Numerical Methods I: Linear least squares

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September 28, 2017
Least-squares problems

Given data points/measurements

\[(t_i, b_i), \quad i = 1, \ldots, m\]

and a model function \(\phi\) that relates \(t\) and \(b\):

\[b = \phi(t; x_1, \ldots, x_n),\]

where \(x_1, \ldots, x_n\) are model function parameters. If the model is supposed to describe the data, the deviations/errors

\[\Delta_i = b_i - \phi(t_i, x_1, \ldots, x_n)\]

should be small. Thus, to fit the model to the measurements, one must choose \(x_1, \ldots, x_n\) appropriately.
Least-squares problems

Example:

1. \( \phi(t; x_1, x_2) = x_1 t^2 + x_2 \exp(t) \) 

\( \bar{b}_2 = b_2 - \phi(t_2; \bar{x}_1, \bar{x}_2) \)

2. \( \tilde{\phi}(t; x_1, x_2) = x_1 t^2 + \log(x_2) t^3 \)

\( x_1, x_2 \) are nonlinearly

Parameters \( x_1, x_2 \) 

Enter linearly

"Linear least squares"
Least-squares problems
Measuring deviations

**Least squares:** Find $x_1, \ldots, x_n$ such that

$$
\frac{1}{2} \sum_{i=1}^{m} \Delta_i^2 \rightarrow \min
$$

From a probabilistic perspective, this corresponds to an underlying Gaussian error model.

**Weighted least squares:** Find $x_1, \ldots, x_n$ such that

$$
\frac{1}{2} \sum_{i=1}^{m} \left( \frac{\Delta_i}{\delta b_i} \right)^2 \rightarrow \min,
$$

where $\delta b_i > 0$ contain information about how much we trust the $i$th data point.
Alternatives to using squares:

$L^1$ error: Find $x_1, \ldots, x_n$ such that

$$\sum_{i=1}^{m} |\Delta_i| \rightarrow \min$$

Result can be very different, other statistical interpretation, more stable with respect to outliers.

$L^\infty$ error: Find $x_1, \ldots, x_n$ such that

$$\max_{1 \leq i \leq m} |\Delta_i| \rightarrow \min$$
Linear least-squares

We assume (for now) that the model depends linearly on \( x_1, \ldots, x_n \), e.g.:

\[
\phi(t; x_1, \ldots, x_n) = a_1(t)x_1 + \ldots + a_n(t)x_n
\]

Example:

\[
\phi(t; x_1, x_2) = x_1t^2 + x_2 \exp(t), \text{ data points } \ (t_i, b_i), \ i = 1, 2, 3
\]

\[
\Delta_1 = b_1 - (x_1t_1^2 + x_2 \exp(t_1))
\]
\[
\Delta_2 = b_2 - (x_1t_2^2 + x_2 \exp(t_2))
\]
\[
\Delta_3 = b_3 - (x_1t_3^2 + x_2 \exp(t_3))
\]

\[
\min \sum_{i=1}^{3} \Delta_i^2 \implies \text{linear least squares problem}
\]

unknowns: \( x_1, x_2 \) (2 unknowns), 3 equations
Linear least-squares

Choosing the least square error, this results in

$$\min_x \|Ax - b\|^2,$$

where $x = (x_1, \ldots, x_n)^T$, $b = (b_1, \ldots, b_m)^T$, and $a_{ij} = a_j(t_i)$.

In the following, we study the overdetermined case, i.e., $m \geq n$.

**Example:**

$$A = \begin{bmatrix} t_1^2 & \exp(t_1) \\ t_2^2 & \exp(t_2) \\ t_3^2 & \exp(t_3) \end{bmatrix} \quad x = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad b = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \end{bmatrix}$$

$A \in \mathbb{R}^{3 \times 2}$, $x \in \mathbb{R}^2$, $b \in \mathbb{R}^3$
Different perspective:
Consider non-square matrices $A \in \mathbb{R}^{m \times n}$ with $m \geq n$ and rank($A$) = $n$. Then the system

$$Ax = b$$

does, in general, not have a solution (more equations than unknowns). We thus instead solve a minimization problem

$$\min_{x} \|Ax - b\|^{2}_{2}.$$ 

The minimum $\bar{x}$ of this optimization problem is characterized by the normal equations:

$$A^{T}A\bar{x} = A^{T}b.$$
Linear least-squares: normal equations

\[ \min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 \]

Geometrical sketch: in 2D:

\[ x = \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 \]

\[ Ax - b \perp \text{Range}(A) \]

**Note:** Such a characterization is only possible for norms that have a corresponding inner product \( \langle \cdot, \cdot \rangle \).

\[ \|x\| = \sqrt{\langle x, x \rangle} \]
Lemma (3.4), $V, \langle \cdot, \cdot \rangle$ finite-dim. vector space, $U \subset V$ subspace

$U^\perp$ is orthogonal complement, i.e. $U^\perp = \{ v \in V | \langle v, u \rangle = 0 \text{ for all } u \in U \}$

Then: $\arg \min_{u \in U} \| u' - u \| = u \leftrightarrow a - u \in U^\perp$

Proof: Let $u \in U$ such that $a - u \in U^\perp$. Then for $u' \in U$:

$\| a - u' \|^2 = \| a - u \|^2 + 2 \langle a - u, u' - u \rangle + \| u - u' \|^2$

$= \| a - u \|^2 + \| u - u' \|^2 \geq \| a - u \|^2$

$\rightarrow \sqrt{\text{ }}$
This unique $u \in U$ is called the orthogonal projection of $v$ onto $U$, $u = P_v v$.

**Thm:** $\bar{x} = \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|^2$ $\implies$ $A^T A \bar{x} = A^T b$

In particular, minimum is unique if $\text{rank}(A) = n$ since then $A^T A$ is invertible.

**Proof:**

$V = \mathbb{R}^m$, $U = \mathbb{R}(A) \subset V$ subspace

$\|b - Ax\| = \min \iff \langle b - Ax, A x' \rangle = 0 \quad \forall x' \in \mathbb{R}^n$

$\iff \langle A^T (b - Ax), x' \rangle = 0 \quad \forall x' \in \mathbb{R}^n$

$\iff A^T A \bar{x} = A^T b$ \quad $\Box$. 
Linear least-squares problems—QR factorization

Solving the normal equations

\[ A^T A \bar{x} = A^T b \]

requires:

- computing \( A^T A \) (which is \( O(mn^2) \))
- condition number of \( A^T A \) is square of condition number of \( A \); (problematic for the Choleski factorization)

Claim:

\[ \kappa_2(A^T A) = \| A^T A \|_2 \| (A^T A)^{-1} \|_2 = \kappa_2(A)^2 \]

Proof: \( \kappa_2(A)^2 \leq \max_{\|x\|_2 = 1} \| A x \|_2^2 = \max_{\|x\|_2 = 1} \frac{\langle A x, A x \rangle}{\| x \|_2} = \frac{\lambda_{\max}(A^T A)}{\lambda_{\min}(A^T A)} = \kappa_2(A^T A) \)

\[ B \in \mathbb{R}^{m \times n} \]

\[ \| B \|_2 = \| \lambda_{\max}(B) \| \]

\[ \| B^{-1} \|_2 = \| \lambda_{\min}(B^{-1}) \| = \frac{1}{\| \lambda_{\max}(B) \|} \]
Conditioning of an orthogonal projection:

**Lemma:** \( P : \mathbb{R}^n \to V \) orthogonal projection onto \( V \subset \mathbb{R}^n \)

For \( b \in \mathbb{R}^n \), define by \( \Theta \) angle between \( b \) and \( V \)

\[ \sin \Theta = \frac{\| b - Pb \|_2}{\| b \|_2} \]

Then, the relative condition number of \( (P, b) \) w.r.t. the 2-norm is

\[ \kappa = \frac{1}{\cos \Theta} \| P \|_2 \]

**Proof:**

\[ \| Pb \|_2^2 = \| b \|_2^2 - \| b - Pb \|_2^2 \]

\[ \frac{\| Pb \|_2^2}{\| b \|_2^2} = 1 - \sin^2 \Theta = \cos^2 \Theta \]

\( P \) is linear, i.e.

\[ \kappa_{rel} = \frac{\| b \|_2}{\| Pb \|_2} \| P'(b) \|_2 = \frac{1}{\cos \Theta} \| P \|_2 \]

\( \blacksquare \)
Solving the normal equation is equivalent to computing $Pb$, the orthogonal projection of $b$ onto the subspace $V$ spanned by columns of $A$.

Let $x$ be the solution of the least square problem and denote the residual by $r = b - Ax$, and

$$\sin(\theta) = \frac{\|r\|_2}{\|b\|_2}.$$
The relative condition number $\kappa$ of $x$ in the Euclidean norm is bounded by

- With respect to perturbations in $b$:

$$\kappa \leq \frac{\kappa_2(A)}{\cos(\theta)}$$

- With respect to perturbations in $A$:

$$\kappa \leq \kappa_2(A) + \kappa_2(A)^2 \tan(\theta)$$

**Small residual problems** $\cos(\theta) \approx 1$, $\tan(\theta) \approx 0$: behavior similar to linear system.

**Large residual problems** $\cos(\theta) \ll 1$, $\tan(\theta) > 1$: behavior essentially different from linear system.
Linear least-squares problems–QR factorization

One would like to avoid the multiplication $A^T A$ and use a suitable factorization of $A$ that aids in solving the normal equation, the QR-factorization:

$$A = QR = [Q_1, Q_2] \begin{bmatrix} R_1 \\ 0 \end{bmatrix} = Q_1 R_1,$$

where $Q \in \mathbb{R}^{m \times m}$ is an orthonormal matrix ($QQ^T = I$), and $R \in \mathbb{R}^{m \times n}$ consists of an upper triangular matrix and a block of zeros.
How can the $QR$ factorization be used to solve the normal equation?

$$Q^T A = Q^T Q R = \begin{bmatrix} R_1 \\ 0 \end{bmatrix}$$

$$\min_x \|Ax - b\|^2 = \min_x \|Q^T(Ax - b)\|^2 = \min_x \left\| \begin{bmatrix} b_1 - R_1 x \\ b_2 \end{bmatrix} \right\|^2,$$

where $Q^T b = \begin{bmatrix} b_1 \\ b_2 \end{bmatrix}$. 

Thus, the least squares solution is $x = R^{-1} b_1$ and the residual is $\|b_2\|$. 

$$= \min_x \|b_1 - R_1 x\|^2 + \|b_2\|^2$$
How can we compute the QR factorization?

**Givens rotations**

Use sequence of rotations in 2D subspaces:

For $m \approx n$: $\sim n^2/2$ square roots, and $4/3n^3$ multiplications

For $m \gg n$: $\sim nm$ square roots, and $2mn^2$ multiplications

**Householder reflections**

Use sequence of reflections in 2D subspaces

For $m \approx n$: $2/3n^3$ multiplications

For $m \gg n$: $2mn^2$ multiplications