Mathematics for Computer Science
Linear Algebra (Part 2)
Linear Regression

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Thanks to Andrei Krokhin and William Moses for use of slides.

Outline

Roadmap for Lectures 5 - 8

- **End Goal:** Application - linear regression.
- **Using:** QR decomposition.
- Requires knowledge of some basics: Inner product spaces.

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Now we recap last lecture & look at what we'll cover today.

Last Lecture Reminder

Definition (Least Squares Problem)

Given a linear system $A\mathbf{x} = \mathbf{b}$ with m equations and n variables, find a vector $\mathbf{x}$ that minimises $||\mathbf{b} - A\mathbf{x}||$ (w.r.t. the Euclidean inner product on $\mathbb{R}^m$).

- We call such a vector $\mathbf{x}$ a least squares solution to the system, the vector $\mathbf{b} - A\mathbf{x}$ is the least squares error vector, and the number $||\mathbf{b} - A\mathbf{x}||$ is the least squares error.
- Let $W = \{A\mathbf{x} \mid \mathbf{x} \in \mathbb{R}^n\}$ be the column space of A.
- $A^T A\mathbf{x} = A^T\mathbf{b}$ is the normal equation (or normal system) associated with $A\mathbf{x} = \mathbf{b}$.
- The solution to $A^T A\mathbf{x} = A^T\mathbf{b}$ is the least squares solution to $A\mathbf{x} = \mathbf{b}$.

Today's Lecture Contents

- **Application:** Least squares fitting to data (aka linear regression)
- The benefit of a QR decomposition

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- The simpler the curve, the better. So try a straight line $y = a + bx$ first.

  (The method extends to more than 2 variables and to more complex curves)

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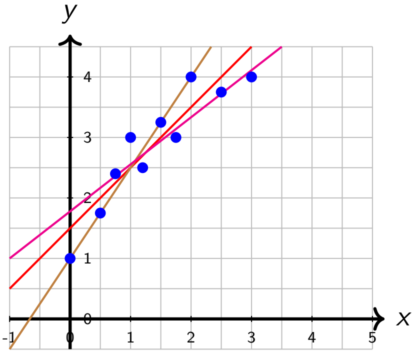

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- This can then be written as a series of equations

$$\begin{aligned} a + bx_1 &= y_1 \\ &\vdots \\ a + bx_n &= y_n \end{aligned}$$

- Or in matrix form $\begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_n \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$

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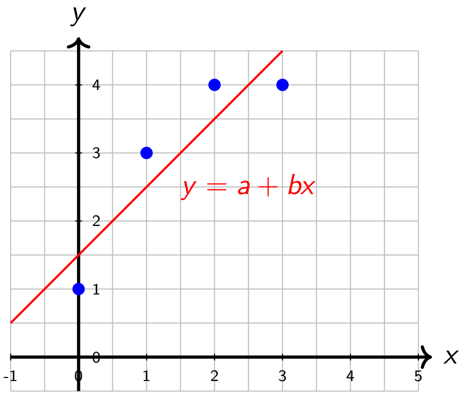
Example



$$\begin{aligned} a + bx_1 &= y_1 \\ a + bx_2 &= y_2 \\ a + bx_3 &= y_3 \\ a + bx_4 &= y_4 \end{aligned}$$

$$\begin{pmatrix} 1 & 0 \\ 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1 \\ 3 \\ 4 \\ 4 \end{pmatrix}$$

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Need to find a least squares solution to the system $A\mathbf{v} = \mathbf{y}$:

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From the associated normal system $A^T A\mathbf{v} = A^T\mathbf{y}$, we get

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From this, $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 1.5 \\ 1 \end{pmatrix}$ so $y = 1.5 + x$ is the least squares straight line fit

(aka the regression line)

Outline

When are Least Squares Solutions Unique?

Equivalently: when does a normal system $A^T A\mathbf{x} = A^T\mathbf{b}$ have a unique solution?

Theorem

For any $m \times n$ matrix A, A has linearly independent columns iff $A^T A$ is invertible.

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- $A^T A$ is square, so it is invertible iff $A^T A\mathbf{x} = \mathbf{0}$ has only the trivial solution.
- Each solution of $A\mathbf{x} = \mathbf{0}$ is a solution of $A^T A\mathbf{x} = \mathbf{0}$.
- Let $\mathbf{x}_0$ be a solution of $A^T A\mathbf{x} = \mathbf{0}$, i.e., $A^T A\mathbf{x}_0 = \mathbf{0}$.

  Then $A\mathbf{x}_0$ is both in the column space of A and in the null space of A^T (which are orthogonal complements of each other). Hence, $A\mathbf{x}_0 = \mathbf{0}$.
- Thus $A\mathbf{x} = \mathbf{0}$ has only the trivial solution iff the same is true for $A^T A\mathbf{x} = \mathbf{0}$.

□

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For the last item, substitute $A = QR$ into the first equation above and simplify:

$$\mathbf{x} = (A^T A)^{-1} A^T \mathbf{b} = ((QR)^T (QR))^{-1} (QR)^T \mathbf{b} = (R^T Q^T QR)^{-1} R^T Q^T \mathbf{b}$$
$$= (R^T IR)^{-1} R^T Q^T \mathbf{b} = (R^T R)^{-1} R^T Q^T \mathbf{b} = R^{-1} (R^T)^{-1} R^T Q^T \mathbf{b} = R^{-1} Q^T \mathbf{b}.$$

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- If $A = QR$ is a QR decomposition (which exists under our assumption), then

$$\mathbf{x} = R^{-1}Q^T\mathbf{b} \quad \text{(or, equivalently, } R\mathbf{x} = Q^T\mathbf{b}\text{)}$$

Projection Matrices

We showed before: for any column vector $\mathbf{b}$, if $W = \mathcal{C}(A)$ is the column space of a matrix A and $\mathbf{x}$ is the least squares solution to $A\mathbf{x} = \mathbf{b}$, then $\mathrm{proj}_W \mathbf{b} = A\mathbf{x}$.

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If A has linearly independent column vectors, then we can use the first formula from the previous slide:

$$\mathrm{proj}_W \mathbf{b} = A\mathbf{x} = A(A^T A)^{-1} A^T \mathbf{b}.$$

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- For any column vector $\mathbf{b}$, the vector $P\mathbf{b}$ is the orthogonal projection of $\mathbf{b}$ onto $W = \mathcal{C}(A)$, the column space of A.
- Such matrices P are used in ML and Data Science to map vectors $\mathbf{b}$ from a high-dimensional space to a suitably chosen small-dimensional space W.

Example 18.2

Given the data points: $(1,-1),(2,2),(0,-6),(3,6),(1,0),(2,3)$, where we weight the experiments as $(4,4,3,3,1,1)$, fit the data to a curve of the form $y = a + bx + cx^2$.

This is equivalent to finding the least squares solution to the system $A\mathbf{x} = \mathbf{y}$:

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 4 \\ 1 & 0 & 0 \\ 1 & 3 & 9 \\ 1 & 1 & 1 \\ 1 & 2 & 4 \end{pmatrix} \begin{pmatrix} a \\ b \\ c \end{pmatrix} = \begin{pmatrix} -1 \\ 2 \\ -6 \\ 6 \\ 0 \\ 3 \end{pmatrix}$$

Example 18.2 ... Gram-Schmidt

N.B inner product is weighted Euclidean dot product with weights $(4, 4, 3, 3, 1, 1)$.

- $\mathbf{v}_1 = (1, 1, 1, 1, 1, 1)$
- $\mathbf{v}_2 = \frac{1}{2}(-1, 1, -3, 3, -1, 1)$
- $\mathbf{v}_3 = \frac{1}{4}(-3, -3, 5, 5, 3, -3)$

Normalising to

- $\mathbf{q}_1 = \frac{1}{4}(1, 1, 1, 1, 1, 1)$
- $\mathbf{q}_2 = \frac{1}{8}(-1, 1, -3, 3, -1, 1)$
- $\mathbf{q}_3 = \frac{1}{4\sqrt{15}}(-3, -3, 5, 5, -3, -3)$

Example 18.2 ... QR decomp

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$$Q = \begin{pmatrix} \frac{1}{4} & \frac{-1}{8} & \frac{-3}{4\sqrt{15}} \\ \frac{1}{4} & \frac{1}{8} & \frac{-3}{4\sqrt{15}} \\ \frac{1}{4} & \frac{-3}{8} & \frac{5}{4\sqrt{15}} \\ \frac{1}{4} & \frac{3}{8} & \frac{5}{4\sqrt{15}} \\ \frac{1}{4} & \frac{-1}{8} & \frac{-3}{4\sqrt{15}} \\ \frac{1}{4} & \frac{1}{8} & \frac{-3}{4\sqrt{15}} \end{pmatrix} R = \begin{pmatrix} 4 & 6 & 13 \\ 0 & 4 & 12 \\ 0 & 0 & \sqrt{15} \end{pmatrix}$$

$$\mathbf{x} = R^{-1} Q^T \mathbf{y} = \frac{1}{160} \begin{pmatrix} -315 \\ 306 \\ -32 \end{pmatrix} \approx \begin{pmatrix} 1.97 \\ 1.91 \\ -0.2 \end{pmatrix}$$

Outline

Exam Question

(d) Given the following points, use the least squares method to find the straight line and quadratic polynomial that best approximate them.

$$P = (0,-1),(0,0),(1,-1),(1,-2),(2,0),(2,2).$$

(e) Which of the two polynomials is the best approximation? Justify your answer. **[3 Marks]**

Wrapping Things Up

Today:

- Least squares solutions for inconsistent linear systems
- Least squares fitting to data (aka linear regression)
- Benefit of a QR decomposition

Next time:

- Orthogonal matrices and spectral decomposition

The End

Supplemental Slide: When are Least Squares Solutions Unique?

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