

6. Approximation and fitting

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

Norm approximation

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

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

Interpretations of solution $x^\star = \operatorname{argmin}_x \|Ax - b\|$

- 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

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

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

- 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

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

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

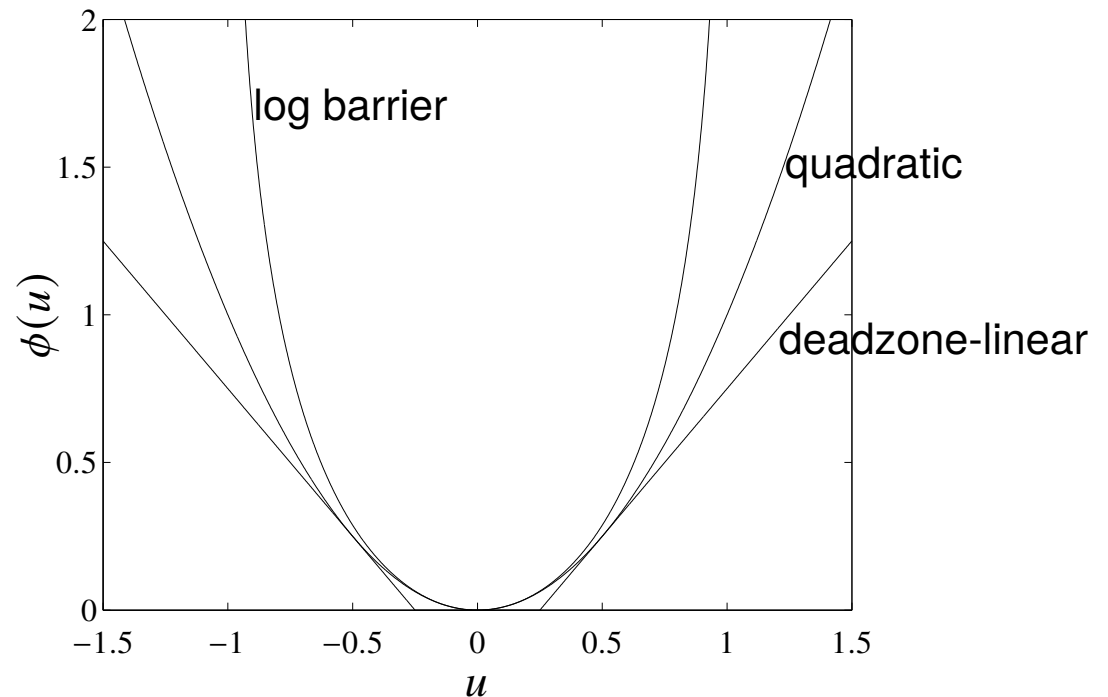
Examples

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

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

- log-barrier with limit a :

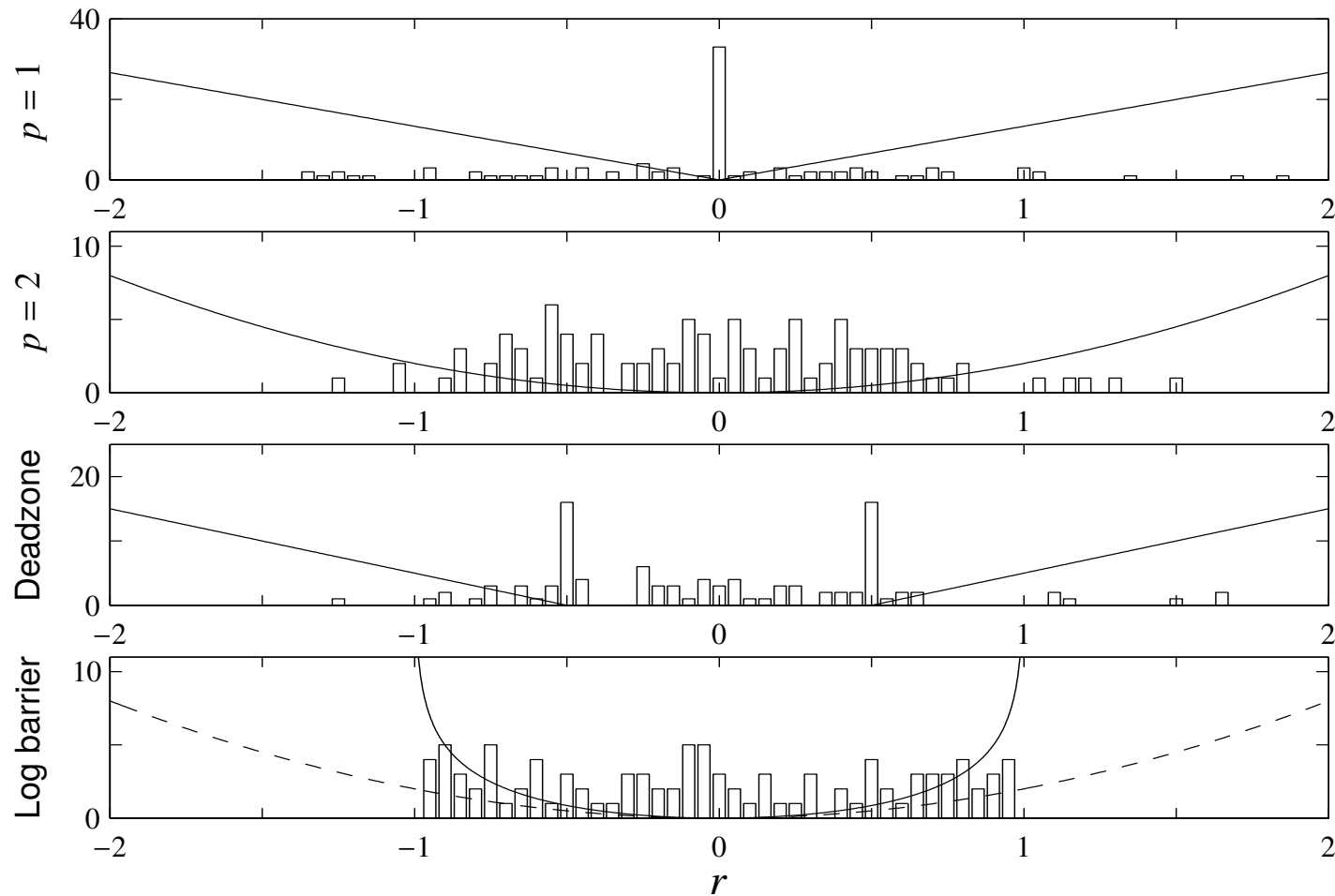
$$\phi(u) = \begin{cases} -a^2 \log(1 - (u/a)^2) & |u| < a \\ \infty & \text{otherwise} \end{cases}$$



Comparison

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

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



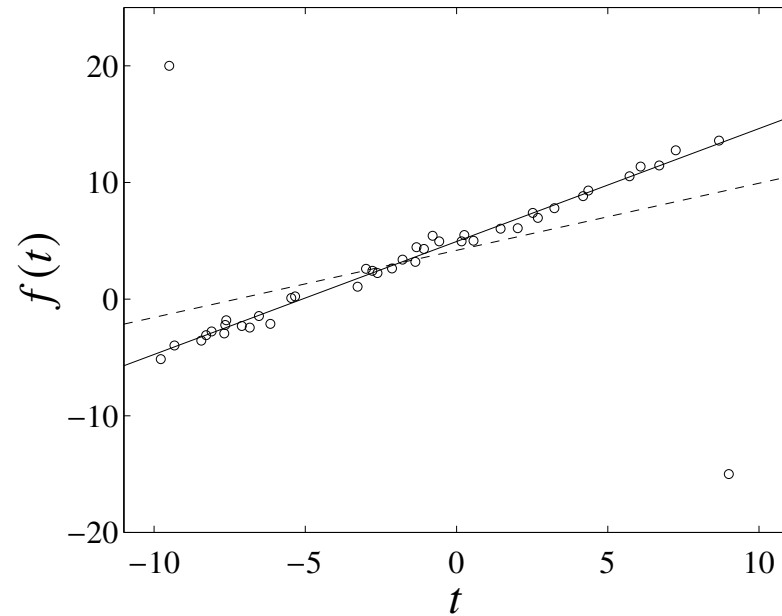
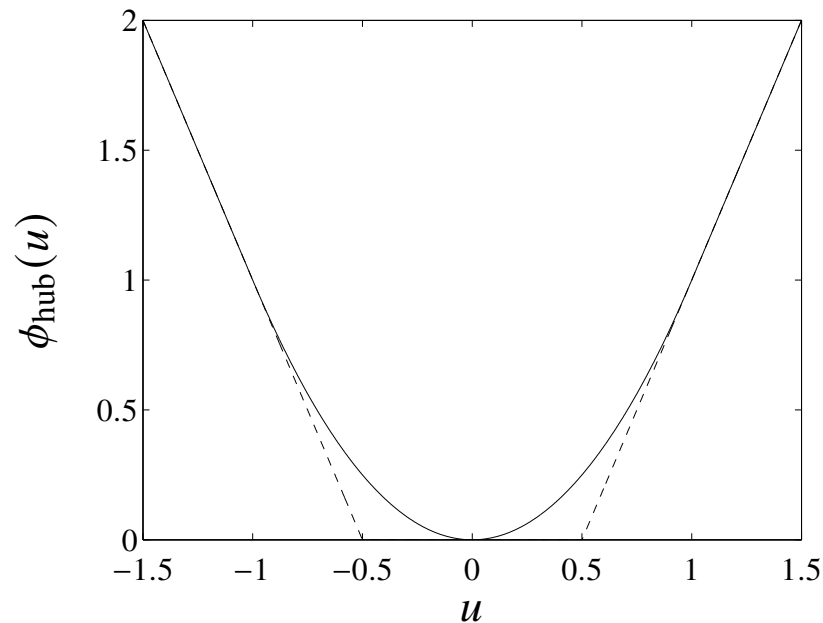
shape of penalty function has large effect on distribution of residuals

Huber penalty

Huber penalty function (with parameter M)

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

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

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

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

Interpretations of solution $x^\star = \operatorname{argmin}_{Ax=b} \|x\|$

- 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

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

- 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

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

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

Regularized approximation

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

$A \in \mathbf{R}^{m \times n}$, norms on \mathbf{R}^m and \mathbf{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

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

- 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

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

can be solved as a least-squares problem

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

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

Optimal input design

Linear dynamical system with impulse response h :

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

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

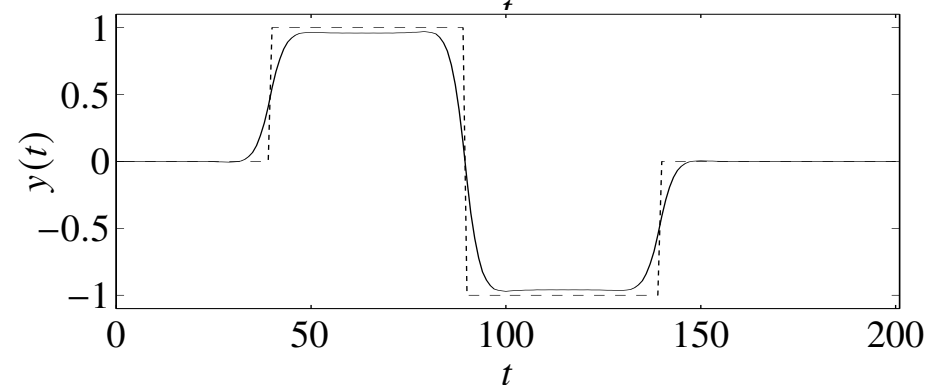
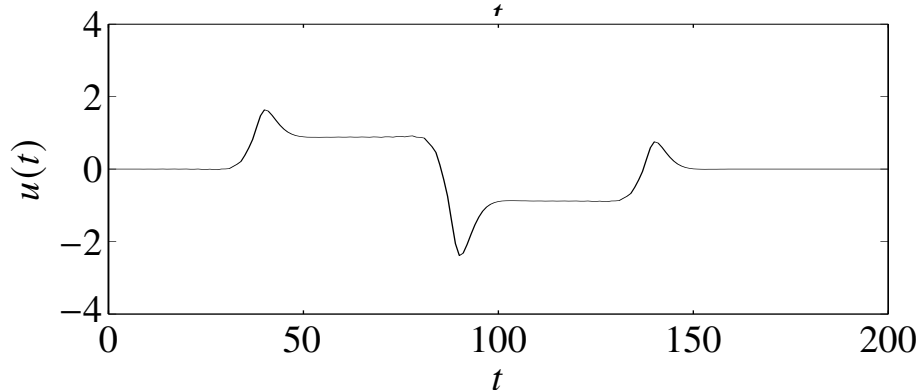
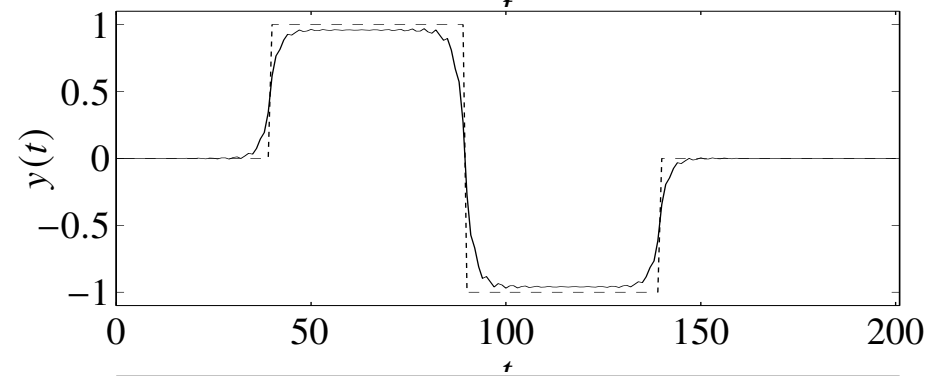
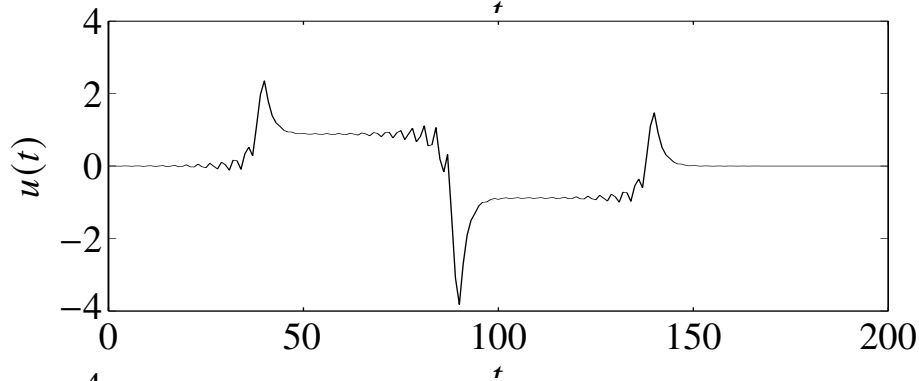
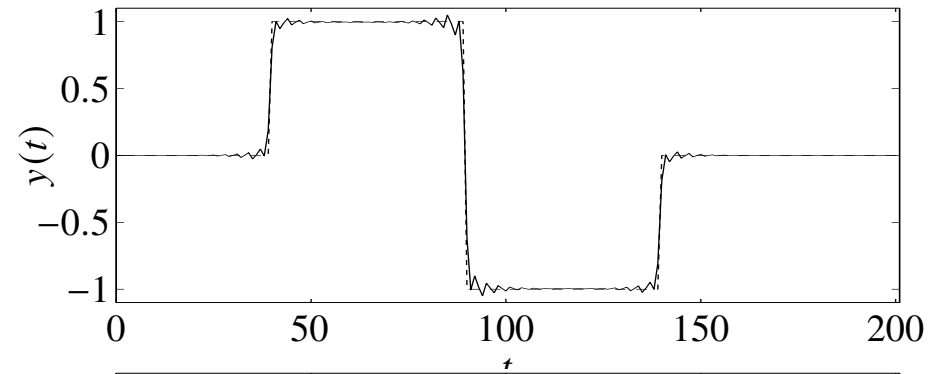
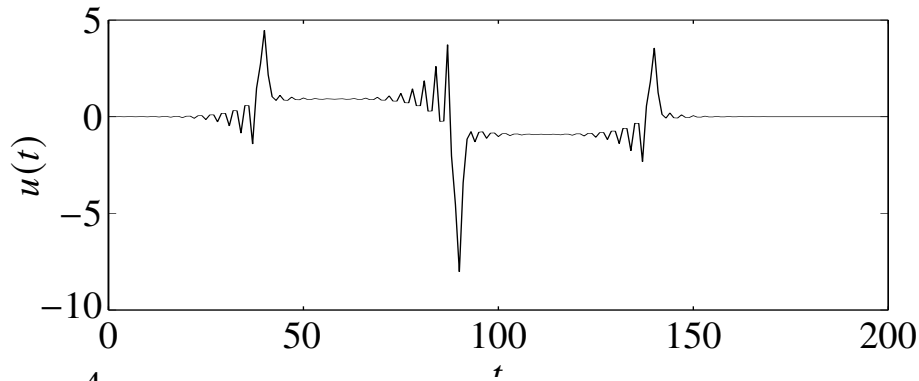
$$\text{minimize} \quad J_{\text{track}} + \delta J_{\text{der}} + \eta J_{\text{mag}}$$

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

Example

3 solutions on optimal trade-off surface

(top) $\delta = 0$, small η ; (middle) $\delta = 0$, larger η ; (bottom) large δ



Signal reconstruction

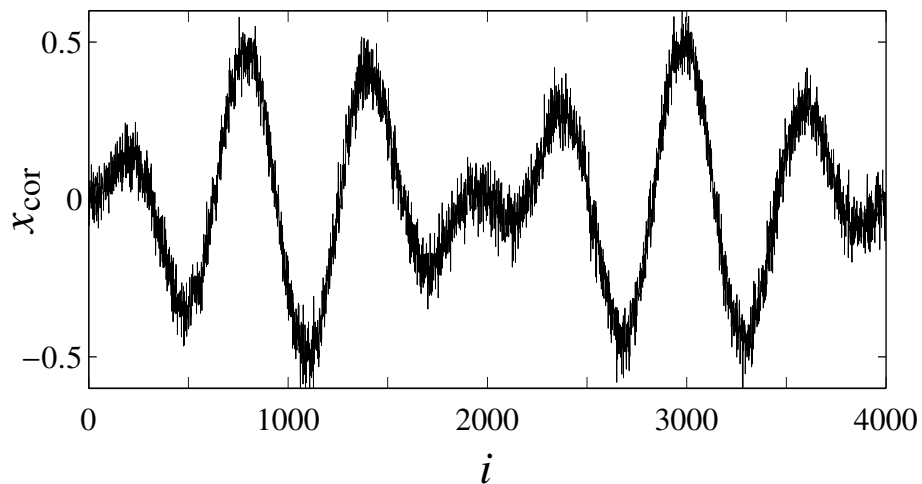
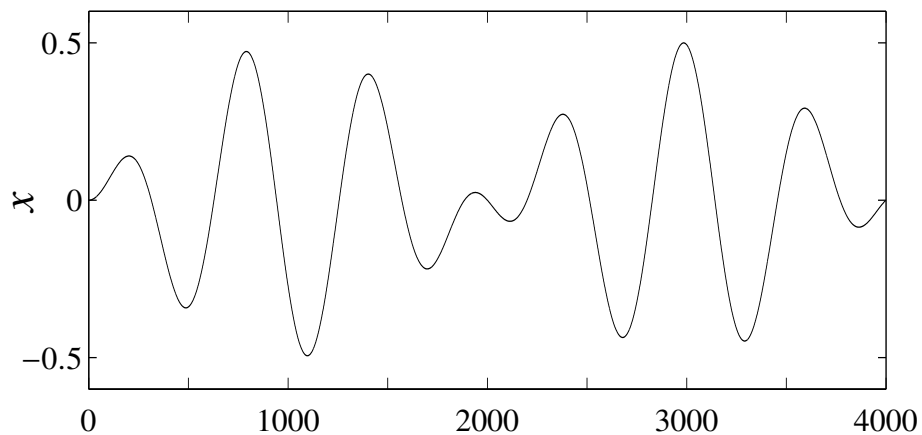
minimize (w.r.t. \mathbf{R}_+^2) $(\|\hat{x} - x_{\text{cor}}\|_2, \phi(\hat{x}))$

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

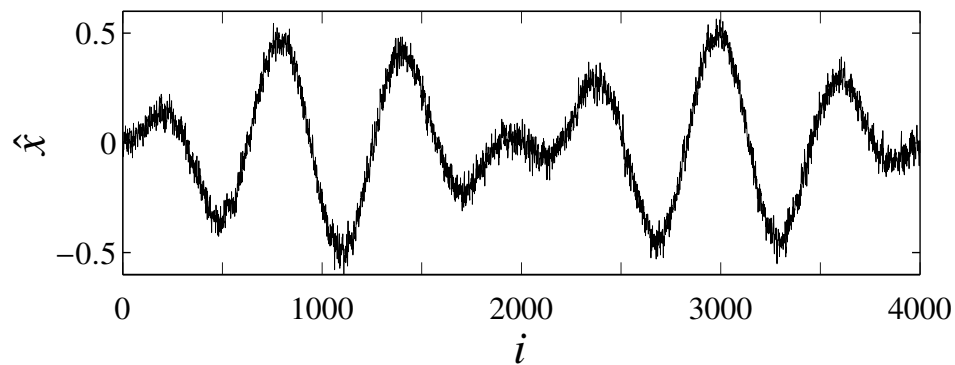
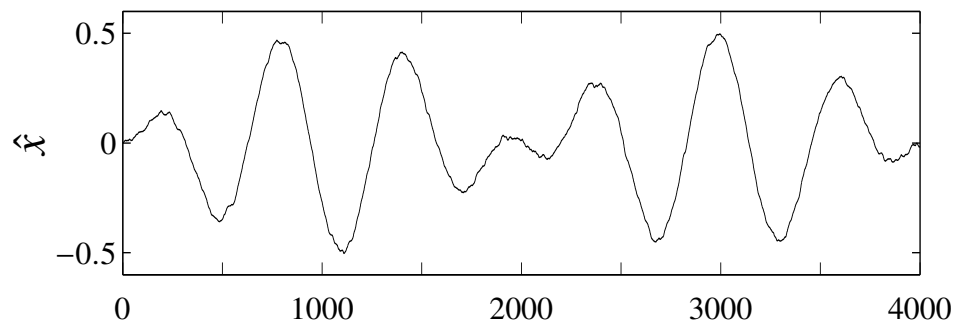
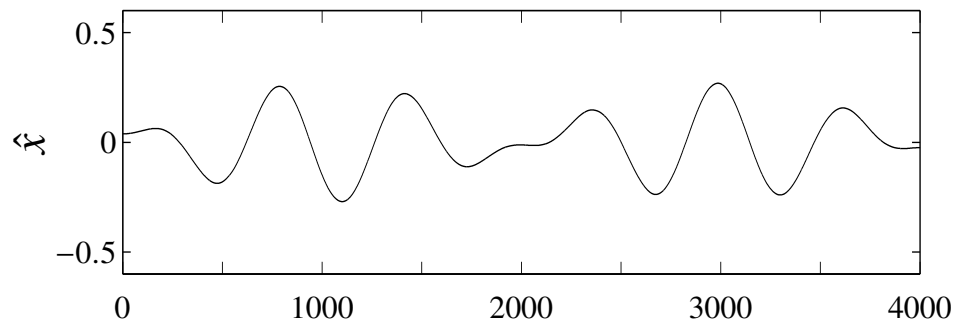
Examples: quadratic smoothing, total variation smoothing:

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

Quadratic smoothing example

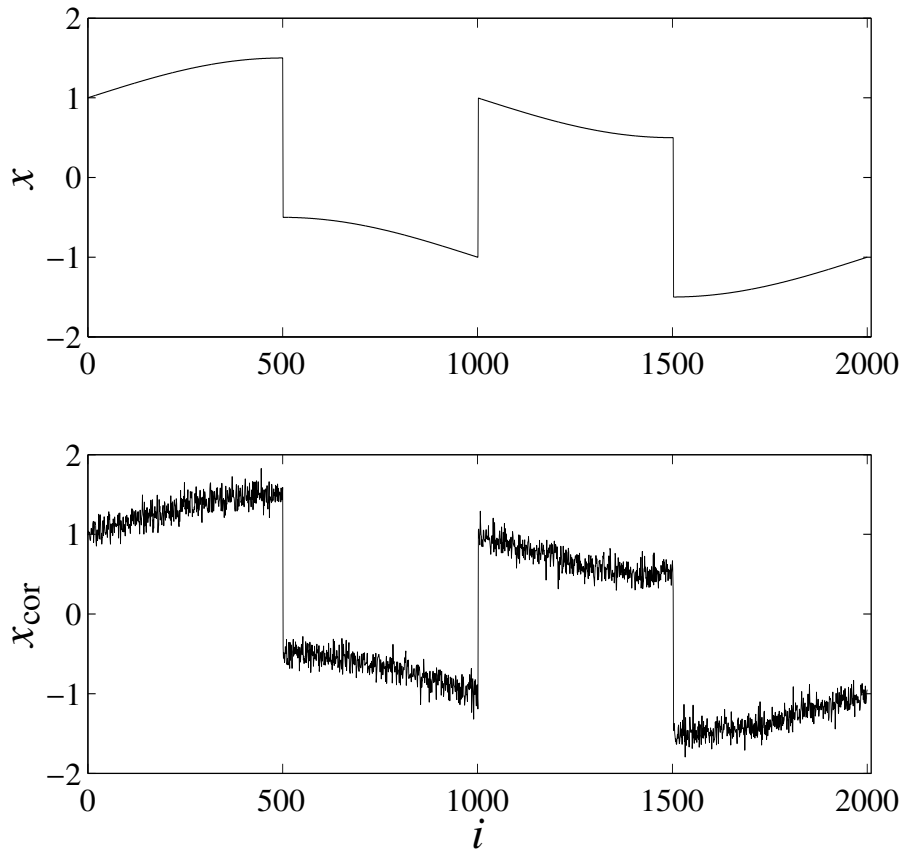


original signal x and noisy signal x_{cor}



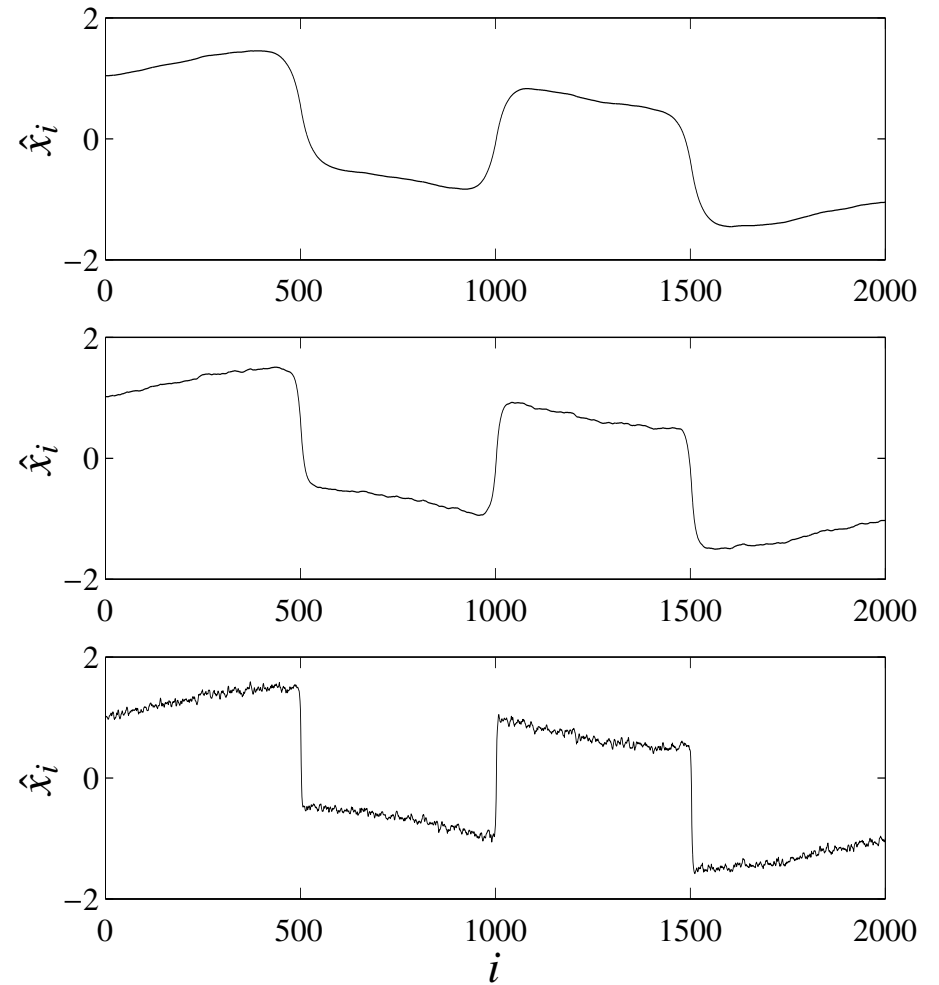
three solutions on trade-off curve
 $\|\hat{x} - x_{\text{cor}}\|_2$ versus $\phi_{\text{quad}}(\hat{x})$

Total variation reconstruction example

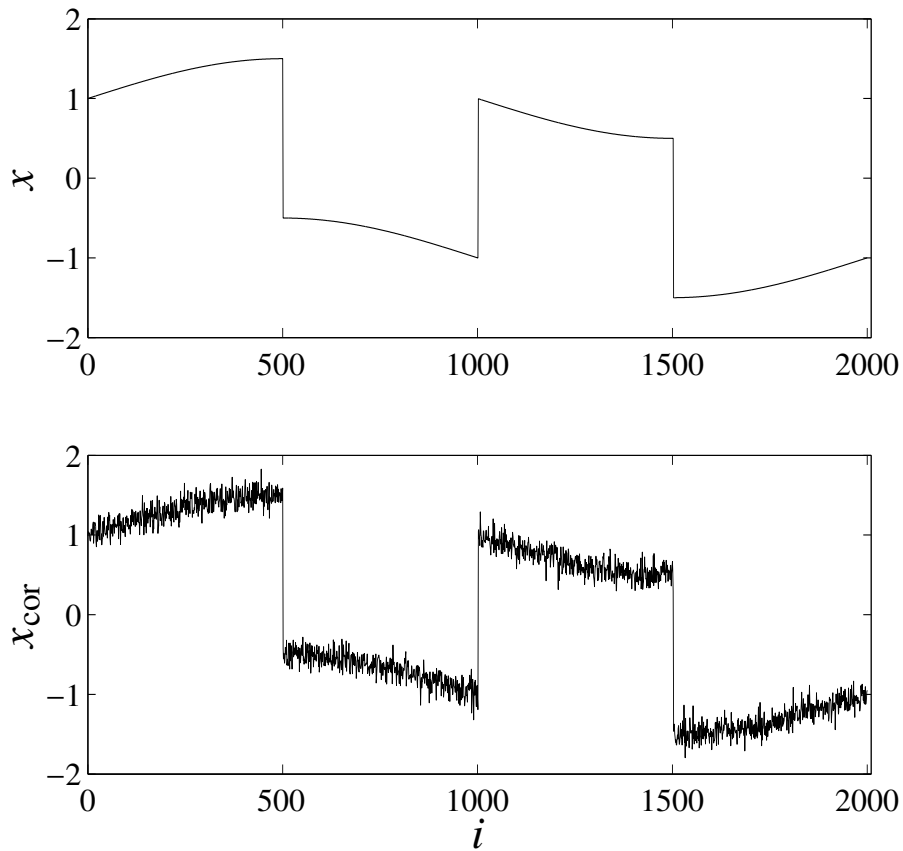


original signal x and noisy signal x_{cor}

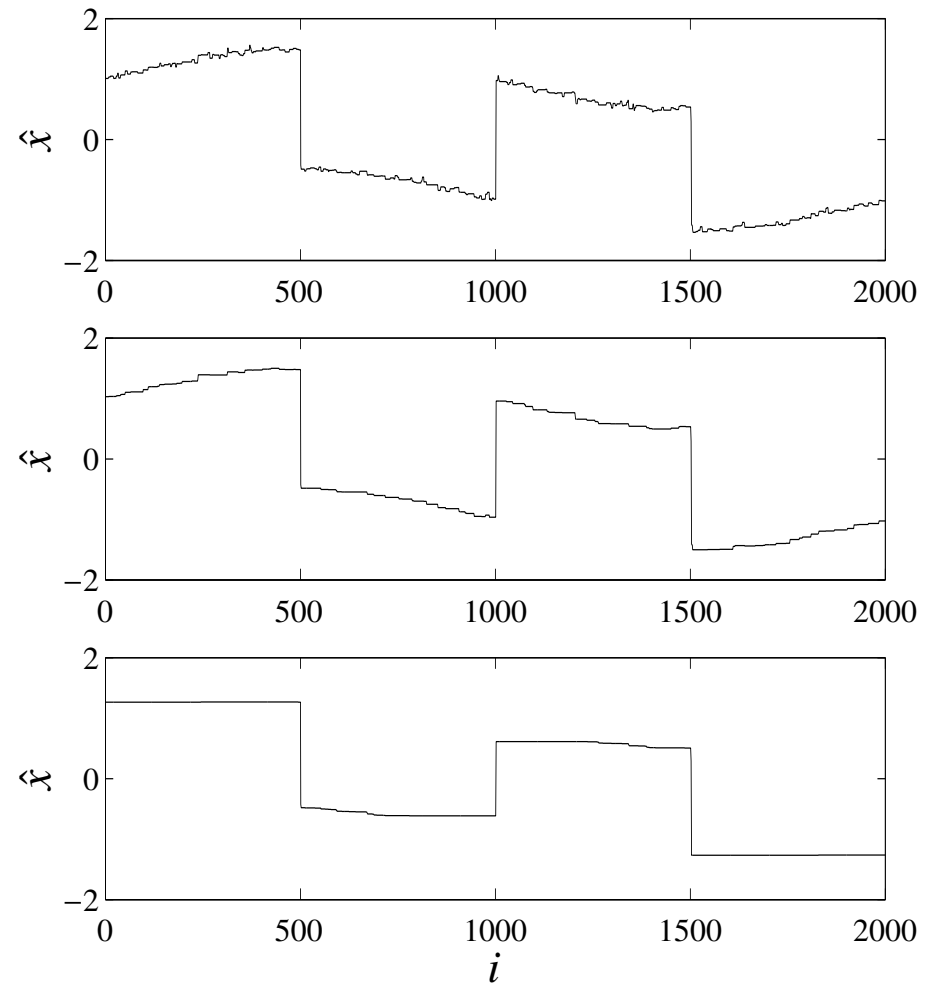
quadratic smoothing smooths out noise **and** sharp transitions in signal



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



original signal x and noisy signal x_{cor}



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

total variation smoothing preserves sharp transitions in signal

Robust approximation

minimize $\|Ax - b\|$ with uncertain A

two approaches:

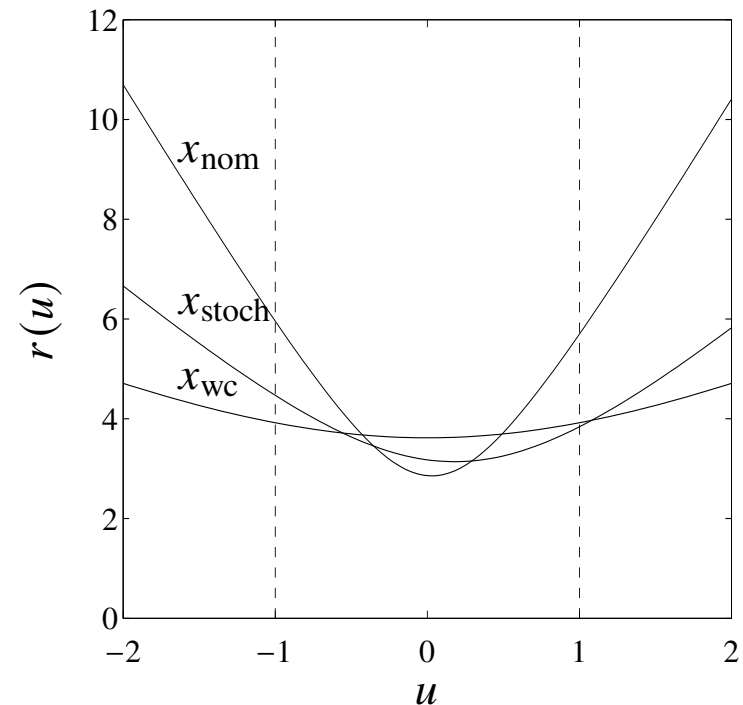
- **stochastic**: assume A is random, minimize $\mathbf{E} \|Ax - b\|$
- **worst-case**: set \mathcal{A} of possible values of A , minimize $\sup_{A \in \mathcal{A}} \|Ax - b\|$

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

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

- x_{nom} minimizes $\|A_0x - b\|_2^2$
- x_{stoch} minimizes $\mathbf{E} \|A(u)x - b\|_2^2$
with u uniform on $[-1, 1]$
- x_{wc} minimizes $\sup_{-1 \leq u \leq 1} \|A(u)x - b\|_2^2$

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



Stochastic robust LS

with $A = \bar{A} + U$, U random, $\mathbf{E} U = 0$, $\mathbf{E} U^T U = P$

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

- explicit expression for objective:

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

- hence, robust LS problem is equivalent to LS problem

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

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

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

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

- from page 5.16, strong duality holds between the following problems

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

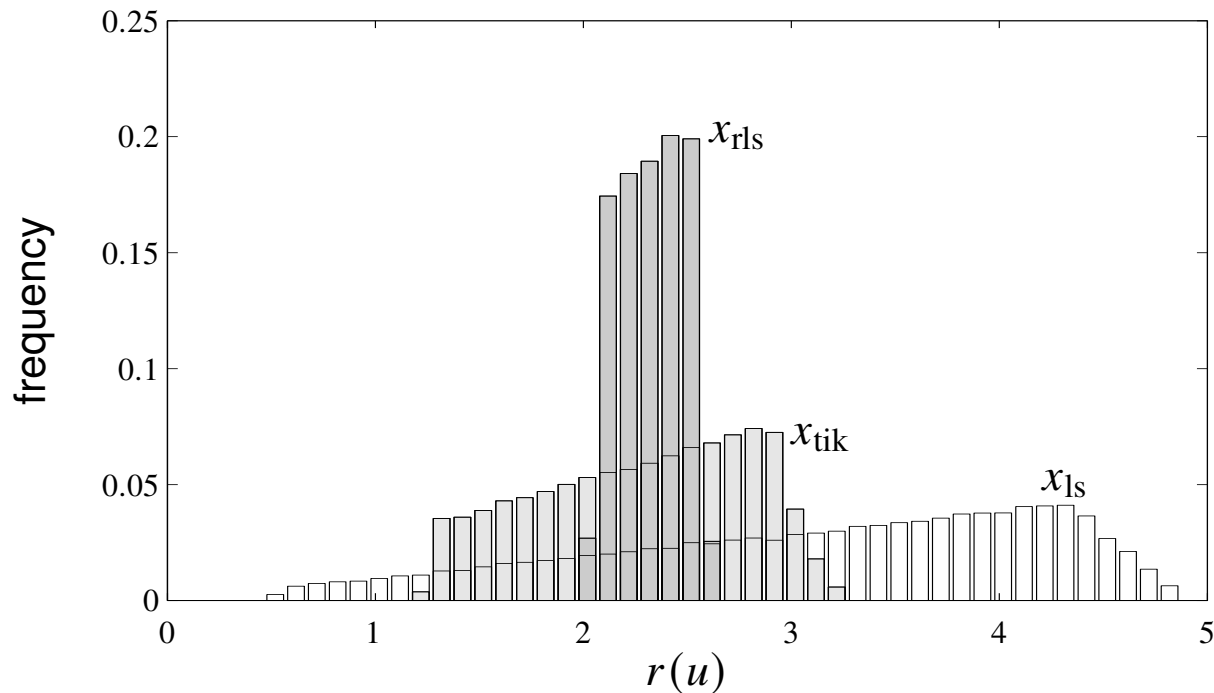
- hence, robust LS problem is equivalent to SDP

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

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_{1s} minimizes $\|A_0 x - b\|_2$
- x_{tik} minimizes $\|A_0 x - b\|_2^2 + \delta \|x\|_2^2$ (Tikhonov solution)
- x_{rls} minimizes $\sup_{A \in \mathcal{A}} \|Ax - b\|_2^2$