Optimization for the information and data sciences

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Approximation and fitting

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Approximation and fitting

- norm approximation
- least-norm problems
- regularized approximation
- robust approximation

Norm approximation

$$\text{minimize} \quad \|Ax - b\|$$

($A \in \mathbb{R}^{m\times n}$ with $m \geq n$, $\|\cdot\|$ is a norm on $\mathbb{R}^m$)

interpretations of solution $x^\star = \arg\min_x \|Ax - b\|$:

- **geometric**: $Ax^\star$ is point in $\mathcal{R}(A)$ closest to b
- **estimation**: linear measurement model

  $$y = Ax + v$$

  y are measurements, x is unknown, v is measurement error
  given $y = b$, best guess of x is $x^\star$
- **optimal design**: x are design variables (input), Ax is result (output)
  $x^\star$ is design that best approximates desired result b

examples

- least-squares approximation ($\|\cdot\|_2$): solution satisfies normal equations

$$A^T A x = A^T b$$

  ($x^\star = (A^T A)^{-1} A^T b$ if **rank**$A = n$)

- Chebyshev approximation ($\|\cdot\|_\infty$): can be solved as an LP

$$\begin{array}{ll} \text{minimize} & t \\ \text{subject to} & -t\mathbf{1} \preceq Ax - b \preceq t\mathbf{1} \end{array}$$

- sum of absolute residuals approximation ($\|\cdot\|_1$): can be solved as an LP

$$\begin{array}{ll} \text{minimize} & \mathbf{1}^T y \\ \text{subject to} & -y \preceq Ax - b \preceq y \end{array}$$

Penalty function approximation

$$\begin{array}{ll} \text{minimize} & \phi(r_1) + \cdots + \phi(r_m) \\ \text{subject to} & r = Ax - b \end{array}$$

($A \in \mathbb{R}^{m \times n}$, $\phi : \mathbb{R} \to \mathbb{R}$ is a convex penalty function)

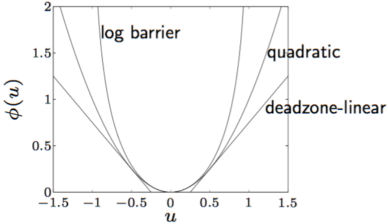
examples

- quadratic: $\phi(u) = u^2$
- deadzone-linear with width a:

$$\phi(u) = \max\{0, |u| - a\}$$

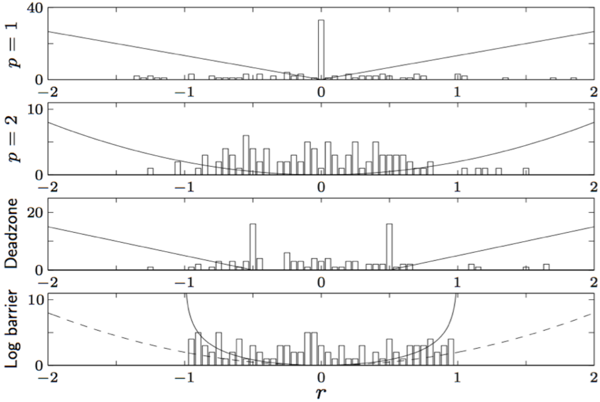
- log-barrier with limit a:

$$\phi(u) = \begin{cases} -a^2 \log(1 - (u/a)^2) & |u| < a \\ \infty & \text{otherwise} \end{cases}$$



example ($m = 100$, $n = 30$): histogram of residuals for penalties

$$\phi(u) = |u|, \quad \phi(u) = u^2, \quad \phi(u) = \max\{0, |u| - a\}, \quad \phi(u) = -\log(1 - u^2)$$

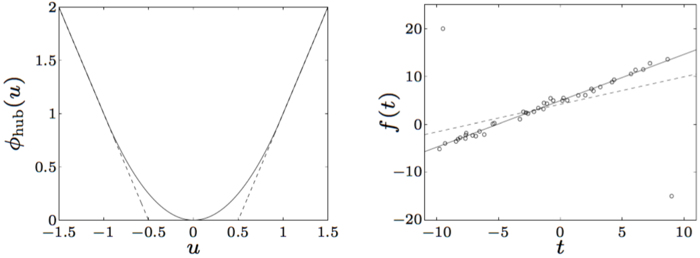


shape of penalty function has large effect on distribution of residuals

Huber penalty function (with parameter M)

$$\phi_{\mathrm{hub}}(u) = \begin{cases} u^2 & |u| \le M \\ M(2|u| - M) & |u| > M \end{cases}$$

linear growth for large u makes approximation less sensitive to outliers



- left: Huber penalty for $M = 1$
- right: affine function $f(t) = \alpha + \beta t$ fitted to 42 points t_i, y_i (circles) using quadratic (dashed) and Huber (solid) penalty

Least-norm problems

$$\begin{array}{ll} \text{minimize} & \|x\| \\ \text{subject to} & Ax = b \end{array}$$

($A \in \mathbb{R}^{m \times n}$ with $m \leq n$, $\|\cdot\|$ is a norm on $\mathbb{R}^n$)

interpretations of solution $x^\star = \arg\min_{Ax=b} \|x\|$:

- **geometric:** $x^\star$ is point in affine set $\{x \mid Ax = b\}$ with minimum distance to 0
- **estimation:** $b = Ax$ are (perfect) measurements of x; $x^\star$ is smallest ('most plausible') estimate consistent with measurements
- **design:** x are design variables (inputs); b are required results (outputs) $x^\star$ is smallest ('most efficient') design that satisfies requirements

examples

- least-squares solution of linear equations ($\|\cdot\|_2$):
  can be solved via optimality conditions

$$2x + A^T\nu = 0, \qquad Ax = b$$

- minimum sum of absolute values ($\|\cdot\|_1$): can be solved as an LP

$$\begin{array}{ll} \text{minimize} & \mathbf{1}^T y \\ \text{subject to} & -y \preceq x \preceq y, \quad Ax = b \end{array}$$

  tends to produce sparse solution $x^\star$

extension: least-penalty problem

$$\begin{array}{ll} \text{minimize} & \phi(x_1) + \cdots + \phi(x_n) \\ \text{subject to} & Ax = b \end{array}$$

$\phi : \mathbb{R} \to \mathbb{R}$ is convex penalty function

Regularized approximation

$$\text{minimize (w.r.t. } \mathbb{R}^2_+) \quad (\|Ax - b\|, \|x\|)$$

$A \in \mathbb{R}^{m \times n}$, norms on $\mathbb{R}^m$ and $\mathbb{R}^n$ can be different

interpretation: find good approximation $Ax \approx b$ with small x

- **estimation:** linear measurement model $y = Ax + v$, with prior knowledge that $\|x\|$ is small
- **optimal design**: small x is cheaper or more efficient, or the linear model $y = Ax$ is only valid for small x
- **robust approximation:** good approximation $Ax \approx b$ with small x is less sensitive to errors in A than good approximation with large x

Scalarized problem

$$\text{minimize} \quad \|Ax - b\| + \gamma\|x\|$$

- solution for $\gamma > 0$ traces out optimal trade-off curve
- other common method: minimize $\|Ax - b\|^2 + \delta\|x\|^2$ with $\delta > 0$

Tikhonov regularization

$$\text{minimize} \quad \|Ax - b\|_2^2 + \delta\|x\|_2^2$$

can be solved as a least-squares problem

$$\text{minimize} \quad \left\| \begin{bmatrix} A \\ \sqrt{\delta} I \end{bmatrix} x - \begin{bmatrix} b \\ 0 \end{bmatrix} \right\|_2^2$$

solution $x^\star = (A^T A + \delta I)^{-1} A^T b$

Optimal input design

linear dynamical system with impulse response h:

$$y(t) = \sum_{\tau=0}^{t} h(\tau)u(t-\tau), \quad t = 0, 1, \ldots, N$$

input design problem: multicriterion problem with 3 objectives

1. tracking error with desired output y_{des}: $J_{\text{track}} = \sum_{t=0}^{N}(y(t) - y_{\text{des}}(t))^2$
2. input magnitude: $J_{\text{mag}} = \sum_{t=0}^{N} u(t)^2$
3. input variation: $J_{\text{der}} = \sum_{t=0}^{N-1}(u(t+1) - u(t))^2$

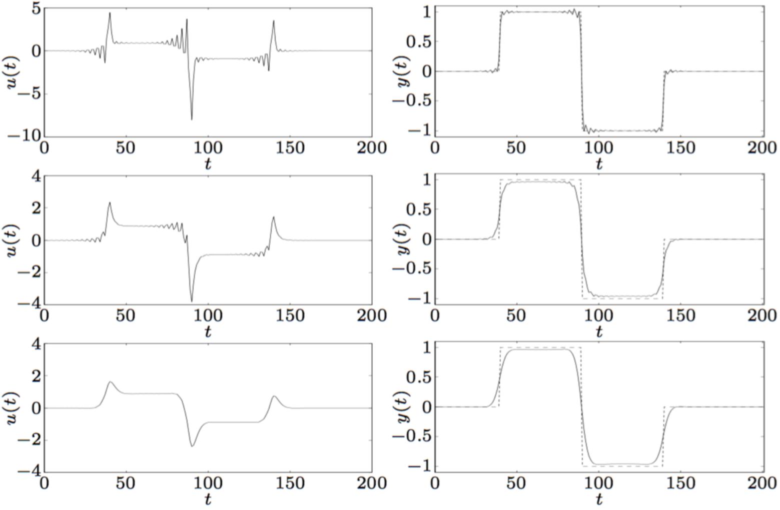
track desired output using a small and slowly varying input signal

regularized least-squares formulation

$$\text{minimize} \quad J_{\text{track}} + \delta J_{\text{der}} + \eta J_{\text{mag}}$$

for fixed δ, η, a least-squares problem in $u(0), \ldots, u(N)$

example: 3 solutions on optimal trade-off surface
(top) $\delta = 0$, small η; (middle) $\delta = 0$, larger η; (bottom) large δ



Signal reconstruction

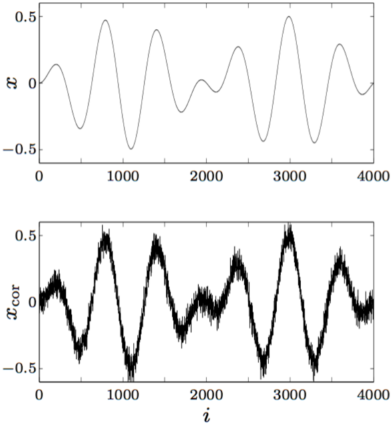
$$\text{minimize (w.r.t. } \mathbb{R}^2_+) \quad (\|\hat{x} - x_{\text{cor}}\|_2, \phi(\hat{x}))$$

- $x \in \mathbb{R}^n$ is unknown signal
- $x_{\text{cor}} = x + v$ is (known) corrupted version of x, with additive noise v
- variable $\hat{x}$ (reconstructed signal) is estimate of x
- $\phi : \mathbb{R}^n \to \mathbb{R}$ is regularization function or smoothing objective

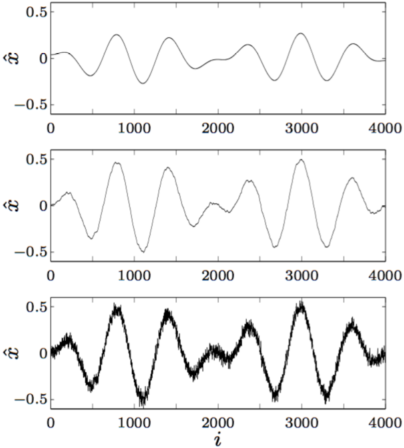
examples: quadratic smoothing, total variation smoothing:

$$\phi_{\text{quad}}(\hat{x}) = \sum_{i=1}^{n-1} (\hat{x}_{i+1} - \hat{x}_i)^2, \qquad \phi_{\text{tv}}(\hat{x}) = \sum_{i=1}^{n-1} |\hat{x}_{i+1} - \hat{x}_i|$$

quadratic smoothing example

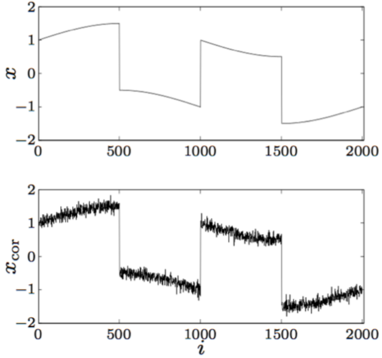


original signal x and noisy signal x_{cor}

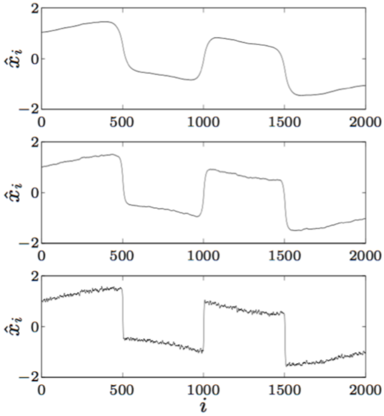


three solutions on trade-off curve $\|\hat{x} - x_{\text{cor}}\|_2$ versus $\phi_{\text{quad}}(\hat{x})$

total variation reconstruction example

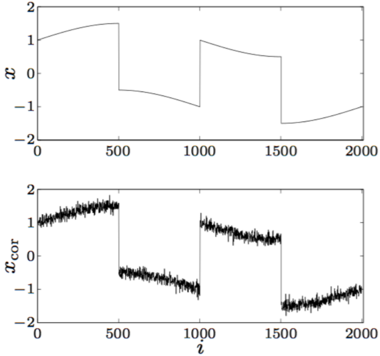


original signal x and noisy signal x_{cor}

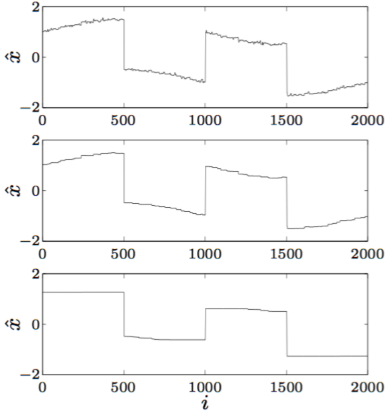


three solutions on trade-off curve $\|\hat{x} - x_{\mathrm{cor}}\|_2$ versus $\phi_{\mathrm{quad}}(\hat{x})$

quadratic smoothing smooths out noise **and** sharp transitions in signal



original signal x and noisy signal x_{cor}



three solutions on trade-off curve $\|\hat{x} - x_{\mathrm{cor}}\|_2$ versus $\phi_{\mathrm{tv}}(\hat{x})$

total variation smoothing preserves sharp transitions in signal

Robust approximation

minimize $\|Ax - b\|$ with uncertain A
two approaches:

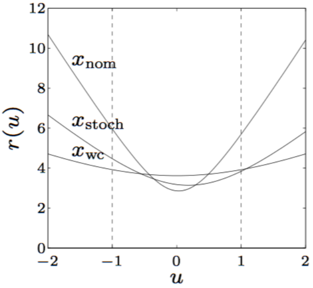
- **stochastic**: assume A is random, minimize $\mathbb{E}\|Ax - b\|$
- **worst-case:** set $\mathcal{A}$ of possible values of A, minimize $\sup_{A \in \mathcal{A}} \|Ax - b\|$

tractable only in special cases (certain norms $\|\cdot\|$, distributions, sets $\mathcal{A}$)

example: $A(u) = A_0 + uA_1$

- x_{nom} minimizes $\|A_0 x - b\|_2^2$
- x_{stoch} minimizes $\mathbb{E}\|A(u)x - b\|_2^2$
  with u uniform on $[-1, 1]$
- x_{wc} minimizes $\sup_{-1 \le u \le 1} \|A(u)x - b\|_2^2$

figure shows $r(u) = \|A(u)x - b\|_2$



stochastic robust LS with $A = \bar{A} + U$, U random, $\mathbb{E}U = 0$, $\mathbb{E}U^T U = P$

$$\text{minimize} \quad \mathbb{E}\|(\bar{A} + U)x - b\|_2^2$$

- explicit expression for objective:

$$\begin{aligned} \mathbb{E}\|Ax - b\|_2^2 &= \mathbb{E}\|\bar{A}x - b + Ux\|_2^2 \\ &= \|\bar{A}x - b\|_2^2 + \mathbb{E}x^T U^T U x \\ &= \|\bar{A}x - b\|_2^2 + x^T P x \end{aligned}$$

- hence, robust LS problem is equivalent to LS problem

$$\text{minimize} \quad \|\bar{A}x - b\|_2^2 + \|P^{1/2}x\|_2^2$$

- for $P = \delta I$, get Tikhonov regularized problem

$$\text{minimize} \quad \|\bar{A}x - b\|_2^2 + \delta\|x\|_2^2$$

worst-case robust LS with $\mathcal{A} = \{\bar{A} + u_1 A_1 + \cdots + u_p A_p \mid \|u\|_2 \leq 1\}$

$$\text{minimize} \quad \sup_{A \in \mathcal{A}} \|Ax - b\|_2^2 = \sup_{\|u\|_2 \leq 1} \|P(x)u + q(x)\|_2^2$$

where $P(x) = \begin{bmatrix} A_1 x & A_2 x & \cdots & A_p x \end{bmatrix}$, $q(x) = \bar{A}x - b$

- strong duality holds between the following problems

$$\begin{array}{ll} \text{maximize} & \|Pu + q\|_2^2 \\ \text{subject to} & \|u\|_2^2 \leq 1 \end{array} \qquad \begin{array}{ll} \text{minimize} & t + \lambda \\ \text{subject to} & \begin{bmatrix} I & P & q \\ P^T & \lambda I & 0 \\ q^T & 0 & t \end{bmatrix} \succeq 0 \end{array}$$

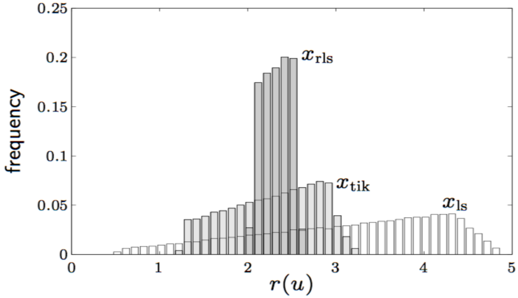
- hence, robust LS problem is equivalent to SDP

$$\begin{array}{ll} \text{minimize} & t + \lambda \\ \text{subject to} & \begin{bmatrix} I & P(x) & q(x) \\ P(x)^T & \lambda I & 0 \\ q(x)^T & 0 & t \end{bmatrix} \succeq 0 \end{array}$$

example: histogram of residuals

$$r(u) = \|(A_0 + u_1 A_1 + u_2 A_2)x - b\|_2$$

with u uniformly distributed on unit disk, for three values of x



- $x_{\rm ls}$ minimizes $\|A_0 x - b\|_2$
- $x_{\rm tik}$ minimizes $\|A_0 x - b\|_2^2 + \delta\|x\|_2^2$ (Tikhonov solution)
- $x_{\rm wc}$ minimizes $\sup_{\|u\|_2 \leq 1} \|A_0 x - b\|_2^2 + \|x\|_2^2$