Numerical Analysis Day 8: Least Squares

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We start with three equations:

$x_1 + x_2 = 2$

$x_1 - x_2 = 1$

$x_1 + x_2 = 3$

$$\begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}$$

We express this overdetermined system as $Ax = b$.

1 Gram-Schmidt Orthogonalization

Two vectors are orthogonal (perpendicular) if $x \cdot y = 0$, where

$(x_1, x_2, x_3) \cdot (y_1, y_2, y_3) = x_1y_1 + x_2y_2 + x_3y_3$

Let's check the columns of our example:

$v_1 = (1, 1, 1), v_2 = (1, -1, 1)$

$v_1 \cdot v_2 = (1, 1, 1) \cdot (1, -1, 1) = 1 - 1 + 1 = 1 \neq 0$

We wish to transform v_2 - we remove all v_1 tendencies from v_2.

Project v_2 onto v_1 to make u, and use u to build a new version of v_2 called y_2.

$$u = \frac{(v_1 \cdot v_2)v_1}{\parallel v_i \parallel^2} = \frac{(1, 1, 1) \cdot (1, -1, 1)}{(1, 1, 1) \cdot (1, 1, 1)}(1, 1, 1) = \frac{1}{3}(1, 1, 1) = (\frac{1}{3}, \frac{1}{3}, \frac{1}{3})$$

$y_2 = v_2 - u = (1, -1, 1) - (1/3, 1/3, 1/3) = (2/3, -4/2, 2/3)$

$v_1 \cdot y_2 = (1, 1, 1) \cdot (2/3, -4/2, 2/3) = 2/3 - 4/3 + 2/3 = 0$

2 Finding the closest point

What value of $a_1x_1 + a_2x_2$ is closest to $b = (2, 1, 3)$?

Project (2, 1, 3) onto the plane spanned by (v_1, v_2) to get nearest point, $\bar{x}$

$(Ax)^T(b - A\bar{x}) = 0$

Since $(Ax)^T = x^T A^T$ we have $x^T A^T(b - A\bar{x}) = 0$

This can only happen for all x if $A^T(b - A\bar{x}) = 0$

Expand and simplify to get $A^T A\bar{x} = A^T b$

$$\begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & -1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & -1 & 1 \end{pmatrix} \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}$$

$$\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 6 \\ 4 \end{pmatrix}$$

$$\bar{x} = \begin{pmatrix} 7/4 \\ 3/4 \end{pmatrix}$$

We will use the Root Mean Squared Error (RMSE) to estimate the error.

$$\sqrt{\frac{e_1^2 + e_2^2 + e_3^2 + \cdots e_n^2}{n}}$$

3 Steps

Pick a model, and parameterize it. For a Linear model, we have: $y = a_1 + a_2x$. For a Quadratic model we have: $y = a_1 + a_2x + a_3x^2$. Build the Vandermonde matrix A.

$$A^T A\bar{x} = A^T b$$

The Vandermonde matrix A has a large condition number, and $A^T A$ has larger one.

Next week, we will find better ways to recover $\bar{x}$ than inverting $M = A^T A$.

In Matlab, rather than take the inverse of matrix M, it is better to use this operator:

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x = M \ b
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