Computational inverse problems

Nuutti Hyvönen and Juha-Pekka Puska

nuutti.hyvonen@aalto.fi, juha-pekka.puska@aalto.fi

First lecture, March 1, 2021.

0 Practical issues

Information and materials

- The main information channel of the course is itse MyCourses homepage:
  `https://mycourses.aalto.fi/course/view.php?id=29656`
- The text books are "J. Kaipio and E. Somersalo, *Statistical and Computational Inverse Problems*, Springer, 2005" (mainly Chapters 2 and 3) and "D. Calvetti and E. Somersalo, *Introduction to Bayesian Scientific Computing. Ten Lectures on Subjective Computing*, Springer, 2007".
- Lecture notes and exercise sheets are posted on the course homepage.

Exercises

- There are no actual exercise sessions, but the assistant is on call in Zulip chat each Friday at 12-16.
- Each week there is one home assignment: The solution to the home assignment in the exercise paper of week m is to be *returned* as instructed in MyCourses before 17.00 on Wednesday of week $m + 1$. (For example, the solution to the home assignment in the first exercise paper should be returned before 17.00 on Wednesday, March 10.)
- Model solutions for the non-homework problems of the current week and the home assignment of the preceding week are published in MyCourses each Thursday.

Evaluation

The course grades will be based on the weekly *home assignments* and a *home exam*.

- The home assignments constitute 25% of the grade. Each returned solution is given $0-3$ points; at the end of the course, the obtained points will be summed and scaled appropriately.
- The home exam constitutes 75% of the grade. It will be held after the lectures have ended — the exact timing will be agreed upon later on. There will be four, more extensive assignments that must be solved within a given time period (e.g., within ten days).

Timetable

The lectures of the course extend over the weeks 9–14, i.e., Period IV (plus the home exam).

- The first half will concentrate on traditional regularization techniques.
- The second half will examine inverse problems from a statistical view point.

1 What is an ill-posed problem?

Well-posed problems

Jacques Salomon Hadamard (1865-1963):

1. A solution exists.
2. The solution is unique.
3. The solution depends continuously on the data, in some *reasonable* topology.

Ill-posed problems

Nuutti Hyvönen: The ill-posed problems are the complement of the well-posed problems in the space of all problems.

Examples:

- Interpolation.
- Finding the cause of a known consequence $\Longrightarrow$ inverse problems.
- Almost all problems encountered in everyday life.

When solving an ill-posed or inverse problem, it is essential to use all possible prior and expert knowledge about the possible solutions.

An example: Heat distribution in an insulated rod

Let us consider the problem

$$\begin{aligned} u_t &= u_{xx} && \text{in } (0,\pi) \times \mathbb{R}_+, \\ u_x(0,\cdot) &= u_x(\pi,\cdot) = 0 && \text{on } \mathbb{R}_+, \\ u(\cdot,0) &= f && \text{on } (0,\pi), \end{aligned}$$

where $u(\cdot,t)$ is the heat distribution at the time $t > 0$, f is the initial heat distribution, and the boundary conditions indicate that the heat cannot flow out of the 'rod' $[0,\pi]$.

Forward problem: Determine the 'final' distribution $u(\cdot,T) \in L^2(0,\pi)$, $T > 0$, if the initial distribution $f \in L^2(0,\pi)$ is known.

Inverse problem: Determine the initial distribution $f \in L^2(0,\pi)$, if the (noisy) 'final' distribution $u(\cdot,T) =: w \in L^2(0,\pi)$ is known.

Forward problem

The solution to the forward problem can be given explicitly:

$$u(x,T) = \sum_{n=0}^{\infty} \hat{f}_n e^{-n^2 T} \cos(nx),$$

where $\{\hat{f}_n\}_{n=0}^{\infty} \subset \mathbb{R}$ are Fourier cosine coefficients of the initial heat distribution f, i.e., $f = \sum_{n=0}^{\infty} \hat{f}_n \cos(nx)$ in the sense of $L^2(0,\pi)$.

It is relatively easy to see that the solution operator

$$E_T : f \mapsto u(\cdot, T), \quad L^2(0,\pi) \to L^2(0,\pi)$$

satisfies the following conditions:

- E_T is linear, bounded and *compact*.
- E_T is injective, i.e., $\mathrm{Ker}(E_T) = \{0\}$.
- $\mathrm{Ran}(E_T)$ is dense in $L^2(0,\pi)$.

Inverse problem

Solving the inverse problem for a general final heat distribution $w \in L^2(0, \pi)$ corresponds to inverting the compact operator $E_T : L^2(0, \pi) \to L^2(0, \pi)$, which is obviously impossible.

The *unbounded* solution operator

$$E_T^{-1} : \mathrm{Ran}(E_T) \to L^2(0, \pi)$$

is, however, well-defined. In other words, the inverse problem has a unique solution if $w = E_T f$ for some $f \in L^2(0, \pi)$, i.e., the measurement contains no noise.

Summary:

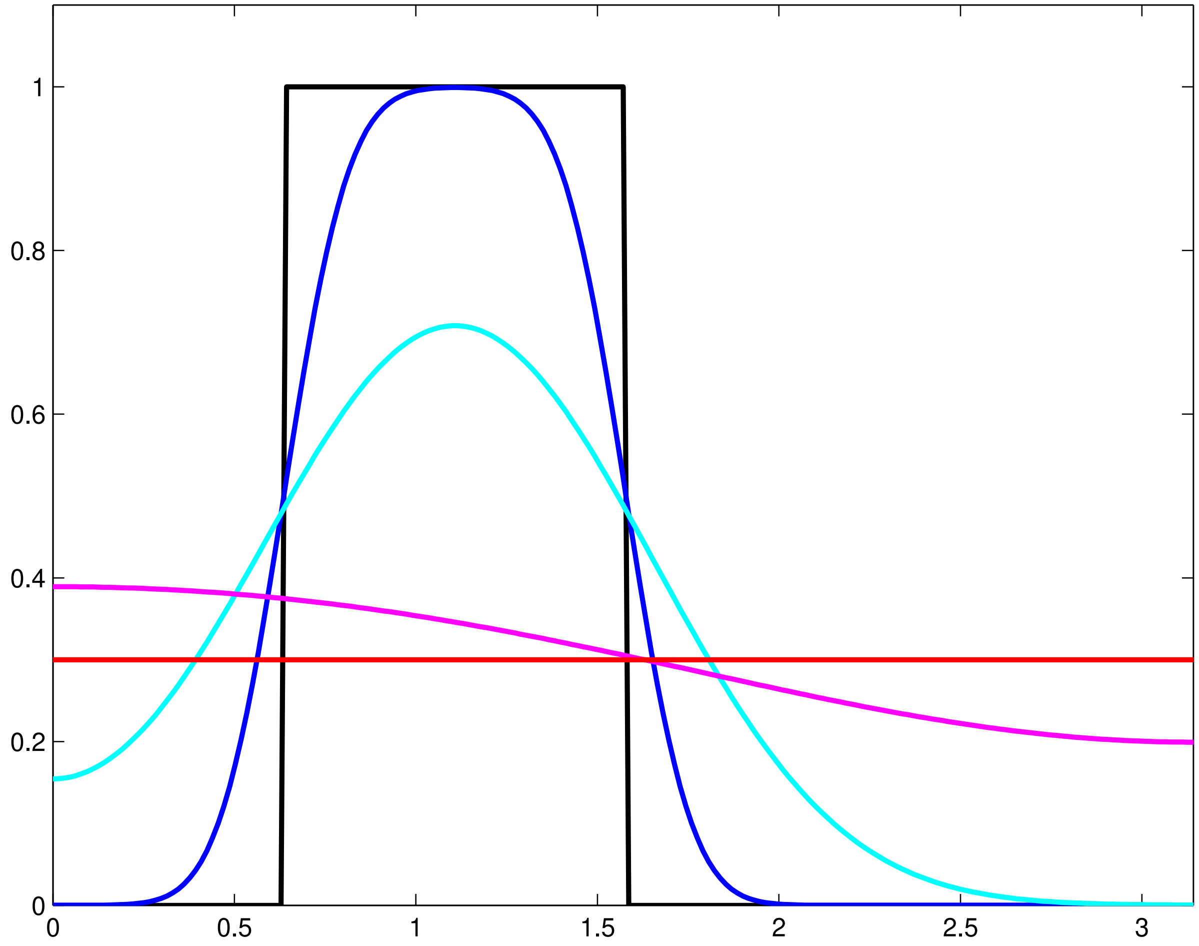
- If $w \in \mathrm{Ran}(E_T)$, the third Hadamard condition is not satisfied.
- If $w \notin \mathrm{Ran}(E_T)$, none of the Hadamard conditions is satisfied.

(Due to noise etc., the latter case is usually the valid one in practice.)

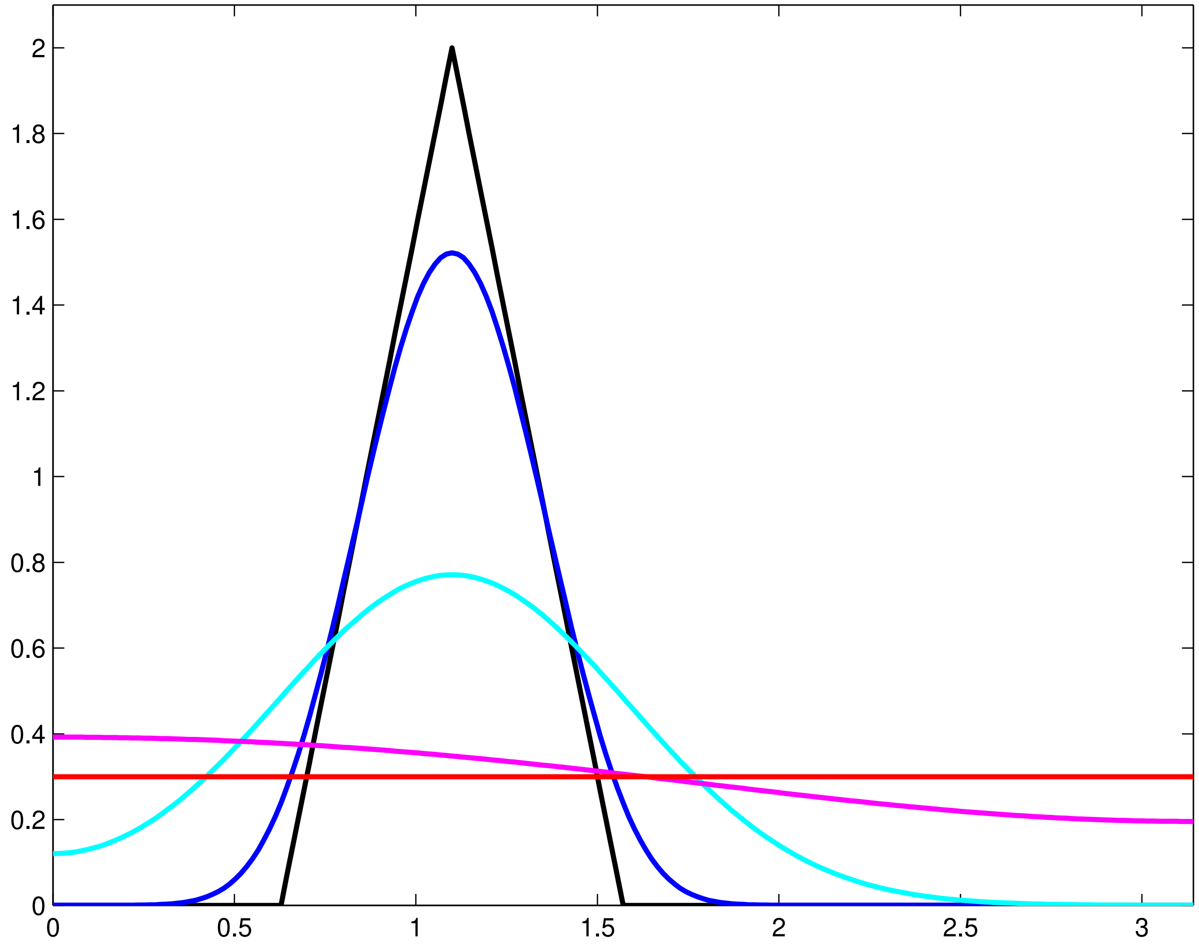
Question: Should one then ignore the ill-posed inverse problem?

Answer: No. The available measurement *always* contains *some* information about the initial heat distribution.

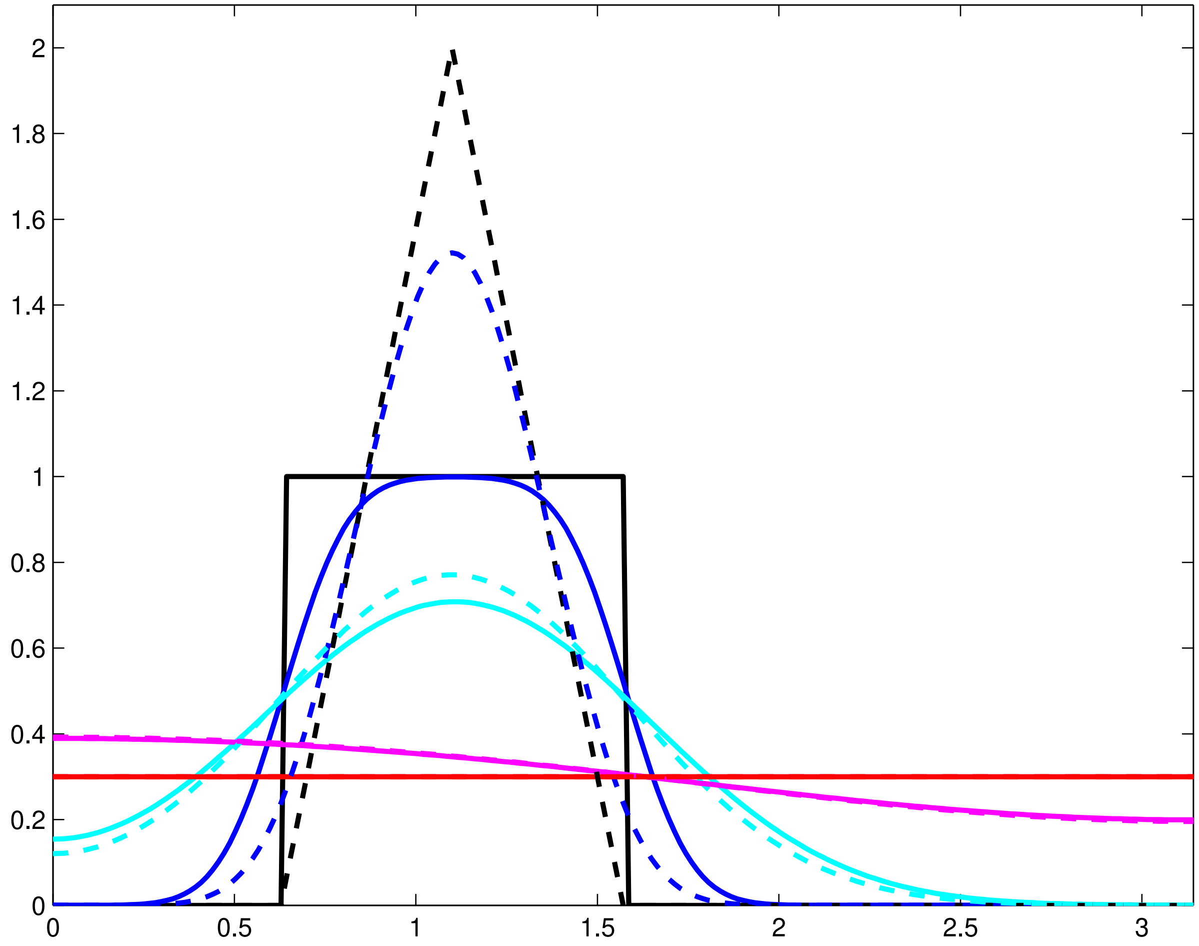
Heat distribution at $t = 0, 0.01, 0.1, 1$ and 10.



Another heat distribution at $t = 0, 0.01, 0.1, 1$ and 10.



Comparison of the two at $t = 0, 0.01, 0.1, 1$ and 10.



2 Classical regularization methods

2.1 Fredholm equation

Separable Hilbert space

A vector space H is a *real inner product space* if there exists a mapping $\langle \cdot, \cdot \rangle : H \times H \to \mathbb{R}$ satisfying

1. $\langle x, y \rangle = \langle y, x \rangle$ for all $x, y \in H$.
2. $\langle ax_1 + bx_2, y \rangle = a\langle x_1, y \rangle + b\langle x_2, y \rangle$ for all $x_1, x_2, y \in H$, $a, b \in \mathbb{R}$.
3. $\langle x, x \rangle \geq 0$, and $\langle x, x \rangle = 0 \Leftrightarrow x = 0$.

Furthermore, H is a *separable real Hilbert space* if, in addition,

1. H is *complete* with respect to the norm $\| \cdot \| = \sqrt{\langle \cdot, \cdot \rangle}$.
2. There exists a *countable orthonormal basis* $\{\varphi_n\}$ of H with respect to the inner product $\langle \cdot, \cdot \rangle$. This means that

$$\langle \varphi_j, \varphi_k \rangle = \delta_{jk} \quad \text{and} \quad x = \sum_n \langle x, \varphi_n \rangle \varphi_n \quad \text{for all } x \in H.$$

Fredholm equation

Let $A : H_1 \to H_2$ be a *compact* linear operator between the real separable Hilbert spaces H_1 and H_2. In the first half of this course, we mainly concentrate on the problem of finding $x \in H_1$ satisfying the equation

$$Ax = y, \tag{1}$$

where $y \in H_2$ is given. (In this setting, compact operators are the closure of the finite-dimensional operators, i.e., loosely speaking matrices, in the operator topology.)

Examples:

- In the example of Section 1, we have $A = E_T$ and $H_1 = H_2 = L^2(0, \pi)$.
- The most important case on this course is $H_1 = \mathbb{R}^n$, $H_2 = \mathbb{R}^m$ and $A \in \mathbb{R}^{m \times n}$ is a matrix.

2.2 Truncated singular value decomposition

Orthogonal decompositions

Let $A^* : H_2 \to H_1$ be the adjoint operator of $A : H_1 \to H_2$, i.e.,

$$\langle Ax, y \rangle = \langle x, A^* y \rangle \quad \text{for all } x \in H_1, y \in H_2.$$

We have the orthogonal decompositions

$$\begin{aligned} H_1 &= \mathrm{Ker}(A) \oplus (\mathrm{Ker}(A))^\perp = \mathrm{Ker}(A) \oplus \overline{\mathrm{Ran}(A^*)}, \\ H_2 &= \overline{\mathrm{Ran}(A)} \oplus (\mathrm{Ran}(A))^\perp = \overline{\mathrm{Ran}(A)} \oplus \mathrm{Ker}(A^*), \end{aligned}$$

where the "bar" denotes the closure of a set and

$$\begin{aligned} \mathrm{Ker}(A) &= \{x \in H_1 \mid Ax = 0\}, \\ \mathrm{Ran}(A) &= \{y \in H_2 \mid y = Ax \text{ for some } x \in H_1\}, \\ (\mathrm{Ker}(A))^\perp &= \{x \in H_1 \mid \langle x, z \rangle = 0 \text{ for all } z \in \mathrm{Ker}(A)\}, \quad \text{etc.} \end{aligned}$$

Characterization of compact operators

There exist (possible countably infinite) orthonormal sets of vectors $\{v_n\} \subset H_1$ and $\{u_n\} \subset H_2$, and a sequence of *positive* numbers $\{\lambda_n\}$, $\lambda_k \geq \lambda_{k+1}$ and $\lim_{n\to\infty} \lambda_n = 0$ in the countably infinite case, such that

$$Ax = \sum_n \lambda_n \langle x, v_n \rangle u_n \qquad \text{for all } x \in H_1 \tag{2}$$

and, in particular,

$$\overline{\mathrm{Ran}(A)} = \overline{\mathrm{span}\{u_n\}} \qquad \text{and} \qquad (\mathrm{Ker}(A))^\perp = \overline{\mathrm{span}\{v_n\}}.$$

(Conversely, if $A : H_1 \to H_2$ has this kind of decomposition, it is compact.)

The system $\{v_n, u_n, \lambda_n\}$ is called a *singular system* of A, and (2) is a *singular value decomposition* (SVD) of A. (Note that $1 \leq n \leq \infty$ or $1 \leq n \leq N < \infty$ depending on $\mathrm{rank}(A) := \dim(\mathrm{Ran}(A))$.)

Solvability of $Ax = y$

It follows from the orthonormality of $\{u_n\}$ that

$$P : H_2 \to \overline{\mathrm{Ran}(A)}, \quad y \mapsto \sum_n \langle y, u_n \rangle u_n,$$

is an orthogonal projection, i.e., $P^2 = P$ and $\mathrm{Ran}(P) \perp \mathrm{Ran}(I - P)$.

The equation $Ax = y$ has a solution *if and only if*

$$y = Py \qquad \text{and} \qquad \sum_n \frac{1}{\lambda_n^2} |\langle y, u_n \rangle|^2 < \infty. \tag{3}$$

In case that (3) is satisfied, all solutions of $Ax = y$ are of the form

$$x = x_0 + \sum_n \frac{1}{\lambda_n} \langle y, u_n \rangle v_n$$

for some $x_0 \in \mathrm{Ker}(A)$.

Intuitive interpretation of the solvability conditions:

- The first condition, $y = Py$, states that y cannot have components in the orthogonal complement of $\overline{\mathrm{Ran}(A)}$ if $y = Ax$.

- The second condition, i.e., the convergence of the series

$$\sum_n \frac{1}{\lambda_n^2} |\langle y, u_n \rangle|^2,$$

is redundant if $\mathrm{rank}(A) < \infty$, in which case $\overline{\mathrm{Ran}(A)} = \mathrm{Ran}(A)$. On the other hand, if $\mathrm{rank}(A) = \infty$, this condition is equivalent to asking that the norm of

$$x = x_0 + \sum_{n=1}^{\infty} \frac{1}{\lambda_n} \langle y, u_n \rangle v_n, \qquad x_0 \in \mathrm{Ker}(A),$$

is finite, i.e., the 'potential solutions' belong to H_1.

An example: Heat distribution in a rod (revisited)

Recall the heat equation

$$\begin{aligned} &u_t = u_{xx} && \text{in } (0,\pi)\times\mathbb{R}_+, \\ &u_x(0,\cdot) = u_x(\pi,\cdot) = 0 && \text{on } \mathbb{R}_+, \\ &u(\cdot,0) = f && \text{on } (0,\pi). \end{aligned}$$

The forward solution operator

$$E_T : f \mapsto u(\cdot,T), \quad H_1 = L^2(0,\pi) \to L^2(0,\pi) = H_2$$

is characterized by

$$E_T : v_n \mapsto \lambda_n v_n,$$

where $\{v_n\}_{n=0}^\infty = \{\sqrt{\frac{1}{\pi}}\} \cup \{\sqrt{\frac{2}{\pi}}\cos(n\,\cdot)\}_{n=1}^\infty$ form an orthonormal basis of $L^2(0,\pi)$, and $\lambda_n = \lambda_n(T) = e^{-n^2 T} > 0$ converges to zero as $n \to \infty$.

In consequence, we have

$$E_T f = \sum_{n=0}^{\infty} \lambda_n \langle f, v_n \rangle v_n,$$

where the inner product of $L^2(0,\pi)$ is defined in the usual way:

$$\langle f, g \rangle = \int_0^{\pi} f g \, dx, \qquad f, g \in L^2(0,\pi).$$

In this case $u_n = v_n$ (because E_T is self-adjoint). Since $\{v_n\}_{n=0}^{\infty}$ are an orthonormal basis for $L^2(0,\pi)$, we have

$$(\mathrm{Ker}(E_T))^{\perp} = \overline{\mathrm{Ran}(E_T)} = L^2(0,\pi),$$

i.e., E_T is injective and has a dense range, as mentioned already earlier. In particular, the projection onto the closure of the range of E_T is the identity operator, i.e., $P = I$.

We thus deduce that there exists $f \in L^2(0,\pi)$ such that

$$E_T f = w,$$

for a given $w \in L^2(0,\pi)$, if and only if

$$\sum_{n=0}^{\infty} \frac{1}{\lambda_n^2} |\langle w, v_n \rangle|^2 = \sum_{n=0}^{\infty} e^{2n^2 T} |\langle w, v_n \rangle|^2 < \infty,$$

which is a very restrictive condition and demonstrates why this inverse problem is extremely ill-posed.