06. Approximation and fitting

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minimize
$$||Ax - b||$$

 $(A \in \mathbf{R}^{m \times n} \text{ with } m \ge n)$

Interpretations of solution $x = \arg\min_{x} ||Ax - b||$:

- 1. **geometric**: Ax^* is point in $\mathcal{R}(A)$ closest to b
- 2. 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^*

- 3. Optimal design: x are design variables(input), Ax is result(output)
- x^* is design that best approximates desired result b

Examples.

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

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

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

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

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

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

minimize
$$\mathbf{1}^T y$$

subject to $-y \leq Ax - b \leq y$

Penalty function approximation.

minimize
$$\phi(r_1) + \cdots + \phi(r_m)$$

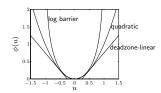
subject to $r = Ax - b$

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

Examples

- 1. quadratic: $\phi(u) = u^2$
- 2. deadzone-linear with width a: $\phi(u) = \max\{0, |u| a\}$
- 3. \log -barrier with limit a:

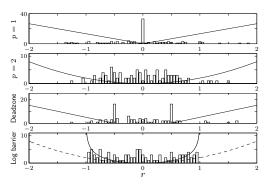
$$\phi(u) = \begin{cases} -a^2 \log(1 - (u/a)^2) & |u| < a \\ \infty & \text{otherwise} \end{cases}$$



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

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

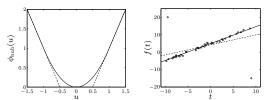
Shape of penalty function has large effect on distribution of residuals



Huber penalty function (with parameter M)

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

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

2 Least-Norm problems

minimize
$$||x||$$
 subject to $Ax = b$

 $(A \in \mathbf{R}^{m \times n} \text{ with } m \leq n)$

Interpretations of solution $x = \arg \min_{Ax=b} ||x||$:

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

2 Least-Norm problems

Examples.

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

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

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

tends to produce sparse solution x^*

extension: least-penalty problem

minimize
$$\phi(x_1) + \cdots + \phi(x_n)$$

subject to $Ax = b$

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



$$\label{eq:minimize} \mbox{ minimize (w.r.t. } \mathbf{R}_+^2) \quad (\|Ax-b\|,\|x\|)$$
 $(A \in \mathbf{R}^{m \times n})$

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

- 1. **estimation**: linear measurement model y = Ax + v, with prior knowledge that ||x|| is small
- 2. **optimal design**: small x is cheaper or more efficient, or the linear model y = Ax is only valid for small x
- 3. 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

$$\text{minimize}\quad \left\|\left[\begin{array}{c}A\\\sqrt{\delta}\mathbf{I}\end{array}\right]x-\left[\begin{array}{c}b\\0\end{array}\right]\right\|_2^2$$

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

Optimal input design

linear dynamical system with impulse response h:

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

Input design problem: multicriterion problem with 3 objectives

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

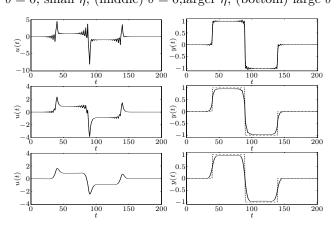
track desired output using a small and slowly varying input signal regularized least-squares formulation

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

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



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



Signal reconstruction

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

 $x \in \mathbf{R}^n$ is unknown signal

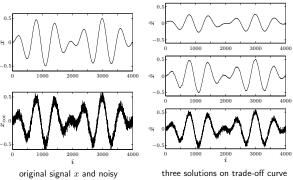
 $x_{\text{cor}} = x + v$ is (known) corrupted version of x, with additive noise v

variable $\hat{\boldsymbol{x}}$ (reconstructed signal) is estimate of \boldsymbol{x}

 $\phi : \mathbf{R}^n \to \mathbf{R}$ is regularization function or smoothing objective **examples**: quadratic smoothing, total variation smoothing:

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

quadratic smoothing example

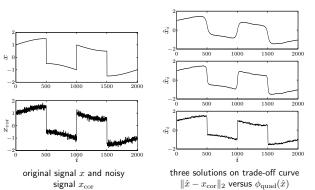


signal x_{cor}

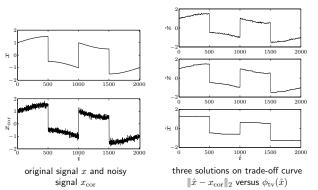
 $\|\hat{x} - x_{cor}\|_2$ versus $\phi_{quad}(\hat{x})$

total variation reconstruction example

quadratic smoothing smooths out noise and sharp transitions in signal



total variation smoothing preserves sharp transitions in signal

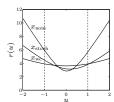


minimize ||Ax-b|| with uncertain A two approaches:

- 1. stochastic: assume A is random, minimize $\mathbf{E} ||Ax-b||$
- 2. worst-case: set \mathcal{A} of possible values of A, minimize $\sup_{A \in A} \|Ax b\|$ tractable only in special cases (certain norms $\|\cdot\|$, distributions, sets \mathcal{A})

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

- 1. x_{norm} minimizes $||A_0x b||_2^2$
- 2. x_{stoch} minimizes $\mathbf{E} ||A(u)x b||_2^2$ with u uniform on [-1, 1]
- 3. 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, $\mathbf{E}\,U=0,\ \mathbf{E}\,U^T\,U=P$

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

1. explicit expression for objective:

$$\mathbf{E} ||Ax - b||_{2}^{2} = \mathbf{E} ||\bar{A}x - b + Ux||_{2}^{2}$$

$$= ||\bar{A}x - b||_{2}^{2} + \mathbf{E}x^{T}U^{T}Ux$$

$$= ||\bar{A}x - b||_{2}^{2} + \mathbf{E}x^{T}px$$

2.hence, robust LS problem is equivalent to LS problem

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

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

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



worst-case robust LS with
$$A = \{\bar{A} + u_1 A_1 + \dots + u_p A_p | \|u\|_2 \le 1\}$$

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

where $P(x) = [A_1 x \ A_2 x \cdots A_p x], q(x) = Ax - b$

1. strong duality holds between the following problems

minimize
$$\|Pu+q\|_2^2$$
 subject to $\|u\|_2^2 \le 1$

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

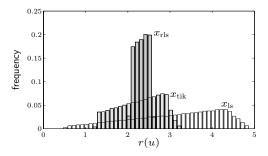
2. hence, robust LS problem is equivalent to SDP

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

example

$$r(u) = ||(A_0 + u_1A_1 + u_2A_2)x - b||2$$

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



- 1. x_{ls} minimizes $||A_0x-b||_2$
- 2. x_{tik} minimizes $||A_0x-b||_2^2 + \delta ||x||_2^2$ (Tikhonov solution)
- 3. x_{wc} minimizes $\sup_{\|u\|_2 < 1} \|A_0 x b\|_2^2 + \|x\|_2^2$