Math 415 - Lecture 25

Multiple linear regression, Gram Schmidt and Orthogonal matrices

Monday October 26th 2015

Textbook reading: Chapters 3.3,3.4

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Suggested practice exercises: Chapter 3.3, 3,5,6,13,22,24,25,26
and Chapter 3.4, 10,11,13,14,16,26

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Khan Academy video: Another Least Squares Example, Gram-Schmidt Example

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Khan Academy video: Another Least Squares Example, Gram-Schmidt Example

Strang lecture: Orthogonal Matrices and Gram-Schmidt Process.

Review

$\hat{\mathbf{x}}$ is a least squares solution of the system $A\mathbf{x} = \mathbf{b}$

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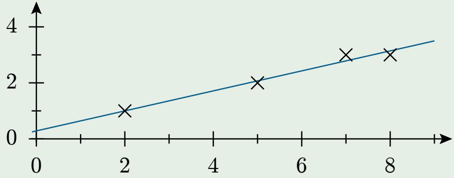
$\overset{FTLA}{\iff}$ $A^T A\hat{\mathbf{x}} = A^T\mathbf{b}$ (the **normal equations**)

Application: fitting data

Least square lines

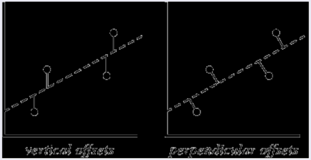
Example

Find β_1, β_2 such that the line $y = \beta_1 + \beta_2 x$ best fits the data points $(2,1), (5,2), (7,3), (8,3)$.



Comment

As usual in practice, we are minimizing the (the sum of the squares of the) vertical offsets.



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Here, we need to find a least squares solution to

$$\begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix}.$$

Solution

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Hence the least squares line is $y = \frac{2}{7} + \frac{5}{14}x$.

Fitting to other curves

What happens if the data just lie close to any line? We can also fit the experimental data using other curves. Try to find $\beta_1, \beta_2, \beta_3$ such that $y = \beta_1 + \beta_2 x + \beta_3 x^2$ fits the data.

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Given data (x_i, y_i), we then find the least squares solution to $X\beta = \mathbf{y}$.

Multiple linear regression

Of course, sometimes the variable y might not just depend on a single variable x, but on two variables, say u and v. So, here you have find the least-squares solution of

$$\underbrace{\begin{bmatrix} 1 & v_1 & w_1 \\ 1 & v_2 & w_2 \\ 1 & v_3 & w_3 \\ \vdots & \vdots & \vdots \end{bmatrix}}_{\text{design matrix}} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix}}_{\text{observation vector}}$$

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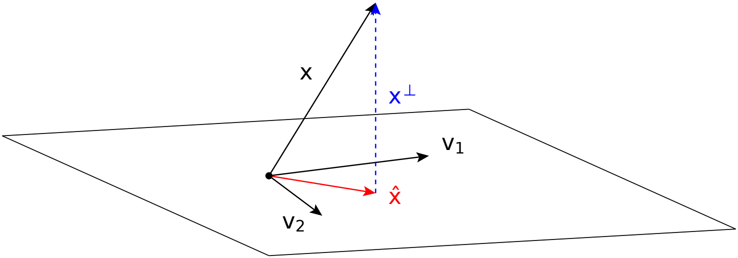
And we again proceed by finding a least squares solution.

Review



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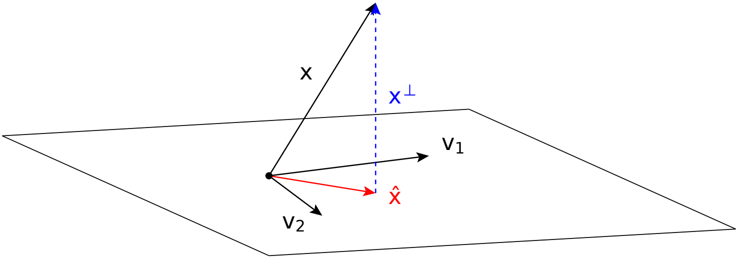

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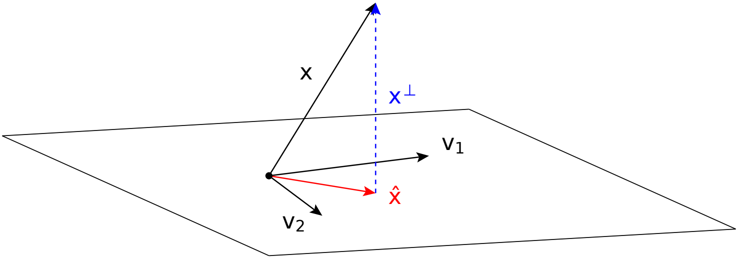

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(To stay agile, we are writing $\langle \mathbf{x}, \mathbf{v}_1 \rangle = \mathbf{x} \cdot \mathbf{v}_1$ for the inner product.)

Gram-Schmidt

Our goal

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* **Gram-Schmidt Process.**

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Recipe. (Gram-Schmidt orthonormalization)

Given a basis $\mathbf{a}_1, \ldots, \mathbf{a}_n$, produce a orthogonal basis $\mathbf{b}_1, \ldots, \mathbf{b}_n$ and an orthonormal basis $\mathbf{q}_1, \ldots, \mathbf{q}_n$.

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$$\begin{aligned}
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\mathbf{b}_3 &= \mathbf{a}_3 - \langle \mathbf{a}_3, \mathbf{q}_1 \rangle \mathbf{q}_1 - \langle \mathbf{a}_3, \mathbf{q}_2 \rangle \mathbf{q}_2, & \mathbf{q}_3 &= \frac{\mathbf{b}_3}{\|\mathbf{b}_3\|} \\
&\dots & &\dots
\end{aligned}$$

Example

Find an orthonormal basis for $V = \text{Span}\left\{ \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 2 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 1 \\ 1 \\ 1 \end{bmatrix} \right\}$.

Solution

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Solution

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We have obtained an orthonormal basis for V: $\mathbf{q}_1, \mathbf{q}_2, \mathbf{q}_3$.

$$\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \frac{1}{\sqrt{2}} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 1 \end{bmatrix}.$$

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$$\mathbf{b}_1 = \mathbf{a}_1, \qquad \mathbf{q}_1 = \underbrace{\frac{\mathbf{b}_1}{\|\mathbf{b}_1\|}}_{\textit{normalize}}$$

Why does Gram-Schmidt work? Recall, if W is a subspace, $\mathbf{b}$ any vector, then

$$\hat{\mathbf{b}} \rightsquigarrow \text{ projection to } W, \ \mathbf{b}^{\perp} = \mathbf{b} - \hat{\mathbf{b}} \rightsquigarrow \text{ orth. to } W$$

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Example

Let $V = \text{Span}\{\begin{bmatrix}2\\1\\2\end{bmatrix}, \begin{bmatrix}0\\0\\3\end{bmatrix}\}$. Find an orthonormal basis for V.

Check that your basis is actually orthonormal.

Orthogonal matrices

Theorem

Let $A = \begin{bmatrix}\mathbf{a_1}, \ldots .\mathbf{a_n}\end{bmatrix}$ be ay matrix. Then $A^T A$ is the matrix of dot products of the columns of A:

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$$A^TA = \begin{bmatrix} \mathbf{a_1}\cdot\mathbf{a_1} & \mathbf{a_1}\cdot\mathbf{a_2} & \mathbf{a_1}\cdot\mathbf{a_3} & \ldots \\ \mathbf{a_2}\cdot\mathbf{a_1} & \mathbf{a_2}\cdot\mathbf{a_2} & \mathbf{a_2}\cdot\mathbf{a_3} & \ldots \\ \mathbf{a_3}\cdot\mathbf{a_1} & \mathbf{a_3}\cdot\mathbf{a_2} & \mathbf{a_3}\cdot\mathbf{a_3} & \ldots \\ \vdots & \vdots & \vdots & \ddots \end{bmatrix}$$

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What happens if the columns of A are orthonormal?

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The columns of Q are orthonormal $\iff$ $Q^T Q = I$

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Proof.

Let $\mathbf{q}_1, \ldots, \mathbf{q}_n$ be the columns of Q.

They orthonormal if and only if $\mathbf{q}_i^T\mathbf{q}_j = \begin{cases} 0, & \text{if } i \neq j, \\ 1, & \text{if } i = j. \end{cases}$

All these products are packaged in $Q^TQ = I$:

$$\begin{bmatrix} -- & \mathbf{q}_1^T & -- \\ -- & \mathbf{q}_2^T & -- \\ & \vdots & \end{bmatrix} \begin{bmatrix} | & | & \\ \mathbf{q}_1 & \mathbf{q}_2 & \cdots \\ | & | & \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \ddots \end{bmatrix}$$

$\square$

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But $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ is an orthogonal matrix.

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But, no example of size 668 is known yet. If you find one you will be famous!