Math 1180, 2009

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1 Further discussion of least squares method

We are discussing systems of the form $A\mathbf{x} = \mathbf{b}$ which have no solution, because $\mathbf{b}$ is not in $C(A)$. (Please be sure you understand why that means there is no solution.) We try to find another vector, $\mathbf{p}$, such that $A\mathbf{x} = \mathbf{p}$ does have a solution, and such that $||\mathbf{b} - \mathbf{p}||$ is as small as possible. We do this by considering what are called the "normal equations", namely the system

$$A^T A\mathbf{x} = \mathbf{A}^T\mathbf{b}.$$

Note that if A is $m \times n$ then $A^T A$ is a symmetric $n \times n$ matrix. Our general theory of systems of n equations in n unknowns tells us that if $A^T A$ is non singular, then the normal equations have a unique solution.

The following Lemma is very useful:
Proof.

Lemma 1 If A is an $m \times n$ matrix, x is in R^n and y is in R^m, then

$$A\mathbf{x} \cdot \mathbf{y} = \mathbf{x} \cdot A^T\mathbf{y}$$

Proof. Note first that both sides of this equation make sense. $A\mathbf{x}$ is in R^m , so $A\mathbf{x} \cdot \mathbf{y}$ is defined. $A^T\mathbf{y}$ is in R^n so $\mathbf{x} \cdot A^T\mathbf{y}$ is defined. The formula follows from the following calculation:

$$\begin{aligned} (A\mathbf{x})_i &= \sum_{j=1}^{n} a_{ij}x_j \text{ for } i = 1..n \\ A\mathbf{x} \cdot \mathbf{y} &= \sum_{i=1}^{m} (A\mathbf{x})_i\, y_i = \sum_{i=1}^{m} \left(\sum_{j=1}^{n} a_{ij}x_j \right) y_i \\ &= \sum_{j=1}^{n} x_j \left(\sum_{i=1}^{M} a_{ij}y_i \right) = \mathbf{x} \cdot \left(A^T\mathbf{y}\right). \end{aligned}$$

Notice that the transpose appears in the last line because the sum in parentheses on the left is over the first index, i. This proves the lemma. ■ ■

Theorem 2 *If the columns of an $m \times n$ matrix A are linearly independent, then the $n \times n$ matrix $A^T A$ is nonsingular.*

Proof. Suppose that $A^T A$ is singular. Then the equation $A^T A\mathbf{x} = \mathbf{0}$ has a non-zero solution $\mathbf{x}$. Take the dot product as follows, using the Lemma (applied to A^Tinstead of A, $A\mathbf{x}$ instead of $\mathbf{x}$ and setting $\mathbf{y} = \mathbf{x}$) :

$$0 = \mathbf{0} \cdot \mathbf{x} = A^T A\mathbf{x} \cdot \mathbf{x} = (A\mathbf{x}) \cdot A\mathbf{x}.$$

This implies that $A\mathbf{x} = \mathbf{0}$, and since A has rank n, we see that $\mathbf{x}$ must be zero, a contradiction. This shows that $A^T A$ is nonsingular. ■

The solution to the normal equations is often called the "least squares" solution to $A\mathbf{x} = \mathbf{b}$. (But keep in mind, it is not a solution to the system.) The reason is that $||\mathbf{b} - \mathbf{p}||$ is as small as possible. The square of this quantity is also as small as possible, and we know that

$$||\mathbf{b} - \mathbf{p}||^2 = (b_1 - p_1)^2 + (b_2 - p_2)^2 + (b_3 - p_3)^2 .$$

In the context of the problem of fitting a straight line to data, the quantity above is the sum of the squares of the differences between the y values in the data (b_1, b_2, b_3), and the y values at the same x values along the line. This will be illustrated graphically in class. The method is called "linear regression" in some areas of application, such as psychology.

In general we can use this method on any system $A\mathbf{x} = \mathbf{b}$. where A is $m \times n$ and $\mathbf{b}$ is $n \times 1$. Suppose that $A\mathbf{x} = \mathbf{b}$ has no solution, and also that A has n linearly independent columns. (Thus, A has rank n. If this is not true, remove columns from A until it is.) Now solve the normal equation

$$A^T A\mathbf{x} = A^T\mathbf{b}.$$

Since $A^T A$ is nonsingular (assuming that A has rank n), we see that

$$\mathbf{x} = \left(A^T A\right)^{-1} A^T\mathbf{b}$$

and that if $\mathbf{p} = A\mathbf{x}$, then

$$\mathbf{p} = A\left(A^T A\right)^{-1} A^T\mathbf{b}.$$

The matrix

$$P = A\left(A^T A\right)^{-1} A^T$$

is called a "projection matrix" because it projects $\mathbf{b}$ onto a subspace of R^m, namely the subspace $C(A)$. This is an "orthogonal projection", because $\mathbf{b} - \mathbf{p}$ is orthogonal to $C(A)$.

In our example above,

$$A = \begin{pmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{pmatrix}, A^T = \begin{pmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \end{pmatrix}$$
$$A^T A = \begin{pmatrix} 14 & 6 \\ 6 & 3 \end{pmatrix}, (A^T A)^{-1} = \frac{1}{6}\begin{pmatrix} 3 & -6 \\ -6 & 14 \end{pmatrix}$$

and the projection matrix is

$$P = A\left(A^T A\right)^{-1} A^T = \begin{pmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{pmatrix} \frac{1}{6} \begin{pmatrix} 3 & -6 \\ -6 & 14 \end{pmatrix} \begin{pmatrix} 1 & 2 & 3 \\ 1 & 1 & 1 \end{pmatrix} = \begin{pmatrix} \frac{5}{6} & \frac{1}{3} & -\frac{1}{6} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ -\frac{1}{6} & \frac{1}{3} & \frac{5}{6} \end{pmatrix}.$$

Note that

$$P \begin{pmatrix} 1 \\ 3 \\ 4 \end{pmatrix} = \begin{pmatrix} \frac{5}{6} & \frac{1}{3} & -\frac{1}{6} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \\ -\frac{1}{6} & \frac{1}{3} & \frac{5}{6} \end{pmatrix} \begin{pmatrix} 1 \\ 3 \\ 4 \end{pmatrix} = \begin{pmatrix} \frac{7}{6} \\ \frac{8}{3} \\ \frac{25}{6} \end{pmatrix}.$$

On the other hand,

$$\mathbf{p} = A \begin{pmatrix} \frac{3}{2} \\ -\frac{1}{3} \end{pmatrix} = \begin{pmatrix} 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{pmatrix} \begin{pmatrix} \frac{3}{2} \\ -\frac{1}{3} \end{pmatrix} = \begin{pmatrix} \frac{7}{6} \\ \frac{8}{3} \\ \frac{25}{6} \end{pmatrix},$$

as expected from the previous line.

Proposition 3 *P has the following properties:*
(i) It is symmetric
(ii) $P^2 = P$.

Proof. The first statement follows from formulas for the transpose of a product of matrices, and the transpose of an inverse.

The second follows because if $\mathbf{b}$ is a vector in $C(A)$ then the projection of $\mathbf{b}$ onto $C(A)$ is simply $\mathbf{b}$ itself. (Obviously, $\mathbf{b}$ is the closest point in $C(A)$ to itself.) If $\mathbf{b}$ is any vector in R^m, then $P\mathbf{b}$ is in $C(A)$ and hence $P(P\mathbf{b}) = P\mathbf{b}$. This proves (ii). ■

In fact, any square matrix with these properties is an orthogonal projection onto the column space of this matrix. For example, consider

$$P = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}.$$

It is symmetric and we easily calculate that $P^2 = P$. For any $\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}$ we have $P \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} x_1 \\ 0 \end{pmatrix}$ and so P is a projection of R^2 to the x_1 axis.

2 more on projections

To repeat:

Definition 4 *A projection on R^n is an $n \times n$ matrix P such that $P^2 = P$.*

Definition 5 *An orthogonal projection on R^n is a projection matrix which is symmetric.*

Theorem 6 *A projection P is orthogonal if and only if for each $\mathbf{x} \in R^n$, $\mathbf{x}-P\mathbf{x}$ is orthogonal to $C(P)$.*

Proof. Any vector in $C(P)$ can be written as $P\mathbf{y}$ for some $\mathbf{y}$ in R^n. This vector is orthogonal to $\mathbf{x}-P\mathbf{x}$ if and only if

$$\langle P\mathbf{y}, \mathbf{x}-P\mathbf{x}\rangle = 0.$$

By the earlier proposition,

$$\langle P\mathbf{y}, \mathbf{x}-P\mathbf{x}\rangle = \langle \mathbf{y}, P^T(\mathbf{x}-P\mathbf{x})\rangle.$$

P is symmetric if and only if $P^T = P$, and P is a projection if and only if $P^2 = P$, and if both of these are true, then

$$P^T(\mathbf{x}-P\mathbf{x}) = P\mathbf{x}-P^2\mathbf{x} = P\mathbf{x}-P\mathbf{x} = \mathbf{0},$$

and $\langle \mathbf{y}, \mathbf{z}\rangle = 0$ for every $\mathbf{y}$ if and only if $\mathbf{z} = \mathbf{0}$. This proves the theorem. ■

We have seen that in the least squares method we encounter an orthogonal projection

$$P = A\left(A^TA\right)^{-1}A^T.$$

We can easily check that it satisfies the conditions of the theorem above. First of all,

$$P^2 = \left(A\left(A^TA\right)^{-1}A^T\right)\left(A\left(A^TA\right)^{-1}A^T\right) = A\left(\left(A^TA\right)^{-1}A^TA\right)\left(A^TA\right)^{-1}A^T = A\left(A^TA\right)^{-1}A^T = P.$$

Also, A^TA is symmetric, because of the formula $(AB)^T = B^TA^T$ and because $\left(A^T\right)^T = A$. This implies that $\left(A^TA\right)^{-1}$ is symmetric, and hence,

$$P^T = \left(A\left(A^TA\right)^{-1}A^T\right)^T = A\left(A^TA\right)^{-1}A^T = P.$$

Now suppose that A is any matrix whose columns are linearly independent. In that case, we saw earlier that A^TA is nonsingular. The matrix

$$P = A\left(A^TA\right)^{-1}A^T$$

is therefore a projection. We can ask: What space does it project onto. Since the matrix on the left in the product defining P is A, P projects into the column space of A. In fact, we can show that P projects **onto** $C(A)$. (What is the difference between “projects into” and “projects onto” ?

Here is an example: Find the matrix which projects P onto the subspace $V = \left\{\begin{pmatrix} x \\ y \\ z \end{pmatrix} \mid x+y+z=0\right\}$.

Note that this subspace is a plane in R^3.

Solution: We need to come up with a matrix A whose columns are a basis for V. This is not hard to do. Check that

$$A = \begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{pmatrix}$$

is such a matrix. Then the desired projection is

$$P = A\left(A^TA\right)^{-1}A^T.$$

But

$$A^TA = \begin{pmatrix} 1 & -1 & 0 \\ 0 & 1 & -1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ -1 & 1 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 2 & -1 \\ -1 & 1 \end{pmatrix}.$$

The inverse of this is a little messy. It turns out that we can get an easier matrix to deal with if we choose our basis for V more carefully. We will look for an **orthogonal basis. It is not hard to see that**

$$\left\{ \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix} \right\}$$

is a basis for V. (Each vector satisfies the equation and there are two of them. Since V is two dimensional (a plane in R^3), any two linearly independent vectors which are in V form a basis.)

Now we have

$$A^T A = \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & -2 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 0 & -2 \end{pmatrix} = \begin{pmatrix} 2 & 0 \\ 0 & 6 \end{pmatrix}.$$

Note that the zeros come because the columns of A are orthogonal. Now the inverse is easy to find:

$$\left(A^T A\right)^{-1} = \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{6} \end{pmatrix}.$$

We then have

$$P = \begin{pmatrix} 1 & 1 \\ -1 & 1 \\ 0 & -2 \end{pmatrix} \begin{pmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{6} \end{pmatrix} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & -2 \end{pmatrix} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{3} & \frac{2}{3} & -\frac{1}{3} \\ -\frac{1}{3} & -\frac{1}{3} & \frac{2}{3} \end{pmatrix}.$$

Note the following about this matrix:

1. It is symmetric.
2. Its columns add up to zero, so each is in V.
3. A calculation shows that $P^2 = P$.