## 6. Approximation and fitting

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


## Norm approximation

$$
\operatorname{minimize}\|A x-b\|
$$

( $A \in \mathbf{R}^{m \times n}$ with $m \geq n,\|\cdot\|$ is a norm on $\mathbf{R}^{m}$ )
interpretations of solution $x^{\star}=\operatorname{argmin}_{x}\|A x-b\|$ :

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

$$
y=A x+v
$$

$y$ 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), $A x$ is result (output) $x^{\star}$ is design that best approximates desired result $b$


## examples

- least-squares approximation $\left(\|\cdot\|_{2}\right)$ : solution satisfies normal equations

$$
A^{T} A x=A^{T} b
$$

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

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

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

- sum of absolute residuals approximation $\left(\|\cdot\|_{1}\right)$ : can be solved as an LP

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

## Penalty function approximation

$$
\begin{array}{ll}
\operatorname{minimize} & \phi\left(r_{1}\right)+\cdots+\phi\left(r_{m}\right) \\
\text { subject to } & r=A x-b
\end{array}
$$

$\left(A \in \mathbf{R}^{m \times n}, \phi: \mathbf{R} \rightarrow \mathbf{R}\right.$ 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 $a$ :


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

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

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


shape of penalty function has large effect on distribution of residuals

Huber penalty function (with parameter $M$ )

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

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

```
minimize |x|
subject to }Ax=
```

$\left(A \in \mathbf{R}^{m \times n}\right.$ with $m \leq n,\|\cdot\|$ is a norm on $\left.\mathbf{R}^{n}\right)$
interpretations of solution $x^{\star}=\operatorname{argmin}_{A x=b}\|x\|$ :

- geometric: $x^{\star}$ is point in affine set $\{x \mid A x=b\}$ with minimum distance to 0
- estimation: $b=A x$ 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 $\left(\|\cdot\|_{2}\right)$ :
can be solved via optimality conditions

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

- minimum sum of absolute values $\left(\|\cdot\|_{1}\right)$ : can be solved as an LP

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

tends to produce sparse solution $x^{\star}$
extension: least-penalty problem

$$
\begin{array}{ll}
\operatorname{minimize} & \phi\left(x_{1}\right)+\cdots+\phi\left(x_{n}\right) \\
\text { subject to } & A x=b
\end{array}
$$

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

## Regularized approximation

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

$A \in \mathbf{R}^{m \times n}$, norms on $\mathbf{R}^{m}$ and $\mathbf{R}^{n}$ can be different
interpretation: find good approximation $A x \approx b$ with small $x$

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


## Scalarized problem

$$
\operatorname{minimize} \quad\|A x-b\|+\gamma\|x\|
$$

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


## Tikhonov regularization

$$
\operatorname{minimize} \quad\|A x-b\|_{2}^{2}+\delta\|x\|_{2}^{2}
$$

can be solved as a least-squares problem

$$
\operatorname{minimize}\left\|\left[\begin{array}{c}
A \\
\sqrt{\delta} I
\end{array}\right] x-\left[\begin{array}{l}
b \\
0
\end{array}\right]\right\|_{2}^{2}
$$

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

## 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 $y_{\text {des }}: J_{\text {track }}=\sum_{t=0}^{N}\left(y(t)-y_{\text {des }}(t)\right)^{2}$
2. input magnitude: $J_{\mathrm{mag}}=\sum_{t=0}^{N} u(t)^{2}$
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 $\delta, \eta$, a least-squares problem in $u(0), \ldots, u(N)$
example: 3 solutions on optimal trade-off curve

$$
\text { (top) } \delta=0, \text { small } \eta \text {; (middle) } \delta=0, \text { larger } \eta ; \text { (bottom) large } \delta
$$








## Signal reconstruction

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

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

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

## quadratic smoothing example


original signal $x$ and noisy signal $x_{\text {cor }}$

three solutions on trade-off curve
$\left\|\hat{x}-x_{\text {cor }}\right\|_{2}$ versus $\phi_{\text {quad }}(\hat{x})$

## total variation reconstruction example


original signal $x$ and noisy signal $x_{\text {cor }}$

three solutions on trade-off curve $\left\|\hat{x}-x_{\text {cor }}\right\|_{2}$ versus $\phi_{\text {quad }}(\hat{x})$
quadratic smoothing smooths out noise and sharp transitions in signal


original signal $x$ and noisy signal $x_{\text {cor }}$



three solutions on trade-off curve

$$
\left\|\hat{x}-x_{\text {cor }}\right\|_{2} \text { versus } \phi_{\mathrm{tv}}(\hat{x})
$$

total variation smoothing preserves sharp transitions in signal

## Robust approximation

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

- stochastic: assume $A$ is random, minimize $\mathbf{E}\|A x-b\|$
- worst-case: set $\mathcal{A}$ of possible values of $A$, minimize $\sup _{A \in \mathcal{A}}\|A x-b\|$ tractable only in special cases (certain norms $\|\cdot\|$, distributions, sets $\mathcal{A}$ )
example: $A(u)=A_{0}+u A_{1}$
- $x_{\text {nom }}$ minimizes $\left\|A_{0} x-b\right\|_{2}^{2}$
- $x_{\text {stoch }}$ minimizes $\mathbf{E}\|A(u) x-b\|_{2}^{2}$ with $u$ uniform on $[-1,1]$
- $x_{\text {wc }}$ 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, $\mathbf{E} U=0, \mathbf{E} U^{T} U=P$

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

- explicit expression for objective:

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

- hence, robust LS problem is equivalent to LS problem

$$
\operatorname{minimize}\|\bar{A} x-b\|_{2}^{2}+\left\|P^{1 / 2} x\right\|_{2}^{2}
$$

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

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

worst-case robust LS with $\mathcal{A}=\left\{\bar{A}+u_{1} A_{1}+\cdots+u_{p} A_{p} \mid\|u\|_{2} \leq 1\right\}$

$$
\operatorname{minimize} \sup _{A \in \mathcal{A}}\|A x-b\|_{2}^{2}=\sup _{\|u\|_{2} \leq 1}\|P(x) u+q(x)\|_{2}^{2}
$$

where $P(x)=\left[\begin{array}{llll}A_{1} x & A_{2} x & \cdots & A_{p} x\end{array}\right], q(x)=\bar{A} x-b$

- from page 5-14, strong duality holds between the following problems

$$
\left.\begin{array}{llll}
\operatorname{maximize} & \|P u+q\|_{2}^{2} & \text { minimize } & t+\lambda \\
\text { subject to } & \|u\|_{2}^{2} \leq 1 & \text { subject to }
\end{array} \begin{array}{ccc}
I & P & q \\
P^{T} & \lambda I & 0 \\
q^{T} & 0 & t
\end{array}\right] \succeq 0
$$

- hence, robust LS problem is equivalent to SDP

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

example: histogram of residuals

$$
r(u)=\left\|\left(A_{0}+u_{1} A_{1}+u_{2} A_{2}\right) x-b\right\|_{2}
$$

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


- $x_{\text {ls }}$ minimizes $\left\|A_{0} x-b\right\|_{2}$
- $x_{\text {tik }}$ minimizes $\left\|A_{0} x-b\right\|_{2}^{2}+\delta\|x\|_{2}^{2}$ (Tikhonov solution)
- $x_{\mathrm{wc}}$ minimizes $\sup _{\|u\|_{2} \leq 1}\left\|A_{0} x-b\right\|_{2}^{2}+\|x\|_{2}^{2}$

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