Basics in Applied Mathematics – Part I: Numerics

Lecture 4: Least squares problems and the QR decomposition

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Last time, and today

Last time: the proofs behind Chapters 1–2 — the norm formulas, the perturbation bound for $Ax = b$, the small pivot, SPD matrices.

Today: more equations than unknowns — $Ax = b$ has no solution, so make $\|Ax - b\|_2$ as small as possible.

After this lecture you can

(i) formulate data fitting as a linear least squares problem and characterise its solutions by the normal equations,

(ii) explain the geometry of least squares (orthogonal projection),

(iii) explain why solving the normal equations squares the condition number,

(iv) construct a QR decomposition by Householder reflections, use it for least squares problems with full column rank, and explain why it is numerically reliable.

3.1 Data fitting · 3.2 Normal equations and geometry · 3.3 Orthogonal matrices and QR
3.5 Householder reflections

Measurements y_i at times t_i, $i = 1, \dots, m$; model $y(t) = x_1\phi_1(t) + \cdots + x_n\phi_n(t)$ with known ϕ_j (e.g. $1, t, t^2$), unknown x_j. One equation per measurement:

$$\sum_{j=1}^{n} \phi_j(t_i)\, x_j = y_i \quad \Longleftrightarrow \quad Ax = b, \qquad A = \big(\phi_j(t_i)\big)_{i,j} \in \mathbb{R}^{m\times n}, \quad b = (y_1, \dots, y_m)^\top.$$

$m \gg n$, measurement errors, approximate model $\Rightarrow$ in general **no solution** ($b \notin \operatorname{Im} A$). Look for the x that fits best.

Definition 3.1 (linear least squares problem)

$A \in \mathbb{R}^{m\times n}$, $b \in \mathbb{R}^m$. Find $x^* \in \mathbb{R}^n$ with

$$\|Ax^* - b\|_2 = \min_{x\in\mathbb{R}^n} \|Ax - b\|_2.$$

Such an x^* is a **least squares solution** of $Ax = b$; $r := b - Ax^*$ is the **residual**.

Remark 3.2. Why the Euclidean norm: a *linear* characterisation of the solutions (Theorem 3.4) and a geometric meaning (projection).

Example 3.3: a projectile

Height $y(t) = v_y\, t - \frac{1}{2} g\, t^2$ (v_y vertical velocity, g gravitational acceleration); unknowns $x = (v_y, g)^\top$.

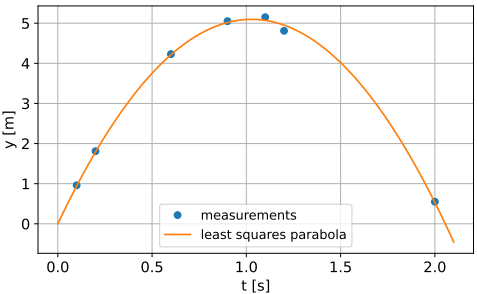
Linear in the parameters, quadratic in t: $\phi_1(t) = t$, $\phi_2(t) = -t^2/2$.

Seven measurements (t in s, y in m):

$t = (0.1,\ 0.2,\ 0.6,\ 0.9,\ 1.1,\ 1.2,\ 2.0)$,
$y = (0.96,\ 1.81,\ 4.23,\ 5.05,\ 5.15,\ 4.81,\ 0.55)$.

`numpy.linalg.lstsq`: $v_y = 9.918$ m/s, $g = 9.652$ m/s^2, $\|r\|_2 = 0.170$.

$g \approx 9.65$ instead of 9.81: the fit is only as good as the data.



The geometry of least squares

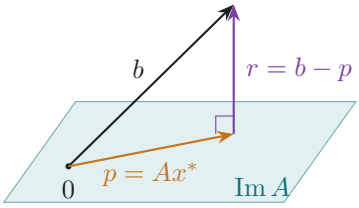
Linear algebra: $A \in \mathbb{R}^{m\times n}, \operatorname{Im} A = \{Ax : x \in \mathbb{R}^n\} \subset \mathbb{R}^m$, $\ker A^\top = \{y \in \mathbb{R}^m : A^\top y = 0\}$, and $(\operatorname{Im} A)^\perp = \ker A^\top$; hence

$$\mathbb{R}^m = \operatorname{Im} A \oplus \ker A^\top : \tag{3.1}$$

every $b = p + q$ uniquely with $p \in \operatorname{Im} A$, $q \in \ker A^\top$, $p \perp q$.

Pythagoras: $u \perp w \;\Rightarrow\; \|u + w\|_2^2 = \|u\|_2^2 + \|w\|_2^2$.

Question: which x minimises $\|Ax - b\|_2$? Think of $\{Ax\}$ as a plane through the origin and b as a point off the plane.



the residual is *normal* to $\operatorname{Im} A$

Theorem 3.4 (normal equations)

Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then $x^* \in \mathbb{R}^n$ is a least squares solution of $Ax = b$ if and only if

$$A^\top A\, x^* = A^\top b \qquad \textbf{(normal equations)}.$$

A least squares solution always exists. It is unique if and only if $\operatorname{rank} A = n$ (the columns are linearly independent, $\ker A = \{0\}$), and then $A^\top A$ is SPD and $x^* = (A^\top A)^{-1} A^\top b$.

Blackboard: proof — decomposition (3.1) and Pythagoras.

- $Ax^* = p$ is the **orthogonal projection** of b onto $\operatorname{Im} A$; $r = b - Ax^* = q$ is orthogonal to all columns of A: $A^\top r = 0$
- p and r are always unique — even when x^* is not
- $\operatorname{rank} A = n$: $P := A(A^\top A)^{-1} A^\top$ satisfies $P^2 = P$, $P^\top = P$, $Ax^* = Pb$

Example 3.5: by hand

$A = \begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 0 & 1 \end{pmatrix}$, $b = \begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix}$: the columns of A span a plane in $\mathbb{R}^3$.

Recipe: $A^\top A = ?$ $\quad A^\top b = ?$ $\quad x^* = ?$

$$A^\top A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}, \quad A^\top b = \begin{pmatrix} 3 \\ 5 \end{pmatrix}, \quad x^* = \begin{pmatrix} 1/3 \\ 7/3 \end{pmatrix}; \quad p = Ax^* = \begin{pmatrix} 1/3 \\ 8/3 \\ 7/3 \end{pmatrix},$$

$$r = b - p = \tfrac{2}{3}\begin{pmatrix} 1 \\ -1 \\ 1 \end{pmatrix}, \quad A^\top r = 0, \quad \|r\|_2 = \frac{2}{\sqrt{3}}\,.$$

We will meet this example again, solved via a QR decomposition, after Theorem 3.13.

$\operatorname{rank} A = n$: $A^\top A$ is SPD $\Rightarrow$ Cholesky (Section 2.5). Cost: $A^\top A$ about mn^2 flops, Cholesky $\frac{1}{3}n^3$.

Definition 3.6 (condition number of a rectangular matrix)

$A \in \mathbb{R}^{m\times n}$ with full column rank; the eigenvalues of the SPD matrix $A^\top A$ are positive, and

$$\sigma_{\max}(A) := \sqrt{\lambda_{\max}(A^\top A)}, \qquad \sigma_{\min}(A) := \sqrt{\lambda_{\min}(A^\top A)}, \qquad \operatorname{cond}_2(A) := \frac{\sigma_{\max}(A)}{\sigma_{\min}(A)}.$$

$\sigma_{\max}(A) = \|A\|_2$ (Theorem 1.22); with $A^+ := (A^\top A)^{-1}A^\top$ (the map $b \mapsto x^*$) one has $\operatorname{cond}_2(A) = \|A\|_2\,\|A^+\|_2$, as in Definition 2.1.

Proposition 3.7

If $A \in \mathbb{R}^{m\times n}$ has full column rank, then $\operatorname{cond}_2(A^\top A) = \operatorname{cond}_2(A)^2$.

$\operatorname{cond}_2(A) = 10^8 \Rightarrow \operatorname{cond}_2(A^\top A) = 10^{16} \approx 1/u$: rounding errors of relative size u in $A^\top A$.

Example 3.9 (Läuchli): the normal equations can fail although $\operatorname{cond}_2(A) \ll 1/u$

$A = \begin{pmatrix} 1 & 1 \\ \varepsilon & 0 \\ 0 & \varepsilon \end{pmatrix}$, $0 < \varepsilon \ll 1$: $A^\top A = \begin{pmatrix} 1+\varepsilon^2 & 1 \\ 1 & 1+\varepsilon^2 \end{pmatrix}$ has the eigenvalues $2+\varepsilon^2$ and ε^2, so $\operatorname{cond}_2(A) = \sqrt{(2+\varepsilon^2)/\varepsilon^2} \approx \sqrt{2}/\varepsilon$; for $\varepsilon = 10^{-8}$: $\operatorname{cond}_2(A) \approx 1.4 \cdot 10^8$, far from $1/u \approx 9 \cdot 10^{15}$. **What can go wrong?**

$\mathrm{fl}(1+\varepsilon^2) = 1$ because $\varepsilon^2 = 10^{-16} < u$: the computed $A^\top A$ is $\left(\begin{smallmatrix} 1 & 1 \\ 1 & 1 \end{smallmatrix}\right)$ — **singular**. With $b = (2, \varepsilon, \varepsilon)^\top$ the solution is $x^* = (1,1)^\top$ (even $Ax^* = b$).

Output (abridged):

```
cond_2(A) = 141421356.2    cond_2(A^T A) computed = 5.96e+16
normal equations + Cholesky failed: leading minor not positive definite
via QR                     : [1. 1.]
```

The information lost in forming $A^\top A$ cannot be recovered by any solver.

The way out: do not form $A^\top A$; work with transformations that preserve $\|\cdot\|_2$ — and hence the least squares problem and its conditioning.

Definition 3.10. $Q \in \mathbb{R}^{m\times m}$ is **orthogonal** if $Q^\top Q = I$. $Q_1 \in \mathbb{R}^{m\times n}$ $(n \le m)$ has *orthonormal columns* if $Q_1^\top Q_1 = I_n$.

Lemma 3.11 (properties of orthogonal matrices)

$Q \in \mathbb{R}^{m\times m}$ orthogonal:

(i) Q is regular with $Q^{-1} = Q^\top$, and $Q^\top$ is orthogonal; the columns of Q form an orthonormal basis of $\mathbb{R}^m$ (and conversely);

(ii) $\|Qx\|_2 = \|x\|_2$ for all x, $\|QA\|_2 = \|A\|_2$ for all $A \in \mathbb{R}^{m\times n}$, $\operatorname{cond}_2(Q) = 1$;

(iii) products of orthogonal matrices are orthogonal;

(iv) Q_1 with orthonormal columns: $\|Q_1 y\|_2 = \|y\|_2$ for all $y \in \mathbb{R}^n$.

All four from $Q^\top Q = I$: e.g. $\|Qx\|_2^2 = x^\top Q^\top Q x = \|x\|_2^2$.

Theorem 3.12 (QR decomposition)

Let $A \in \mathbb{R}^{m\times n}$ with $m \geq n$. There are an orthogonal $Q \in \mathbb{R}^{m\times m}$ and an upper triangular $R_1 \in \mathbb{R}^{n\times n}$ with

$$A = Q \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = \begin{pmatrix} Q_1 & Q_2 \end{pmatrix} \begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 R_1,$$

where $Q_1 \in \mathbb{R}^{m\times n}$ holds the first n columns of Q and $Q_2 \in \mathbb{R}^{m\times(m-n)}$ the rest. If $\operatorname{rank} A = n$, then R_1 is regular, and Q_1, R_1 are unique once the diagonal entries of R_1 are required to be positive.

- $A = Q_1 R_1$: the **reduced** QR decomposition;
- regularity: $n = \operatorname{rank}(Q_1 R_1) \leq \operatorname{rank} R_1 \leq n$; uniqueness: in the notes
- existence: **constructively**, by Householder reflections (Section 3.5, Proposition 3.23)

Theorem 3.13 (least squares via QR)

Let $\operatorname{rank} A = n$ and $A = Q\begin{pmatrix} R_1 \\ 0 \end{pmatrix} = Q_1 R_1$ as in Theorem 3.12. Then the least squares solution of $Ax = b$ is the solution of the regular triangular system

$$R_1 x^* = Q_1^\top b, \qquad \text{and} \qquad \min_{x \in \mathbb{R}^n} \|Ax - b\|_2 = \|Q_2^\top b\|_2.$$

Blackboard: proof — multiply by $Q^\top$ and split.

Remark 3.14 (no loss of conditioning). $A^\top A = R_1^\top Q_1^\top Q_1 R_1 = R_1^\top R_1 \;\Rightarrow\; A$ and R_1 have the same $\sigma_{\max}, \sigma_{\min}$, so

$$\operatorname{cond}_2(R_1) = \operatorname{cond}_2(A) \qquad \text{instead of} \qquad \operatorname{cond}_2(A^\top A) = \operatorname{cond}_2(A)^2.$$

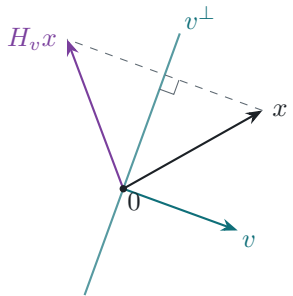
The matrix of the triangular system has the condition number of A, not its square.

Householder reflections

Idea: *triangularise* A by orthogonal transformations — elimination with reflections in place of the E_k (Lemma 2.11).

Definition 3.19. For $v \in \mathbb{R}^m \setminus \{0\}$ the **Householder reflection** is

$$H_v := I - 2\,\frac{vv^\top}{v^\top v} \in \mathbb{R}^{m\times m}.$$



mirror image of x in $v^\perp$

Lemma 3.20 (properties)

(i) H_v is symmetric and orthogonal, and $H_v^2 = I$;

(ii) $H_v v = -v$ and $H_v w = w$ for $w \perp v$: H_v is the **reflection** in the hyperplane $v^\perp$;

(iii) $H_v x = x - 2\,\frac{v^\top x}{v^\top v}\,v$ costs $O(m)$ flops — the matrix H_v is never formed.

Choosing the reflection

Lemma 3.21 (choice of the reflection)

$x \in \mathbb{R}^m \setminus \{0\}$, $\operatorname{sgn}(x_1) \in \{\pm 1\}$ with $\operatorname{sgn} 0 := 1$, $\alpha := -\operatorname{sgn}(x_1)\,\|x\|_2$, $v := x - \alpha e_1$. Then $v \neq 0$ and $H_v x = \alpha e_1 = -\operatorname{sgn}(x_1)\,\|x\|_2\, e_1$.

Proof: $|v_1| = |x_1| + \|x\|_2 > 0$, so $v \neq 0$;
$v^\top v = \|x\|_2^2 - 2\alpha x_1 + \alpha^2 = 2\big(\|x\|_2^2 - \alpha x_1\big) = 2\, v^\top x$, so $H_v x = x - v = \alpha e_1$.

Why this sign: $v_1 = x_1 + \operatorname{sgn}(x_1)\|x\|_2$ adds numbers of the same sign — *no cancellation* (compare Example 1.5); likewise $v^\top v = 2\big(\|x\|_2^2 + |x_1|\,\|x\|_2\big)$.

$x = (3,4)^\top$: $\|x\|_2 = 5$, $\alpha = -5$, $v = (8,4)^\top$,

$$H_v = I - \frac{2\,vv^\top}{80} = \frac{1}{5}\begin{pmatrix} -3 & -4 \\ -4 & 3 \end{pmatrix}, \qquad H_v x = \begin{pmatrix} -5 \\ 0 \end{pmatrix} = \alpha e_1.$$

Algorithm 3.22 (Householder QR decomposition)

$A \in \mathbb{R}^{m\times n}$, $m \geq n$, $A^{(1)} := A$. For $k = 1, \ldots, p := \min(n, m-1)$:
$x^{(k)} := \left(a_{kk}^{(k)}, \ldots, a_{mk}^{(k)}\right)^\top \in \mathbb{R}^{m-k+1}$;
if $x^{(k)} = 0$: $H_k := I$; otherwise v_k for $x^{(k)}$ by Lemma 3.21 and

$$H_k := \begin{pmatrix} I_{k-1} & 0 \\ 0 & H_{v_k} \end{pmatrix}, \qquad A^{(k+1)} := H_k A^{(k)},$$

that is, H_{v_k} is applied to rows $k, \ldots, m$ of columns $k, \ldots, n$.

$m = 4$, $n = 3$ ($*$: final entries, $\times$: still to be changed):

$$\begin{pmatrix} \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \\ \times & \times & \times \end{pmatrix} \xrightarrow{H_1} \begin{pmatrix} * & * & * \\ 0 & \times & \times \\ 0 & \times & \times \\ 0 & \times & \times \end{pmatrix} \xrightarrow{H_2} \begin{pmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & \times \\ 0 & 0 & \times \end{pmatrix} \xrightarrow{H_3} \begin{pmatrix} * & * & * \\ 0 & * & * \\ 0 & 0 & * \\ 0 & 0 & 0 \end{pmatrix}$$

Householder QR gives Theorem 3.12 — and solves least squares problems

Proposition 3.23

In Algorithm 3.22 every H_k is symmetric and orthogonal, step k leaves rows $1, \dots, k-1$ unchanged, and $A^{(k+1)}$ has zeros below the diagonal in columns $1, \dots, k$. Hence

$$H_p \cdots H_1 A = \begin{pmatrix} R_1 \\ 0 \end{pmatrix}, \qquad Q := H_1 \cdots H_p \text{ orthogonal}, \qquad A = Q \begin{pmatrix} R_1 \\ 0 \end{pmatrix}:$$

Theorem 3.12 holds for every $A \in \mathbb{R}^{m \times n}$ with $m \geq n$.

Order of the factors: $Q = H_1 \cdots H_p$, but $Q^\top = H_p \cdots H_1$ (the H_k are symmetric) — applying H_1 first and H_p last to a vector y gives $Q^\top y$. Proof: induction on k (notes).

$\operatorname{rank} A = n$: **do not form Q.**

- apply $H_1, \dots, H_p$ to b as well (in this order) $\Rightarrow$ $Q^\top b$
- solve the regular triangular system $R_1 x = (Q^\top b)_{1:n}$ (backward substitution)
- the remaining components give the minimal residual: $\|(Q^\top b)_{n+1:m}\|_2 = \|Q_2^\top b\|_2$ (Theorem 3.13)

Example 3.25: Householder QR by hand

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 0 & -\sqrt{2} & \sqrt{2}/2 \\ 0 & \sqrt{2} & 5/\sqrt{2} \end{pmatrix}, \qquad b = \begin{pmatrix} 3\sqrt{2} \\ -1 \\ 7 \end{pmatrix}.$$

Blackboard: two reflection steps, $Q^\top b$, backward substitution.

$$R = \begin{pmatrix} -1 & -1 & -1 \\ 0 & 2 & 2 \\ 0 & 0 & 3 \end{pmatrix}, \qquad Q^\top b = \begin{pmatrix} -3\sqrt{2} \\ 4\sqrt{2} \\ 3\sqrt{2} \end{pmatrix}, \qquad x = \begin{pmatrix} \sqrt{2} \\ \sqrt{2} \\ \sqrt{2} \end{pmatrix} \qquad \text{(check: } Ax = b\text{)}.$$

$r_{11} = -1 < 0$: Householder's sign choice does not give the positive diagonal of Theorem 3.12 — flip the signs of row 1 of R and column 1 of Q.
Computed (`householder_qr` in the notes): $\|A - QR\|_F = 5 \cdot 10^{-16}$, $\|Q^\top Q - I\|_F = 1 \cdot 10^{-17}$.

Cost and stability — normal equations versus QR

	normal equations + Cholesky	Householder QR (Remark 3.24)
cost ($m \geq n$)	$mn^2 + \frac{1}{3}n^3$ flops	$2mn^2 - \frac{2}{3}n^3$ flops for R_1; $Q^\top b$ costs $O(mn)$; Q is not needed
system solved	$A^\top A x = A^\top b$ with $\operatorname{cond}_2(A^\top A) = \operatorname{cond}_2(A)^2$	$R_1 x = Q_1^\top b$ with $\operatorname{cond}_2(R_1) = \operatorname{cond}_2(A)$
rounding errors	forming $A^\top A$ loses information once $u \operatorname{cond}_2(A)^2 \gtrsim 1$ (Example 3.9)	backward stable: $A + \Delta A = \tilde{Q}\left(\begin{smallmatrix}\hat{R}_1\\0\end{smallmatrix}\right)$ with the computed $\hat{R}_1$ and some exactly orthogonal $\tilde{Q}$ (not the computed $\hat{Q}$), $\|\Delta A\|_F \lesssim c\,mn\,u\,\|A\|_F$ (Higham, Thm 19.4)
orthogonality	—	$\hat{Q}$, if formed, is orthogonal to working precision whatever $\operatorname{cond}_2(A)$
software	—	`numpy.linalg.qr` (LAPACK `geqrf`); `lstsq` uses the SVD

$m = n$: about $\frac{4}{3}n^3$ flops, twice Gaussian elimination — the price for orthogonality. Neither method changes the conditioning of the least squares problem *itself* (Remark 3.8*, reading).

Summary

- **least squares**: minimise $\|Ax - b\|_2$; solutions $\iff$ normal equations $A^\top A x = A^\top b$; the residual is orthogonal to $\operatorname{Im} A$; unique $\iff$ $\ker A = \{0\}$
- $\operatorname{rank} A = n$: solving the normal equations **squares the condition number**, $\operatorname{cond}_2(A^\top A) = \operatorname{cond}_2(A)^2$ — information is lost when $A^\top A$ is formed once $u \operatorname{cond}_2(A)^2 \gtrsim 1$ (Example 3.9)
- **QR** ($\operatorname{rank} A = n$): $A = Q_1 R_1$ reduces the problem to the regular triangular system $R_1 x = Q_1^\top b$ with $\operatorname{cond}_2(R_1) = \operatorname{cond}_2(A)$; the minimal residual is $\|Q_2^\top b\|_2$
- **Householder**: $H_v = I - 2vv^\top/(v^\top v)$, $v = x - \alpha e_1$, $\alpha = -\operatorname{sgn}(x_1)\|x\|_2$ maps $x \mapsto \alpha e_1$ without cancellation; column by column gives R_1 in $2mn^2 - \frac{2}{3}n^3$ flops, backward stable; $Q^\top b$ by applying the reflections to b
- blackboard proofs of today: Theorem 3.4 (normal equations), Theorem 3.13 (least squares via QR); by hand: Householder QR (Example 3.25)