Least Squares Problems

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Goal of Least Squares

Find an *approximate solution* that best fits the data.

Least Squares: Problem Statement

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Define the **residual vector**

$$r = y - Ac$$

and solve:

$$\boxed{\min_c \|r\|_2^2}$$

Interpretation

- Ac lies in the column space $\mathrm{Im}(A)$,
- y generally does not,
- least squares finds the closest point in $\mathrm{Im}(A)$ to y.

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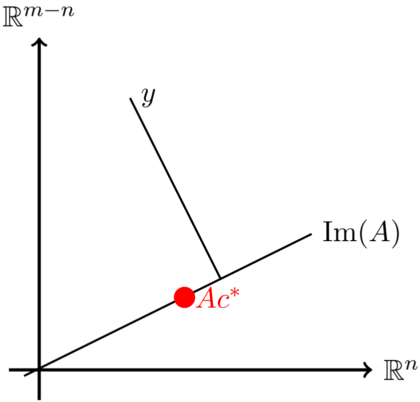
Key idea

Minimizing the residual norm is equivalent to minimizing the Euclidean distance between y and its approximation.

Geometric Intuition: Projection



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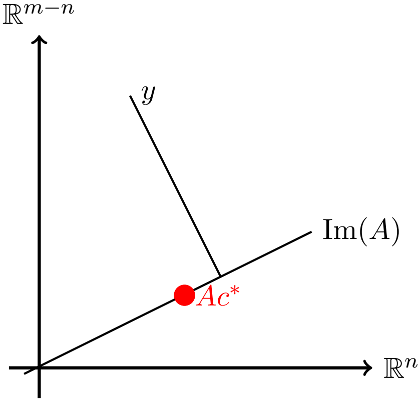

$$\boxed{r = y - Ac^* \perp \mathrm{Im}(A)}$$

Orthogonality Condition (Theorem)

c^* minimizes $\|y - Ac\|_2^2$ if and only if:

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This implies:

$$\boxed{A^\top r = 0}$$

Normal Equations

Since $r = y - Ac^*$:

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$$\boxed{A^\top A c^* = A^\top y}$$

Normal equations

They characterize the least-squares solution.

Derivation via Objective Expansion

$$\|Ac - y\|_2^2 = (Ac - y)^\top (Ac - y)$$

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$$\nabla_c = 2A^\top Ac - 2A^\top y$$

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Setting it to zero yields:

$$\boxed{A^\top Ac^* = A^\top y}$$

Explicit Solution and Pseudo-Inverse

If $\mathrm{rank}(A) = n$, then $A^\top A$ is invertible and:

$$\boxed{c^* = (A^\top A)^{-1} A^\top y = A^+ y}$$

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Moore–Penrose pseudo-inverse

Maps $y \in \mathbb{R}^m$ to the least-squares optimal $c^* \in \mathbb{R}^n$.

Numerical Considerations

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In practice

Use QR or SVD decompositions.

Least Squares via QR Decomposition

If $A = QR$ with:

- $Q^\top Q = I$,
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Advantages

Stable and efficient.

Least Squares via SVD

For general matrices:

$$A = U\Sigma V^\top$$

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Least Squares via SVD

For general matrices:

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$$\boxed{A^+ = V\Sigma^{-1}U^\top}$$

- handles rank deficiency,
- reveals effective dimensionality,
- yields minimum-norm solution.

Summary

- Least squares handles overdetermined systems
- Solution $=$ orthogonal projection onto $\mathrm{Im}(A)$
- Leads to normal equations
- Computed stably using QR or SVD

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Key message

Least squares is both a geometric projection and a numerical optimization problem.