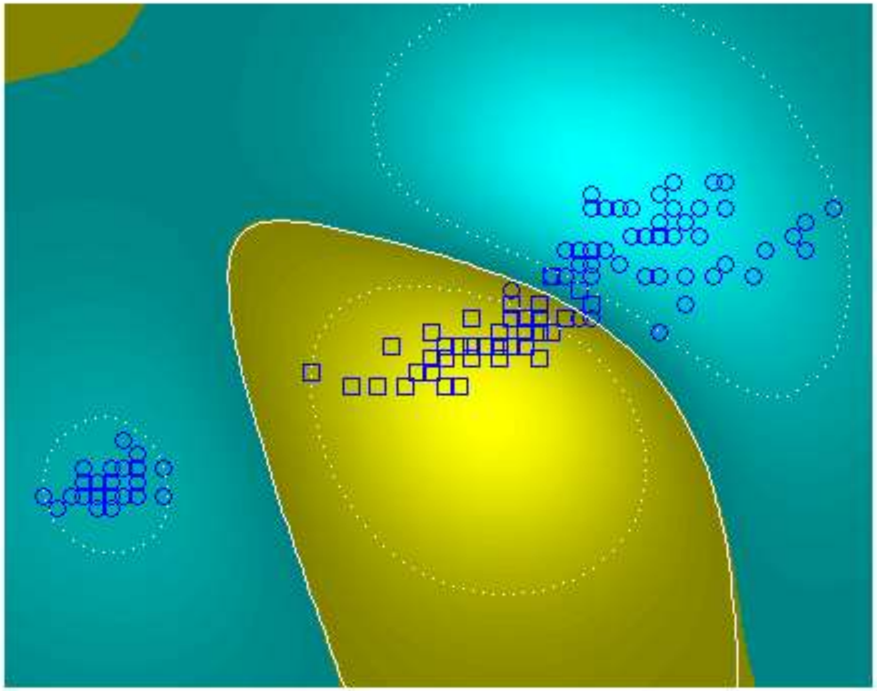
RBF Gaussian Kernel C=10 / σ= 1



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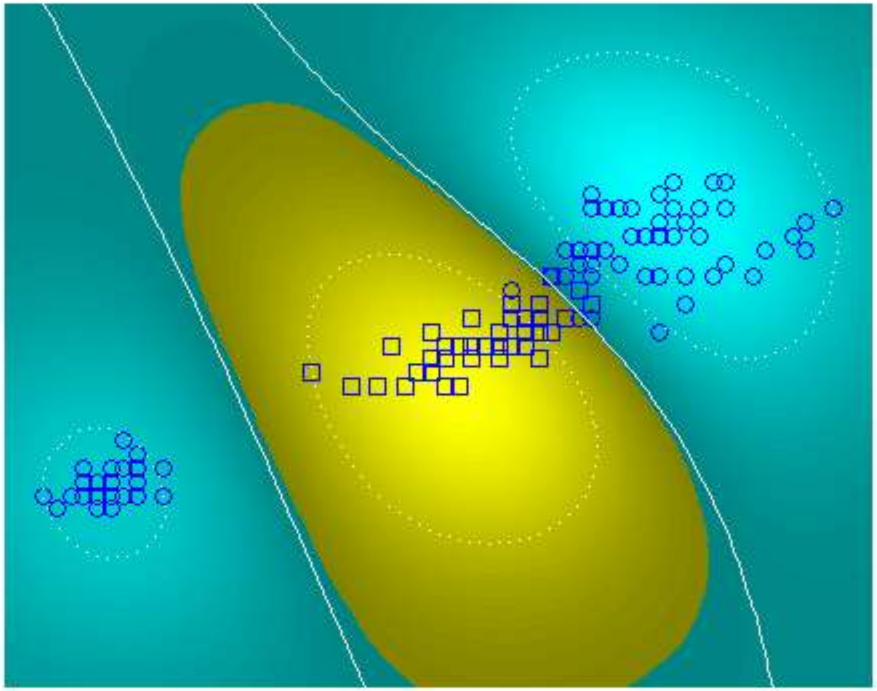
RBF Gaussian Kernel C=1 / σ= 1



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Learning data base

2233 animal particles:

- **meat & bone meal**
- **fish meal**
- **poultry meal**

3288 plant particles:

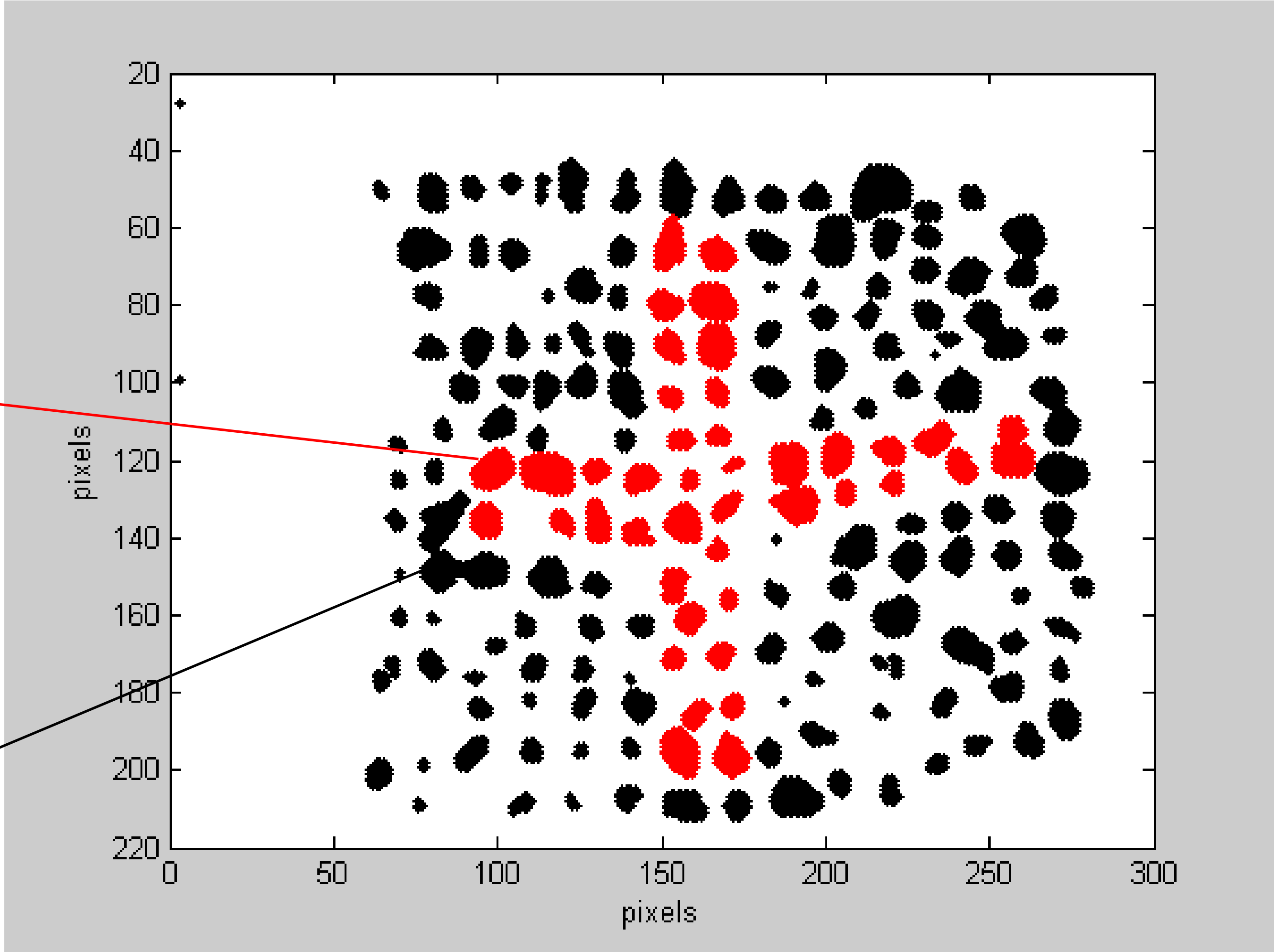
> **to compute the SVM model by optimisation of**
>
> **C : regularisation factor**
>
> **σ : width of the Gaussian**

- **cereals (wheat, oats, barley, corn, ..)**
- **protein sources** *(rapeseed meal, peas, soya meal,…)*
- **tropical by-products** *(peanuts, cocoa, coconut, manioc, palm kernel)*
- **other vegetal meals** *(sugar beet by-products, bakery by-products, chicory, lucern, potatoes by-products,..*

Test image : data set with separated particles

Animal particles

Vegetal particles



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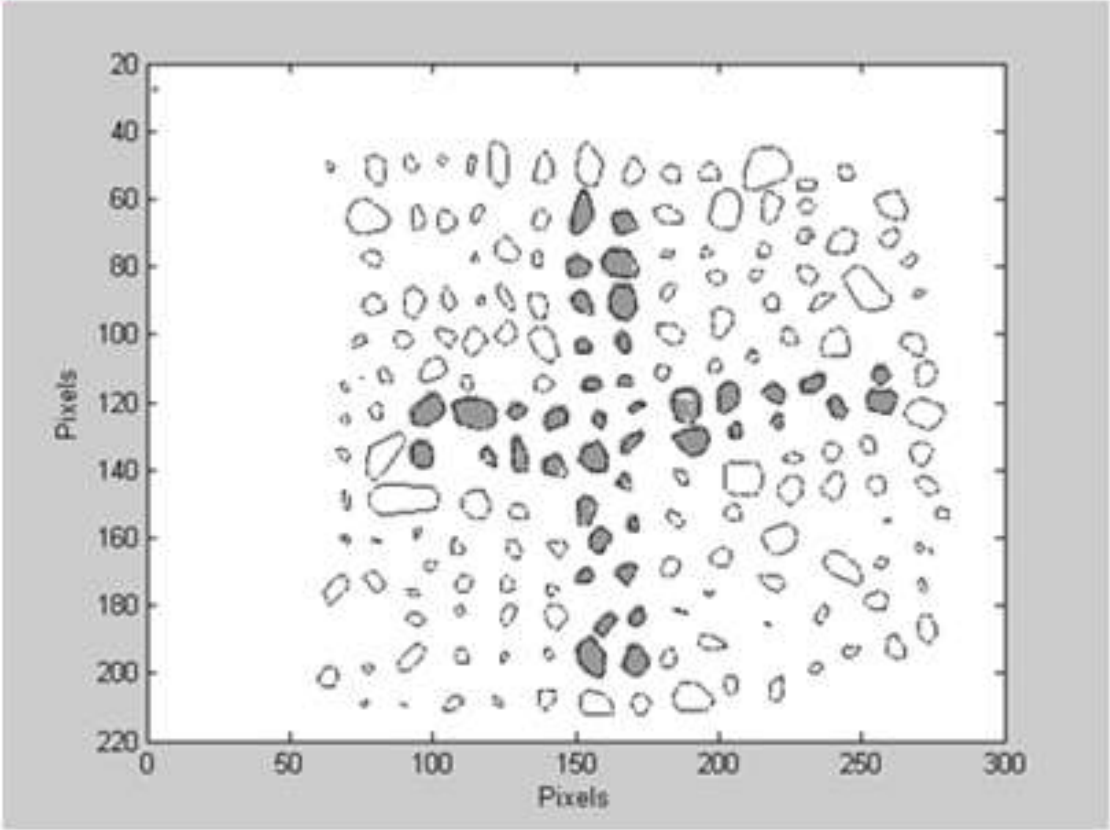
Prediction by SVM

Grey=animal

White=vegetal

(C=1000, σ=25)



84,88 % of pixels -> 100% animal particles

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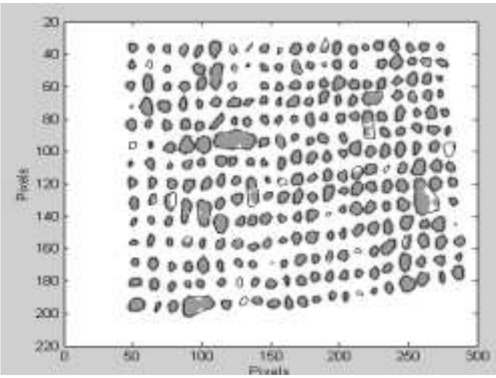
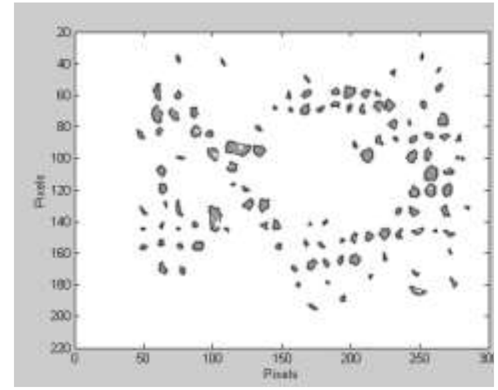
Detection of Fish meal in MBM

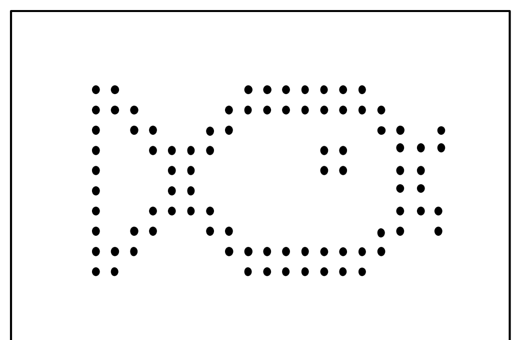


Discriminant models



Animal *vs.* Vegetal
Fish *vs.* Terrestrial animal

Distribution of the fish particles



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Hyperspectral imaging and support vector machines for the trace back of compound feeds

Plant ←→ animal : easy, LOD : 0.1%

Fish ←→ terrestrial animal : OK, but difficult

Mammalian ←→ Poultry : even more difficult

Bovine ←→ Pig : impossible by NIR microscopy

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Screening of plant ingredients in feed

This research is decisive in the support of the Proposal for a European Parliament and Council Directive amending Directive 79/373/EC on the marketing of compound feedstuffs.
In this document, the Commission underlines the advantages of the labelling previsions of compound feedstuffs for production animals in order to facilitate the trace back of compound feed.

Not only : composition percentage, Protein, Fat, …
Energy, …
+ % of ingredients (cereals, soyameal, …)

←→ Industry interests;
- **secret formulas,**
- **many types of feed,**

NIRS in food and Agriculture

- **use of ‘universal’ and recognized data bases (models)** **(+ wireless & internet)**
- **chemometrics** **(new algorithms & computing power)**
- **increase of on-line installations**
- **new low cost portable spectrometers**
- **new applications for imaging spectroscopy**

Merci bramin p'o m'awès choutè

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Today's Needs for Tomorrow's Hardware

- Sensitivity
- Dynamic range
- Stability and ruggedness
- Spectral reproducibility
- Spectral resolution
- Speed
- Portability
- Reduced cost

Ed. Stark
12th ICNIRS
Auckland, April 05

Conflicting needs require tradeoffs

* Time Resolved Spectroscopy, *Véronique Bellon-Maurel*

-A laser pulse of a few pico-seconds irradiates the sample

-The light signal reflected by the sample at a given distance from the irradiation point is then temporally recorded

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*** Time Resolved Spectroscopy,** *Véronique Bellon-Maurel*

*** Surface Plasmon Resonance NIRS,** *Akifumi Ikehata*

*** Infrared Micro-spectrometers based on MEMS,** *Adrian Keating*

*** Hadamard Coding with mechanical shutters,** *Robert Burling-Claridge*

*** Near Infrared Emission Spectroscopy (NIRES),** *Celio Pasquini*

The background

Mad cow crisis (BSE)

↓

'Processed animal proteins (meat and bone meal (MBM)) are totally banned in feedingstuffs destined to farmed animals which are kept, fattened or bred for the production of food'
(Council Decision 2000/776/EC – 4/12/2000)

↓

lots of legal decisions to ensure the safety and quality of feedingstuffs

↓

DETECTION METHODS

http://stratfeed.cra.wallonie.be

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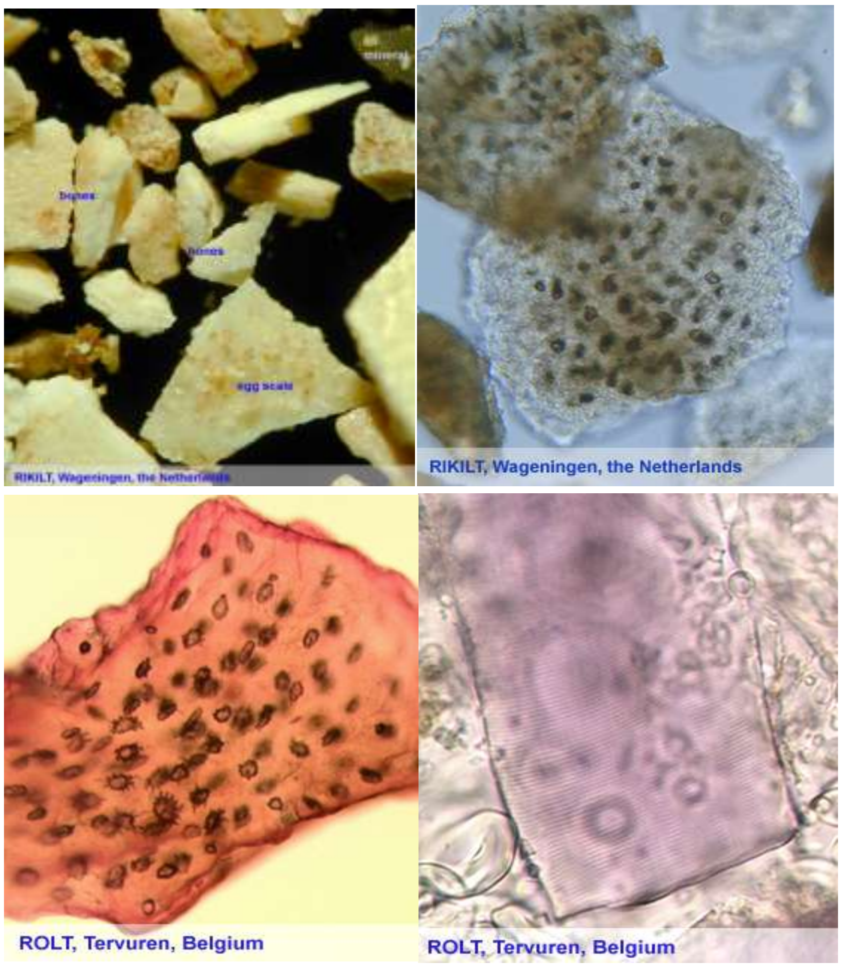
EU Reference method : classical microscopy



Classical Microscopy is based on visual observations of the morphological characteristic of the particles of bones.

➔

- time consuming
- well trained microscopists
- subjectivity
- quite poor reproducibility

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- ***Classical microscopy is based on the visual observation of morphologic features of ingredient particles***

- ***NIR miscroscopy is based on the organic composition of ingredient particles***

- ***Our objective => replace the eyes of the analyst (i.e. visible detectors) by infrared detectors and the expertise of the microscopist by discriminant equations***

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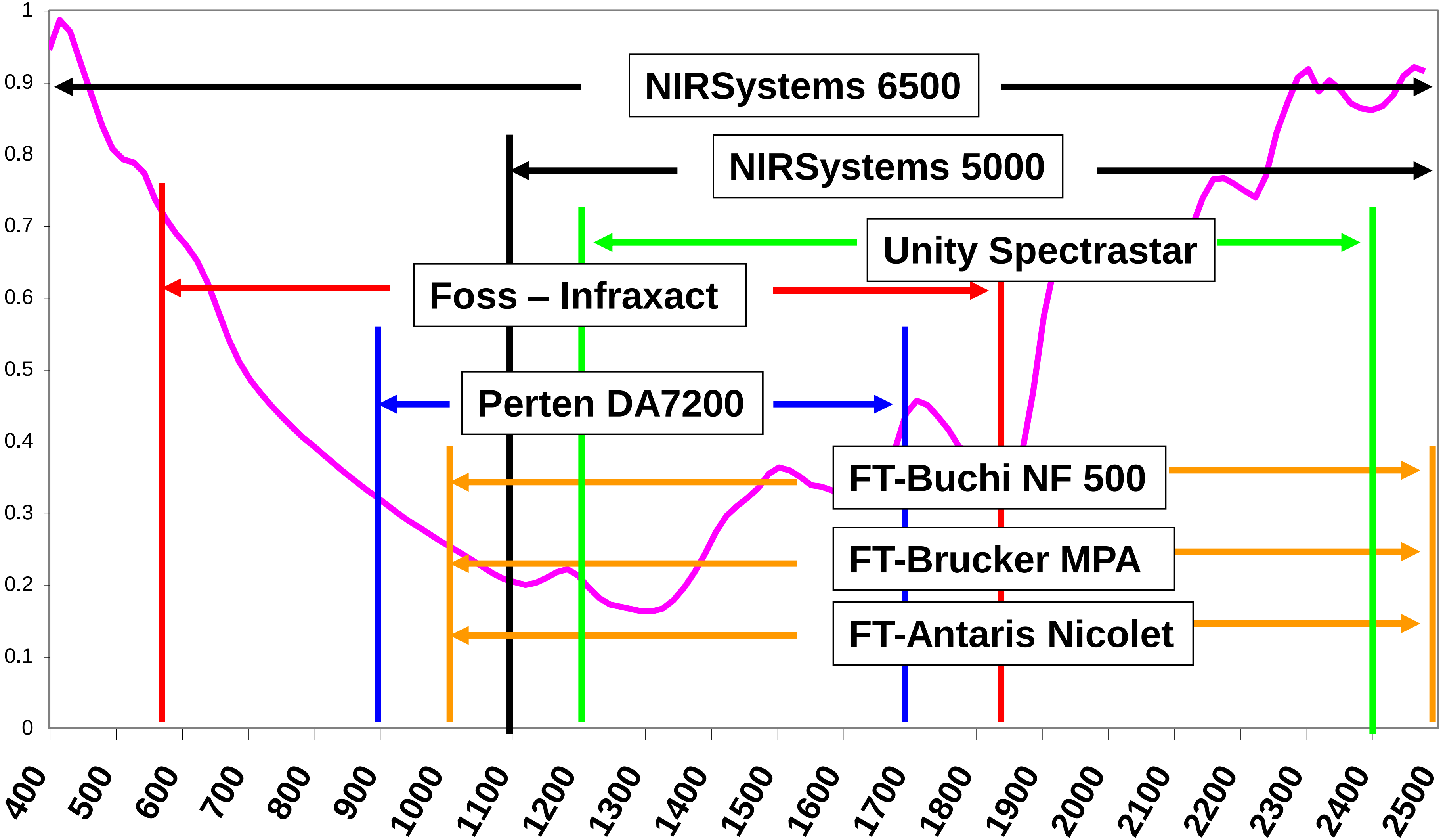
http://www.central-labs.co.uk/



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