Condition Numbers and Inverse Problems

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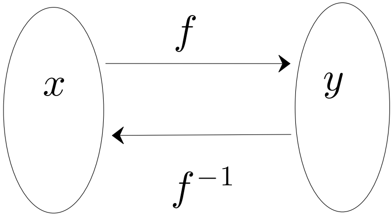
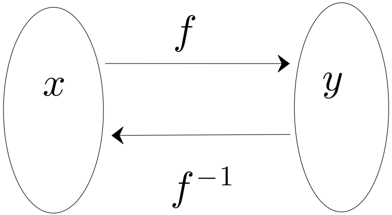
Inverse Problems vs Forward Problems



input for f $\longrightarrow$ output

output $\longleftarrow$ (approximate or incomplete) input for f^{-1}

Inverse Problems vs Forward Problems



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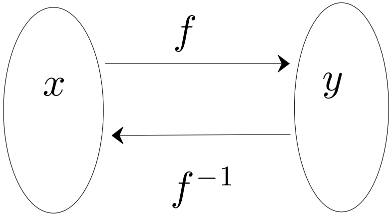
Inverse problems are typically ill-conditioned.

Inverse Problems vs Forward Problems



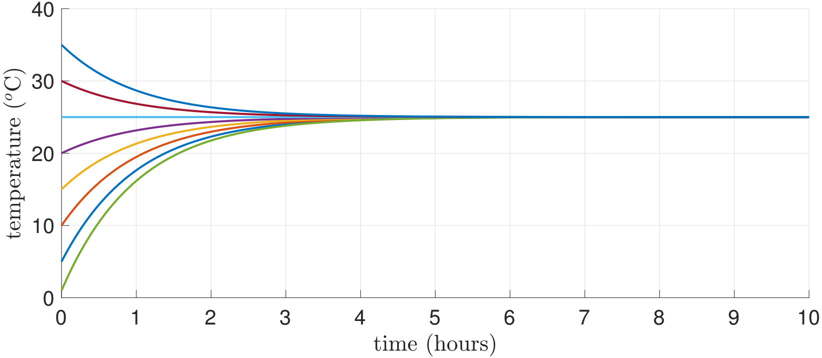
input for f $\longrightarrow$ output

output $\longleftarrow$ (approximate or incomplete) input for f^{-1}

Inverse problems are typically ill-conditioned.
Therefore, further regularization is usually required!

Inverse Problems vs Forward Problems: Example

Forward problem: given $T(0)$, find $T(t^*)$.
Inverse problem: given $T(t^*)$, find $T(0)$.



Consider the mapping A which takes the solution f to output data g. $Af = g$. Inverse problem: find f given g and A.

Definition (well-posed)

The problem of finding f from g is called well-posed (Hadamard, 1923) if all

- Existence - a solution exists for any data g in data space
- Uniqueness - the solution is unique
- Stability - continuous dependence of f on g: the inverse mapping $g \to f$ is continuous

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The first two conditions are equivalent to saying that the operator A has a well defined inverse A^{-1}.
Moreover, we require that the domain of A^{-1} is all of data space.

Ill-posed problem

Definition (Ill-Posed: according to Hadamard)

A problem is ill-posed if it does not satisfy all three conditions for well-posedness. Alternatively an ill-posed problem is one in which

1. $g \notin \text{range}(A)$
2. inverse is not unique because more than one image is mapped to the same data, or
3. an ~~arbitrarily~~ small change in the data can cause an ~~arbitrarily~~ large change in the image.

(Relative) Condition Numbers (scalar case)

Main idea:

Rel variation in the output $\approx \kappa(x)$(Rel perturbation in the input)

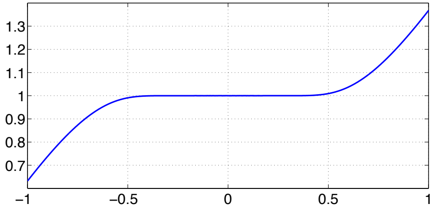
Definition: Forward problem:

$$\kappa(x) = \lim_{\epsilon \to 0} \sup_{|\delta x| \le \epsilon} \left| \frac{\frac{f(x+\delta x) - f(x)}{f(x)}}{\frac{\delta x}{x}} \right| = \left| \frac{x f'(x)}{f(x)} \right|$$

Inverse problem: $\kappa(y) = |y/(g(y) f'(g(y))|$

A simple example (scalar)

Let $f(x) = x\exp(-1/x^2) + 1$. Find x such that $1 = f(x)$.

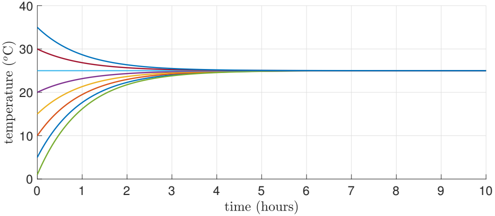


Forward problem:

$$\kappa(x) = \left|\frac{xf'(x)}{f(x)}\right|$$

Inverse problem: $\kappa(y) \approx |y/(g(y)f'(g(y))|$ $\qquad (\kappa(1) = \infty)$

Another example (scalar)



Model: $T(t) = 25(1 - e^{-\alpha t}) + T(0)e^{-\alpha t}$

Condition number of the forward problem:

$$T'(t) = (25 - T(0))\alpha e^{-\alpha t}$$

$$k(t) = |t(25 - T(0))\alpha e^{-\alpha t}|/|25(1 - e^{-\alpha t}) + T(0)e^{-\alpha t}|$$

Condition number of the inverse problem:

$$T(0) = T(t^*)e^{\alpha t^*} - 25(e^{\alpha t^*} - 1)$$

$$\kappa_0 = \left| \frac{T(t^*)e^{\alpha t^*}}{T(0)} \right|$$

Matrix condition number

Let A be an $n \times n$ matrix, then

$$\kappa(A) = \|A\| \|A^{-1}\|$$

if A is invertible and $\kappa(A) = \infty$ otherwise.

If the errors are measured with the 2-norm, then

$$\kappa(A) = \sigma_1/\sigma_n,$$

where $\{\sigma_k\}$ are the singular values of A.

A simple example (discrete)

Consider the linear system

$$A = \begin{bmatrix} 0.16 & 0.10 \\ 0.17 & 0.11 \\ 2.02 & 1.29 \end{bmatrix}, \quad b = \begin{bmatrix} 0.26 \\ 0.28 \\ 3.31 \end{bmatrix}, \quad x = \begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

The least squares solution yields

$$x_{ls} = [1, 1]^T, \ \|Ax_{ls} - b\|^2 = 0, \ \|x - x_{ls}\|^2 = 0$$

Perturbing b by $\delta b = [.01, .01, .001]^T$ gives

$$x'_{ls} = [1.6857, -0.0718]^T, \ \|Ax'_{ls} - b\|^2 = 0.0018, \ \|x - x'_{ls}\|^2 = 1.6189$$

- A small residual does not imply a realistic solution
- Ill-conditioning of A leads to a poor solution ($\kappa(A) = \|A\| \|A^\dagger\|$)
- Perturbing b leads to a larger perturbation in x.

A PDE example (diffusion equation)

$$u_t = u_{xx}, \quad (t, x) \in (0, \infty) \times (-1, 1)$$

$$u(t, -1) = u(t, 1) = 0, \;\; u(0, x) = u_0(x)$$

Forward problem: given u_0 find $u(t, x)$ for some $t > 0$.

Backward problem: given $u(T, x)$ find u_0.

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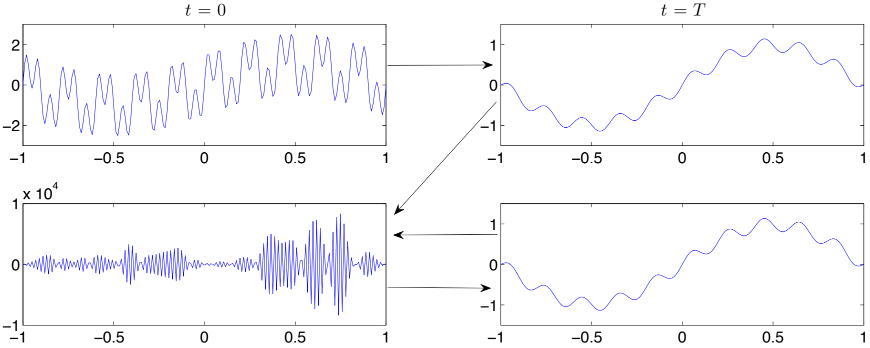

Heat equation - Fourier expansion

$$u_t = u_{xx}, \quad (t, x) \in (0, \infty) \times (-\pi, \pi)$$

$$u(t, -\pi) = u(t, \pi), \;\; u_x(t, -\pi) = u_x(t, \pi) \;\; u(0, x) = u_0(x)$$

Let

$$u(t, x) \approx \sum_{k=-N}^{N} \hat{u}_k(t) \exp(ikx)$$

Then

$$u_t(t, x) \approx \sum_{k=-N}^{N} \hat{u}_k'(t) \exp(ikx) \quad \text{and} \quad u_{xx}(t, x) \approx \sum_{k=-N}^{N} -k^2 \hat{u}_k(t) \exp(ik$$

Therefore, $\hat{u}_k'(t) = -k^2 \hat{u}_k(t)$ and $\hat{u}_k(t) = \exp(-k^2 t)\hat{u}_k(0)$,

$$u(t, x) \approx \sum_{k=-N}^{N} \exp(-k^2 t)\hat{u}_k(0) \exp(ikx)$$

Heat equation - Fourier expansion (inverse problem)

Now suppose that we want to recover $u(0,x)$ from $u(T,x)$.
Then $\hat{u}_k(T) = \exp(-k^2 T)\hat{u}_k(0)$ gives

$$\hat{u}_k(0) = \exp(k^2 T)\hat{u}_k(T).$$

And

$$u(0,x) \approx \sum_{k=-N}^{N} \exp(k^2 T)\hat{u}_k(T)\exp(ikx).$$

Heat equation - Fourier expansion (inverse problem)

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And

$$u(0, x) \approx \sum_{k=-N}^{N} \exp(k^2 T)\hat{u}_k(T)\exp(ikx).$$

In the presence of noise,

$$\begin{aligned} u_{recovered}(0, x) &= \sum_{k=-N}^{N} \exp(k^2 T)(\hat{u}_k(T) + \eta_k))\exp(ikx) \\ &= u(0, x) + \sum_{k=-N}^{N} \exp(k^2 T)\eta_k \exp(ikx) \end{aligned}$$

Noise in highest modes are amplified first (exponentially).

Blurring/deblurring of images

original

blurred

We consider the linear problem $Ax \approx b$.
Existence: (possible fix) Least squares $A^T Ax = A^T b$ (overdetermined or underdetermined).

Uniqueness and stability:

Tikhonov regularization, named after Andrey Tikhonov (1906-1993), has been on of the most commonly used methods of regularization of ill-conditioned problems.

Tikhonov regularization

One Introduces a regularization parameter $\alpha > 0$ in such a way that small α gives us a problem that is "close" to the original. The problem now is to minimize the functional:

$$J_\alpha(x) = \|b - Ax\|^2 + \alpha\|x\|^2,$$

or more generally

$$J_B(x) = \|b - Ax\|^2 + \|Bx\|^2.$$

The solution is given by the linear system $(A^T A + B^T B)x = A^T b$.

B can be a differential operator and $\|Bx\|$ an approximation to a Sobolev norm.

Tikhonov regularization

Numerically, the best way to minimize

$$J_B(x) = \|b - Ax\|^2 + \|Bx\|_2^2.$$

is to solve the concatenated least-squares problem,

$$J_B(x) = \left\| \begin{bmatrix} A \\ B \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_2^2.$$

- For small problems, a QR factorization of $\begin{bmatrix} A \\ B \end{bmatrix}$ works well.
- For large (sparse) problems, iterative algorithms can be used.
  - LSQR or LSMR (Paige and Saunders) (click here)

Choice of regularization parameter α

This is one of the main topics in the are of inverse problems. The optimal regularization parameter α is usually unknown and often in practical problems is determined by an ad hoc method. Approaches include the discrepancy principle, (leave-one-out) cross-validation, L-curve method, restricted maximum likelihood, unbiased predictive risk estimator, etc .

Morozov's discrepancy principle (MDP)

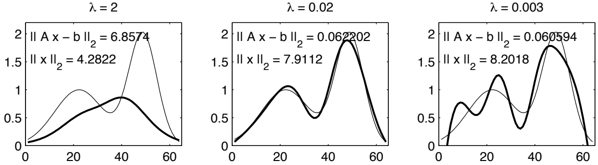
A-priori: $\alpha(\delta b) \sim \delta b$

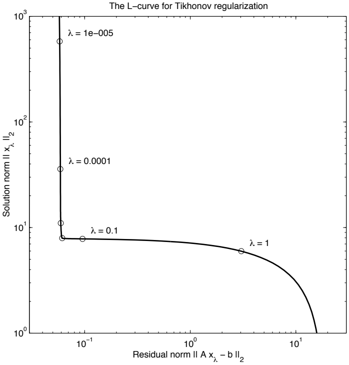
More specifically:

In this principle, α is chosen as the solution of the equation

$$\|Ax_\alpha^\delta - b^\delta\| = C\delta b, \text{ with } C \geq 1.$$

Choice of regularization parameter α (L-curve mehod)





(graphs by P.C. Hansen - click here)

Regularization by SVD filtering

Example

$$u_t = u_{xx}, \quad -\infty \leq x \leq \infty \quad u(0,x) = f(x), \quad f \in L_2(-\infty,\infty)$$

$$u(x,t) = \frac{1}{2\sqrt{t\pi}} \int_{-\infty}^{\infty} e^{-(x-\tau)^2/(4t)} f(\tau) d\tau$$

Fredholm first kind integral equation

$$g(x) = \int_a^b k(x,\tau) f(\tau) d\tau, \quad a < x, \tau < b$$

For image deblurring, typically $k(x,\tau) = k(x-\tau)$

- Gaussian $k(x) = \frac{1}{\sigma\sqrt{2\pi}} \exp(-x^2/(2\sigma^2)), \ \sigma > 0$.
- Out of focus: $k(x) = \begin{cases} C, & x_1 \leq x \leq x_2 \\ 0, & \text{otherwise} \end{cases}$

SVD decomposition and filtering

$$b = Ax_{true} + \eta$$
$$\delta := \|\eta\|$$
$$A = U\Sigma V^T \quad \text{invertible}$$
$$A^{-1}b = V\Sigma^{-1}U^T b = x_{true} + \sum_{i=1}^{n} \sigma_i^{-1}(u_i^T\eta)v_i$$

Remark: Instability arises due to division by small singular values.

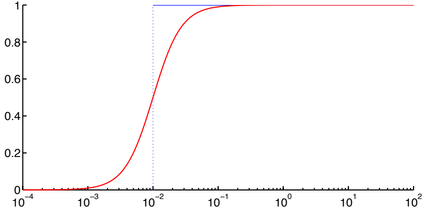
Filter: Multiply σ_i^{-1} by a regularizing filter function $w_\alpha(\sigma_i^2)$ for which

$$w_\alpha(\sigma^2)\sigma^{-1} \to 0 \;\text{ as }\; \sigma \to 0.$$

Regularized Solution

$$x_\alpha = \sum_{i=1}^{n} w_\alpha(\sigma_i^2)\sigma_i^{-1}(u_i^T b)v_i.$$

SVD decomposition and filtering



SVD truncation:

$$w_\alpha(\sigma^2) = \begin{cases} 1, & \sigma^2 > \alpha \\ 0, & \text{otherwise} \end{cases}$$

Tikhonov filter: (equivalent to regularization $\alpha\|x\|$)

$$w_\alpha(\sigma^2) = \frac{\sigma^2}{\sigma^2 + \alpha}$$

Remark: This can be derived more generally for compact operators.

References

- Prof. Renaut slides:
  http://math.la.asu.edu/ rosie/classes/index.html
- Computational Methods for Inverse Problem, Vogel, SIAM 2002. http://www.math.montana.edu/ vogel/Book/
- Rank Deficient and Discrete Ill-Posed Inverse Problems, Hansen, SIAM 1997
  http://www2.imm.dtu.dk/ pch/Regutools/