An informal walk in the world of mathematical optimization

Oliver Smithies and Leverhume Lecture I, November 2015

Thanks

- Leverhulme Trust, UK
- Balliol College, Oxford
- Belgian Fund for Scientific Research (FNRS)
- University of Florence, Italy
- University of Namur, Belgium

Mathematics : a universal language

My objectives :

- Show (by examples) that optimization is a language in which a large number of complex and interesting problems can be solved.
- Share my enthousiasm and amazement at the variety and scope of its applications.
- Spend some intellectually stimulating moments in your company.

The menu

1. Objectives and concepts
2. Methods et means
3. An history-rich discipline
4. Optimization in action
   - in industry and technology
   - in sciences
   - in human society
5. Conclusions

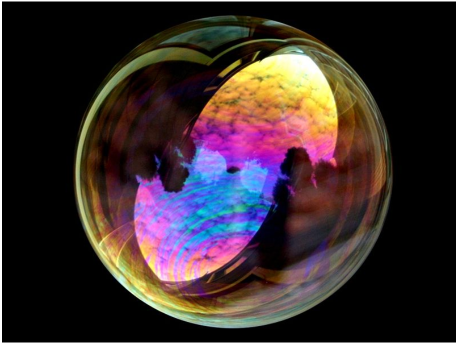
What is mathetamical optimization ?

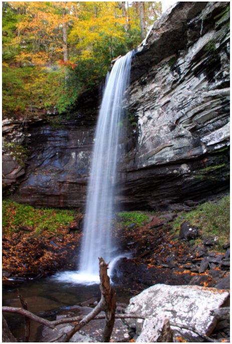
Use mathematics to

> make the best choice under constraints

best	$\Rightarrow$	criterion, objective function (maximize/minimize)
choice	$\Rightarrow$	variables whose values we are free to choose
constraints	$\Rightarrow$	restrictions on the admissible variables' values

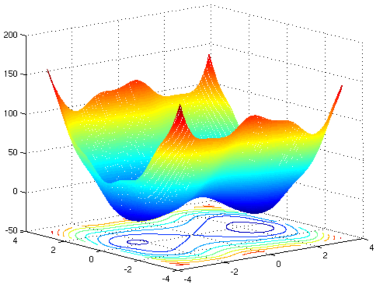
Nature optimizes

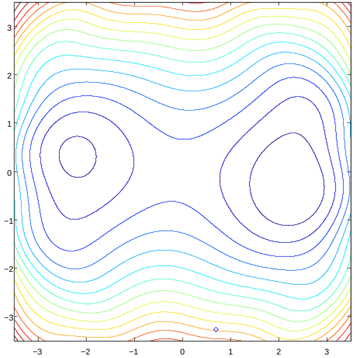




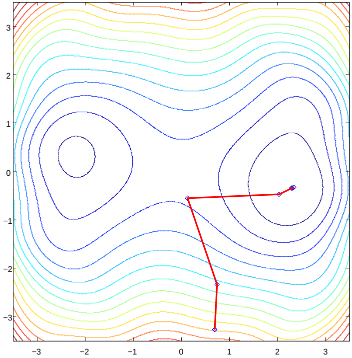
Humans optimize (every day)

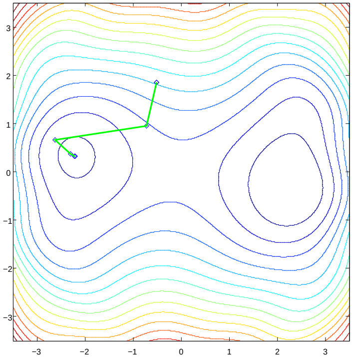
Methods : a mountaineering vision . . .





Methods : the path to the lake





The means

Powerful computers :

IBM Blue Gene

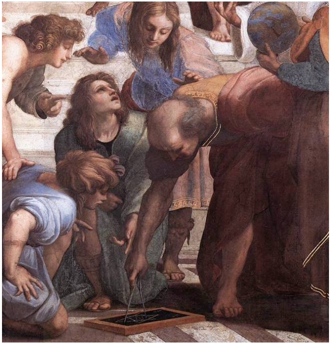
Optimization pioneers

"Nous sommes comme des nains juchés sur des épaules de géants, de telle sorte que nous puissions voir plus de choses et de plus éloignées que n'en voyaient ces derniers. Et cela, non point parce que notre vue serait puissante ou notre taille avantageuse, mais parce que nous sommes portés et exhaussés par la haute stature des géants."

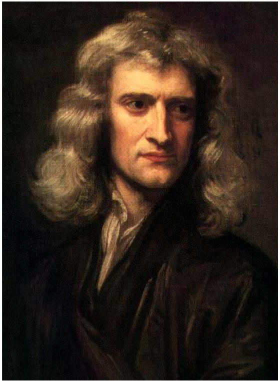
"We are like dwarves standing on the shoulders of giants, so that we may see more and further afar than they could. And not because our sight is powerful or because we are tall, but only because we are carried and raised by the high stature of the giants."

Bernard de Chartres (1130-1160)

Euclide (300 BC) Al-Khwarizmi (783-850)

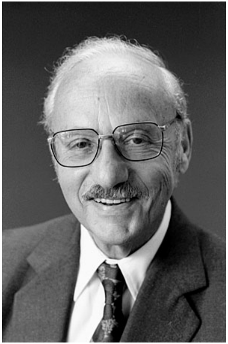


Isaac Newton (1642-1727) Leonhard Euler (1707-1783)



J. de Lagrange (1735-1813) Friedrich Gauss (1777-1855)

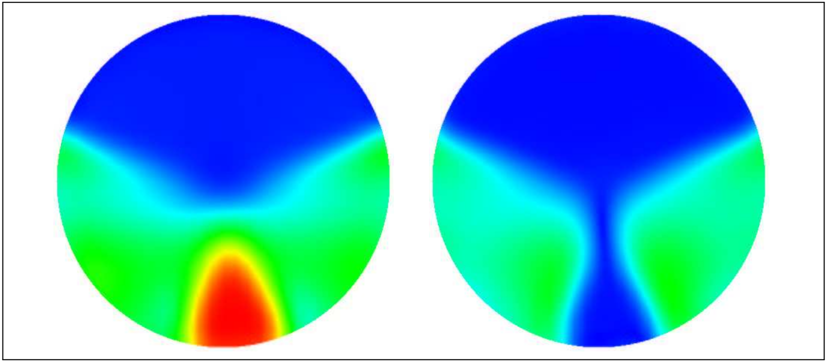
Augustin Cauchy (1789-1857) George Dantzig (1914-2005)



Design of progressive lenses (1)

Specification of modern progressive lenses :

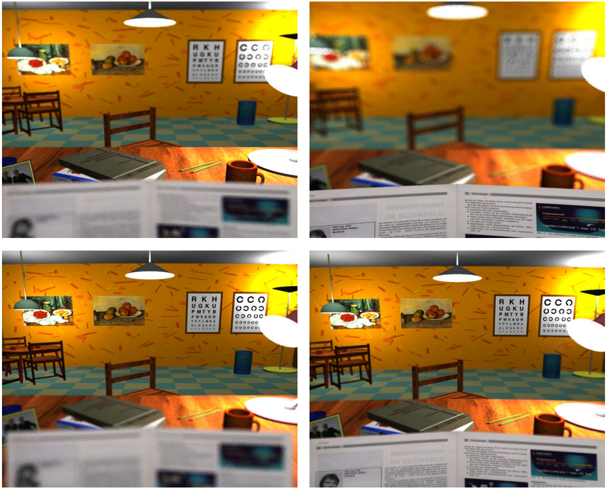
vary the lens's optical power while minimizing astigmatism



Loos, Greiner, Seidel (1997)

Design of progressive lenses (2)

What can be done :



without correction　　short distance

long distance　　with progressive lenses

Design of progressive lenses (3)

Is this problem nonlinear ($\approx$ difficult) ?

If the urface of the lens is given by $z = z(x,y)$, the optical power is

$$p(x,y) = \frac{N^3}{2}\left[\left(1+\left[\frac{\partial z}{\partial x}\right]^2\right)\frac{\partial^2 z}{\partial y^2} + \left(1+\left[\frac{\partial z}{\partial y}\right]^2\right)\frac{\partial^2 z}{\partial x^2} - 2\frac{\partial z}{\partial x}\,\frac{\partial z}{\partial y}\,\frac{\partial^2 z}{\partial x \partial y}\right]$$

where

$$N = N(x,y) = \frac{1}{\sqrt{1+\left[\frac{\partial z}{\partial x}\right]^2 + \left[\frac{\partial z}{\partial y}\right]^2}}.$$

The surface astigmatism is then given by

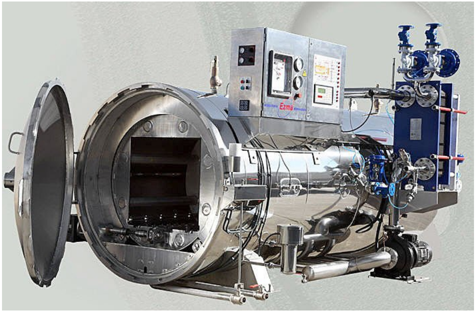
$$a(x,y) = -2\sqrt{p(x,y) - N^4\left(\frac{\partial z}{\partial x}\,\frac{\partial z}{\partial y} - \left[\frac{\partial^2 z}{\partial x \partial y}\right]^2\right)}$$

Sterilization of baby food (1)

A very standard problem in the food industry :

keep a max of vitamines while eliminating a given fraction of the bacteries

heat the food in vapour- or hot-water autoclaves



Sachs (2003)

Sterilization of baby food (2)

Model : coupled partial differential equations (PDEs)

Concentration of micro-organisms and other nutriments :

$$\frac{\partial C}{\partial t}(x,t) = -K[\theta(x,t)]C(x,t),$$

where $\theta(x,t)$ is temperature, and where

$$K[\theta] = K_1 e^{-K_2\left(\frac{1}{\theta}-\frac{1}{\theta_r}\right)} \quad \text{(Arrhenius equation)}$$

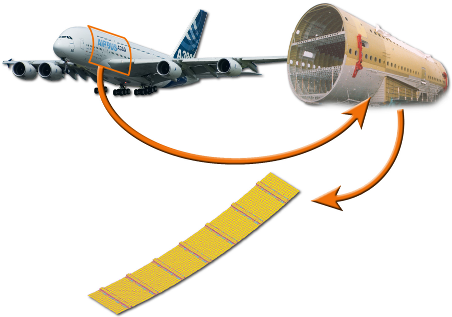
Temperature evolution :

$$\rho c(\theta)\frac{\partial \theta}{\partial t} = \nabla \cdot [k(\theta)\nabla\theta],$$

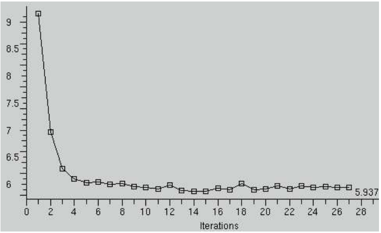
(with suitable boundary conditions : refrigerant, initial temperature, ldots)

Structural design for aeronautics

minimize fuselage weight while maintaining structural integrity



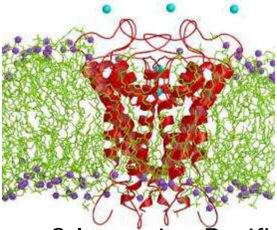
SAMTECH (2009)



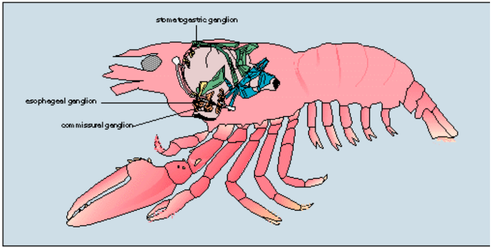
mass reduction
during optimization

A parameter estimation problem in biology (1)

A model for a potassic channel in a neurone's membrane :
Sansom (2001)



But where are these neurones ? In a spiny Pacific lobster (*Panulirus interruptus*) ! Simmers, Meyrand and Moulin (1995)



A parameter estimation problem in biology (2)

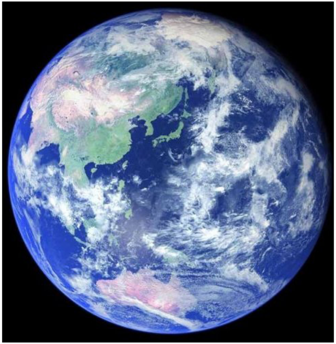
After collecting experimental data
(applying a current to the cell) :

estimate the model's parameters in order to best fit the data

The model (for the biologists) :

- Activation : p independent gates
- Deactivation : n_h gatess with different dynamics
- $n_h + 2$ coupled PDEs for voltage, activation level and partial inactivation levels
- 5-points BDF integrator for $\approx$ 50000 time steps
- $\Rightarrow$ very nonlinear !

Data assimilation in weather forecasting (1)

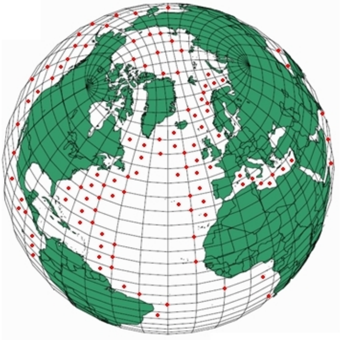


(Attempt to) predict. . .

- tomorrow's weather
- average temperature in the ocean for the coming month
- future gravity field
- next currents in the ionosphère
- . . .

Data assimilation in weather forecasting (2)

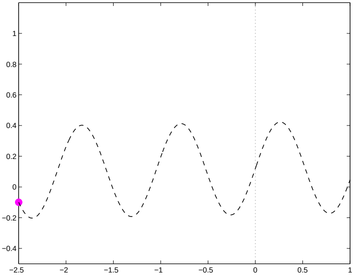
Data : temperature, wind, pressure, . . . everywhere and at all times !



Contains more than 1.000.000.000 variables !

Data assimilation in weather forecasting (3)

The principle :

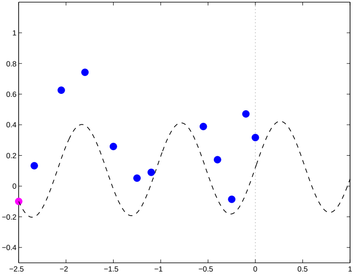


temperature/days

- Situation known 2.5 days ago and “background” forecast

Data assimilation in weather forecasting (3)

The principle :



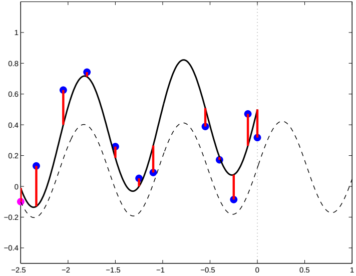
temperature/days

- Situation known 2.5 days ago and "background" forecast
- Temperature for the past 2.5 days

Data assimilation in weather forecasting (3)

The principle :

Minimize the error between model and past observations



temperature/days

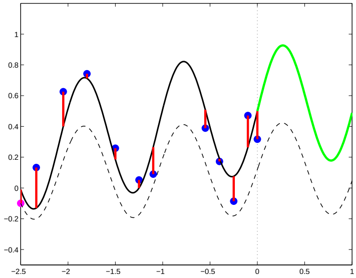
- Situation known 2.5 days ago and "background" forecast
- Temperature for the past 2.5 days
- Run the model to minimiser distance between model prediction and observations

$$\min_{x_0} \frac{1}{2}\|x_0 - x_b\|^2_{B^{-1}} + \frac{1}{2}\sum_{i=0}^{N} \|\mathcal{H}\mathcal{M}(t_i, x_0) - b_i\|^2_{R_i^{-1}}.$$

Data assimilation in weather forecasting (3)

The principle :

Minimize the error between model and past observations

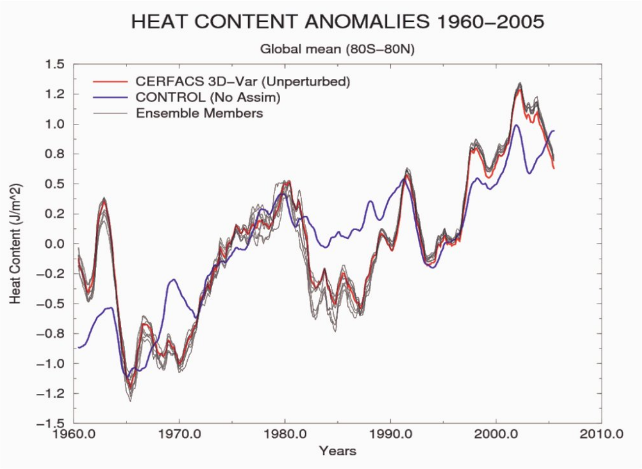


temperature/days

- Situation known 2.5 days ago and "background" forecast
- Temperature for the past 2.5 days
- Run the model to minimiser distance between model prediction and observations
- Predict tomorrow's temperature

Data assimilation in weather forecasting (4)

Analysis of the heat content in the ocean : CERFACS (2009)



Musch better fit !

Image denoising (1)

Consider an image with random noise (incorrect of pixel blackness) proportional to signal strength.

HQuestion ; reconstruct the original blackness levels

use the pixels' values as much as possible
while minimizing sharp transitions (gradients)

This yields the optimization problem

$$\min_u \sum_{ij\in\Omega} (u_{ij} - z_{ij}\log(u_{ij})) + \alpha \int_\Omega \|\nabla u\|$$

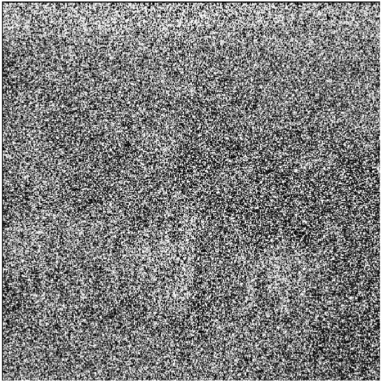
where

$$z_{ij} = u_{ij} + n f(u_{ij})$$

and n is a Gaussian noise.

Image denoising (2)

Some spectacular results : an 512 $\times$ 512 image with 95% noise



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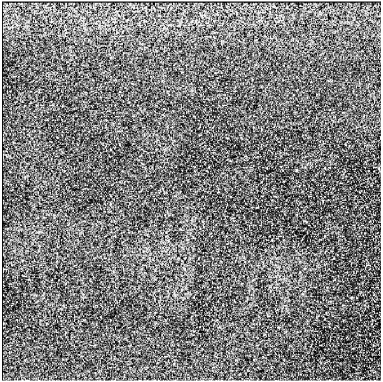


Chan and Chen (2007)

Reconstruction of hidden objects (2)

- an object $\mathcal{O}$ hidden in an opaque medium (ground, water, body ...)
- one "illuminates" this object with an electromagnetic plane wave in "all" directions

$$u^{inc}(x,d) = e^{ik\langle x,d\rangle} \quad d \in \mathcal{S}$$

- one measures the waves reflected $u^s(x,d)$ by the object in "all" directions

$$\Delta u^s + k^2 u^s = 0 \quad \text{(outside } \mathcal{O}\text{)}$$

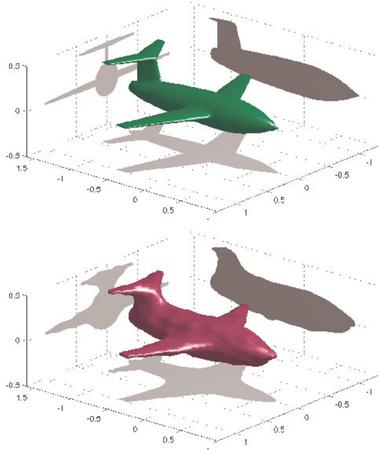
with

$$u = u^{inc} + u^s, \quad u = 0 \text{ on } \partial\mathcal{O} \quad \text{et} \quad \lim_{r\to\infty} \frac{\partial u^s}{\partial r} = iku^s.$$

Optimize the object's shape $\mathcal{O}$ from the measurements $u^s(x,d)$

Illustration : reconstruction of a plane

The original and its reconstructions ($N = 1002, p = 5, 20, 50$)



Optimization, transport et mobility

The context

Analyse de la mobilité quotidienne en Belgique

Modelling the displacements

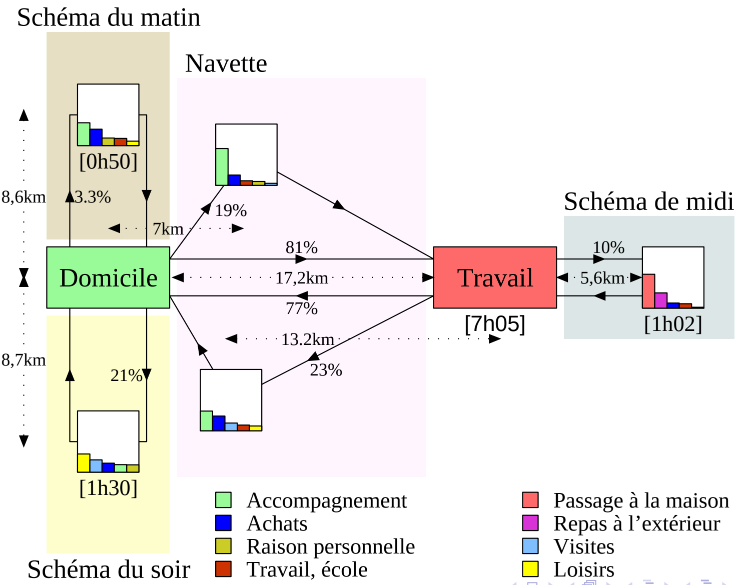
⇓

Modelling the activities

⇓

Modelling behaviours of individuals/households

Daily mobility : a complex system



Understanding choice strategies in society

Context : simulation of individuals' mobility choices (mode, route, start time, ...)

Random utility theory

Individual i assigns to alternative j the "utility"

$$U_{ij} = [\text{ parameters } \times \text{ explaining factors}] + [\text{ random error }]$$

Illustration :

$$U_{bus} = \text{distance} - 1.2 \times \text{ticket price} - 2.1 \times \text{delay w.r.t. trip by car} + \epsilon$$

Discrete choice models (1)

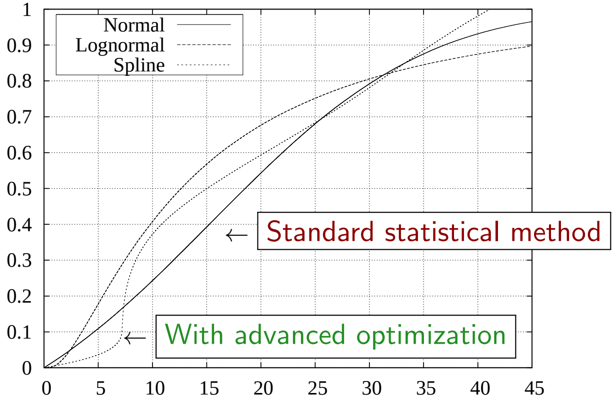
Probability that the individual i chooses alternative j rather than alternative k is given by

$$\text{prob}\,(U_{ij} \geq U_{ik} \quad \text{for all} \quad k)$$

Data : mobility surveys (MOBEL, BELDAM, etc.)

find the utility's parameters which
maximize the likelihood of observed behaviours

Discrete choice models (2)



Estimation of the value of lost time in traffic congestion
(with and without advanced optimization)

Modelling individuals ?

A major difficulty

- Individual data (often) unavailable/incoherent...
  (cost, privacy regulations, variable sources)

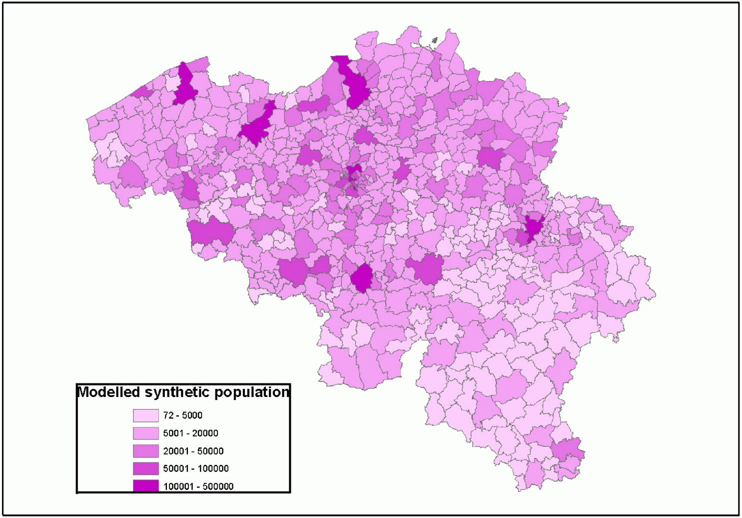
Build a syntetic population

Method

- maximize the likelihood of individuals/housholds descriptions
- while maitaining known statistics for the real population

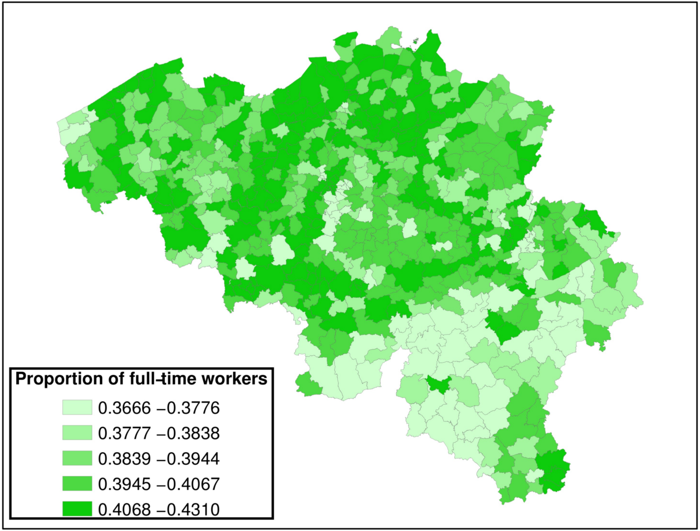
A synthetic population for Belgium

One gets ≈ 10.600.000 individuals in 4.400.000 housholds



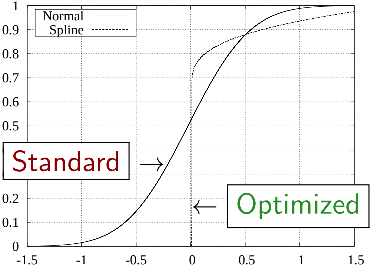
A synthetic population for Belgium

From which one can deduce (using other optimization techniques)



and in finance. . .

1. risk management
2. portfolio analysis
3. forex markets



Distribution of the BoJ investments 1991-2004

4. . . .

Everybody likes an optimizer !

Some conclusions

The mathematical language is astonishingly *flexible, adaptable, elegant and efficient*.

Applied mathematics is a booming area of expertise.

Optimisation and complex system analysis are in the forefront.

A regret : not being able to share (yet) the fulgurence of the theory. . .