6. Approximation and fitting

- norm approximation

- least-norm problems

- regularized approximation

- robust approximation

Norm approximation

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

($A \in \mathbf{R}^{m \times n}$ 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

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

$(x^\star = (A^T A)^{-1} A^T b$ 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

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

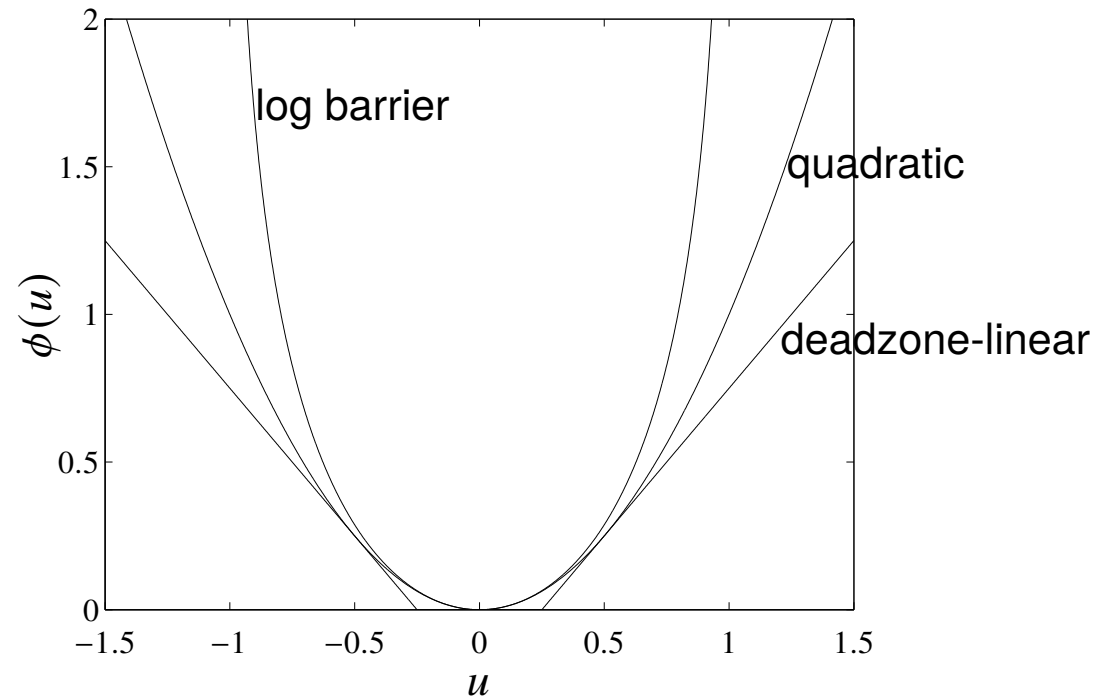$(A \in \mathbf{R}^{m \times n}, \phi : \mathbf{R} \to \mathbf{R}$ is a convex penalty function$)$

Examples

- quadratic: $\phi(u) = u^2$

- deadzone-linear with width a:

$$\phi(u) = \max\{0, |u| - a\}$$
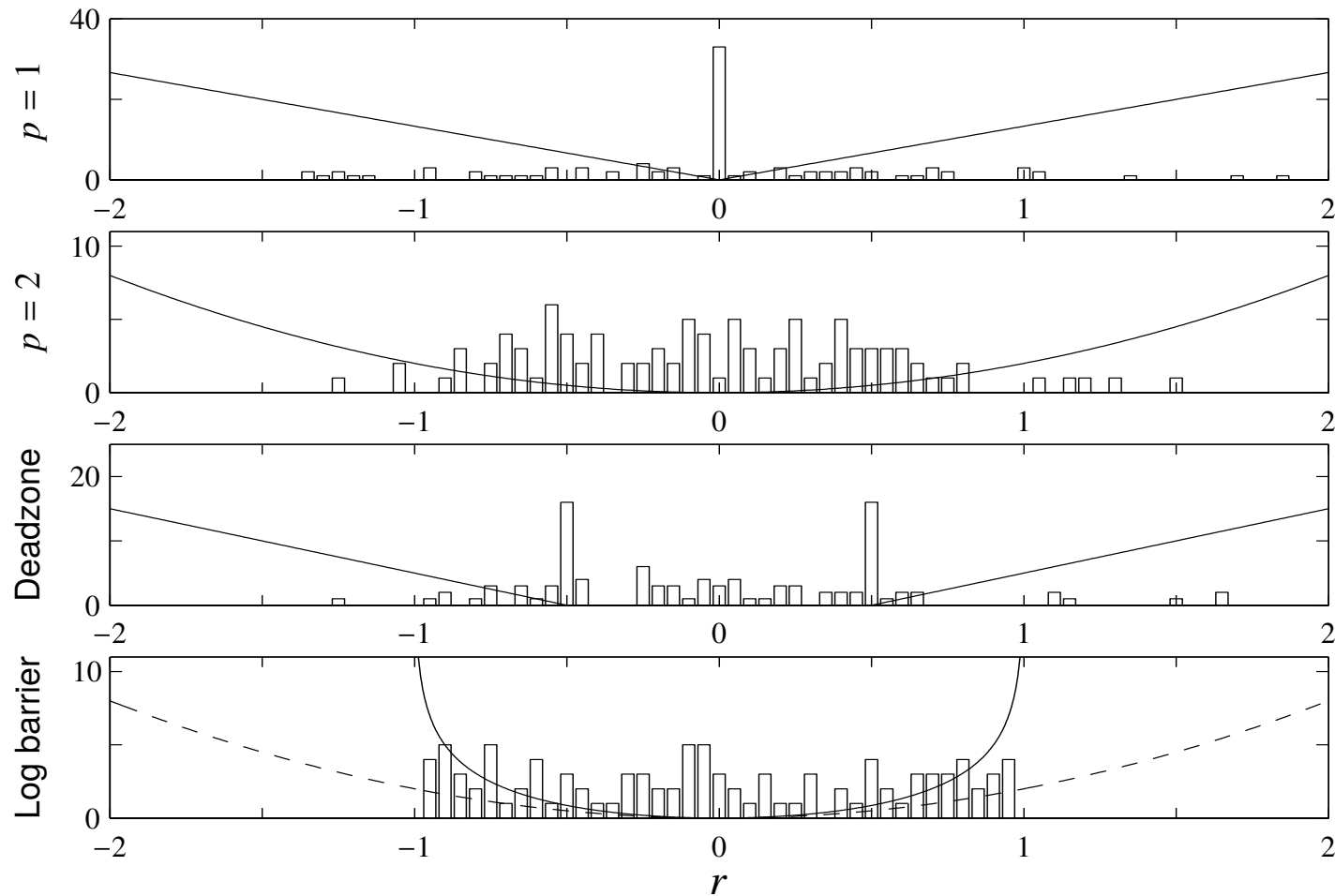
- log-barrier with limit a:

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

Comparison

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

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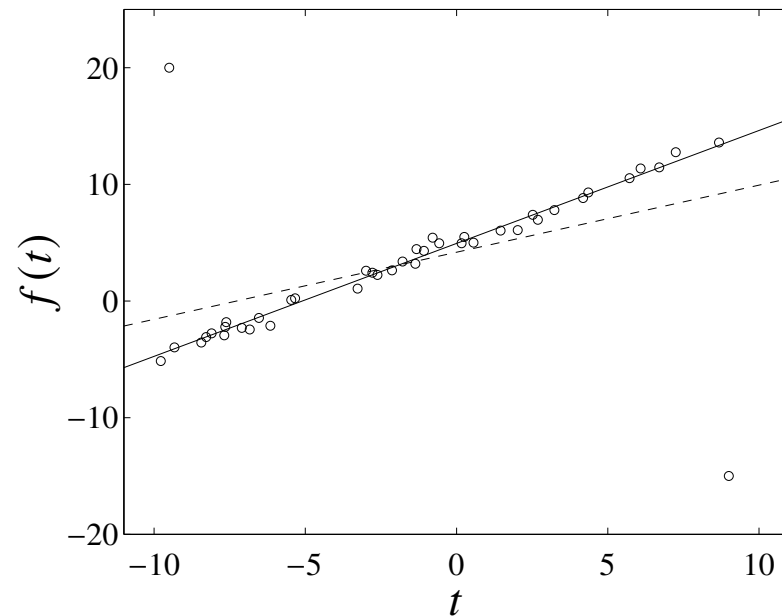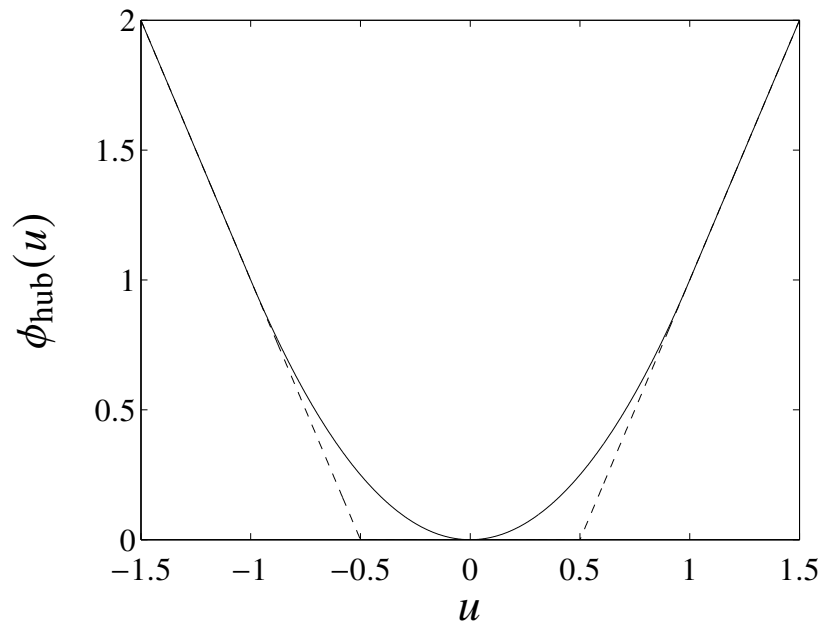

shape of penalty function has large effect on distribution of residuals

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

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

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

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

  tends to produce sparse solution $x^\star$

Extension: least-penalty problem

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

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

Regularized approximation

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

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

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

- 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}: $J_{\text{track}} = \Sigma_{t=0}^{N}(y(t) - y_{\text{des}}(t))^2$

2. input magnitude: $J_{\text{mag}} = \Sigma_{t=0}^{N} u(t)^2$

3. input variation: $J_{\text{der}} = \Sigma_{t=0}^{N-1}(u(t + 1) - u(t))^2$

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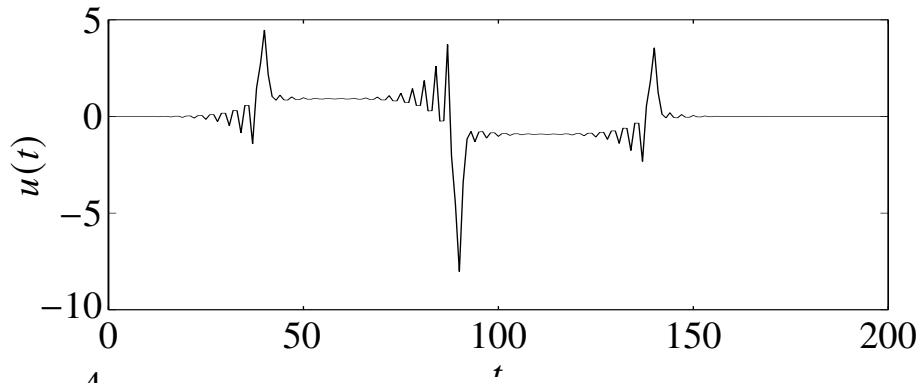
Regularized least-squares formulation

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

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
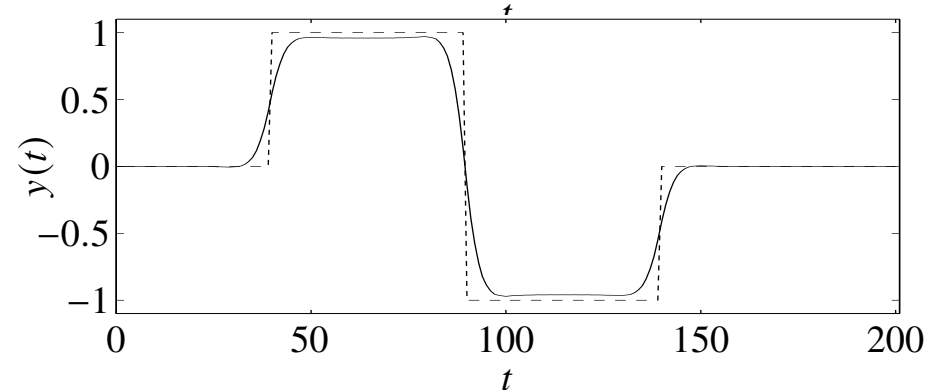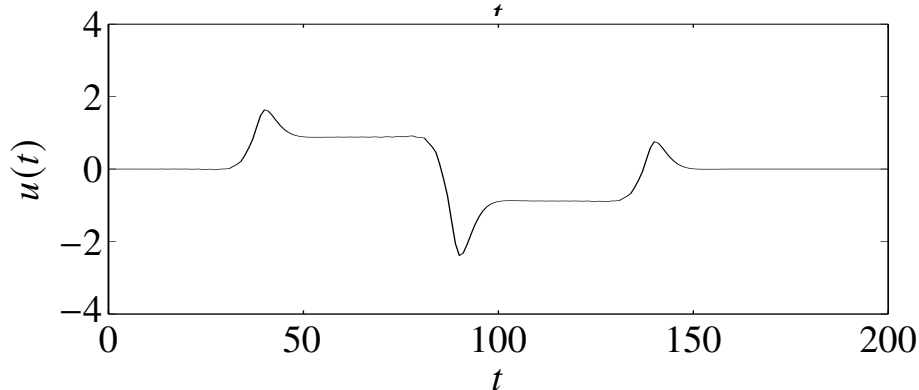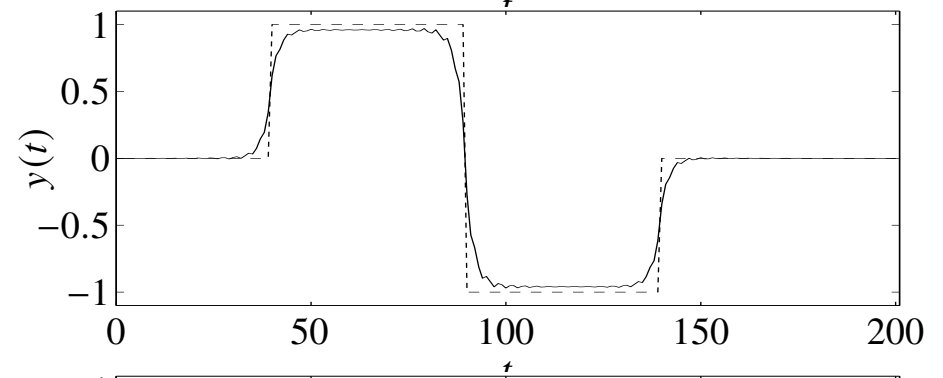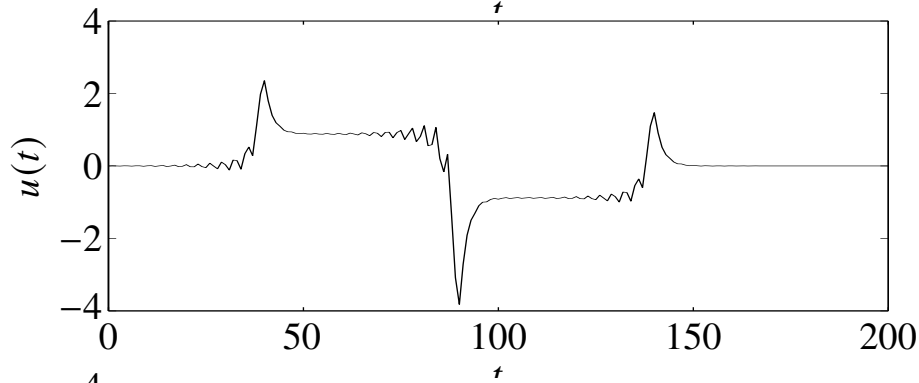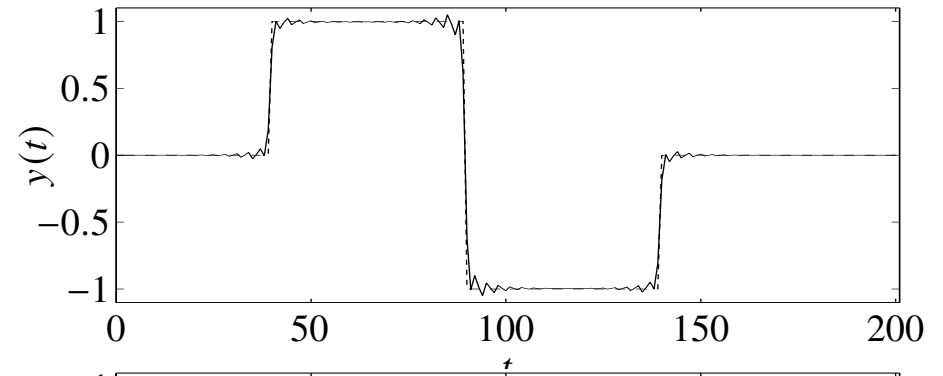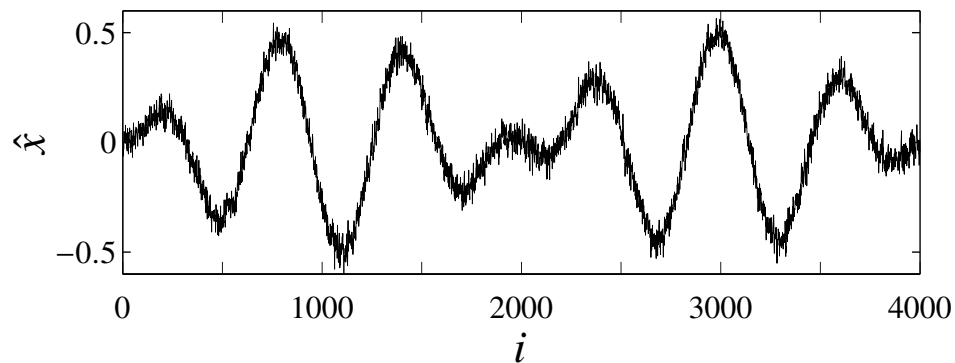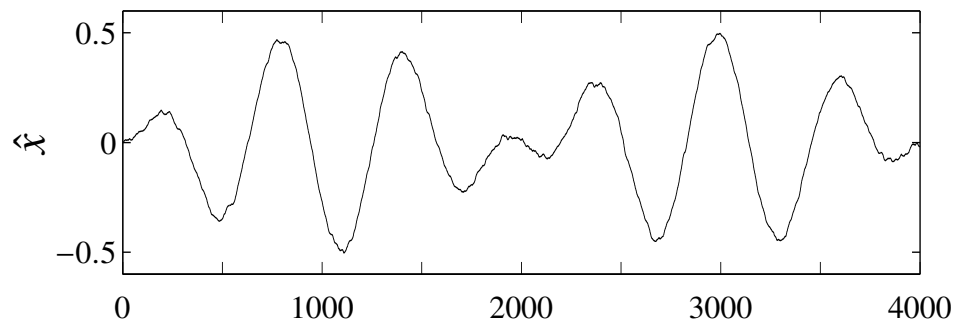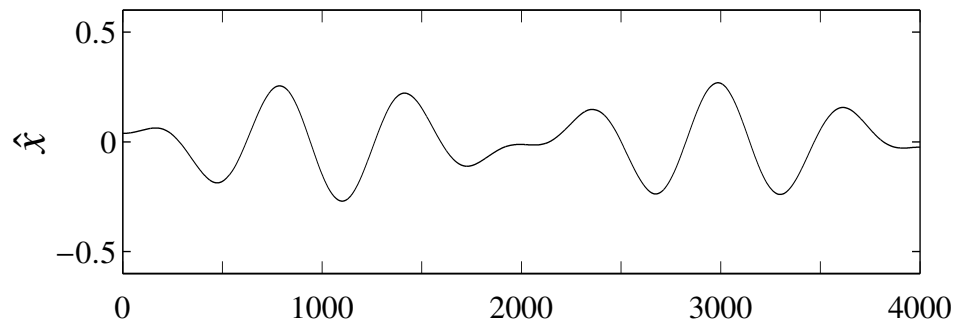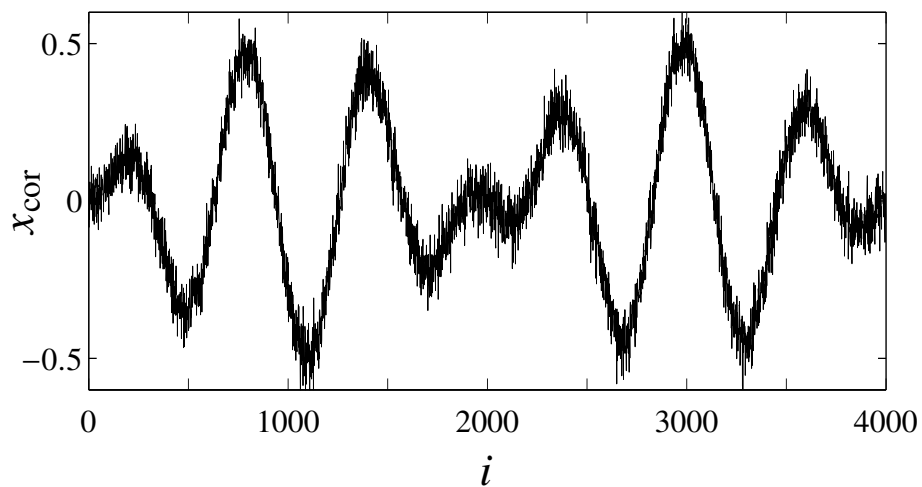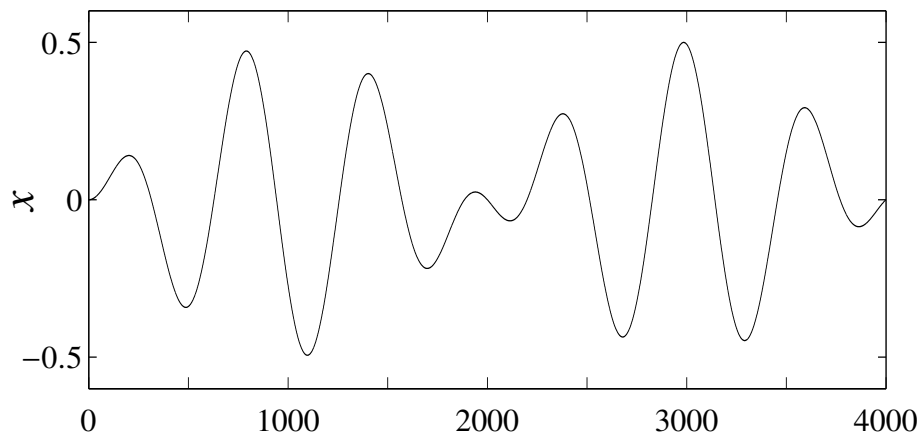
Signal reconstruction

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

- $x \in \mathbf{R}^n$ 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

- $\phi : \mathbf{R}^n \to \mathbf{R}$ is regularization function or smoothing objective

Examples: quadratic smoothing, total variation smoothing:

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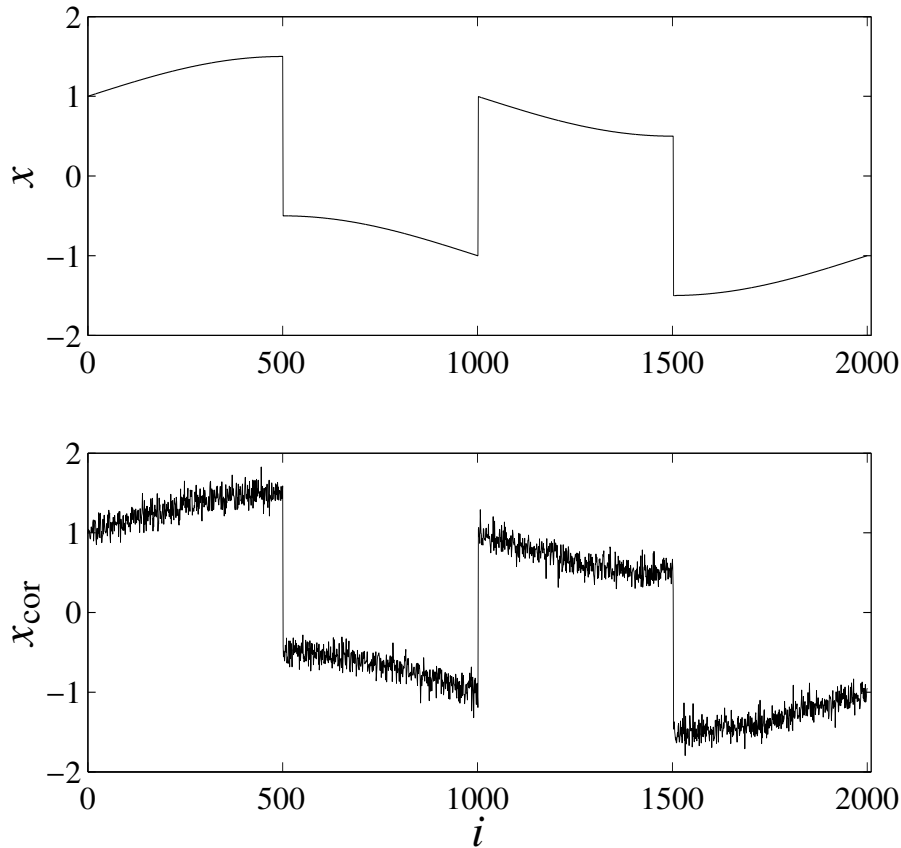
Quadratic smoothing example

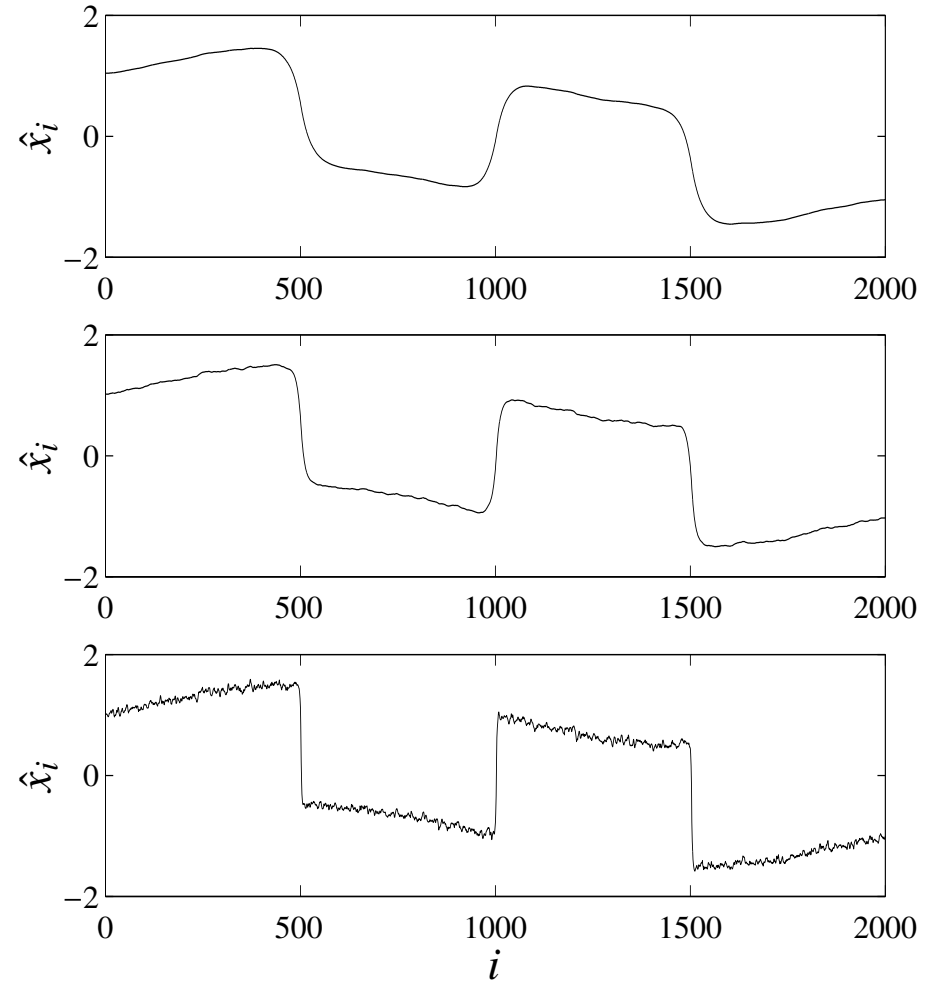original signal x and noisy signal x_{cor}

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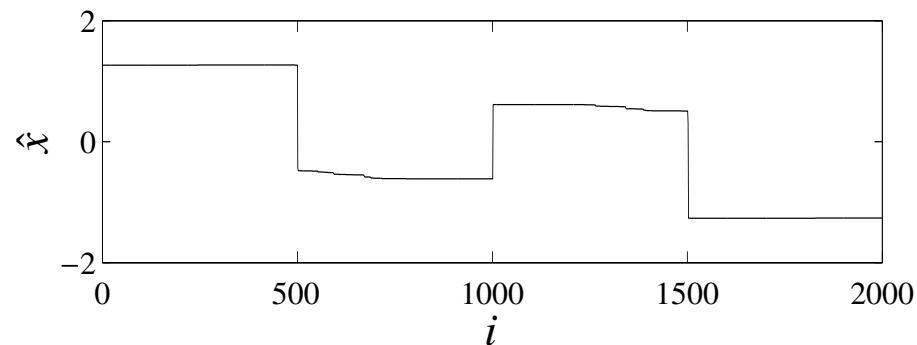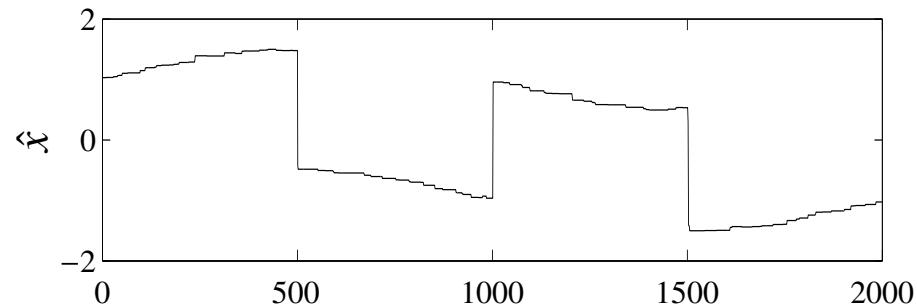
Total variation reconstruction example

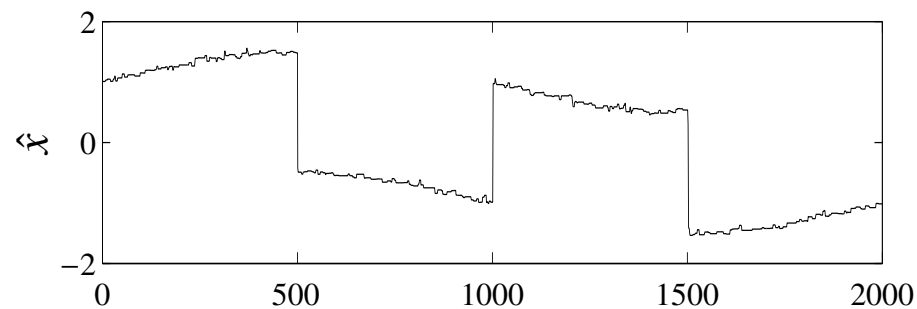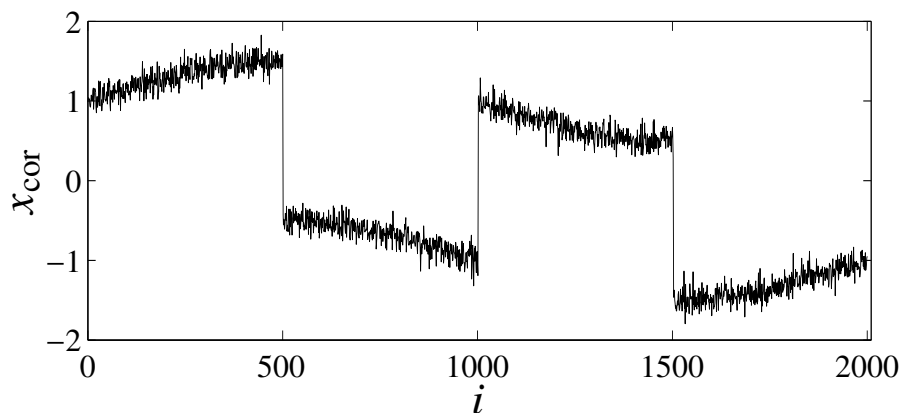

original signal x and noisy signal x_{cor}

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

quadratic smoothing smooths out noise **and** sharp transitions in signal
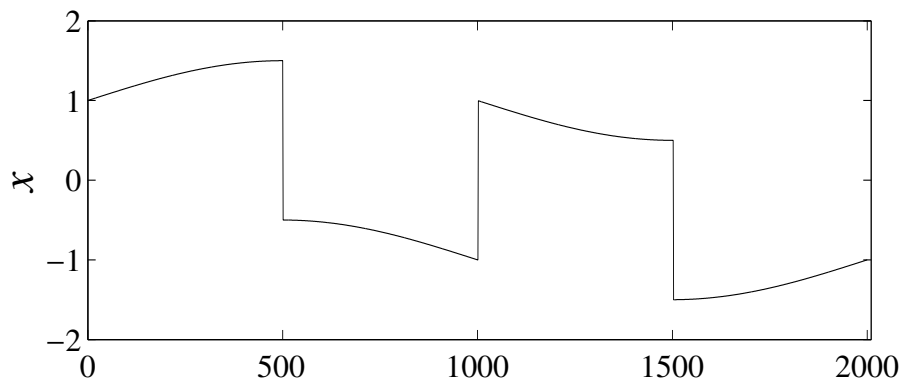
original signal x and noisy signal x_{cor}

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
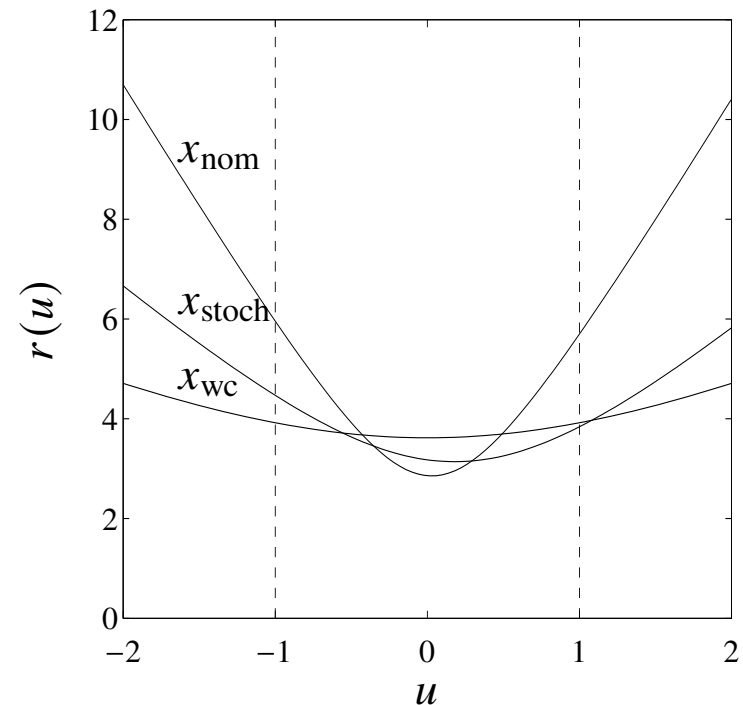
two approaches:

- **stochastic**: assume A is random, minimize $\mathbf{E}\,\|Ax - b\|$

- **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 $\|A_0 x - b\|_2^2$

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

- x_{wc} minimizes $\sup_{-1 \le u \le 1} \|A(u)x - b\|_2^2$

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

Stochastic robust LS

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

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

- 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

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

- 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 $\mathcal{A} = \{\bar{A} + u_1 A_1 + \cdots + u_p A_p \mid \|u\|_2 \le 1\}$

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

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

$$\begin{array}{ll} \text{maximize} & \|Pu + q\|_2^2 \\ \text{subject to} & \|u\|_2^2 \le 1 \end{array} \qquad \begin{array}{ll} \text{minimize} & t + \lambda \\ \\ \text{subject to} & \begin{bmatrix} I & P & q \\ P^T & \lambda I & 0 \\ q^T & 0 & t \end{bmatrix} \ge 0 \end{array}$$
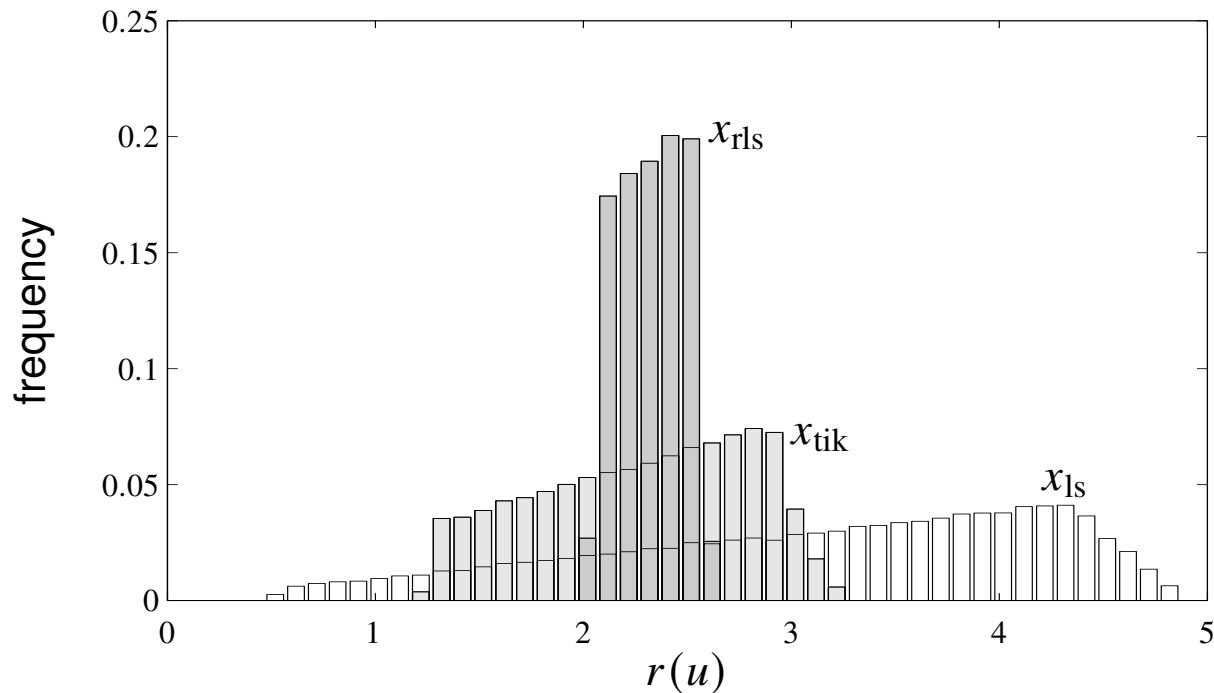
- hence, robust LS problem is equivalent to SDP

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

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