EE263 Autumn 2014–15 Sanjay Lall

Lecture 5 Least-squares

- least-squares (approximate) solution of overdetermined equations
- projection and orthogonality principle
- least-squares estimation
- BLUE property

Overdetermined linear equations

consider y = Ax where $A \in \mathbf{R}^{m \times n}$ is (strictly) skinny, i.e., m > n

- called overdetermined set of linear equations (more equations than unknowns)
- for most y, cannot solve for x

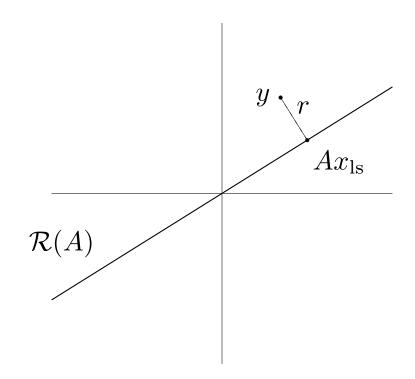
one approach to approximately solve y = Ax:

- define *residual* or error r = Ax y
- find $x = x_{ls}$ that minimizes ||r||

 $x_{\rm ls}$ called *least-squares* (approximate) solution of y = Ax

Geometric interpretation

 Ax_{ls} is point in $\mathcal{R}(A)$ closest to y (Ax_{ls} is projection of y onto $\mathcal{R}(A)$)



Least-squares (approximate) solution

- assume A is full rank, skinny
- to find x_{ls} , we'll minimize norm of residual squared,

$$||r||^2 = x^T A^T A x - 2y^T A x + y^T y$$

• set gradient w.r.t. x to zero:

$$\nabla_x ||r||^2 = 2A^T A x - 2A^T y = 0$$

- yields the normal equations: $A^TAx = A^Ty$
- ullet assumptions imply A^TA invertible, so we have

$$x_{\rm ls} = (A^T A)^{-1} A^T y$$

... a very famous formula

- $x_{\rm ls}$ is linear function of y
- $x_{ls} = A^{-1}y$ if A is square
- x_{ls} solves $y = Ax_{ls}$ if $y \in \mathcal{R}(A)$
- ullet $A^\dagger = (A^TA)^{-1}A^T$ is called the *pseudo-inverse* of A
- A^{\dagger} is a *left inverse* of (full rank, skinny) A:

$$A^{\dagger}A = (A^T A)^{-1}A^T A = I$$

Projection on $\mathcal{R}(A)$

 Ax_{ls} is (by definition) the point in $\mathcal{R}(A)$ that is closest to y, i.e., it is the projection of y onto $\mathcal{R}(A)$

$$Ax_{ls} = \mathcal{P}_{\mathcal{R}(A)}(y)$$

ullet the projection function $\mathcal{P}_{\mathcal{R}(A)}$ is linear, and given by

$$\mathcal{P}_{\mathcal{R}(A)}(y) = Ax_{ls} = A(A^T A)^{-1} A^T y$$

ullet $A(A^TA)^{-1}A^T$ is called the *projection matrix* (associated with $\mathcal{R}(A)$)

Orthogonality principle

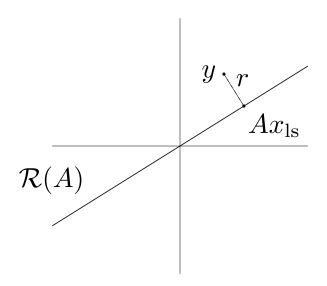
optimal residual

$$r = Ax_{ls} - y = (A(A^{T}A)^{-1}A^{T} - I)y$$

is orthogonal to $\mathcal{R}(A)$:

$$\langle r, Az \rangle = y^T (A(A^T A)^{-1} A^T - I)^T Az = 0$$

for all $z \in \mathbf{R}^n$



Completion of squares

since $r = Ax_{\rm ls} - y \perp A(x - x_{\rm ls})$ for any x, we have

$$||Ax - y||^2 = ||(Ax_{ls} - y) + A(x - x_{ls})||^2$$
$$= ||Ax_{ls} - y||^2 + ||A(x - x_{ls})||^2$$

this shows that for $x \neq x_{ls}$, $||Ax - y|| > ||Ax_{ls} - y||$

Least-squares via ${\it QR}$ factorization

- $A \in \mathbf{R}^{m \times n}$ skinny, full rank
- factor as A=QR with $Q^TQ=I_n$, $R\in \mathbf{R}^{n\times n}$ upper triangular, invertible
- pseudo-inverse is

$$(A^T A)^{-1} A^T = (R^T Q^T Q R)^{-1} R^T Q^T = R^{-1} Q^T$$

so
$$x_{\rm ls} = R^{-1}Q^Ty$$

ullet projection on $\mathcal{R}(A)$ given by matrix

$$A(A^{T}A)^{-1}A^{T} = AR^{-1}Q^{T} = QQ^{T}$$

Least-squares via full ${\it QR}$ factorization

• full *QR* factorization:

$$A = [Q_1 \ Q_2] \left[\begin{array}{c} R_1 \\ 0 \end{array} \right]$$

with $[Q_1 \ Q_2] \in \mathbf{R}^{m \times m}$ orthogonal, $R_1 \in \mathbf{R}^{n \times n}$ upper triangular, invertible

• multiplication by orthogonal matrix doesn't change norm, so

$$||Ax - y||^2 = ||[Q_1 Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - y||^2$$

$$= ||[Q_1 Q_2]^T [Q_1 Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - [Q_1 Q_2]^T y||^2$$

$$= \left\| \begin{bmatrix} R_1 x - Q_1^T y \\ -Q_2^T y \end{bmatrix} \right\|^2$$

$$= \left\| R_1 x - Q_1^T y \right\|^2 + \| Q_2^T y \|^2$$

- this is evidently minimized by choice $x_{ls} = R_1^{-1}Q_1^Ty$ (which makes first term zero)
- ullet residual with optimal x is

$$Ax_{ls} - y = -Q_2Q_2^T y$$

- $Q_1Q_1^T$ gives projection onto $\mathcal{R}(A)$
- $Q_2Q_2^T$ gives projection onto $\mathcal{R}(A)^{\perp}$

Least-squares estimation

many applications in inversion, estimation, and reconstruction problems have form

$$y = Ax + v$$

- x is what we want to estimate or reconstruct
- y is our sensor measurement(s)
- v is an unknown *noise* or *measurement error* (assumed small)
- *i*th row of *A* characterizes *i*th sensor

least-squares estimation: choose as estimate \hat{x} that minimizes

$$||A\hat{x} - y||$$

i.e., deviation between

- what we actually observed (y), and
- what we would observe if $x = \hat{x}$, and there were no noise (v = 0)

least-squares estimate is just $\hat{x} = (A^T A)^{-1} A^T y$

BLUE property

linear measurement with noise:

$$y = Ax + v$$

with A full rank, skinny

consider a *linear estimator* of form $\hat{x} = By$

• called *unbiased* if $\hat{x} = x$ whenever v = 0 (*i.e.*, no estimation error when there is no noise)

same as BA = I, *i.e.*, B is left inverse of A

estimation error of unbiased linear estimator is

$$x - \hat{x} = x - B(Ax + v) = -Bv$$

obviously, then, we'd like B 'small' (and BA = I)

• fact: $A^{\dagger} = (A^T A)^{-1} A^T$ is the *smallest* left inverse of A, in the following sense:

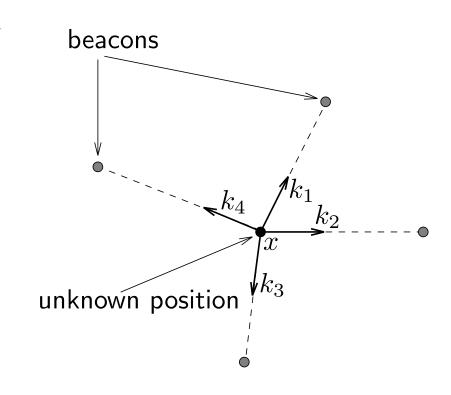
for any B with BA = I, we have

$$\sum_{i,j} B_{ij}^2 \ge \sum_{i,j} A_{ij}^{\dagger 2}$$

i.e., least-squares provides the best linear unbiased estimator (BLUE)

Navigation from range measurements

navigation using range measurements from distant beacons



beacons far from unknown position $x \in \mathbf{R}^2$, so linearization around x = 0 (say) nearly exact

ranges $y \in \mathbf{R}^4$ measured, with measurement noise v:

$$y = -\begin{bmatrix} k_1^T \\ k_2^T \\ k_3^T \\ k_4^T \end{bmatrix} x + v$$

where k_i is unit vector from 0 to beacon i

measurement errors are independent, Gaussian, with standard deviation 2 (details not important)

problem: estimate $x \in \mathbb{R}^2$, given $y \in \mathbb{R}^4$

(roughly speaking, a 2:1 measurement redundancy ratio)

actual position is x = (5.59, 10.58); measurement is y = (-11.95, -2.84, -9.81, 2.81)

Just enough measurements method

 y_1 and y_2 suffice to find x (when v=0)

compute estimate \hat{x} by inverting top (2×2) half of A:

$$\hat{x} = B_{je}y = \begin{bmatrix} 0 & -1.0 & 0 & 0 \\ -1.12 & 0.5 & 0 & 0 \end{bmatrix} y = \begin{bmatrix} 2.84 \\ 11.9 \end{bmatrix}$$

(norm of error: 3.07)

Least-squares method

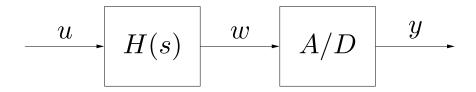
compute estimate \hat{x} by least-squares:

$$\hat{x} = A^{\dagger} y = \begin{bmatrix} -0.23 & -0.48 & 0.04 & 0.44 \\ -0.47 & -0.02 & -0.51 & -0.18 \end{bmatrix} y = \begin{bmatrix} 4.95 \\ 10.26 \end{bmatrix}$$

(norm of error: 0.72)

- ullet $B_{
 m je}$ and A^\dagger are both left inverses of A
- ullet larger entries in B lead to larger estimation error

Example from overview lecture



• signal u is piecewise constant, period $1 \sec$, $0 \le t \le 10$:

$$u(t) = x_j, \quad j - 1 \le t < j, \quad j = 1, \dots, 10$$

• filtered by system with impulse response h(t):

$$w(t) = \int_0^t h(t - \tau)u(\tau) d\tau$$

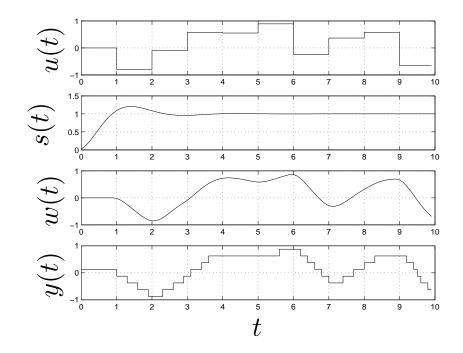
ullet sample at $10 \mathrm{Hz}$: $\tilde{y}_i = w(0.1i)$, $i=1,\ldots,100$

• 3-bit quantization: $y_i = Q(\tilde{y}_i)$, $i = 1, \dots, 100$, where Q is 3-bit quantizer characteristic

$$Q(a) = (1/4) (\mathbf{round}(4a + 1/2) - 1/2)$$

• problem: estimate $x \in \mathbf{R}^{10}$ given $y \in \mathbf{R}^{100}$

example:

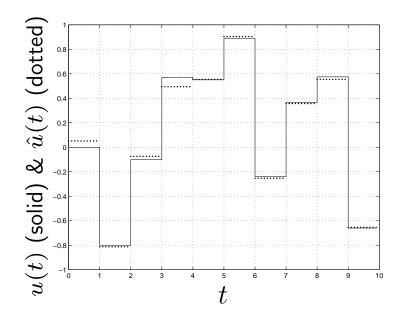


we have y = Ax + v, where

•
$$A \in \mathbf{R}^{100 \times 10}$$
 is given by $A_{ij} = \int_{j-1}^{j} h(0.1i - \tau) \ d\tau$

• $v \in \mathbf{R}^{100}$ is quantization error: $v_i = Q(\tilde{y}_i) - \tilde{y}_i$ (so $|v_i| \le 0.125$)

least-squares estimate: $x_{ls} = (A^T A)^{-1} A^T y$

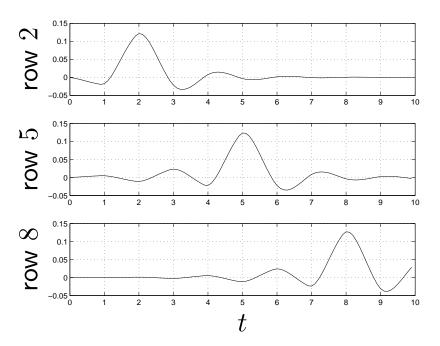


RMS error is
$$\frac{\|x - x_{\rm ls}\|}{\sqrt{10}} = 0.03$$

better than if we had no filtering! (RMS error 0.07)

more on this later . . .

some rows of $B_{ls} = (A^T A)^{-1} A^T$:



- ullet rows show how sampled measurements of y are used to form estimate of x_i for i=2,5,8
- to estimate x_5 , which is the original input signal for $4 \le t < 5$, we mostly use y(t) for $3 \le t \le 7$