

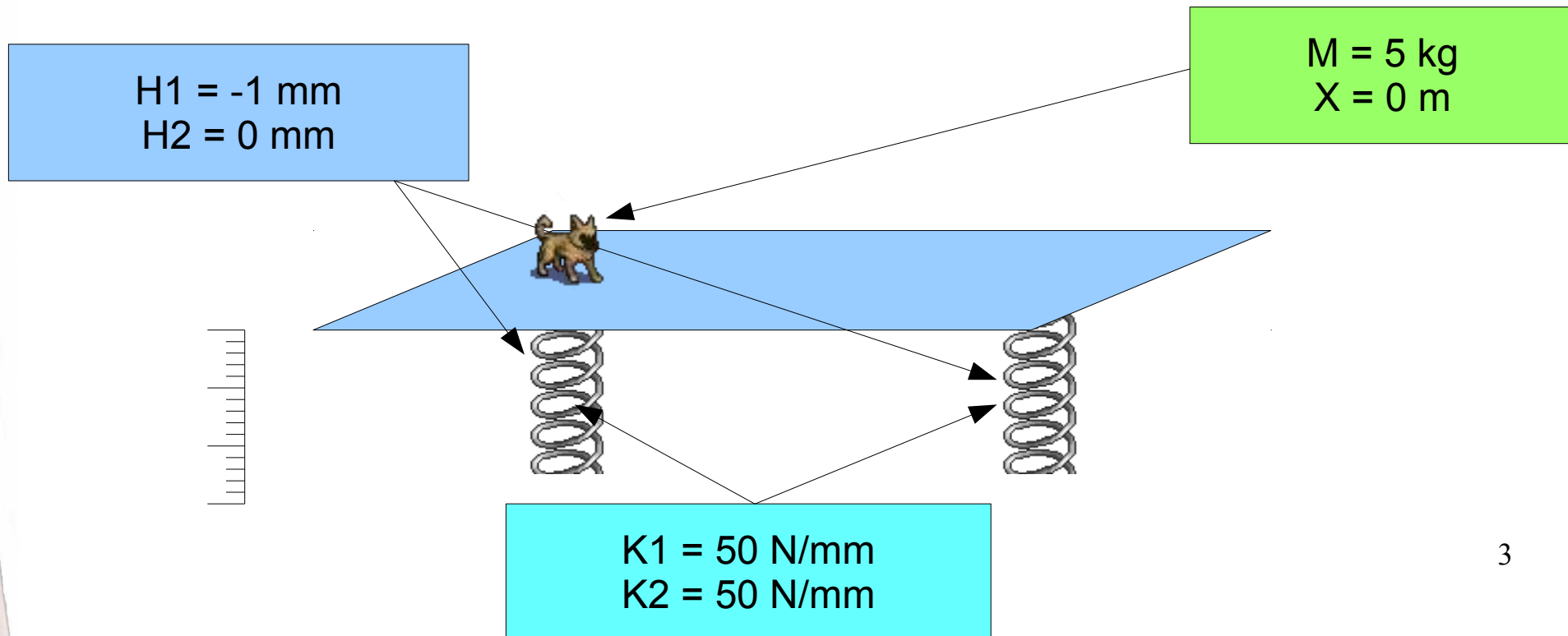
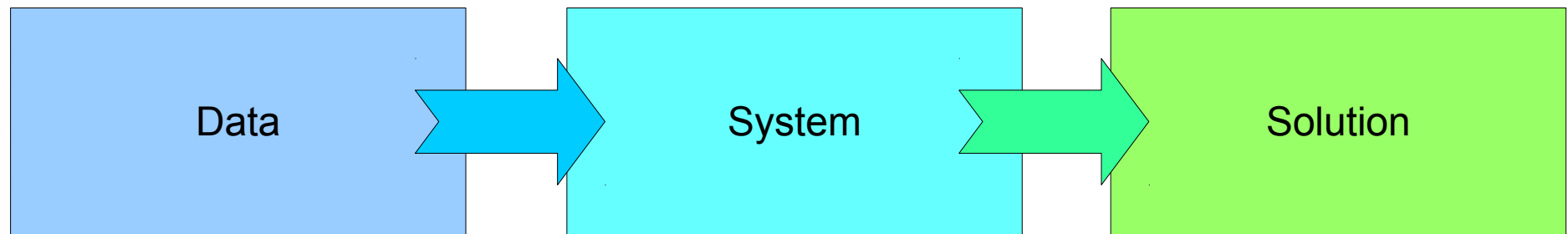
Inversion of ill-conditioned systems



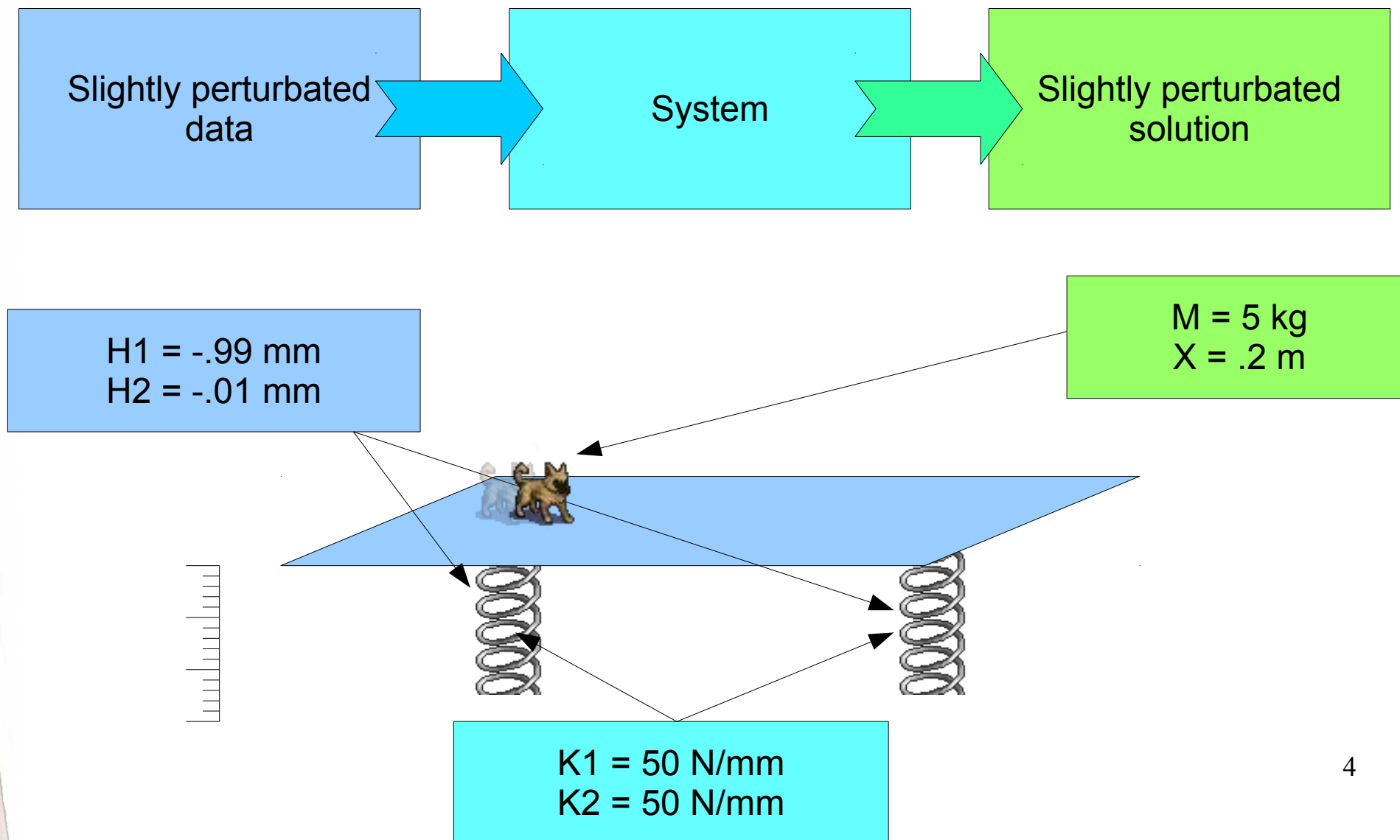
What is an ill-conditioned system ?



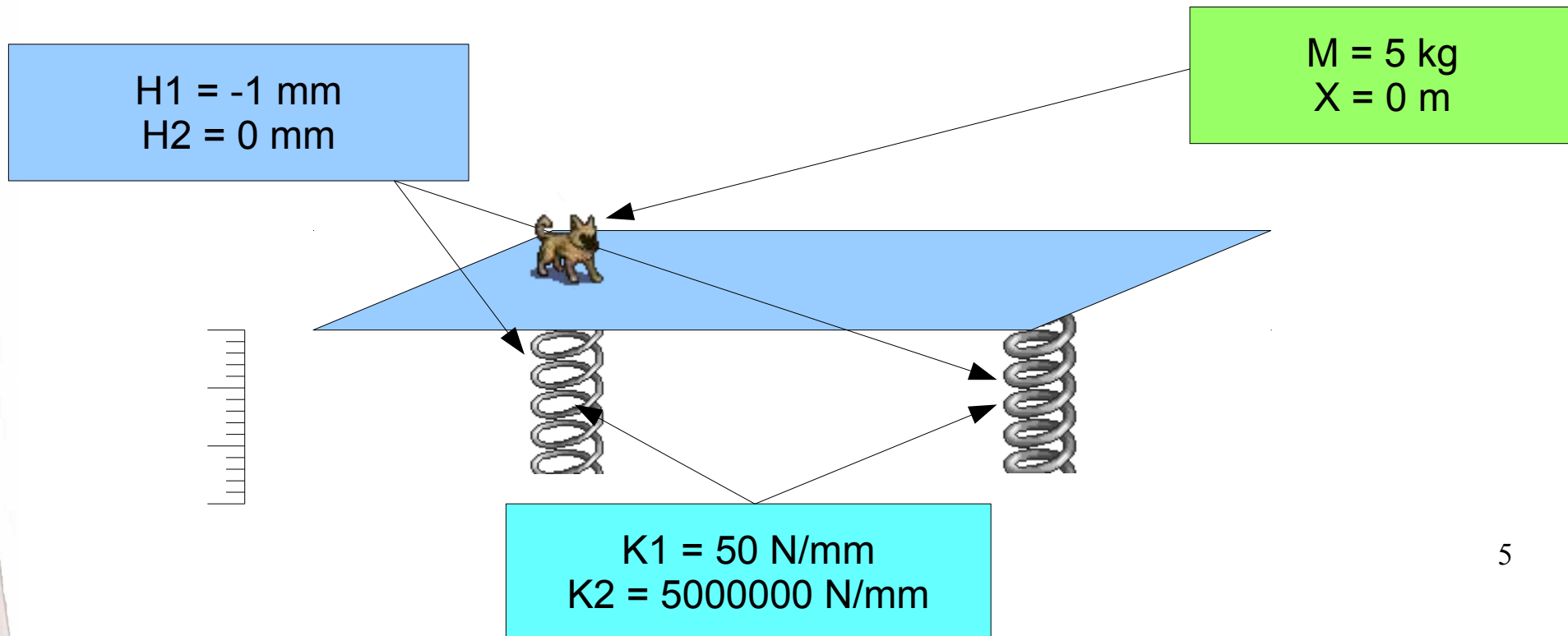
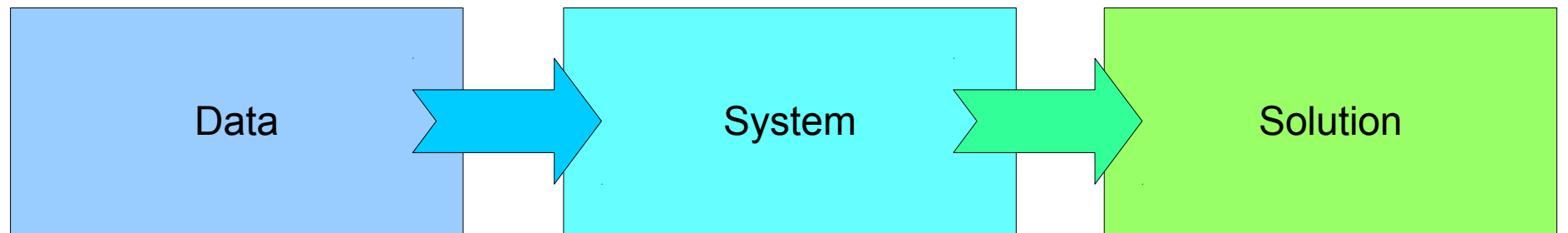
What is a well-conditioned system ?



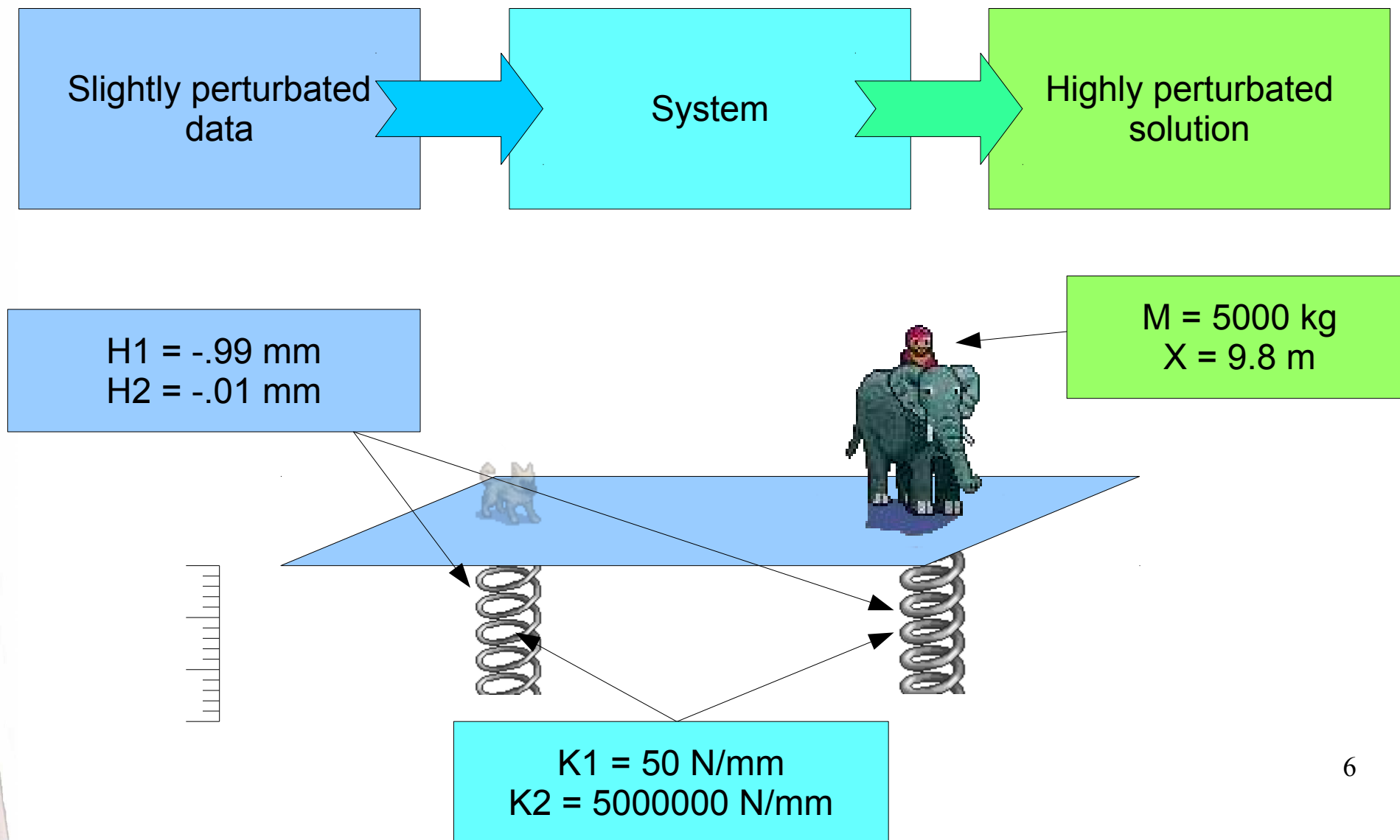
What is a well-conditioned system ?



What is an ill-conditioned system ?



What is an ill-conditioned system ?



What is an ill-conditioned matrix ?

A is a SDP matrix

$$Ax = b$$

Rem : if A is not SDP, work on the normal system

$$A^T Ax = A^T b$$

Perturbated system :

$$A(x + \delta x) = b + \delta b$$

We have then :

$$A\delta x = \delta b$$

Goal : find a stability inequality

$$\frac{\|\delta x\|}{\|x\|} \leq \text{???} \frac{\|\delta b\|}{\|b\|}$$

Relative error on the solution

Relative error on the input

A constant to find

What is an ill-conditioned matrix ?

$$\delta x = A^{-1} \delta b$$

$$Ax = b$$

By definition of the induced 2-norm :

$$\begin{aligned} \|A^{-1}\| &= \max \text{eig}(A^{-1}) = \frac{1}{\min \text{eig}(A)} = \max_{\delta b} \frac{\|A^{-1} \delta b\|}{\|\delta b\|} \\ &= \max_{A^{-1} \delta b = \delta x} \frac{\|\delta x\|}{\|\delta b\|} \end{aligned}$$

$$\|A\| = \max \text{eig}(A) = \max_x \frac{\|Ax\|}{\|x\|} = \max_{Ax=b} \frac{\|b\|}{\|x\|}$$

$$\|b\| \leq \max \text{eig}(A) \|x\|$$

$$\|\delta x\| \leq \frac{1}{\min \text{eig}(A)} \|\delta b\|$$

What is an ill-conditioned matrix ?

$$\|b\| \leq \max \text{eig}(A) \|x\| \qquad \|\delta x\| \leq \frac{1}{\min \text{eig}(A)} \|\delta b\|$$

$$\frac{\|\delta x\|}{\|x\|} \leq \frac{\max \text{eig}(A)}{\min \text{eig}(A)} \frac{\|\delta b\|}{\|b\|}$$

Condition number of the Matrix

What is the limit ?

100 ?

10^{10}

10^{3567}

1 ?

It depends



What is an ill-conditioned matrix ?

The acceptable condition number depends on your right hand side.

Extreme case : image denoising [Chambolle 04]



$$\begin{array}{c} \text{Identity} \nearrow \quad \nwarrow \text{Noised image} \\ Ix = b \\ \uparrow \\ \text{De-noised image} \end{array}$$

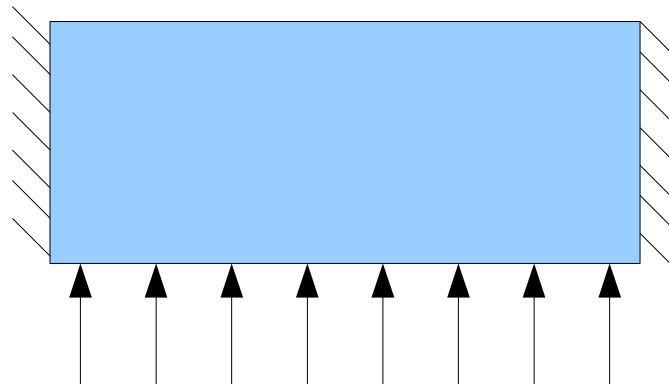
What is an ill-conditioned matrix ?

Other extreme case : control problem



In that case, there is no noise on the right hand side

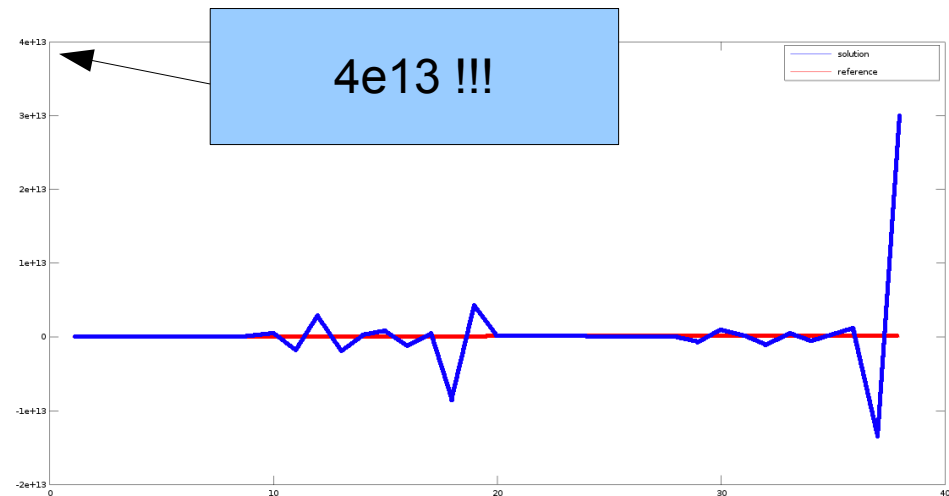
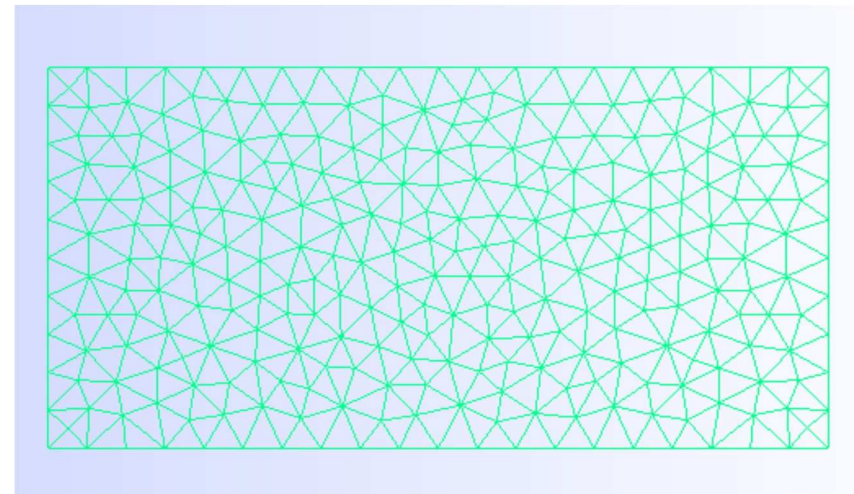
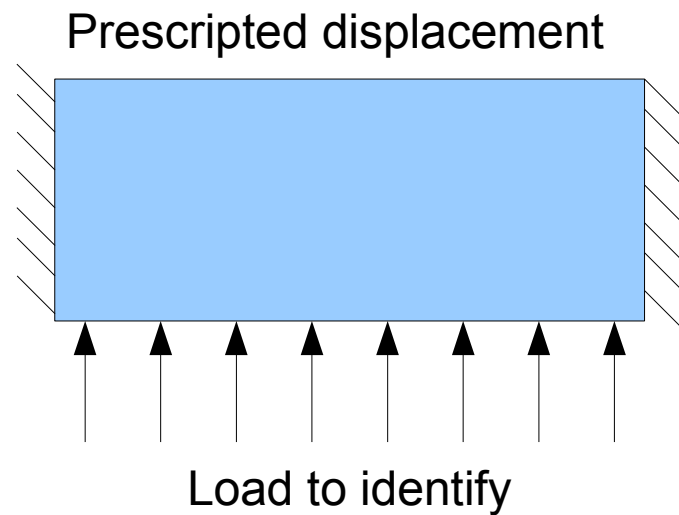
Prescribed displacement & 0 Neumann condition



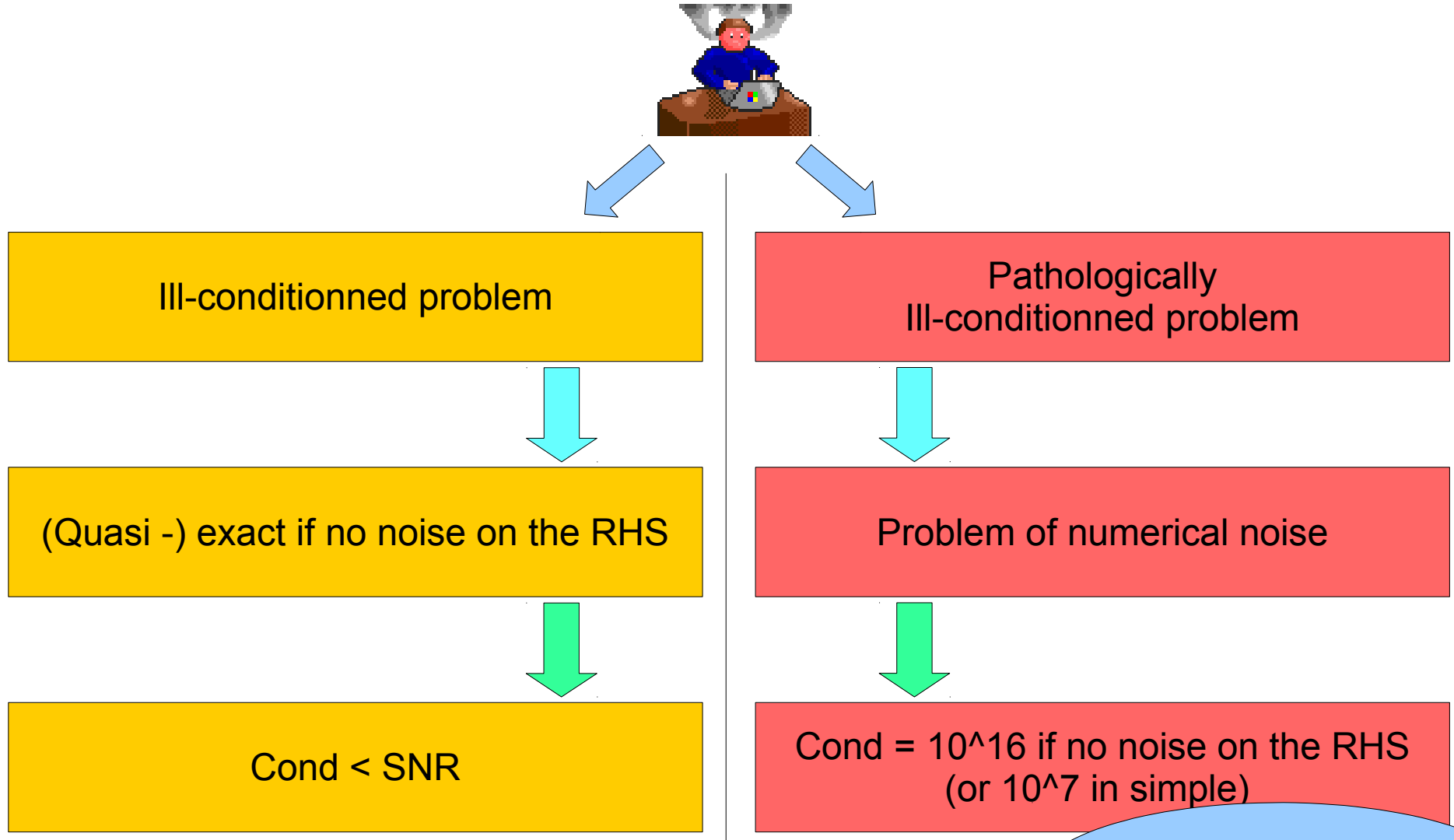
Load to identify

What is an ill-conditioned matrix ?

Numerical inversion of the system



What is an ill-conditioned matrix ?



Attention :
Not systematic

When do you get ill-conditioned matrices ?



When you mix data that don't have the same magnitude
Exemple : imposing Dirichlet BCs by Lagrange multipliers

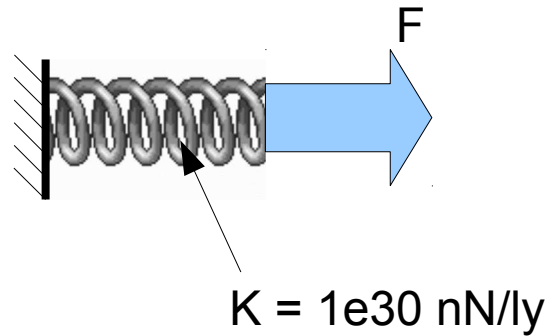


When you are modelling an instable physical phenomenon



When you try to do something morally reprehensible
Exemple : inverse problems in general

Example of benign ill-conditioned system



Equivalent system :

$$\begin{pmatrix} 10^{30} & -10^{30} & 1 \\ -10^{30} & 10^{30} & 0 \\ 1 & 0 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ \lambda \end{pmatrix} = \begin{pmatrix} 0 \\ f \\ 0 \end{pmatrix}$$

Equilibrated system :

$$\begin{pmatrix} 10^{30} & -10^{30} & 10^{30} \\ -10^{30} & 10^{30} & 0 \\ 10^{30} & 0 & 0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ 10^{-30}\lambda \end{pmatrix} = \begin{pmatrix} 0 \\ f \\ 0 \end{pmatrix}$$

How to invert ill-conditioned systems ?



How to invert ill-conditioned systems ?

First idea : try to see if the case is benign

Try scaling the lines and columns

The Frobenius norm
Is very good for that

Try permutating lines or columns



Linear solvers won't necessary do it for you

How to invert ill-conditioned systems ?

General idea for inverse problems



$$Ax = b$$



Full-rank system

Only 1 solution : the aberrant one

Rank deficient system

An infinity of solutions,
all of them are likely to be aberrant

And none of them is the solution of the underlying physical problem

We don't trust the system : we need extra information

Careful balance between extra information and the system

How to invert ill-conditioned systems ?

Choice of the balance parameter

Methods that use the noise level

Efficient if the condition number is $< 10^{16}$

Fairly stable in that case

Methods that don't use the noise level

Bakushinsky veto [Bakushinsky 84]
The method will not converge in the worst case

Quite used and reliable in practice



Tikhonov Regularization



Tikhonov regularization

$$Ax = b$$

Normal equations :

$$x = \arg \min_{x^*} \|Ax^* - b\|^2 \iff A^T Ax = A^T b$$

We'd like to control the distance to a reference x_0 wrt. a certain norm.

$$\|x - x_0\|_n$$

Final minimization problem [Tikhonov 63]

$$x = \min_{x^*} \underbrace{\|Ax^* - b\|^2}_{\text{Residual}} + \underbrace{\mu}_{\text{Balance parameter}} \underbrace{\|x^* - x_0\|_n^2}_{\text{Regularization term}}$$

Tikhonov regularization

Choice of x_0 and n

$$x = \min_{x^*} \|Ax^* - b\|^2 + \mu \|x^* - x_0\|_n^2$$

Ex : Young modulus of a variant of steel
 $x_0 = 210\,000 \text{ MPa}$

In some cases, we don't know what x_0 to use

In those cases, $x_0 = 0$

n can be the L2 norm

Or, for mechanical fields, a norm penalizing the gradients
Or the gap to equilibrium [Claire 04]

Tikhonov regularization

Quadratic Tikhonov regularization

$$x = \min_{x^*} \|Ax^* - b\|^2 + \mu \|Lx^* - Lx_0\|^2$$

The functionnal is convex (if $\mu > 0$)

Minimum atteigned for the zero of the gradient :

$$(A^T A + \mu L^T L)x = A^T b + \mu L^T Lx_0$$

Rem : is case A is SDP, the following problem is also relevant :

$$(A + \mu L^T L)x = b + \mu L^T Lx_0$$

And even if A is only squared, this may work

But it's dirty !



Tikhonov regularization

Remark on the normal equation for squared matrices :

$$Ax = b$$

vs

$$A^T Ax = A^T b$$

$$\text{cond}(A^T A) = \text{cond}(A)^2$$

If A is reasonably well-conditioned,
Working on one or the other system is equivalent

Because the error comes from the noise on b
That is multiplied by A'

If A is too badly conditioned
(ie float point errors enter into consideration),
The simple system is preferable

Because the error comes from every operation

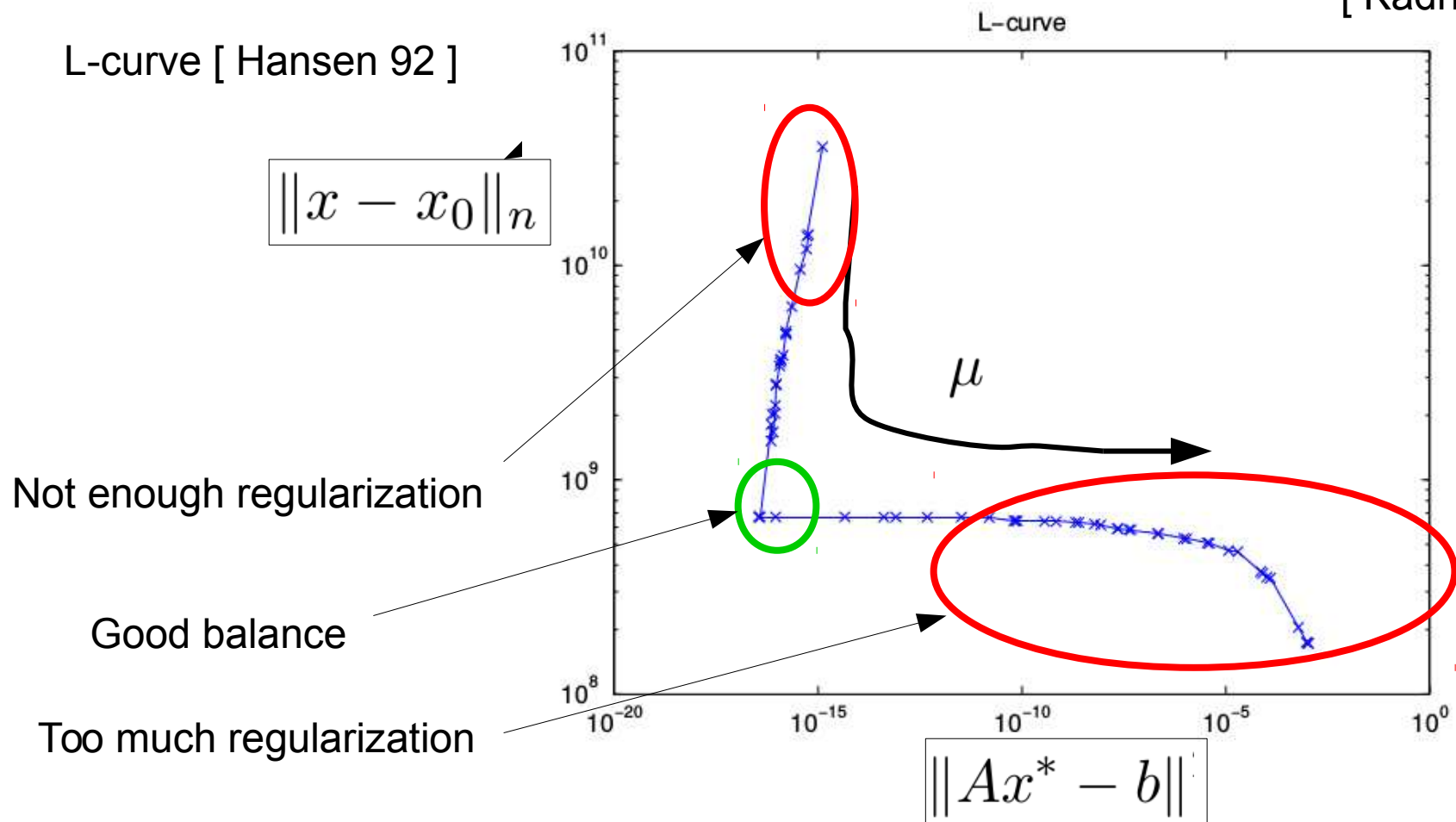
Tikhonov regularization

Determination of the regularization parameter μ

$$x = \min_{x^*} \|Ax^* - b\|^2 + \mu \|x^* - x_0\|_n^2$$

[Kadri 11]

L-curve [Hansen 92]



Tikhonov regularization

Determination of the regularization parameter μ

$$x = \min_{x^*} \|Ax^* - b\|^2 + \mu \|x^* - x_0\|_n^2$$

Morozov :

$$\|Ax - b\|^2 = \|\delta b\|^2$$

Arcangeli :

$$\|Ax - b\|^2 = \frac{\|\delta b\|^2}{\mu}$$

Arcangeli's criterion
Works only if $L = 1$



And was proven to have a
good convergence wrt
the noise

Rem : $\|\delta b\|^2$ Is the residual of the solution of the noise free problem

Truncated Generalized Singular Values Decomposition



Truncated Generalized Singular Values Decomposition

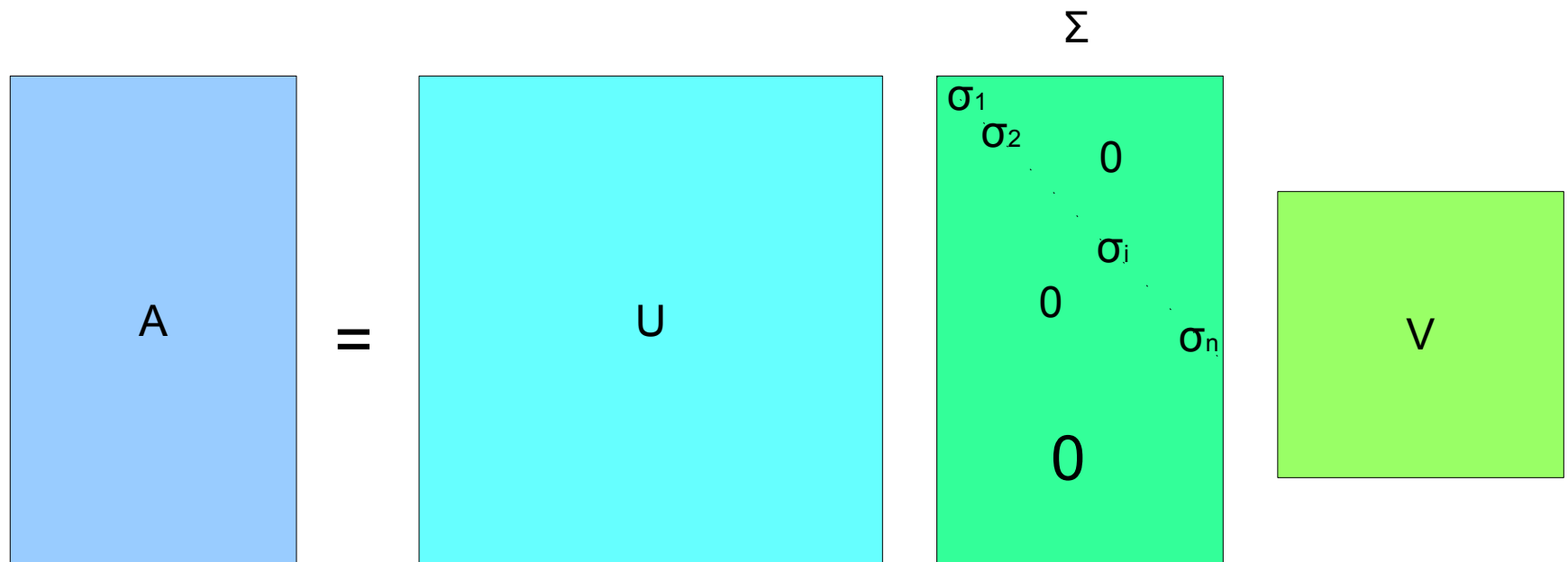
$$Ax = b$$

$$A = U\Sigma V^T$$

With :

$$U^T U = 1 \quad V^T M_v V = 1$$

$$M_v^T = M_v$$



Truncated Generalized Singular Values Decomposition [Hansen 87]

$$Ax = b$$

$$A = U\Sigma V^T$$

$$U\Sigma V^T x = b$$

$$x = M_v V \Sigma^{-1} U^T b$$

$$\Sigma^{-1} = \begin{pmatrix} \frac{1}{\sigma_1} & & \\ & \frac{1}{\sigma_2} & \\ & & \ddots \\ & & & \frac{1}{\sigma_n} \end{pmatrix}$$

Corresponding terms
are supposed to be small

But the noise
makes them

Not so small

Inverse of small values => Big

Huge (and false)
terms appear

Truncated Generalized Singular Values Decomposition [Hansen 87]

$$x = M_v V \Sigma^{-1} U^T b$$

$$\tilde{\Sigma}_k^{-1} = \begin{pmatrix} \frac{1}{\sigma_1} & & & & \\ & \ddots & & & \\ & & \frac{1}{\sigma_k} & & \\ & & & 0 & \\ & & & & \ddots \\ & & & & & 0 \end{pmatrix}$$

No terms,
No problem



$$x_k = M_v V \tilde{\Sigma}_k^{-1} U^T b$$

Truncated Generalized Singular Values Decomposition

$$Ax = b$$

$$x_k = M_v V \tilde{\Sigma}_k^{-1} U^T b$$

Parameter of the method

Rem : it is possible to add an a-priori known term in
 $\text{Span}(\Sigma - \tilde{\Sigma}_k)$



PB : generalization for non-linear problems

Truncated Generalized Singular Values Decomposition

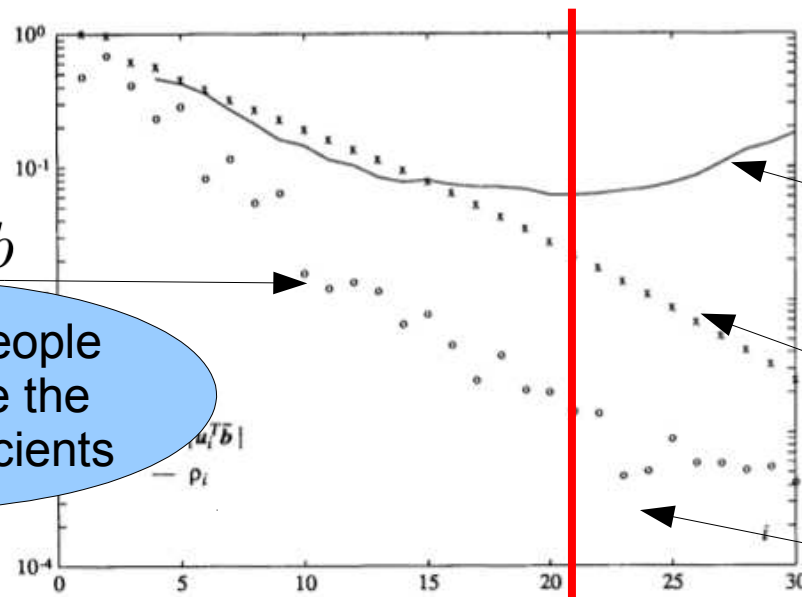
Choice of the nb of singular values (k)

L-curve

Picard Plot [Hansen 90]

Right hand side $U^T b$

In practice, people
Prefer to use the
Fourier coefficients



Solution $\tilde{\Sigma}_k^{-1} U^T b$

Singular values

Stagnation of the Rhs

The Morozov criterion is still available

Truncated Generalized Singular Values Decomposition

Remark : The damped GSVD [Ekstrom 74]

$$\tilde{\Sigma}_{\mu}^{-1} = \begin{pmatrix} \frac{1}{\sigma_1 + \mu} & & & & \\ & \frac{1}{\sigma_2 + \mu} & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & \frac{1}{\sigma_n + \mu} \end{pmatrix}$$

This is equivalent to the Tikhonov regularization

This gives a new method to compute the optimal parameter for Tikhonov (adaptation of Picard)

And generalization to NL problems is then trivial

Early-stopped iterative algorithm



Early-stopped iterative algorithm

$$\{x_i\}_{i=0..n}, \lim_{i \rightarrow +\infty} x_i \text{ Solution of } Ax = b$$

Usual criterion on the residual ($<1e-12$)

In case we don't let the algorithm finish :

Exemple : Richardson algorithm : $\text{eig}(A) < 1$

$$\begin{aligned}x_{i+1} &= (\mathcal{I} - A)x_i + b \\x_{i+1} &= V(\mathcal{I} - \Theta)V^T x_i + b \\ \tilde{x}_{i+1} &= (\mathcal{I} - \Theta)\tilde{x}_i + \tilde{b}\end{aligned}$$

The small eigenvalues converge slowly

Early-stopping doesn't take them into account

Early-stopped iterative algorithm

Usually, in iterative algorithms, last eigenvalues converge more slowly

Link with the truncated eigenvalues method

Mainly for Krylov solvers

(Block-) Conjugate Gradient

GMRES / Orthodir [Calvetti 02]

Conjugate Residuals

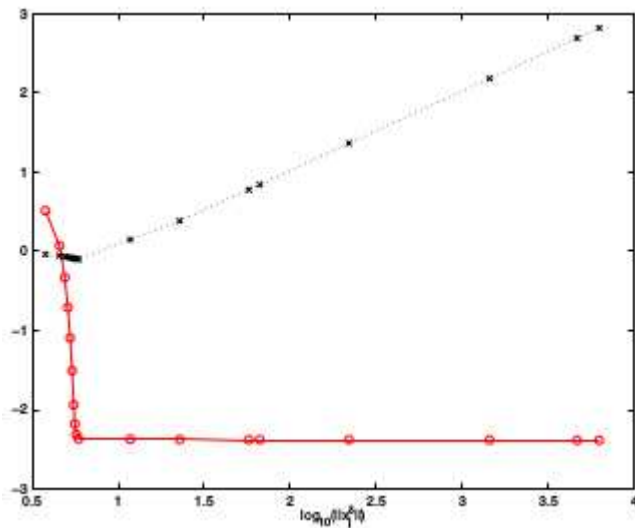
But also for Steepest descent
(that is not a Krylov)



Early-stopped iterative algorithm

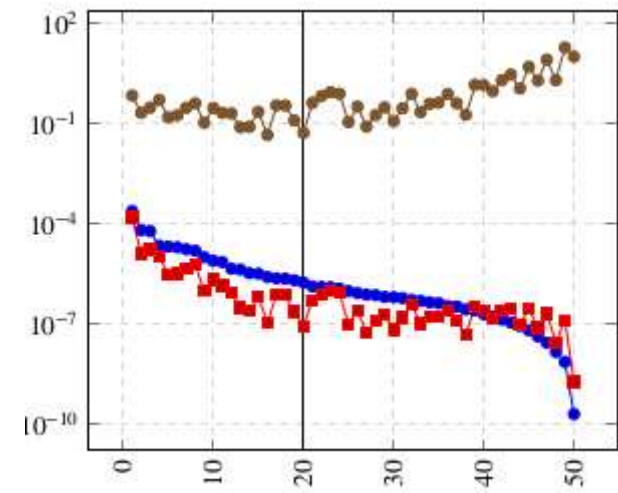
Choice of the stopping criterion

L-curve



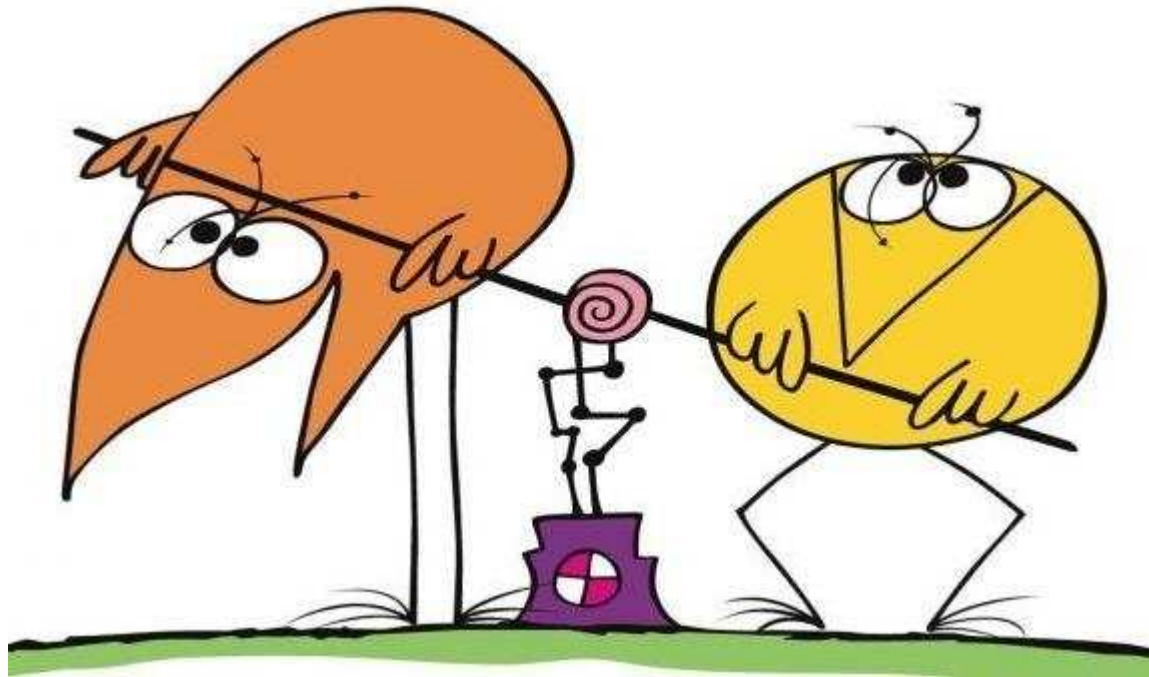
[Calvetti 02]

Picard plot
(in some cases)



[🦘 18]

Bayesian inversion



Bayesian inversion

$$Ax = b$$

we are set in the
linear setting
but the method is
more general

In the probabilistic setting

$$\tilde{x} \quad \tilde{b}$$

A-priori probability law of the unknown (ex : isoprobability)

$$p(\tilde{x} = x)$$

Probability law of the right hand side (from the measurement uncertainty)

$$p(\tilde{b} = b | \tilde{x} = x)$$

Bayes theorem gives the a-posteriori law of the unknown

$$p(\tilde{x} = x | \tilde{b} = b)$$



Bayesian inversion

$$Ax = b$$

Bayes theorem :

a-posteriori

measure

a-priori

$$p(\tilde{x} = x | \tilde{b} = b) = \frac{p(\tilde{b} = b | \tilde{x} = x) p(\tilde{x} = x)}{p(\tilde{b} = b)}$$

Normalization constant

Bayesian inversion

Remark on the probability law of the right hand side

$$p(\tilde{b} = b | \tilde{x} = x)$$

If there is no measurement noise, $b = Ax$

The probability is function of the distance between b and Ax
And of the measurement noise level

Estimated correlation of the measurement noise

$$p(\tilde{b} = b | \tilde{x} = x) = \frac{1}{(2\pi)^{n_b/2} \sqrt{\det(C_b)}} e^{-\frac{1}{2}(b-Ax)^T C_b^{-1} (b-Ax)}$$

Normalization stuff

Residual between x and b



For each value of x
An evaluation of Ax is required

Bayesian inversion

$$Ax = b$$

We know thanks to Bayes theorem : $p(\tilde{x} = x | \tilde{b} = b)$

But a numerical result is needed. For that we can compute :

The mean

The arg max of the probability law

The median

The covariance matrix

Upper order statistical moments

Bayesian inversion

Computation of the mean (similar for the other quantities)

$$\mathfrak{E}(\tilde{x}|\tilde{b} = b) = \int_{\mathcal{R}^n} x \mathfrak{p}(\tilde{x} = x|\tilde{b} = b) dx$$

$$\mathfrak{E}(\tilde{x}|\tilde{b} = b) = \int_{\mathcal{R}^n} x \frac{\mathfrak{p}(\tilde{b} = b|\tilde{x} = x) \mathfrak{p}(\tilde{x} = x)}{\mathfrak{p}(\tilde{b} = b)} dx$$

$$\int_{\mathcal{R}^n} \mathfrak{F}(x) \mathfrak{p}(\tilde{x} = x) dx$$

► Monte-Carlo integration

Bayesian inversion

Monte-Carlo integration

$$\int_{\mathcal{R}^n} \mathfrak{F}(x) p(\tilde{x} = x) dx$$

Sample the a-priori probability density

Compute the associated $\mathfrak{F}(x)$
including the probability of an output knowing the input

That's why we are pumping

Because each
evaluation of $\mathfrak{F}(x)$ includes
a forward resolution

Shut up and pump



Sum the $\mathfrak{F}(x)$ and divide by the nb of samples

Bayesian inversion

Monte-Carlo integration convergence properties

$$\int_{\mathcal{R}^n} \mathfrak{F}(x) p(\tilde{x} = x) dx$$

Converges p - almost surely with rate $K n^{1/2}$
(n is the number of samples)

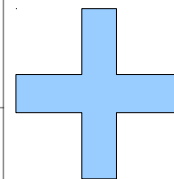
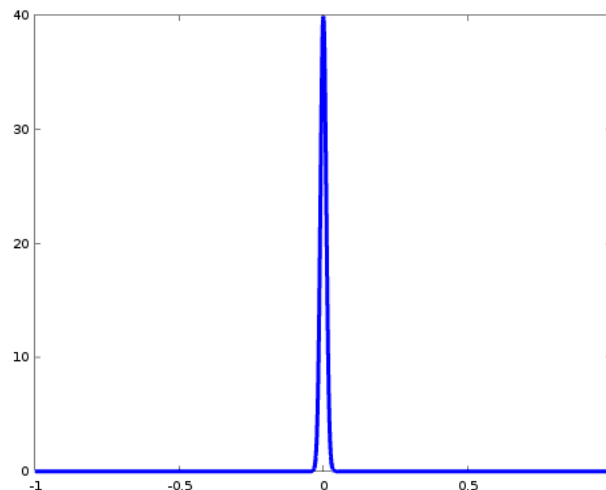
And K may be very small if p is « large »
And \mathfrak{F} is « small »



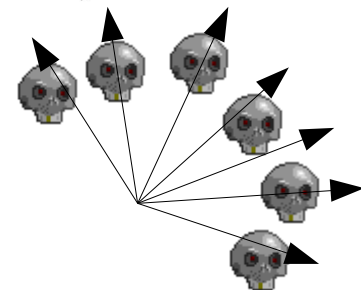
Exemple :

$p(x)$ is the
equiprobable law
on $[-1;1]$

\mathfrak{F} is gaussian of
variance $1/100$



Curse Of Dimensionality



Bayesian inversion

How to cure those bad properties ?

Multilevel Monte-Carlo [Giles 08]

Markov Chain [Gilks 95]

Kalman Filter [Kalman 60]

Though Kalman claimed that
his method had nothing
to do with Bayesian inversion

Transport Maps method / Variational Bayesian

Reduced forward model [Rubio 18]



Bayesian inversion

Remark in the case of Gaussian probabilities (1/2)

Because of the
Central Limit Theorem
Many people use gaussian
probabilities

$$p(\tilde{x} = x) = \frac{1}{(2\pi)^{n_x/2} \sqrt{\det(C_x)}} e^{-\frac{1}{2}(x-x_0)^T C_x^{-1} (x-x_0)}$$

$$p(\tilde{b} = b | \tilde{x} = x) = \frac{1}{(2\pi)^{n_b/2} \sqrt{\det(C_b)}} e^{-\frac{1}{2}(b-Ax)^T C_b^{-1} (b-Ax)}$$



$$p(\tilde{x} = x | \tilde{b} = b) = Cte \cdot e^{-\frac{1}{2}(x^T (A^T C_b^{-1} A + C_x) x - 2(x_0^T C_x^{-1} + b^T C_b^{-1} A) x + x_0^T C_x^{-1} x_0 + b^T C_b^{-1} b)}$$

Bayesian inversion

Remark in the case of Gaussian probabilities (2/2)

The mean of x respects :

$$\min_x x^T (A^T C_b^{-1} A + C_x) x - 2(x_0^T C_x^{-1} + b^T C_b^{-1} A) x + x_0^T C_x^{-1} x_0 + b^T C_b^{-1} b$$

$$(A^T C_b^{-1} A + C_x^{-1}) x = (C_x^{-1} x_0 + A^T C_b^{-1} b)$$

We study the particular case where :

$$C_b^{-1} = \nu \mathcal{I}$$

$$C_x^{-1} = \eta \mathcal{I}$$

$$\mu = \frac{\nu}{\eta}$$

$$(A^T A + \mu \mathcal{I}) x = (\mu x_0 + A^T b)$$

In the gaussian case, Bayesian inversion can be seen as a way to determine the regularization parameter

But how do you find the variance of the prior law ?



Relaxtion of the constraint



Relaxation of the constraint [Ladevèze 93]

$$\min_{Cx=d} \|Ax - b\|^2$$

Noisy

$$\min_x \|Ax - b\|^2 + \mu \|Cx - d\|^2$$

Useful only in the case where
(A ; C) is overdetermined



Illustrative examples



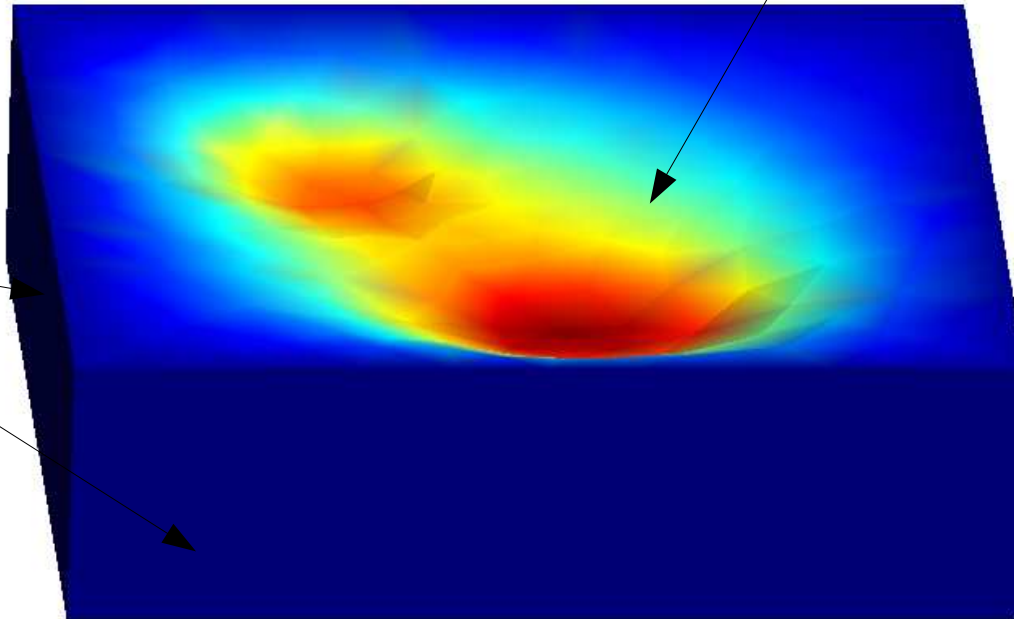
Illustrative examples

Identification of BCs (Cauchy problem)



Identification of U and F

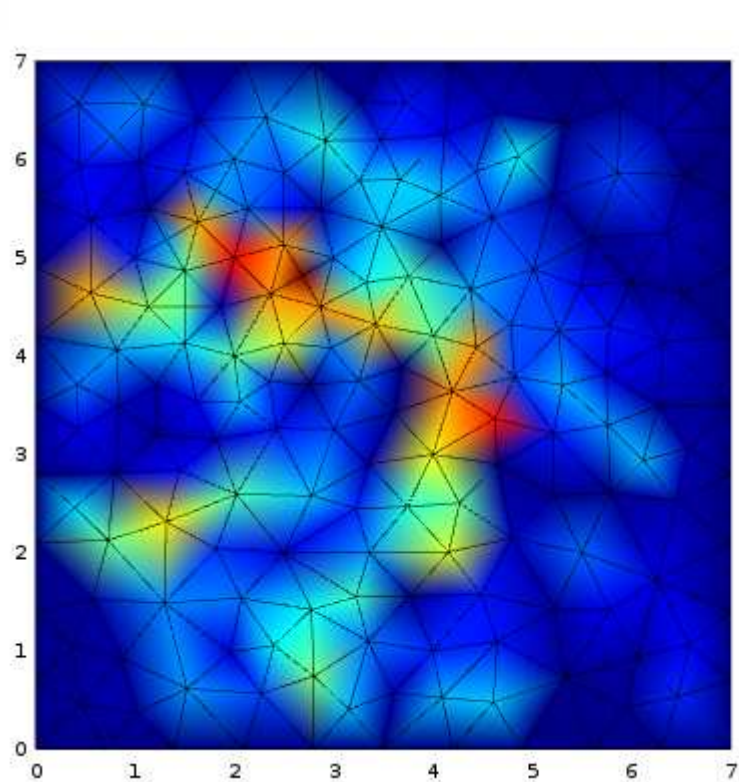
$U = 0$



$F = 0$ & Measurement of U

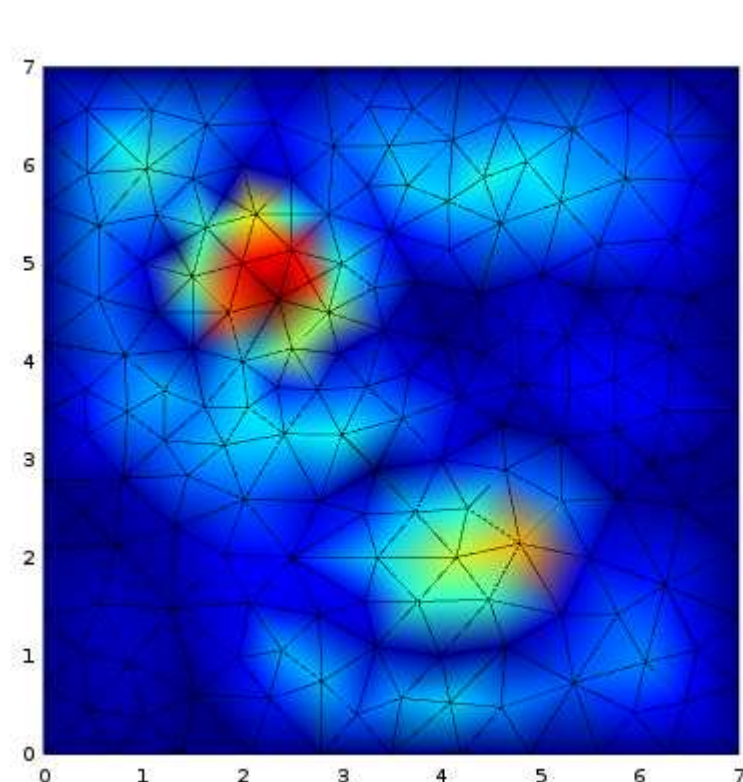
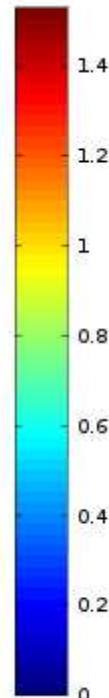
Illustrative examples

Identification of BCs (Cauchy problem)



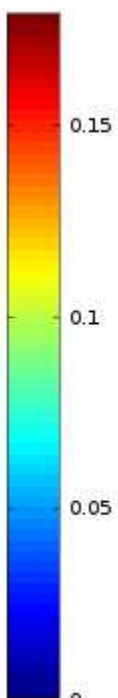
10 % noise, no regularization

error



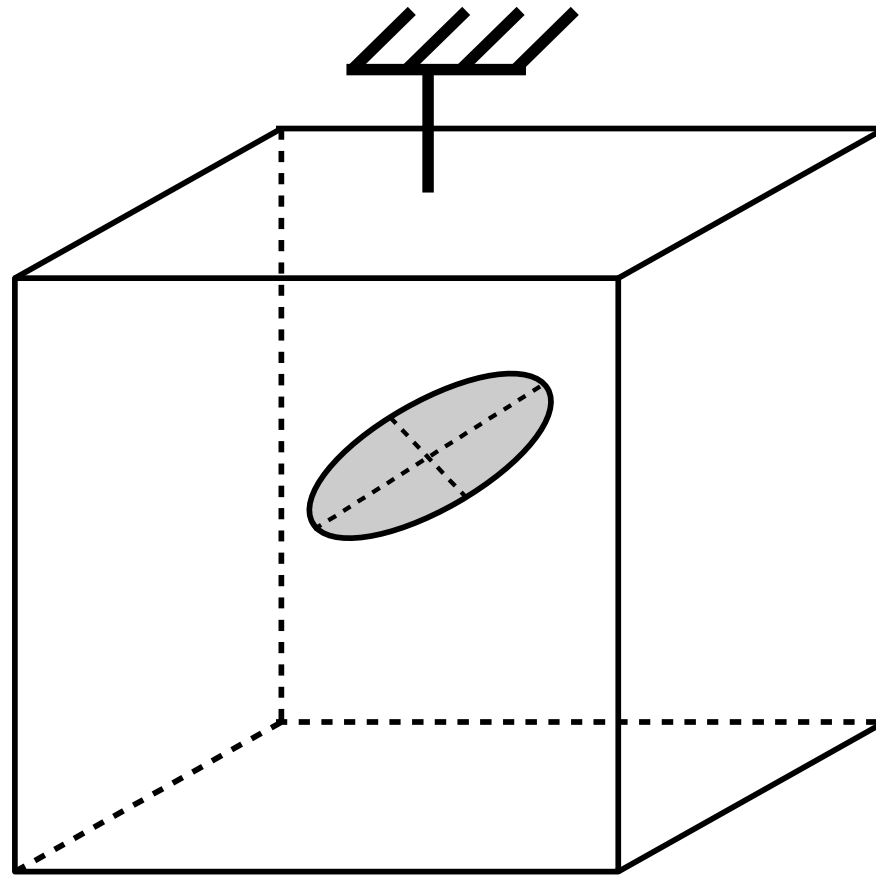
10 % noise,
Regularization by early-stopped
conjugate gradient and Ritz post-
analysis

error



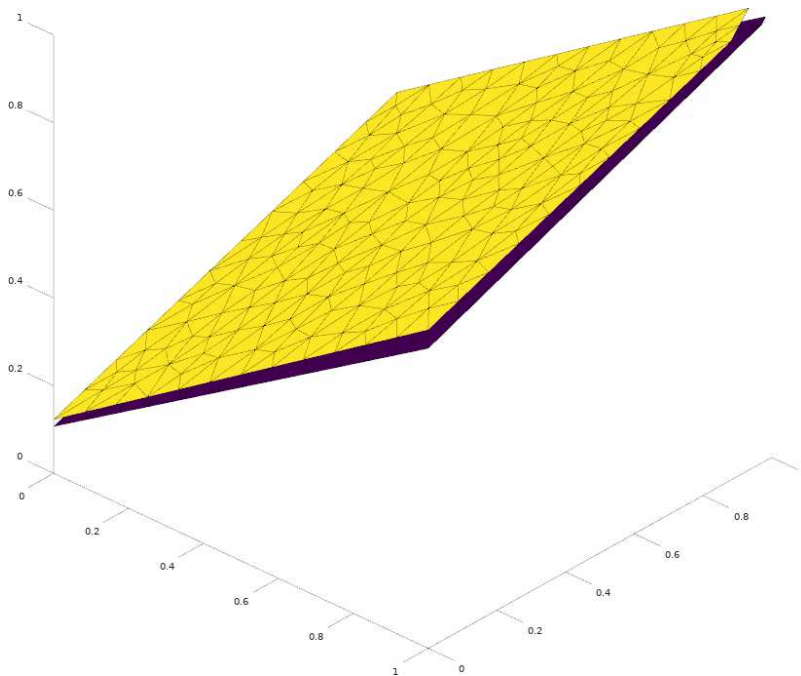
Illustrative examples

Identification of a displacement gap (crack)

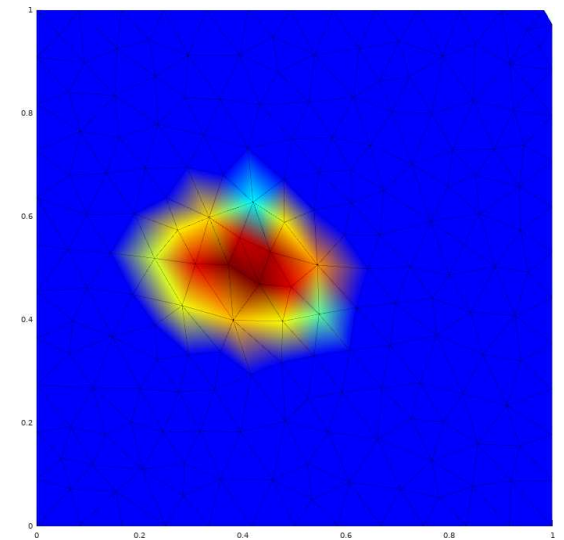
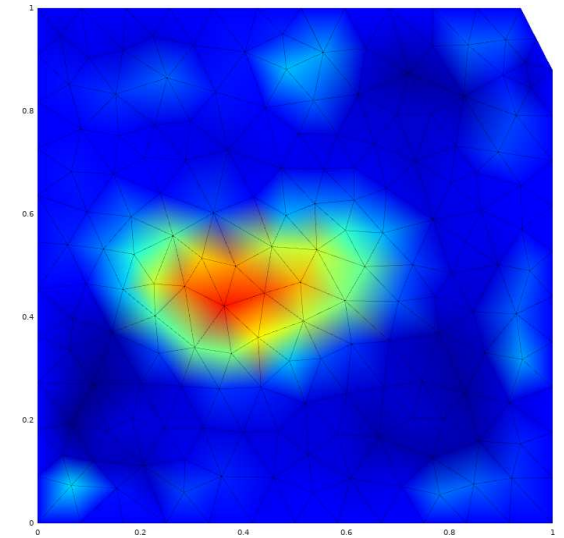


Illustrative examples

Identification of a displacement gap (crack)



Identification of the plane
(Tikhonov regularization)



Identification of the gap 55
(Identification and reference)

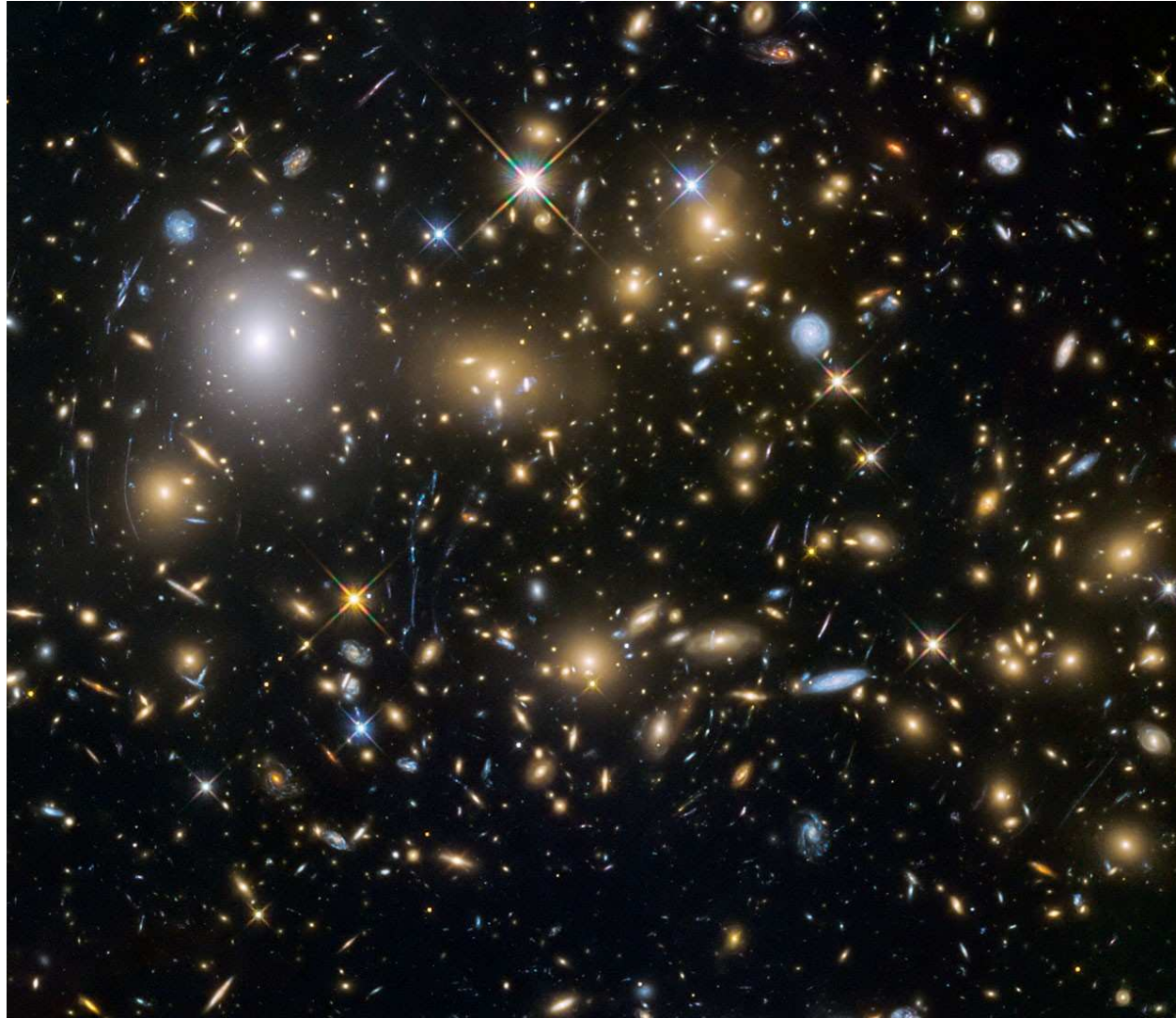
Remark : library for regularization By Christian Hansen

Featuring tools to implement in practice the presented methods
And many other nice features as well !

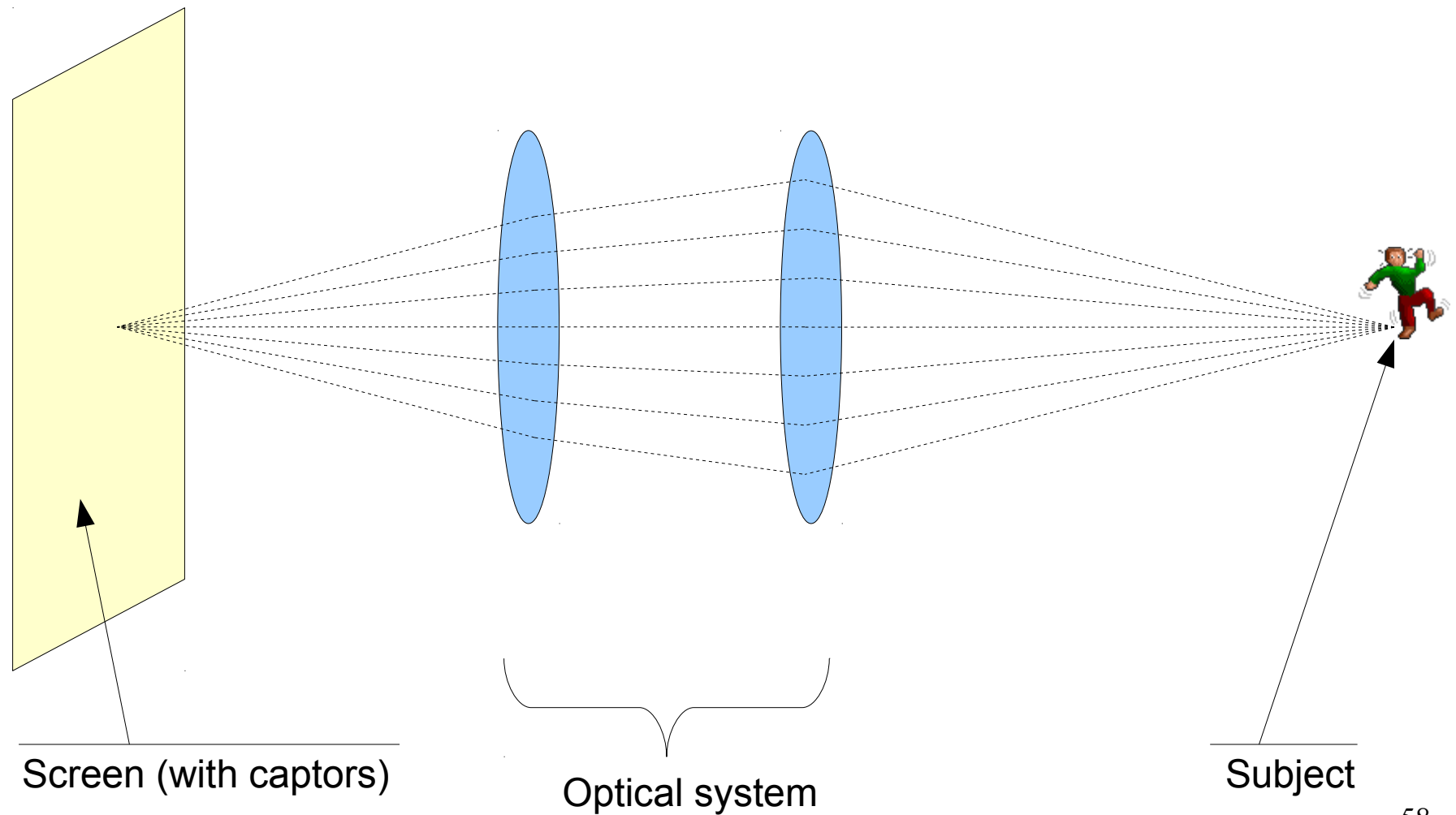
<http://www.imm.dtu.dk/~pcha/Regutools/>



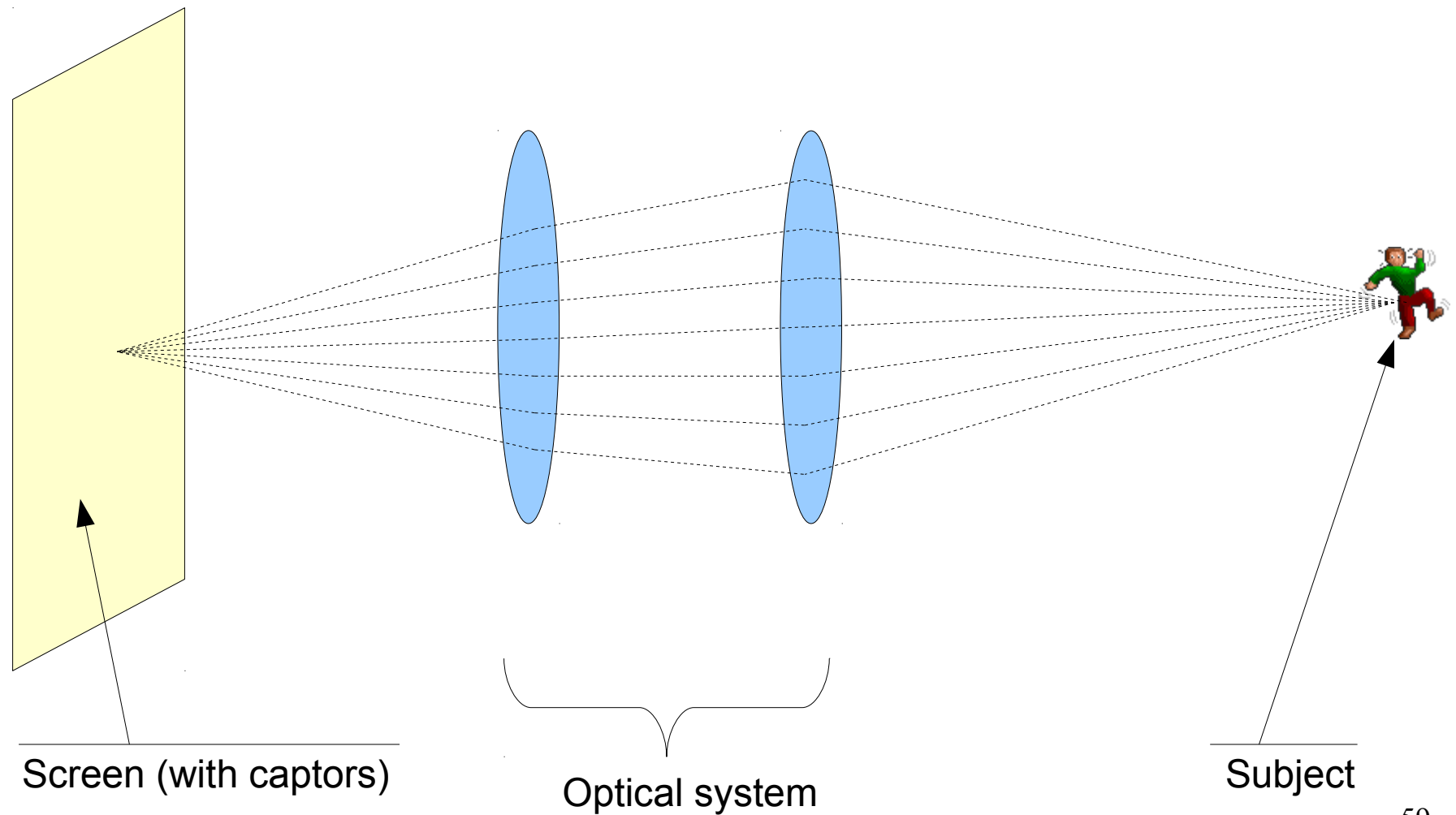
Applicative example : correction of blurred images



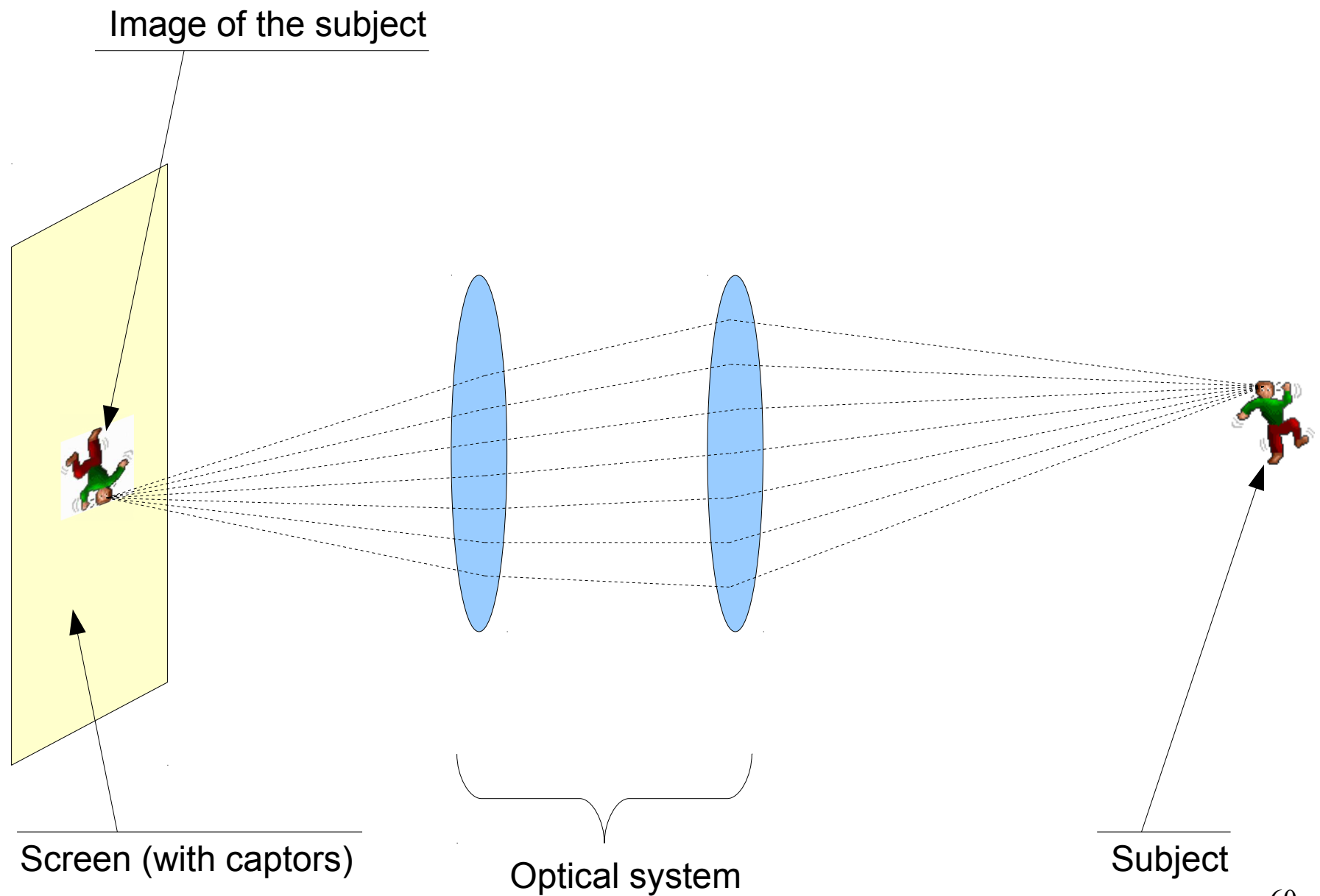
Applicative example : Correction of blurred images



Applicative example : Correction of blurred images

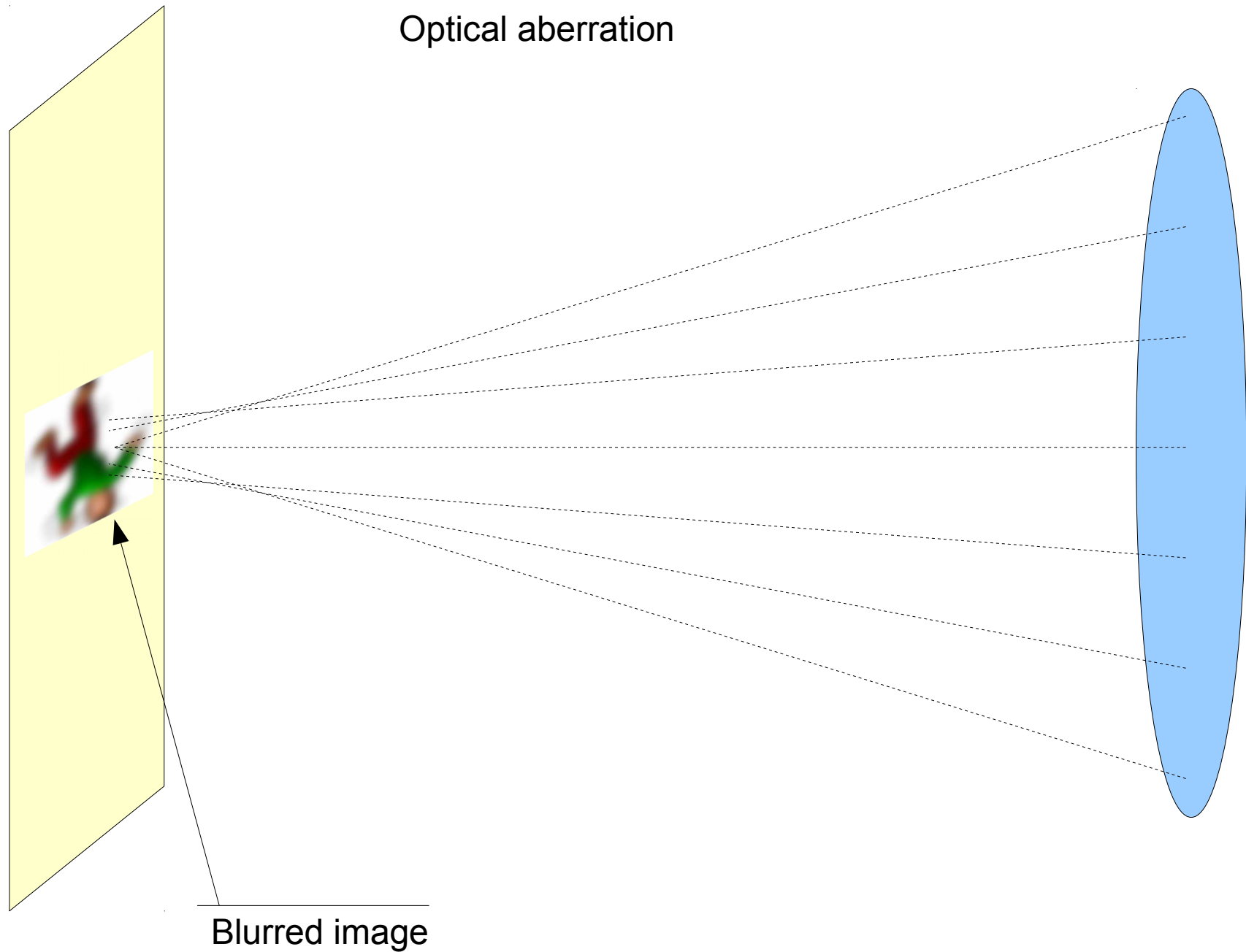


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Optical aberration



Applicative example : Correction of blurred images

In some applications, it is necessary to post-process the image

Need of very precise pictures



Or

Very bad optics



Model the blur as a linear operator.
Invert that operator in order to recover the image

Problem :

This operator is
Pathologically
Ill-conditionned

Other
Problem :

There is also
noise



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In normal applications, high quality images ($\sim 3000 \times 3000$ pix)

Full operator of size $9 \cdot 10^6$

High spec hardware & optimized (and compiled) code
(Matrix-free methods, GPU computing...)

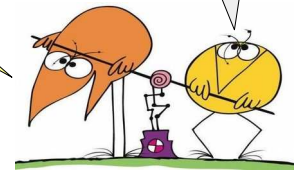
We use laptops on an unoptimized code (pedagogically optimized)

Nice excuse

Looks like
someone here is coding
with his ass...

Our pictures are very small

The behaviour of real images wrt the algos
May be slightly different to the behaviour of
The proposed ones



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The gaussian blur model (one among many) :

$$I_B(\underline{x}) = \frac{1}{N(\underline{x})} \int_{\Omega} e^{\frac{-(\underline{x} - \underline{\tilde{x}})^2}{2\sigma^2}} I(\underline{\tilde{x}}) d\underline{\tilde{x}}$$

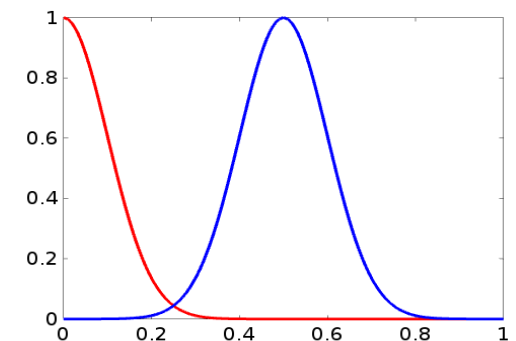
Blurred image
Normalization factor
Unblurred image

Fredholm integral
↓
Trouble

$$N(\underline{x}) = \int_{\Omega} e^{\frac{-(\underline{x} - \underline{\tilde{x}})^2}{2\sigma^2}} d\underline{\tilde{x}}$$

$$\mathcal{B}(\underline{x}, \underline{y}) = \frac{1}{N(\underline{x})} e^{\frac{-(\underline{x} - \underline{y})^2}{2\sigma^2}}$$

Attention :
This operator is not symmetric
 $N(x) \neq N(y)$
Because of the bounds



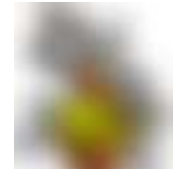
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Proposed images :

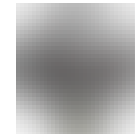
1) 11 X 11 noiseless picture (for debugging), detail of picture 2



2) 62 X 65 noiseless picture



3) 31 X 34 0.1 % noised picture



4) 16 X 15 0.1 % noised picture (for calibrating the NL solver)



5) 16 X 15 noiseless picture the same as the previous one



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Proposed solvers :

- 1) Tikhonov regularization
- 2) Total Variation regularization (non-quadratic Tikhonov)
- 3) Early-stopped Krylov solver
- 4) Truncated SVD

As it is, there are
too much unknowns to do
Bayesian inversion

Unless we try to do
weird things that are
out of the scope
for today

And it's not an
overdetermined system
So, no relaxation



And also out
of the scope
of competences
of the guy who
coded all
the stuff



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Suggestion of funny things to do (1/2) :

Fun points

1) For Tikhonov : compare the solutions of $A'Ax = A'b$ and $Ax = b$



2) For all : Compare the deblurring from a picture and from a matrix
Is it different ? Why ?



3) Test the Morozov method for noisy data $\|Ax - b\|^2 = \|\delta b\|^2$



4) For the picture etnono.png, understand why the blue is behaving so strange



5) See what happens when the operator is modified (the model is false)



6) For Krylov, try to use a conjugate gradient on the normal equation. Compare it on the quality and CPU point of view.



6 1/2) If you really want to compare, implement a MRHS CG



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Suggestion of funny things to do (2/2) :

Fun points

7) Try using the data from a .png and compare with the .mat
What is the difference ?



8) Modify the truncated SVD method to make a damped SVD
Compare the result with Tikhonov



9) On TSVD with the image 2-cr, does the function findPicard really
choose the best number of modes ?
Understand what's wrong and cure the function



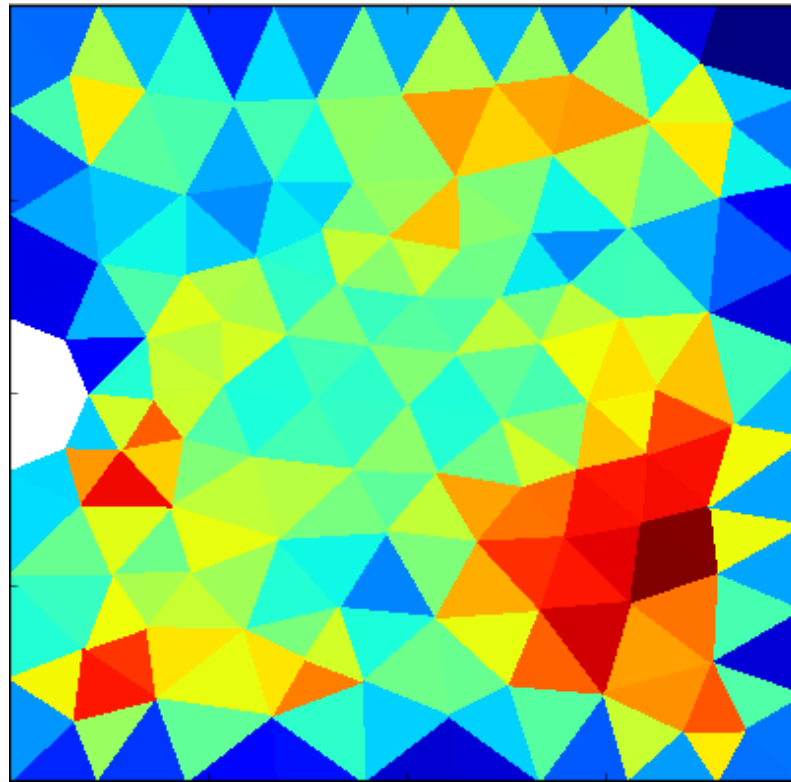
10) Why does the total variation tend to give better results than
quadratic Tikhonov ?

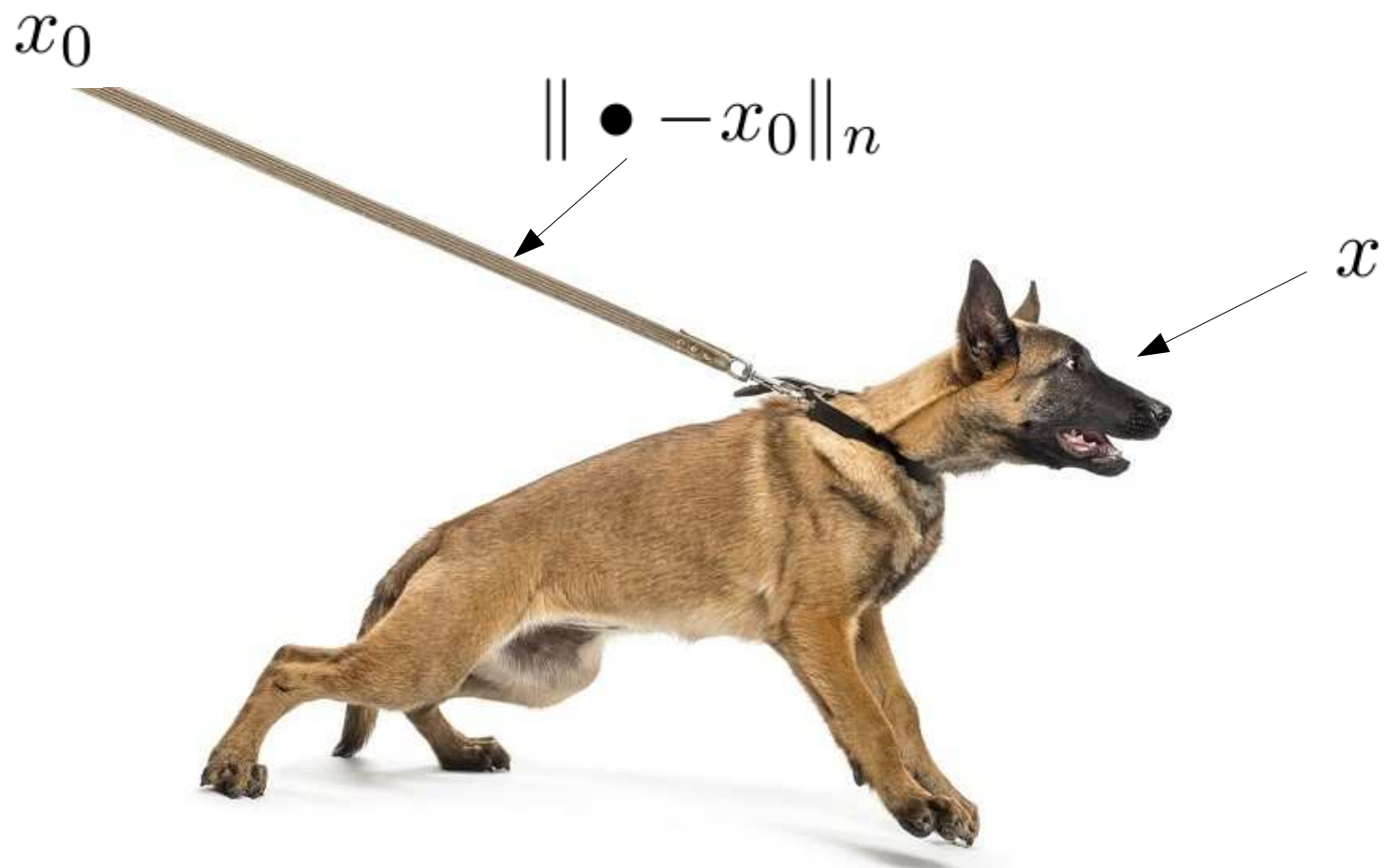


11) By inverting the Morozov principle, estimate an equivalent noise
level for unnoised pictures. Is it stable between the pictures ?
Do the same for the normal equation



Thank you for your attention





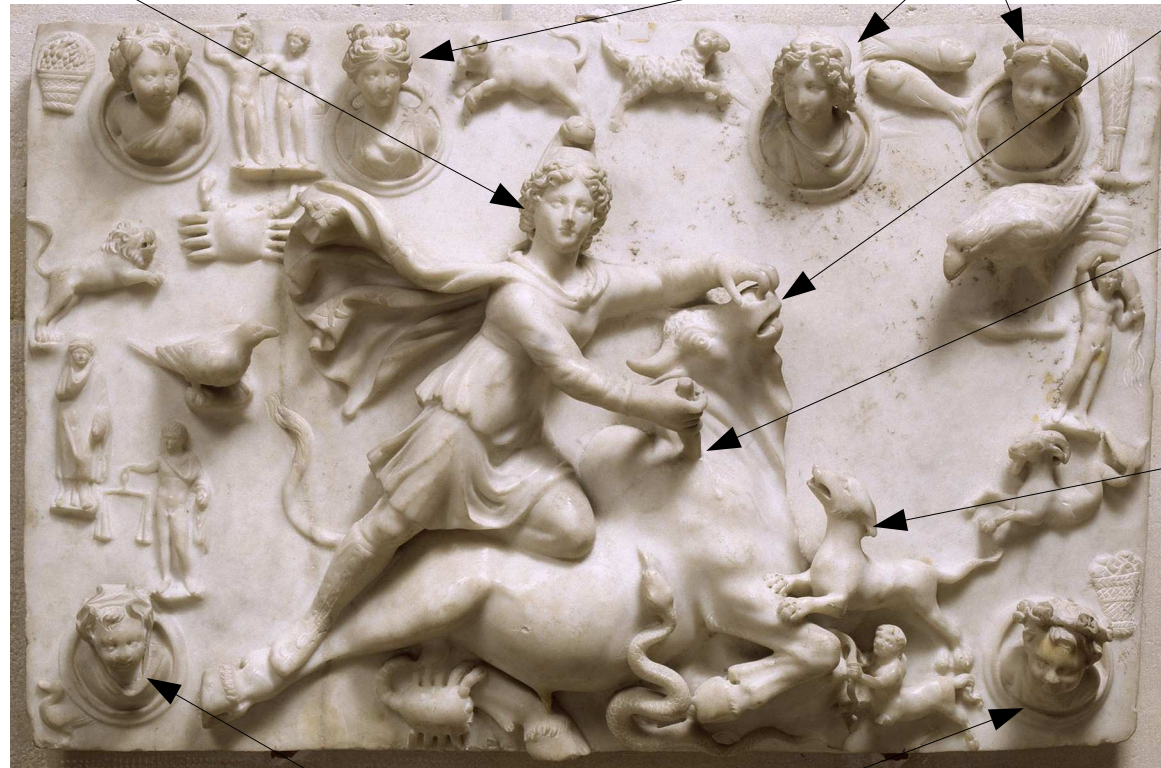
You

The jury of your PhD

An ill-conditioned matrix

The regularization toolbox

The guy who has stupid questions, but you have to answer because he is part of the jury



Your parents : they don't understand anything, but look happy