Linear least squares problems (§12.1)

- Least squares: a special class of optimization problems.
- Well studied because:
 - Many applications
 - Easy to solve
- Basic idea: want to solve

$$Ax = b$$

even when there is no solution (!).

• Consider the system of linear equations

$$Ax = b$$

where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$, $m \ge n$, and rank A = n (full rank).

- Number of unknowns \leq number of equations (overdetermined).
- If $b \notin \mathcal{R}(A)$, then no solution (inconsistent).
- Alternative goal:

$$\text{minimize } \frac{1}{2} \| \boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} \|^2.$$

• The reason for the factor of 1/2 will be clear later.

Examples of linear least squares problems

- Linear regression (line fitting)
- Discrete Fourier series
- Linear system identification
- Optimal filtering
- ... others
- Detailed examples later.

A note about quadratics

• Consider a quadratic

$$f(\boldsymbol{x}) = \frac{1}{2} \boldsymbol{x}^T \boldsymbol{Q} \boldsymbol{x} - \boldsymbol{x}^T \boldsymbol{b} + c,$$

where Q > 0.

 \bullet We can write f as

$$f(x) = \frac{1}{2}(x - x^*)^T Q(x - x^*) + \left(c - \frac{1}{2}x^{*T}Qx^*\right),$$

where $\boldsymbol{x}^* = \boldsymbol{Q}^{-1}\boldsymbol{b}$.

• Hence, $x^* = Q^{-1}b$ is the unique global minimizer.

Quadratic formulation of least squares problem

• Rewrite $f(\boldsymbol{x}) = \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|^2/2$ as

$$f(\boldsymbol{x}) = \frac{1}{2}(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})^T(\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b})$$
$$= \frac{1}{2}\boldsymbol{x}^T(\boldsymbol{A}^T\boldsymbol{A})\boldsymbol{x} - \boldsymbol{x}^T(\boldsymbol{A}^T\boldsymbol{b}) + \frac{\boldsymbol{b}^T\boldsymbol{b}}{2}.$$

- \bullet Thus, f is a quadratic.
- It is clear that $A^T A$ is positive semidefinite. (Why?)
- But, is $A^T A > 0$? For if it is, then the unique global minimizer is $x^* = (A^T A)^{-1} A^T b$.

Lemma (12.1): rank $\mathbf{A} = n \Leftrightarrow \mathbf{A}^T \mathbf{A} > 0$.

Proof:

• Given $\boldsymbol{x} \in \mathbb{R}^n$, we have

$$\boldsymbol{x}^T(\boldsymbol{A}^T\boldsymbol{A})\boldsymbol{x} = \|\boldsymbol{A}\boldsymbol{x}\|^2.$$

• By property of norm,

$$\|\mathbf{A}\mathbf{x}\|^2 = 0 \qquad \Leftrightarrow \qquad \mathbf{A}\mathbf{x} = \mathbf{0}.$$

• Hence,

$$\mathbf{A}^{T} \mathbf{A} \geqslant 0 \Leftrightarrow \exists \mathbf{x} \neq \mathbf{0} : \mathbf{x}^{T} (\mathbf{A}^{T} \mathbf{A}) \mathbf{x} = 0$$

 $\Leftrightarrow \exists \mathbf{x} \neq \mathbf{0} : \mathbf{A} \mathbf{x} = \mathbf{0}$
 $\Leftrightarrow \operatorname{rank} \mathbf{A} < n.$

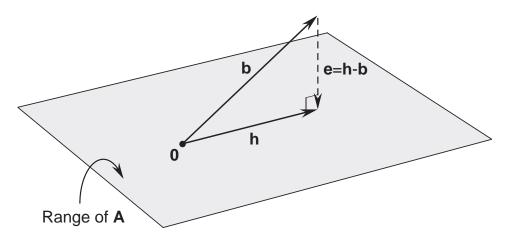
Version: Initial distribution

Solution to least squares problem

- Theorem: The unique (global) minimizer to the least squares problem is $x^* = (A^T A)^{-1} A^T b$.
- Proof: Follows immediately from the quadratic formulation of the problem.

Orthogonality principle

- Prop. (12.1): The vector Ax^* is orthogonal to $Ax^* b$.
- Proof: By simple algebra.
- Least squares problem \equiv approximating b by a point in $\mathcal{R}(A)$.
- $h = Ax^*$ is the projection of b onto $\mathcal{R}(A)$.
- The projection Ax^* is orthogonal to the error in the approximation e = h b.



- Let a_i represent the *i*th column of A; i.e., $A = [a_1, a_2, \dots, a_n]$.
- We have

$$m{A}^Tm{A} = egin{bmatrix} \langle m{a}_1, m{a}_1
angle & \cdots & \langle m{a}_n, m{a}_1
angle \ dots & dots \ \langle m{a}_1, m{a}_n
angle & \cdots & \langle m{a}_n, m{a}_n
angle \end{bmatrix}$$

Name: Gram matrix (or Grammian).

• Also,

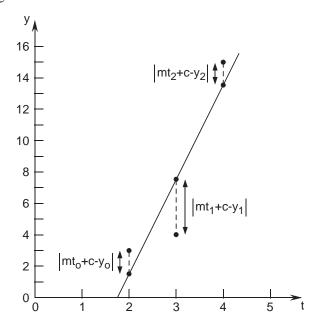
$$oldsymbol{A}^Toldsymbol{b} = egin{bmatrix} \langle oldsymbol{a}_1, oldsymbol{b}
angle \ dots \ \langle oldsymbol{a}_n, oldsymbol{b}
angle \end{bmatrix}.$$

Example (12.1): Linear Regression

• Given data:

i	0	1	2
t_i	2	3	4
y_i	3	4	15

• Want to find straight line of best fit.



- Equation of straight line: y = mt + c.
- If a straight line passed through all three points, we would have

$$2m + c = 3$$

$$3m + c = 4$$

$$4m + c = 15.$$

- The above is an inconsistent (overdetermined) set of equations.
- The total squared error between the line and the given data points is

$$f(m,c) = \sum_{i=0}^{2} (mt_i + c - y_i)^2$$

= $\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$

where

$$m{A} = egin{bmatrix} 2 & 1 \ 3 & 1 \ 4 & 1 \end{bmatrix}, \quad m{b} = egin{bmatrix} 3 \ 4 \ 15 \end{bmatrix}, \quad m{x} = egin{bmatrix} m \ c \end{bmatrix}.$$

- The above is a least squares problem. Note that rank A = 2.
- We compute

$$(\boldsymbol{A}^T \boldsymbol{A})^{-1} = \frac{1}{6} \begin{bmatrix} 3 & -9 \\ -9 & 29 \end{bmatrix}, \qquad \boldsymbol{A}^T \boldsymbol{b} = \begin{bmatrix} 78 \\ 22 \end{bmatrix}.$$

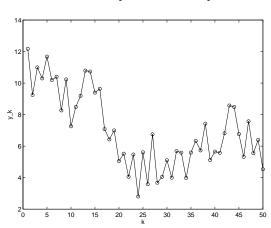
• Solution:

$$\boldsymbol{x}^* = \begin{bmatrix} m^* \\ c^* \end{bmatrix} = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{b} = \begin{bmatrix} 6 \\ -32/3 \end{bmatrix}.$$

Example: Signal representation

• Given: a discrete time signal

$$\boldsymbol{b} = [b_1, b_2, \dots, b_m]^T.$$



- Want to "represent" this signal using other prespecified signals.
- Specifically, want to write this signal as

$$b \approx x_1 s^{(1)} + x_2 s^{(2)} + \dots + x_n s^{(n)},$$

where $s^{(1)}, \dots, s^{(n)}$ are prespecified signals.

- What coefficients x_1, \ldots, x_n should we use?
- Examples of prespecified signals: sinusoids (Fourier), square waves, wavelets, sigmoids (neural nets).
- Specific example: (Haar basis)

$$s^{(1)} = [1, -1, 1, -1, 1, -1, 1, -1]^T$$

$$s^{(2)} = [1, 1, -1, -1, 1, 1, -1, -1]^T$$

$$s^{(3)} = [1, 1, 1, 1, -1, -1, -1, -1]^T.$$

- Note that the above signals are mutually orthogonal.
- Formulate as least squares problem.
- Want to find x_1, \ldots, x_n to minimize

$$\|(x_1\mathbf{s}^{(1)}+x_2\mathbf{s}^{(2)}+\cdots+x_n\mathbf{s}^{(n)})-\mathbf{b}\|^2$$
.

• Define

$$oldsymbol{A} = \begin{bmatrix} oldsymbol{s}^{(1)}, oldsymbol{s}^{(2)}, \dots, oldsymbol{s}^{(n)} \end{bmatrix}, \ oldsymbol{x} = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}.$$

- Objective function becomes $\|Ax b\|^2$.
- To find the solution, we first compute $A^T A$.
- Note that the (i, j)th entry of $\mathbf{A}^T \mathbf{A}$ is

$$\left\langle oldsymbol{s}^{(i)}, oldsymbol{s}^{(j)}
ight
angle = oldsymbol{s}^{(i)T} oldsymbol{s}^{(j)}.$$

• We use the following identities:

$$m{s}^{(i)T}m{s}^{(j)} = \sum_{k=1}^m s_k^{(i)} s_k^{(j)} = 0 \text{ for } i \neq j$$
 $m{s}^{(i)T}m{s}^{(i)} = \sum_{k=1}^m (s_k^{(i)})^2 = m.$

• With the aid of the previous identities, we find that

$$m{A}^Tm{A} = mm{I}_n = egin{bmatrix} m & & 0 \\ & \ddots & \\ 0 & & m \end{bmatrix}$$

which is clearly nonsingular, with inverse

$$(\boldsymbol{A}^T\boldsymbol{A})^{-1} = \frac{1}{m}\boldsymbol{I}_n.$$

• We next compute $A^T b$:

$$m{A}^Tm{b} = egin{bmatrix} m{s}^{(1)T}m{b} \ dots \ m{s}^{(n)T}m{b} \end{bmatrix}.$$

• The solution is

$$\boldsymbol{x}^* = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{b} = \frac{1}{m} \begin{bmatrix} \boldsymbol{s}^{(1)T} \boldsymbol{b} \\ \vdots \\ \boldsymbol{s}^{(n)T} \boldsymbol{b} \end{bmatrix}.$$

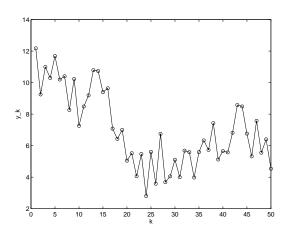
• Hence, the *i*th component is:

$$x_i^* = \frac{1}{m} \mathbf{s}^{(i)T} \mathbf{b} = \frac{1}{m} \sum_{k=1}^m s_k^{(i)} b_k.$$

• Interpretation: x_i^* is the "correlation" between the signals b and $s^{(i)}$.

Example: Linear system identification

• Consider a discrete time signal, $\{y_k\}$. (E.g., speech signal, stock price, etc.)



• We model the signal using a linear model:

$$y_k = a_1 y_{k-1} + a_2 y_{k-2}$$

Name: second order autoregressive (or AR(2)) model.

- Given measurements of y, we want to determine (estimate) the values of a_1 and a_2 .
- Estimate \equiv parameter values that minimize total squared error.
- Suppose we are given $y_1, y_2, \ldots, y_{m+2}$.
- To formulate as a least squares problem, we write objective function as

$$f(a_1, a_2) = \sum_{k=3}^{m+2} (a_1 y_{k-1} + a_2 y_{k-2} - y_k)^2.$$

• So, define

$$oldsymbol{x} = egin{bmatrix} a_1 \ a_2 \end{bmatrix}, \qquad oldsymbol{A} = egin{bmatrix} y_2 & y_1 \ y_3 & y_2 \ dots & dots \ y_{m+1} & y_m \end{bmatrix}, \qquad oldsymbol{b} = egin{bmatrix} y_3 \ y_4 \ dots \ y_{m+2} \end{bmatrix}.$$

- Objective function becomes $f(x) = ||Ax b||^2$.
- Solution: $\boldsymbol{x}^* = (\boldsymbol{A}^T \boldsymbol{A})^{-1} \boldsymbol{A}^T \boldsymbol{b}$.
- We have

$$m{A}^Tm{A} = egin{bmatrix} \sum_{i=1}^m y_{i+1}^2 & \sum_{i=1}^m y_i y_{i+1} \\ \sum_{i=1}^m y_i y_{i+1} & \sum_{i=1}^m y_i^2 \end{bmatrix}, \ m{A}^Tm{b} = egin{bmatrix} \sum_{i=1}^m y_{i+1} y_{i+2} \\ \sum_{i=1}^m y_i y_{i+2} \end{bmatrix}. \end{cases}$$

• Solution:

$$\begin{bmatrix} a_1^* \\ a_2^* \end{bmatrix} = \frac{1}{(\overline{Y_0^2})(\overline{Y_1^2}) - (\overline{Y_0Y_1})^2} \begin{bmatrix} (\overline{Y_0^2})(\overline{Y_1Y_2}) - (\overline{Y_0Y_1})(\overline{Y_0Y_2}) \\ (\overline{Y_1^2})(\overline{Y_0Y_2}) - (\overline{Y_0Y_1})(\overline{Y_1Y_2}) \end{bmatrix},$$

where

$$\overline{Y_j Y_k} = \sum_{i=1}^m y_{i+j} y_{i+k}.$$

• Can easily generalize the previous technique to autoregressive models of higher order:

$$y_n = a_1 y_{n-1} + a_2 y_{n-2} + \dots + a_p y_{n-p}$$

AR(p) model.

• We can even include external inputs:

$$y_n = a_1 y_{n-1} + a_2 y_{n-2} + \dots + a_p y_{n-p} + b_1 u_{n-1} + \dots + b_a u_{n-a}$$

(autoregressive moving average (ARMA(p,q)) model).

Recursive least squares (RLS) algorithm (§12.2)

- Consider the line fitting problem.
- Given data $(t_0, y_0), (t_1, y_1), (t_2, y_2)$, we can find line of best fit: m^*, c^* . We use

$$m{A} = egin{bmatrix} t_0 & 1 \ t_1 & 1 \ t_2 & 1 \end{bmatrix}, \qquad m{b} = egin{bmatrix} y_0 \ y_1 \ y_2 \end{bmatrix}.$$

Version: Initial distribution

- Solution: $[m^*, c^*]^T = (A^T A)^{-1} A^T b$.
- Suppose we are now given another data point (t_3, y_3) . Wish to find the line of best fit through all the data points so far.
- New matrices have extra row:

$$m{A} = egin{bmatrix} t_0 & 1 \ t_1 & 1 \ t_2 & 1 \ t_3 & 1 \end{bmatrix}, \qquad m{b} = egin{bmatrix} y_0 \ y_1 \ y_2 \ y_3 \end{bmatrix}.$$

- We have already calculated m^* and c^* for the first three data points.
- RLS: we can update the previous m^* and c^* to incorporate the new data point (without having to calculate the new m^* and c^* from scratch).

Formulation of RLS algorithm

• Given A_0 and $b^{(0)}$, suppose we solve the least squares problem

minimize
$$\| \boldsymbol{A}_0 \boldsymbol{x} - \boldsymbol{b}^{(0)} \|^2$$
.

- Solution: $x^{(0)} = (A_0^T A_0)^{-1} A_0^T b^{(0)}$.
- For simplicity, write $G_0 = A_0^T A_0$.
- So, solution is

$$\boldsymbol{x}^{(0)} = \boldsymbol{G}_0^{-1} \boldsymbol{A}_0^T \boldsymbol{b}^{(0)}.$$

- Suppose we now add an extra "data point": (a_1, b_1) , where $a_1 \in \mathbb{R}^n$, $b_1 \in \mathbb{R}$.
- New matrices have extra row:

$$m{A}_1 = egin{bmatrix} m{A}_0 \ m{a}_1^T \end{bmatrix}, \qquad m{b}^{(1)} = egin{bmatrix} m{b}^{(0)} \ b_1 \end{bmatrix}.$$

• New problem

minimize
$$\|\boldsymbol{A}_1\boldsymbol{x}-\boldsymbol{b}^{(1)}\|^2$$
.

• New solution:

$$x^{(1)} = G_1^{-1} A_1^T b^{(1)}.$$

where $\boldsymbol{G}_1 = \boldsymbol{A}_1^T \boldsymbol{A}_1$.

• Goal: write $x^{(1)}$ in terms of $x^{(0)}$, G_0 , and the new data (a_1, b_1) .

• Now,

$$egin{array}{lll} oldsymbol{G}_1 &=& egin{bmatrix} oldsymbol{A}_0^T & oldsymbol{a}_1 \end{bmatrix} egin{bmatrix} oldsymbol{A}_0^T & oldsymbol{a}_1 oldsymbol{A}_1 oldsymbol{a}_1^T \ &=& oldsymbol{G}_0 + oldsymbol{a}_1 oldsymbol{a}_1^T. \end{array}$$

- Hence, we have a formula for G_1 in terms of G_0 and a_1 .
- Also,

$$egin{aligned} oldsymbol{A}_1^T oldsymbol{b}^{(1)} &=& \left[oldsymbol{A}_0^T oldsymbol{a}_1
ight] egin{bmatrix} oldsymbol{b}^{(0)} & oldsymbol{a}_1 oldsymbol{b}^{(0)} \ & b_1 \end{bmatrix} \ &=& oldsymbol{A}_0^T oldsymbol{b}^{(0)} + oldsymbol{a}_1 b_1. \end{aligned}$$

• We now write

$$egin{array}{lcl} m{A}_0^T m{b}^{(0)} & = & m{G}_0 m{G}_0^{-1} m{A}_0^T m{b}^{(0)} \ & = & m{G}_0 m{x}^{(0)} \ & = & (m{G}_1 - m{a}_1 m{a}_1^T) m{x}^{(0)} \ & = & m{G}_1 m{x}^{(0)} - m{a}_1 m{a}_1^T m{x}^{(0)}. \end{array}$$

• Hence,

$$egin{array}{lll} m{x}^{(1)} & = & m{G}_1^{-1} m{A}_1^T m{b}^{(1)} \ & = & m{G}_1^{-1} \left(m{A}_0^T m{b}^{(0)} + m{a}_1 b_1
ight) \ & = & m{G}_1^{-1} \left(m{G}_1 m{x}^{(0)} - m{a}_1 m{a}_1^T m{x}^{(0)} + m{a}_1 b_1
ight) \ & = & m{x}^{(0)} + m{G}_1^{-1} m{a}_1 \left(b_1 - m{a}_1^T m{x}^{(0)}
ight), \end{array}$$

where G_1 can be calculated using

$$\boldsymbol{G}_1 = \boldsymbol{G}_0 + \boldsymbol{a}_1 \boldsymbol{a}_1^T.$$

- ullet Ideally, we need an update formula for G_1^{-1} .
- Use Sherman-Morrison formula:

$$(A + uv^T)^{-1} = A^{-1} - \frac{(A^{-1}u)(v^TA^{-1})}{1 + v^TA^{-1}u}.$$

• We have

$$egin{array}{lcl} m{G}_1^{-1} &=& (m{G}_0 + m{a}_1 m{a}_1^T)^{-1} \ &=& m{G}_0^{-1} - rac{m{G}_0^{-1} m{a}_1 m{a}_1^T m{G}_0^{-1}}{1 + m{a}_1^T m{G}_0^{-1} m{a}_1}. \end{array}$$

For simplicity of notation, we rewrite G^{-1} as P.

- We now have an update formula for updating from $x^{(0)}$ and P_0 to $x^{(1)}$ and P_1 , given a_1 and b_1 .
- We can generalize the above to $k = 2, 3, 4, \ldots$

Summary of RLS algorithm

$$egin{array}{lcl} m{P}_{k+1} & = & m{P}_k - rac{m{P}_k m{a}_{k+1} m{a}_{k+1}^T m{P}_k}{1 + m{a}_{k+1}^T m{P}_k m{a}_{k+1}} \ m{x}^{(k+1)} & = & m{x}^{(k)} + m{P}_{k+1} m{a}_{k+1} \left(b_{k+1} - m{a}_{k+1}^T m{x}^{(k)}
ight). \end{array}$$

- ullet The term $b_{k+1} oldsymbol{a}_{k+1}^T oldsymbol{x}^{(k)}$ is called the *innovation*.
- If innovation is zero, then $x^{(k+1)} = x^{(k)}$.

Example: Line fitting

• Recall line fitting example. Original data:

i	0	1	2
t_i	2	3	4
y_i	3	4	15

• We have

$$m{A} = egin{bmatrix} 2 & 1 \ 3 & 1 \ 4 & 1 \end{bmatrix}, \quad m{b} = egin{bmatrix} 3 \ 4 \ 15 \end{bmatrix}, \quad m{x} = egin{bmatrix} m \ c \end{bmatrix}.$$

• We compute

$$(\boldsymbol{A}^T \boldsymbol{A})^{-1} = \frac{1}{6} \begin{bmatrix} 3 & -9 \\ -9 & 29 \end{bmatrix}, \qquad \boldsymbol{A}^T \boldsymbol{b} = \begin{bmatrix} 78 \\ 22 \end{bmatrix}.$$

• Hence,

$$oldsymbol{x}^* = \left[egin{array}{c} m^* \ c^* \end{array}
ight] = (oldsymbol{A}^Toldsymbol{A})^{-1}oldsymbol{A}^Toldsymbol{b} = \left[egin{array}{c} 6 \ -32/3 \end{array}
ight].$$

- Given a new data point: $(t_3, y_3) = (5, 18)$.
- Recursive formulation:

$$m{P}_0 = rac{1}{6} \begin{bmatrix} 3 & -9 \\ -9 & 29 \end{bmatrix}, \qquad \quad m{x}^{(0)} = \begin{bmatrix} 6 \\ -32/3 \end{bmatrix}$$
 $m{a}_1 = \begin{bmatrix} 5 \\ 1 \end{bmatrix}, \qquad \quad b_1 = 18.$

• Hence,

$${m P}_1 = {m P}_0 - rac{{m P}_0 {m a}_1 {m a}_1^T {m P}_0}{1 + {m a}_1^T {m P}_0 {m a}_1} = egin{bmatrix} 0.2 & -0.7 \ -0.7 & 2.7 \end{bmatrix},$$

and

$$\boldsymbol{x}^{(1)} = \boldsymbol{x}^{(0)} + \boldsymbol{P}_1 \boldsymbol{a}_1 \left(b_1 - \boldsymbol{a}_1^T \boldsymbol{x}^{(0)} \right) = \begin{bmatrix} 5.6 \\ -9.6 \end{bmatrix}.$$

Matlab demo

Related to Kalman filtering.