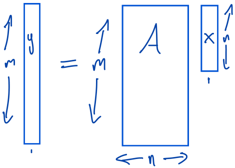
# 2: Least-squares

- approximate solutions of **overdetermined** systems
  - projection and orthogonality
  - QR decomposition
  - BLUE property
- least-norm solutions of **underdetermined** systems

# Overdetermined system of linear equations

consider the system of equations

$$y = Ax, \quad \text{where } A \in \mathbb{R}^{m \times n} \text{ with } m > n$$




- more equations (rows of $A, y$) than unknowns ($x$)
- typically no solution: no $x$ s.t. $y = Ax$

instead, find $x$ s.t. $y \approx Ax$:

- define the **residual** $r = Ax - y$
- make $r$ small by minimizing $\|r\|$
- denote $x_{\rm ls}$ as the $x$ that minimizes $\|r\|$: **least-squares approximate solution**

# Norms

the **Euclidean** norm of a vector $z \in \mathbb{R}^n$

$$\|z\| = \sqrt{z_1^2 + z_2^2 + \cdots + z_n^2} = \sqrt{z^T z}$$

- $\|z\|$ measures the length of a vector (from the origin)
- $\|z - x\|$ measures the distance between vectors $z$ and $x$

more generally, a norm is *any* function $f : V \to \mathbb{R}$ that satisfies

1. $f(x) \geq 0$ for all $x \in V$ with $f(x) = 0$ if and only if $x = 0$
2. $f(x + y) \leq f(x) + f(y)$ for all $x, y \in V$
3. $f(\lambda x) = |\lambda| f(x)$ for all $\lambda \in \mathbb{C}$ and $x \in V$

when satisfied, we replace $f$ with $\| \cdot \|$

# Least-squares approximate solution

- for simplicity, assume $\mathrm{rank}(A) = n$
- finding $x_{\mathrm{ls}}$ is an unconstrained optimization problem:

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

- set gradient w.r.t. $x$ to zero:

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

- produces the **normal equations**:

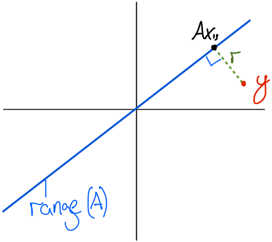
$$A^T A x = A^T y$$

- by assumption the inverse exists, giving

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

# Geometry

- $Ax_{\text{ls}}$ is the point in $\text{range}(A)$ closest to $y$
- $Ax_{\text{ls}}$ is the **projection** of $y$ onto the **subspace** $\text{range}(A)$
- the projection is **orthogonal** (see later)




the range of $A \in \mathbb{R}^{m \times n}$ is defined as

$$\text{range}(A) = \{Ax \mid x \in \mathbb{R}^n\} \subseteq \mathbb{R}^m$$

- the set of vectors that can be reached by applying $A$ to vectors in $\mathbb{R}^n$

in summary, in general there is no $x$ such that $y = Ax$

- the least-squares approximate solution is

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

  provides the smallest residual error in the Euclidean norm

- $x_{\mathrm{ls}}$ is a linear function of $y$

- *if* $A$ is square ($m = n$), then $x_{\mathrm{ls}} = A^{-1} y$

- *if* $y \in \mathrm{range}(A)$, then $y = A x_{\mathrm{ls}}$

- $A^\dagger = (A^T A)^{-1} A^T$ is called the **pseudo-inverse** of $A$

- $A^\dagger$ is a **left inverse** of (full rank, tall) $A$, *i.e.*, it satisfies

$$A^\dagger A = I$$

- many other left inverses exist: $BA = I \iff B$ is a left inverse

# Orthogonality

the **unsigned angle** between two vectors $x$ and $y$ in $\mathbb{R}^n$ is defined as

$$\theta = \cos^{-1}\left(\frac{x^T y}{\|x\|\|y\|}\right)$$

thus $x^T y = \|x\|\|y\| \cos\theta$

the term $x^T y$ defines an **inner product** on $\mathbb{R}^n$, usually denoted by $\langle x, y\rangle$

special cases:

- $x$ and $y$ are aligned: $\theta = 0$, then $x^T y = \|x\|\|y\|$
- $x$ and $y$ are antialigned: $\theta = \pi$, then $x^T y = -\|x\|\|y\|$
- $x$ and $y$ are orthogonal: $\theta = \pm\pi/2$, then $x^T y = 0$

orthogonal vectors are often denoted by $x \perp y$

# Projection onto a subspace

$Ax_{\text{ls}}$ is the point in $\text{range}(A)$ closest to $y$, it is the projection of $y$ onto $\text{range}(A)$:

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

- $\mathcal{P}_{\text{range}(A)}$ is a linear function:

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

- the matrix $A(A^T A)^{-1} A^T$ is called the **projection matrix** (associated with $\text{range}(A)$) or **projector**

**properties of projection matrices**

- If $P$ is a projecor (onto $\mathcal{V}$), then $I - P$ is a projector matrix
- $I - P$ projects on $\mathcal{V}^\perp$
- $P^2 = P$ and so $(I - P)P = 0 = P(I - P)$

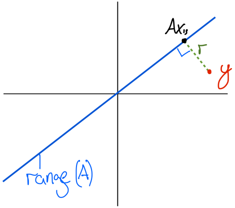
# Orthogonal projections

the optimal residual

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

is orthogonal to $\text{range}(A)$: to see this, observe that for all $z \in \mathbb{R}^n$,

$$\langle r, Az\rangle = y^T(A(A^TA)^{-1}A^T - I)^T Az = 0, \quad \text{i.e., } r \perp \text{range}(A)$$




**properties of orthogonal projectors**

- a projector $P$ provides an orthogonal projection *if and only if* $P = P^T$

# Optimality of $x_{\mathrm{ls}}$

for any $x \in \mathbb{R}^n$, we have

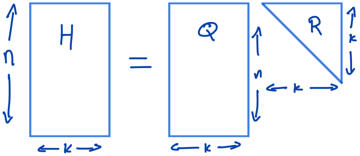
$$\begin{aligned} \|Ax - y\|^2 &= \|(Ax_{\mathrm{ls}} - y) + A(x - x_{\mathrm{ls}})\|^2 \\ &= \|Ax_{\mathrm{ls}} - y\|^2 + \|A(x - x_{\mathrm{ls}})\|^2 \end{aligned}$$

therefore, for any $x \neq x_{\mathrm{ls}}$, $\|Ax - y\| > \|Ax_{\mathrm{ls}} - y\|$

show using properties of norms and the fact that $r \perp \mathrm{range}(A)$

# QR decomposition

given $H \in \mathbb{R}^{n\times k}$, $n \geq k$, $\mathrm{rank}(H) = k$, then $H = QR$




- dimensions: $Q \in \mathbb{R}^{n\times k}$, $R \in \mathbb{R}^{k\times k}$
- $Q^TQ = I_k$, $R$ is upper-triangular
- $R_{ii}$'s are non-zero
- most definitions require $R_{ii} > 0$, in this case, $Q$ and $R$ are unique
- express $Q$ in terms of it's columns: $Q = \begin{bmatrix} q_1 & q_2 & \dots & q_k \end{bmatrix}$, the column vectors form an **orthonormal** set:

$$\|q_i\| = 1, \quad q_i^Tq_j = 0 \text{ if } i \neq j$$

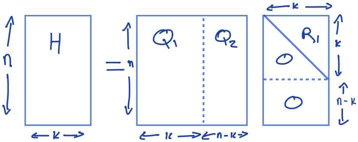
- columns of $Q$ form an **orthonormal basis** for $\mathrm{range}(H)$

# Full QR decomposition

the **full** QR decomposition of a full-rank matrix $H \in \mathbb{R}^{n\times k}$ is defined as

$$H = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix}, \quad \text{where } [Q_1\ Q_2] \in \mathbb{R}^{n\times n} \text{ is orthogonal,}$$

and $R_1$ is upper-triangular and invertible




- $H = Q_1 R_1$ is the QR factorization defined previously
- the additional $n-k$ columns that form $Q_2$ are orthogonal to $\mathrm{range}(H)$
- `>>[Q,R]=qr(H)  %gives full qr factorization`
- `>>[Q,R]=qr(H,0)  %gives qr factorization`

## Notes

- the above QR decompositions assume $H$ is full-rank and tall
- rank deficiency produces non-invertible $R$ ($R_1$)
- every tall $m \times n$ matrix has a full QR decomposition, and hence a QR decomposition
- every full-rank, tall matrix has a unique QR decomposition with an invertible $R$
- the projector $A(A^TA)^{-1}A^T$ written in terms of the QR factorization is $QQ^T$

# Solving least-squares via QR decomposition

assuming $A$ is full rank and tall, rewrite $x_{\text{ls}}$ in terms of QR factorization $A = QR$

$$\begin{aligned} x_{\text{ls}} &= (A^T A)^{-1} A^T y \\ &= ((QR)^T (QR))^{-1} (QR)^T y \\ &= R^{-1} Q^T y \end{aligned}$$

**Algorithm**

1. compute QR factorization $A = QR$
2. compute $w = Q^T y$
3. solve $Rx = w$ `// triangular system, use back substitution`

there are many ways to compute $x_{\text{ls}}$:

```
>>[Q,R]= qr(A,0)
>>xls = R\(Q'*y)
```

# Least-squares via full QR decomposition

full QR factorization of $A$:

$$A = \begin{bmatrix} Q_1 & Q_2 \end{bmatrix} \begin{bmatrix} R_1 \\ 0 \end{bmatrix}, \quad Q = [Q_1 \ Q_2] \in \mathbb{R}^{m \times m} \text{ is orthogonal,}$$

- multiplication by an orthogonal matrix doesn't affect the norm:

$$\|Uz\|^2 = z^T U^T U z = z^T z = \|z\|^2$$

- substitute QR factorization to get

$$\begin{aligned}
\|Ax - y\|^2 &= \left\| [Q_1 \ Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - y \right\|^2 \\
&= \left\| [Q_1 \ Q_2]^T [Q_1 \ Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} x - [Q_1 \ Q_2]^T y \right\|^2 \\
&= \left\| \begin{bmatrix} R_1 x - Q_1^T y \\ -Q_2^T y \end{bmatrix} \right\|^2 \\
&= \|R_1 x - Q_1^T y\|^2 + \|Q_2^T y\|^2
\end{aligned}$$

recall, least-squares objective is to minimize $\|r\|^2$

- shown that $\|r\|^2 = \|Ax - y\|^2 = \|R_1 x - Q_1^T y\|^2 + \|Q_2^T y\|^2$

no optimization performed yet - this involves selecting $x$:

- clearly selecting $x = x_{\mathrm{ls}} = R_1^{-1} Q_1^T y$ achieves optimality

the residual at $x_{\mathrm{ls}}$ is

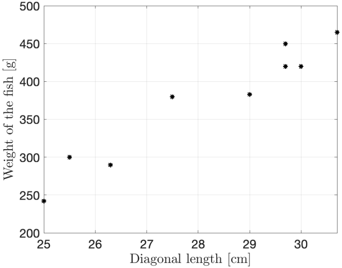
$$Ax_{\mathrm{ls}} - y = -Q_2 Q_2^T y$$

# Example: linear regression

objective: estimate the weight of a fish based on its width

- sample size $N = 10$
- data consists of points $(x_i, y_i)$ where $x_i$ is the diagonal width and $y_i$ the weight

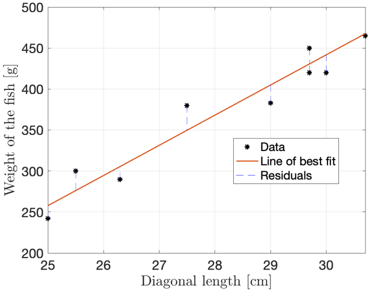
| diagonal width [cm] | weight [g] |
|---|---|
| 25 | 242 |
| 26.3 | 290 |
| 25.5 | 300 |
| 29 | 383 |
| 32 | 530 |
| 29.7 | 450 |
| 29.7 | 420 |
| 30 | 420 |
| 27.5 | 380 |
| 30.7 | 465 |




suggests an approximately linear relationship: $y \approx mx + b$, find $m, b$ that minimize

$$\underset{m,b}{\text{minimize}} \quad \sum_{i=1}^{N} (mx_i + b - y_i)^2$$

solving the least squares problem provides estimates $(\bar{m}, \bar{b}) = (36.8, -662.3)$




line of best fit, $y = 36.8x - 662.3$ minimizes the sum of the square of the residuals

# Estimation

many signal reconstruction and estimation problems take the form

$$y = Ax + v, \quad A \in \mathbb{R}^{m \times n}, \quad m \geq n$$

- $x \in \mathbb{R}^n$ is the vector we want to estimate/recover/reconstruct
- $y \in \mathbb{R}^m$ is the sensor measurement/observable
- $v \in \mathbb{R}^m$ is the unknown measurement error/noise

If $v$ was known exactly, or $v = 0$, then any left inverse of $A$ recovers $x$

$$y = Ax + v = Ax \quad \Rightarrow \quad By = BAx = x$$

one such choice is $B = A^\dagger$

# Least-squares estimation

choose an estimate $\hat{x}$ (of $x$) that minimizes

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

captures the magnitude of the difference between

- the observation
- what would be observed if we could run the model with no noise/error

a **linear estimator** is any mapping from $y$ to $\hat{x}$ that can be written as $\hat{x} = By$

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

# Best Linear Unbiased Estimate (BLUE) property

- **linear:** map from observation to estimate is represented by a linear function

$$f(\alpha x + \beta y) = \alpha f(x) + \beta f(y), \quad \alpha, \beta \in \mathbb{R}, \quad x, y \in \mathbb{R}^l$$

- **unbiased:** no estimation error when there is no noise:

$$\hat{x} = x \text{ when } v = 0$$

estimation error of an estimator is $x - \hat{x}$, for **unbiased linear estimators**:

$$x - \hat{x} = x - By = -Bv$$

clearly, we should make $B$ "small" subject to the constraint $BA = I$

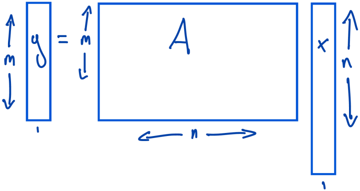
- **best**: $A^\dagger = (A^T A)^{-1} A^T$ is the smallest left inverse of $A$ in the sense that: for any $B$ such that $BA = I$, it can be shown that

$$\|B\|_F^2 \geq \|A^\dagger\|_F^2$$

# Underdetermined systems of linear equations

consider the system of equations

$$y = Ax, \quad \text{where } A \in \mathbb{R}^{m \times n} \text{ with } m < n$$




- more unknowns ($x$) than equations (rows of $A, b$)
- $x$ is *underspecified*; many (infinite) choices of $x$ satisfy the equation
- $A$ has a nontrivial nullspace

assume that $\operatorname{rank}(A) = m$, so for every $y \in \mathbb{R}^m$, there is a solution

# Nullspace

the **nullspace** of the matrix $A \in \mathbb{R}^{m\times n}$ is defined as

$$\operatorname{null}(A) = \{x \in \mathbb{R}^n \mid Ax = 0\} \subseteq \mathbb{R}^n$$

- the set of vectors mapped to $0$ by the map $Az$
- $\operatorname{null}(A)$ characterizes ambiguity in $x$ when $y = Ax$:

$$y = Ax \text{ and } z \in \operatorname{null} A \quad \Rightarrow \quad y = A(x+z)$$

- conversely, if $x$ and $\bar{x}$ are solutions, then $\bar{x} = x + z$ with $z \in \operatorname{null}(A)$

all dimensions are related:

$$n = \operatorname{rank}(A) + \dim\left(\operatorname{null}(A)\right)$$

# Nullspace parameterization of solutions

assuming $A$ is wide and full-rank, set of all solutions has the form

$$\{x \mid y = Ax\} = \{x_{\mathrm{p}} + z \in \mathrm{null}(A) \text{ and } y = Ax_{\mathrm{p}}\}$$

where $x_{\mathrm{p}}$ is any "particular" solution

- the vextor $z$ characterizes the choices available
- the dimension of the nullspace gives the number of degrees of freedom in the solution
- choose $z$ to optimize over solutions

# Least-norm solution

a particular solution of interest is

$$x_{\mathrm{ln}} = A^T(AA^T)^{-1}y$$

which can be verified by direct substitution: $Ax_{\mathrm{ln}} = y$

the solution $x_{\mathrm{ln}}$ solves the constrained optimization problem

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

($x_{\mathrm{ln}}$ is the unique solution to this optimization problem)

# Optimal least-norm solution

we've directly verified that $x_{\text{ln}}$ is feasible, now show it's optimal

suppose $y = Ax$, then we must have $A(x - x_{\text{ln}}) = 0$

consider the inner product

$$\begin{aligned}(x - x_{\text{ln}})^T x_{\text{ln}} &= (x - x_{\text{ln}})^T A^T (AA^T)^{-1} y \\ &= (A(x - x_{\text{ln}}))^T (AA^T)^{-1} y \\ &= 0\end{aligned}$$

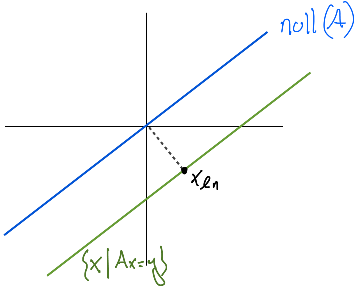
the result above shows $(x - x_{\text{ln}}) \perp x_{\text{ln}}$, so

$$\|x\|^2 = \|x_{\text{ln}} + x - x_{\text{ln}}\|^2 = \|x_{\text{ln}}\|^2 + \|x - x_{\text{ln}}\|^2 \geq \|x_{\text{ln}}\|^2$$

which means $x_{\text{ln}}$ has the smallest norm amongst all solutions

# Geometry

- $x_{\text{ln}}$ is the **orthogonal projection** of $0$ onto the set $\{x \mid Ax = y\}$
- $x_{\text{ln}} \perp \text{null}(A)$




- $A^\dagger - A^T(AA^T)^{-1}$ is a **right inverse** of (full rank, wide) $A$: $AA^\dagger = I$

# Solution via QR factorization

apply a QR decomposition to $A^T$, so that $A^T = QR$

assumed that $m < n$ and $\mathrm{rank}(A) = m$, then

- $R \in \mathbb{R}^{m \times m}$ is invertible
- $Q \in \mathbb{R}^{n \times m}$ with $Q^T Q = I_m$

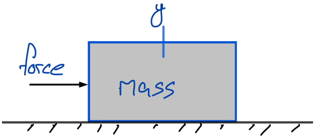
substituting the factorization into $x_{\mathrm{ln}} = A^T(AA^T)^{-1}y$ we see that

$$x_{\mathrm{ln}} = QR^{-T}y \quad \text{and} \quad \|x_{\mathrm{ln}}\| = \|R^{-T}y\|$$

note: $Z^{-T}$ is shorthand for $(Z^T)^{-1}$

# Example: optimal mass transfer

unit mass subject to force $x_i$ at time $i$, initially at rest




- $y_t$ and $v_t$: position and velocity at time $t$
- $x_t$: constant force applied for time interval $[t, t+1]$

dynamics given by

$$
\begin{aligned}
v_{t+1} - v_t &= x_t \quad \text{(force equals } \Delta v\text{)} \\
y_{t+1} - y_t &= v_t \quad \text{(velocity equals } \Delta y\text{)}
\end{aligned}
$$

objective: choose force $x$ to move mass 1 unit of distance in $10$s, leaving it at rest

[Example from Boyd & Lall]

- initial conditions: $y_0 = 0$, $v_0 = 0$
- target: $y_{10} = 1$, $v_{10} = 0$
- expand the system dynamics and express target in terms of initial conditions and the $x_i$s:

$$\begin{bmatrix} v_{10} \\ y_{10} \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & \dots & 1 & 1 \\ 9 & 8 & 7 & \dots & 1 & 0 \end{bmatrix} \begin{bmatrix} x_0 \\ x_1 \\ \vdots \\ x_9 \end{bmatrix} + \begin{bmatrix} v_0 \\ y_0 \end{bmatrix}$$

solve for least-norm solution

simulated solution