Math 415 - Lecture 25

Multiple linear regression, Gram Schmidt and Orthogonal matrices

Monday October 26th 2015

Textbook reading: Chapters 3.3,3.4

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

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

Strang lecture: Orthogonal Matrices and Gram-Schmidt Process.

1 Review

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

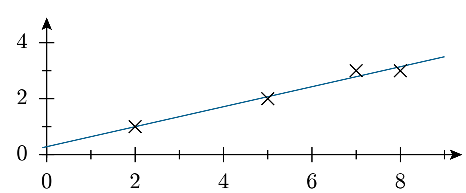
$\iff$ $\hat{\mathbf{x}}$ is such that $A\hat{\mathbf{x}} - \mathbf{b}$ is as small as possible

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

2 Application: fitting data

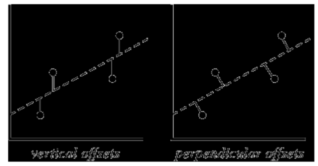
2.1 Least square lines

Example 1. 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.



2.2 Solution

The equations $y = \beta_1 + \beta_2 x$ in matrix form:

$$\underbrace{\begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix}}_{\text{design matrix } X} \begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}}_{\text{observation vector } \mathbf{y}}$$

Here, we need to find a least squares solution to

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

$$X^T X = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 2 \\ 1 & 5 \\ 1 & 7 \\ 1 & 8 \end{bmatrix} = \begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix}$$

$$X^T \mathbf{y} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 2 & 5 & 7 & 8 \end{bmatrix} \begin{bmatrix} 1 \\ 2 \\ 3 \\ 3 \end{bmatrix} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$$

Solving $\begin{bmatrix} 4 & 22 \\ 22 & 142 \end{bmatrix} \hat{\beta} = \begin{bmatrix} 9 \\ 57 \end{bmatrix}$, we find $\begin{bmatrix} \beta_1 \\ \beta_2 \end{bmatrix} = \begin{bmatrix} 2/7 \\ 5/14 \end{bmatrix}$.

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

2.3 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. To fit: $y_i \approx \beta_1 + \beta_2 x_i + \beta_3 x_i^2$ with parameters $\beta_1, \beta_2, \beta_3$. The equations $y_i = \beta_1 + \beta_2 x_i + \beta_3 x_i^2$ in matrix form:

$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ \vdots & \vdots & \vdots \end{bmatrix}}_{\text{design matrix } X} \begin{bmatrix} \beta_1 \\ \beta_2 \\ \beta_3 \end{bmatrix} = \underbrace{\begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ \vdots \end{bmatrix}}_{\text{observation vector } \mathbf{y}}$$

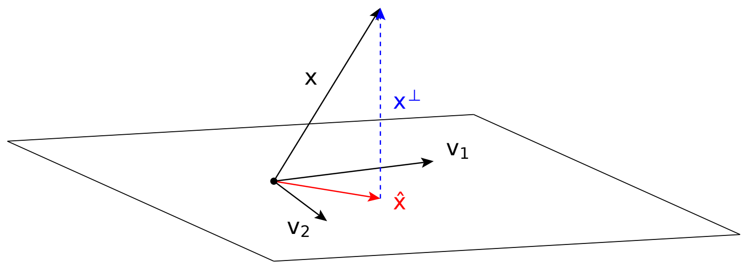
Given data (x_i, y_i), we then find the least squares solution to $X\beta = \mathbf{y}$.

2.4 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

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

And we again proceed by finding a least squares solution.



3 Review

Suppose $\mathbf{v}_1, \ldots, \mathbf{v}_m$ is an orthonormal basis of W. The **orthogonal projection** of $\mathbf{x}$ onto W is :

$$\hat{\mathbf{x}} = \underbrace{\langle \mathbf{x}, \mathbf{v}_1 \rangle \mathbf{v}_1}_{\text{proj. of } \mathbf{x} \text{ onto } \mathbf{v}_1} + \ldots + \underbrace{\langle \mathbf{x}, \mathbf{v}_m \rangle \mathbf{v}_m}_{\text{proj. of } \mathbf{x} \text{ onto } \mathbf{v}_m}$$

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

4 Gram-Schmidt

4.1 Our goal

* In calculating projections we used an *orthogonal basis* and the easy formula for the coefficients.
* What if we are given an arbitrary basis, not orthogonal?
* Turn the starting basis into an orthogonal (or orthonormal) basis.
* **Gram-Schmidt Process.**

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 $\mathbf{q}_1, \ldots, \mathbf{q}_n$.

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

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

Solution.

$$\mathbf{b}_1 = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}, \qquad \mathbf{q}_1 = \begin{bmatrix}1\\0\\0\\0\end{bmatrix}$$

$$\mathbf{b}_2 = \begin{bmatrix}2\\1\\0\\0\end{bmatrix} - \langle \begin{bmatrix}2\\1\\0\\0\end{bmatrix}, \mathbf{q}_1\rangle \mathbf{q}_1 = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}, \qquad \mathbf{q}_2 = \begin{bmatrix}0\\1\\0\\0\end{bmatrix}$$

$$\mathbf{b}_3 = \begin{bmatrix}1\\1\\1\\1\end{bmatrix} - \langle \begin{bmatrix}1\\1\\1\\1\end{bmatrix}, \mathbf{q}_1\rangle \mathbf{q}_1 - \langle \begin{bmatrix}1\\1\\1\\1\end{bmatrix}, \mathbf{q}_2\rangle \mathbf{q}_2 = \begin{bmatrix}0\\0\\1\\1\end{bmatrix}, \quad \mathbf{q}_3 = \tfrac{1}{\sqrt{2}} \begin{bmatrix}0\\0\\1\\1\end{bmatrix}$$

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

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

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

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

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 orthonor-

mal basis $\mathbf{q}_1, \dots, \mathbf{q}_n$.

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

$$\mathbf{b}_2 = \mathbf{a}_2 - \underbrace{\langle \mathbf{a}_2, \mathbf{q}_1 \rangle \mathbf{q}_1}_{\hat{\mathbf{a}_2} \rightsquigarrow \text{projection to Span}\{\mathbf{q_1}\}} \quad \underbrace{\mathbf{a}_2 - \langle \mathbf{a}_2, \mathbf{q}_1 \rangle \mathbf{q}_1}_{\mathbf{a}_2^\perp \rightsquigarrow \text{orth. to Span}\{\mathbf{q_1}\}}, \qquad \mathbf{q}_2 = \underbrace{\frac{\mathbf{b}_2}{\|\mathbf{b}_2\|}}_{normalize}$$

$$\mathbf{b}_3 = \underbrace{\mathbf{a}_3 - (\langle \mathbf{a}_3, \mathbf{q}_1 \rangle \mathbf{q}_1 + \langle \mathbf{a}_3, \mathbf{q}_2 \rangle \mathbf{q}_2)}_{\mathbf{a}_3^\perp \text{ orth. to Span}\{\mathbf{q_1},\mathbf{q_2}\}} \qquad \underbrace{\mathbf{q}_3 = \frac{\mathbf{b}_3}{\|\mathbf{b}_3\|}}_{normalize}$$

$$\dots \qquad \dots$$

Example 3. 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.

4.2 Orthogonal matrices

Theorem 1. *Let $A = \begin{bmatrix}\mathbf{a_1}, \dots . \mathbf{a_n}\end{bmatrix}$ be ay matrix. Then $A^T A$ is the matrix of dot products of the columns of A:*

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

What happens if the columns of A are orthonormal?

Theorem 2. *The columns of Q are orthonormal $\iff Q^T Q = I$*

Proof. Let $\mathbf{q}_1, \dots, \mathbf{q}_n$ 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 $Q^T Q = I$:

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

□

Definition. An **orthogonal matrix** is a square matrix Q with orthonormal columns.

It is historical convention to restrict to square matrices, and to say orthogonal matrix even though "orthonormal matrix" might be better.

An $n \times n$ matrix Q is orthogonal $\iff Q^T Q = I$ In other words, $Q^{-1} = Q^T$.

Example 4. $P = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$ is orthogonal.Why?

Why is $P = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}$ orthogonal?

Solution. Because their columns are a permutation of the standard basis. And so we always have $P^T P = I$. So what is P^{-1}?

Example 5. $Q = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix}$ is orthogonal, Why?

Solution.

- $\begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix}, \begin{bmatrix} -\sin\theta \\ \cos\theta \end{bmatrix}$ is an orthonormal basis of $\mathbb{R}^2$. Just to make sure: why length 1? Because $\| \begin{bmatrix} \cos\theta \\ \sin\theta \end{bmatrix} \| = \sqrt{\cos^2\theta + \sin^2\theta} = 1$.
- Alternatively: $Q^T Q = \begin{bmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{bmatrix} \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$

So what is Q^{-1}?

Example 6. Is $H = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ orthogonal?

Solution. No, the columns are orthogonal but not normalized. But $\frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$ is an orthogonal matrix.

Example 7. (Just for fun) an $n \times n$ matrix with entries ± 1 whose columns are orthogonal is called a *Hadamard matrix* of size n. A size 4 example: $\begin{bmatrix} H & H \\ H & -H \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{bmatrix}$ Continuing this construction, we get examples of size $8, 16, 32, \ldots$. It is believed that Hadamard matrices exist for all sizes $4n$. But, no example of size 668 is known yet. If you find one you will be famous!