## **Chapter 4: Orthogonality**

4.2. Projections

**Proposition.** Let A be a matrix. Then  $N(A^T A) = N(A)$ .

*Proof.* If  $A\mathbf{x} = \mathbf{0}$ , then of course  $A^T A \mathbf{x} = \mathbf{0}$ . Conversely, if  $A^T A \mathbf{x} = \mathbf{0}$ , then

$$0 = \boldsymbol{x} \cdot (A^T A \boldsymbol{x}) = \boldsymbol{x}^T A^T A \boldsymbol{x} = (A \boldsymbol{x})^T A \boldsymbol{x} = (A \boldsymbol{x}) \cdot (A \boldsymbol{x}) ,$$

so  $A\mathbf{x} = \mathbf{0}$  also.

**Corollary.** If the columns of the matrix A are independent, then  $A^T A$  is invertible.

*Proof.* Suppose A is  $m \times n$ , so that its rank is  $r(\leq m, \text{ of course})$ . Then  $A^T A$  is an  $n \times n$  matrix, and  $N(A^T A) = N(A)$  consists only the zero vector, so it is invertible.

Take a subspace V of  $\mathbb{R}^m$ . We want to figure out how to find the orthogonal projection of each vector  $\boldsymbol{b}$  in  $\mathbb{R}^m$  onto V, i.e., the closest point  $\boldsymbol{p}$  in V to  $\boldsymbol{b}$ . (That the closest  $\boldsymbol{p}$  to  $\boldsymbol{b}$  really makes  $\boldsymbol{b} - \boldsymbol{p}$  perpendicular to V is clear by geometry, but we can also do it as a minimization problem in multivariate calc — see the next section.) We can see from geometry that the function that assigns to each  $\boldsymbol{b}$  its projection  $\boldsymbol{p}$  is a linear transformation — it respects addition and scalar multiplication — so there is an  $m \times m$  matrix P for which  $P\boldsymbol{b} = \boldsymbol{p}$  for each  $\boldsymbol{b}$ . [WARNING: In the display on page 210, Strang has a typo: P is  $m \times m$ , not  $n \times n$ .] To find this P, it's enough to find a matrix that does what we want to an invertible matrix B (because if PB = MB, then we can multiply on the right by  $B^{-1}$  and say P = M.

Choose a basis for V and use it as the columns of a matrix A; suppose  $\dim(V) = n$ , so that A is  $m \times n$ . We claim that the projection matrix P that we want is

$$P = A(A^T A)^{-1} A^T .$$

This product at least does make sense: Because the columns of A are a basis for V, they are independent, so  $A^T A$  is an invertible  $n \times n$  matrix; and the dimensions of the factors are right for multiplication. Now let's form a basis for  $\mathbb{R}^m$  starting with the columns of A and adding in a basis  $c_1, \ldots, c_{m-n}$  for the orthogonal complement  $V^{\perp}$  of V. The projection should leave the columns of A unchanged and turn the c's to  $\theta$ :

$$\begin{bmatrix} A \quad \boldsymbol{c}_1 \quad \dots \quad \boldsymbol{c}_{m-n} \end{bmatrix} \xrightarrow{P} \begin{bmatrix} A \quad O_{m \times (m-n)} \end{bmatrix};$$

so let's check that the P given by the (ugly) formula above does that:

Multiplying the columns of A by  $A^T$  gives  $A^T A$  (a matrix of dot products of the columns of A with each other, but we don't need that right now), and multiplying the c's by  $A^T$  gives columns of 0's because the c's were orthogonal to the columns of A. So multiplying by the factors in the product gives the sequence of block matrices

$$\begin{bmatrix} A & \boldsymbol{c}_1 & \dots & \boldsymbol{c}_{m-n} \end{bmatrix} \stackrel{A^T}{\rightarrow} \begin{bmatrix} A^T A & \boldsymbol{0} & \dots & \boldsymbol{0} \end{bmatrix} \stackrel{(A^T A)^{-1}}{\rightarrow} \begin{bmatrix} I_n & O_{n \times (m-n)} \end{bmatrix}$$
$$\stackrel{A}{\rightarrow} \begin{bmatrix} A & O_{m \times (m-n)} \end{bmatrix}.$$

So  $A(A^TA)^{-1}A^T$  is the P we want.

Notation: Strang consistently uses **b** for a general vector  $\mathbb{R}^m$ , A for the matrix whose columns are a basis for the subspace onto which we are projecting, **p** for the projection of **b** onto that subspace and **e** for the "error vector"  $\mathbf{b} - \mathbf{p}$  (orthogonal to V). He also uses  $\hat{\mathbf{x}} = (x_1, \ldots, x_n)$  for the column of coefficients that gives **p** in terms of the columns of A, i.e.,  $A\hat{\mathbf{x}} = \mathbf{p}$ . So, because we know  $A\hat{\mathbf{x}} = P\mathbf{b} = A(A^TA)^{-1}A^T\mathbf{b}$ , and that A can be cancelled from the left (its nullspace is just the 0 vector), we see that  $\hat{\mathbf{x}} = (A^TA)^{-1}A^T\mathbf{b}$ , i.e.,  $\hat{\mathbf{x}}$  is the solution to  $A^TA\mathbf{x} = A^T\mathbf{b}$ .

**Example.** We want to find the orthogonal projection p of b = (2, 0, 3) on the subspace of  $\mathbb{R}^3$  with basis (1, 1, 1) and (1, 0, -1), and to find the projection matrix, and to verify that e = b - p is orthogonal to the subspace:

$$A = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 1 & -1 \end{bmatrix}, \quad (A^{T}A)^{-1} = \begin{bmatrix} 3 & 0 \\ 0 & 2 \end{bmatrix}^{-1} = \begin{bmatrix} 1/3 & 0 \\ 0 & 1/2 \end{bmatrix}$$
$$P = \begin{bmatrix} 1 & 1 \\ 1 & 0 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1/3 & 0 \\ 0 & 1/2 \end{bmatrix} \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 5/6 & 1/3 & -1/6 \\ 1/3 & 1/3 & 1/3 \\ -1/6 & 1/3 & 5/6 \end{bmatrix},$$
$$p = P \begin{bmatrix} 2 \\ 0 \\ 3 \end{bmatrix} = \begin{bmatrix} 7/6 \\ 5/3 \\ 13/6 \end{bmatrix}, \quad A^{T}(b-p) = \begin{bmatrix} 1 & 1 & 1 \\ 1 & 0 & -1 \end{bmatrix} \begin{bmatrix} 5/6 \\ -5/3 \\ 5/6 \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

Special Case (silly): A is invertible, i.e.,  $V = \mathbb{R}^m$ : The closest point in V to any **b** in  $\mathbb{R}^m$  is **b** itself, so  $\mathbf{p} = \mathbf{b}$ , P = I and  $\hat{\mathbf{x}} = A^{-1}\mathbf{b}$ .

Special Case (not silly): A is a single nonzero vector  $\boldsymbol{a}$ , i.e., V is a line: Then  $A^T A = \boldsymbol{a} \cdot \boldsymbol{a}$  is a nonzero number, so its inverse is just its reciprocal, and

$$P = \frac{aa^T}{a \cdot a}$$

Moreover,

$$p = \frac{aa^T}{a \cdot a}b = \frac{a(a^Tb)}{a \cdot a} = \frac{a \cdot b}{a \cdot a}a$$
, so  $\hat{x} = \frac{a \cdot b}{a \cdot a}$ ,

because in this case  $\hat{x}$  is a single number, the coefficient of a when writing p.

**Example.** We want to find the projection p of b = (1, 2, 3) onto (the span of) a = (1, 0, -1) and the corresponding  $\hat{x}$ , and to check that e = b - p is orthogonal to a:

$$P = \frac{1}{1+0+1} \begin{bmatrix} 1\\0\\-1 \end{bmatrix} \begin{bmatrix} 1 & 0 & -1 \end{bmatrix} = \begin{bmatrix} 1/2 & 0 & -1/2\\0 & 0 & 0\\-1/2 & 0 & 1/2 \end{bmatrix}, \quad p = P \begin{bmatrix} 1\\2\\3 \end{bmatrix} = \begin{bmatrix} -1\\0\\1 \end{bmatrix},$$
$$\hat{x} = \frac{a \cdot b}{a \cdot a} = \frac{1+0+(-3)}{1+0+1} = -1, \qquad a \cdot e = \begin{bmatrix} 1\\0\\-1 \end{bmatrix} \cdot \begin{bmatrix} 2\\2\\2 \end{bmatrix} = 0$$

Note that any projection matrix P, onto the subspace V, say, multiplies all the vectors in  $\mathbb{R}^m$  into V, and if we multiply again by P, they don't change. Thus,

$$P^2 \boldsymbol{b} = P \boldsymbol{b}$$
 for every  $\boldsymbol{b}$  in  $\mathbb{R}^m$ , i.e.,  $P^2 = P$ 

The term for a matrix that equals its own square is *idempotent*. There is more about idempotent matrices in the exercises.

## 4.3. Least Squares Approximation

In this section the objective is to find the *n*-dimensional subspace of  $\mathbb{R}^{n+1}$  that best approximates a set of *m* points in  $\mathbb{R}^m$ , with "best" being measured as "minimizing the sum of the squares of the <u>vertical</u> distances from the points to the subspace", where vertical means in the direction of the axis for the last variable. This is the *least squares approximation* to the points. It seemed to me that this question, with <u>vertical</u> distances, was basically different from the last section, which measures <u>orthogonal</u> distances; but by writing both problems in neutral variables (so that I can keep straight which are the constants and which are the variables), we can see they are the same: Sticking to 3-dimensional space, so that we can visualize things, we can write

The projection problem: Given vectors  $(p_1, p_2, p_3), (q_1, q_2, q_3), (r_1, r_2, r_3)$  in  $\mathbb{R}^3$ , find the point  $(\hat{r}_1, \hat{r}_2, \hat{r}_3) = g(p_1, p_2, p_3) + h(q_1, q_2, q_3)$  closest to  $(r_1, r_2, r_3)$ , i.e., minimizing

$$E = (r_1 - \hat{r}_1)^2 + (r_2 - \hat{r}_2)^2 + (r_3 - \hat{r}_3)^2$$
  
=  $(r_1 - (gp_1 + hq_1))^2 + (r_2 - (gp_2 + hq_2))^2 + (r_3 - (gp_3 + hq_3))^2$ 

In our earlier notation r = b, p and q are the columns of A, and we seek  $\hat{r} = p$  and  $\hat{x} = (g, h)$ .

The least squares problem: Given points  $(p_1, q_1, r_1), (p_2, q_2, r_2), (p_3, q_3, r_3)$  in  $\mathbb{R}^3$ , with r on the vertical axis, find the subspace, given by the equation  $\hat{r} = gp + hq$ , that minimizes the sum of the squares of the vertical distances from the given points to the corresponding points on the subspace, i.e., minimizing

$$E = (r_1 - \hat{r}_1)^2 + (r_2 - \hat{r}_2)^2 + (r_3 - \hat{r}_3)^2$$
  
=  $(r_1 - (gp_1 + hq_1))^2 + (r_2 - (gp_2 + hq_2))^2 + (r_3 - (gp_3 + hq_3))^2$ .

The least squares problem, though, arises in a different way: Given data values with n "input" (or "explanatory", or "predictor") variables  $x_1, x_2, \ldots, x_n$  and one "output" (or "response") variable y, find the coefficients  $c_i$  of the linear equation

$$\hat{y} = c_1 x_1 + c_2 x_2 + \dots + c_n x_n$$

that best approximates the data. From this point of view, the x-values of the data points become the <u>constants</u>, the entries in the matrix X (which used to be A), the y-values of the data points become **b**, the c's become the coefficients for writing the approximation  $\hat{y}$  for y in terms of x-values of the data points — in other words, what  $\hat{x}$  was in the other version of the problem (ARGH!).

So this time we aren't interested as much in what corresponds to p or P as what corresponds to  $\hat{x}$ , i.e., the solution c to  $X^T X c = y$ , where

$$X = \begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,n} \\ x_{2,1} & x_{2,2} & \dots & x_{2,n} \\ \vdots & \vdots & \ddots & \vdots \\ x_{m,1} & x_{m,2} & \dots & x_{m,n} \end{bmatrix}$$

At least, m, the number of data points, is usually much larger than n, the number of variables, and we can often control those values in an experiment, so the columns of X are usually independent. Thus,  $X^T X$  is usually invertible, and we can solve for  $\boldsymbol{c} = (X^T X)^{-1} X^T \boldsymbol{y}$ .

**Example.** Find the plane  $\hat{y} = cx_1 + dx_2$  that is the least squares approximation to the data points (0,1,4), (1,0,5), (1,1,8), (-1,2,7):

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \\ 1 & 1 \\ -1 & 2 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 4 \\ 5 \\ 8 \\ 7 \end{bmatrix}, \quad (X^T X)^{-1} = \begin{bmatrix} 3 & -1 \\ -1 & 6 \end{bmatrix}^{-1} = (1/17) \begin{bmatrix} 6 & 1 \\ 1 & 3 \end{bmatrix}$$
$$\mathbf{c} = (X^T X)^{-1} X^T \mathbf{y} = (1/17) \begin{bmatrix} 6 & 1 \\ 1 & 3 \end{bmatrix} \begin{bmatrix} 6 \\ 26 \end{bmatrix} = \begin{bmatrix} 62/17 \\ 84/17 \end{bmatrix};$$

so the best approximation to these points is  $\hat{y} = (62/17)x_1 + (84/17)x_2$ .

**Example.** Find the line  $\hat{y} = mx + b$  in  $\mathbb{R}^2$  that is the least squares approximation to (i.e., is the regression line for) the data points (0,1), (1,2), (2,5), (3,6):

There seems to be only one input variable here, but we can create a second having the value 1 at each data point, to take care of the constant term b that means the line is not a subspace:

$$X = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 2 & 1 \\ 3 & 1 \end{bmatrix}, \quad \mathbf{y} = \begin{bmatrix} 1 \\ 2 \\ 5 \\ 6 \end{bmatrix}, \quad (X^T X)^{-1} = \begin{bmatrix} 14 & 6 \\ 6 & 4 \end{bmatrix}^{-1} = \begin{bmatrix} 0.2 & -0.3 \\ -0.3 & 0.7 \end{bmatrix}$$
$$\mathbf{c} = (X^T X)^{-1} X^T \mathbf{y} = \begin{bmatrix} 0.2 & -0.3 \\ -0.3 & 0.7 \end{bmatrix} \begin{bmatrix} 42 \\ 24 \end{bmatrix} = \begin{bmatrix} 1.8 \\ 0.8 \end{bmatrix};$$

so the best approximation to these points is  $\hat{y} = 1.8x + 0.8$ .

**Example.** The heights h in feet of a ball t seconds after it is thrown upward are (0,0.2), (0.2,3.0), (0.4,5.3), (0.6,7.0), (0.8,7.5), (1.0,5.5). Of course the height should be related to the time by an equation of the form  $h = a + bt + ct^2$  where c is negative. What are best approximations for the values of a, b, c? These are the initial height, initial velocity, and half the gravitational constant respectively — we don't know that the ball was thrown on Earth.

Besides the column of 1's, we also add a column of  $t^2$ 's. Then we use R again:

$$T = \begin{bmatrix} 1 & 0 & 0 \\ 1 & 0.2 & 0.04 \\ 1 & 0.4 & 0.16 \\ 1 & 0.6 & 0.36 \\ 1 & 0.8 & 0.64 \\ 1 & 1 & 1 \end{bmatrix}, \quad \mathbf{h} = \begin{bmatrix} 0.2 \\ 3.0 \\ 5.3 \\ 7.0 \\ 7.5 \\ 5.5 \end{bmatrix}, \quad (T^T T)^{-1} = \begin{bmatrix} 0.8214286 & -2.946429 & 2.232143 \\ -2.9464286 & 18.169643 & -16.741071 \\ 2.2321429 & -16.741071 & 16.741071 \end{bmatrix}$$
$$\begin{bmatrix} \hat{a} \\ \hat{b} \\ \hat{c} \end{bmatrix} = (T^T T)^{-1} T^T \mathbf{h} = \begin{bmatrix} -0.08571429 \\ 19.88571429 \\ -13.92857143 \end{bmatrix}$$

Apparently the ball was <u>not</u> thrown on Earth; it was thrown out of a shallow hole on a smaller planet.

## 4.4. Orthogonal Bases and Gram-Schmidt

Vectors are orthonormal iff they are pairwise orthogonal and they all have length 1. If the columns of the matrix Q (traditionally that letter) and Q is  $m \times n$  where  $m \ge n$ , then  $Q^T Q = I_n$ . In particular, if Q is  $n \times n$  — and still has orthonormal columns — then Q is invertible with inverse its transpose; it is then called orthogonal. (Why not "orthonormal", I don't know, and apparently neither does Strang.)

Suppose we have a basis  $q_1, \ldots, q_n$  for  $\mathbb{R}^n$  consisting of orthonormal vectors. What does that do for us? Well, for any vector v in  $\mathbb{R}^n$ , suppose we have written v in terms of the q's:

$$\boldsymbol{v} = c_1 \boldsymbol{q}_1 + \dots + c_n \boldsymbol{q}_n$$
 .

Then for each k from 1 to n:

$$\boldsymbol{q}_{k}^{T}\boldsymbol{v} = c_{1}\boldsymbol{q}_{k}^{T}\boldsymbol{q}_{1} + \dots + c_{n}\boldsymbol{q}_{k}^{T}\boldsymbol{q}_{n} \qquad \qquad = c_{1}(0) + \dots + c_{k}(1) + \dots + c_{n}(0) = c_{k} \ .$$

So we can find the coefficients to write v in terms of  $q_1, \ldots, q_n$  just by taking dot products with the q's

We want to start with a basis  $a_1, \ldots, a_n$  for  $\mathbb{R}^n$  and build a new basis  $q_1, \ldots, q_n$  that consists of orthonormal vectors.

How do we get from the a's to the q's? Well, the first step is easy: We just "normalize"  $a_1$ , i.e., give it length 1, by dividing by its length:

$$m{q}_1 = m{a}_1 / || m{a}_1 ||$$
 .

Then we have to replace  $a_2$  with one that is orthogonal to  $q_1$ . By Section 4.2, we have a way to get one: project  $a_2$  onto  $q_1$ , and subtract the result from  $a_2$ . Then we normalize that result:

$$m{e}_2 = m{a}_2 - rac{m{q}_1^Tm{a}_2}{m{q}_1^Tm{q}_1}m{q}_1 = m{a}_2 - (m{q}_1^Tm{a}_2)m{q}_1 \;, \qquad m{q}_2 = m{e}_2/||m{e}_2|| \;;$$

the projection formula is simpler because  $q_1$  have length 1. Then the next step: subtract from  $a_3$  its projections on  $q_1$  and  $q_2$  (which gives something orthogonal to the first two q's), and normalize the result.

$$m{e}_3 = m{a}_3 - (m{q}_1^T m{a}_3)m{q}_1 - (m{q}_2^T m{a}_3)m{q}_2 \;, \qquad m{q}_3 = m{e}_3/||m{e}_3|| \;.$$

And so on.

And what is the process of going back from the q's to the a's? Using the dot product fact that we noted earlier, we get

$$oldsymbol{a}_k = \sum_{i=1}^n (oldsymbol{q}_i^Toldsymbol{a}_k)oldsymbol{q}_i \; .$$

If we write this in terms of matrices, we get

If we call A the matrix with columns the  $\mathbf{a}$ 's, Q the matrix with columns the  $\mathbf{q}$ 's, and R the matrix of dot products, then A = QR. Moreover, look at the entries  $\mathbf{q}_i^T \mathbf{a}_j$  in the lower triangle of R, i.e., i > j. Then  $\mathbf{a}_j$  can be written as a combination of the  $\mathbf{q}$ 's up to j; and  $\mathbf{q}_i$  is orthogonal to the earlier  $\mathbf{q}$ 's, so it is orthogonal to  $\mathbf{a}_j$ . So the lower triangle is all 0's, i.e., R is upper triangular.

**Example.** The vector (1, -2, 2)/3 has length 1. We want to find an basis for  $\mathbb{R}^3$  that includes it, and then write the corresponding A as QR where Q is orthogonal and R is upper triangular:

The given vector together with (0,1,0) and (0,0,1) is a basis for  $\mathbb{R}^3$ , so we can use this basis

$$\boldsymbol{a}_1 = \boldsymbol{q}_1 = \begin{bmatrix} 1/3 \\ -2/3 \\ 2/3 \end{bmatrix}, \ \boldsymbol{a}_2 = \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \ \boldsymbol{a}_3 = \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}, \ \boldsymbol{A} = \begin{bmatrix} 1/3 & 0 & 0 \\ -2/3 & 1 & 0 \\ 2/3 & 0 & 1 \end{bmatrix}.$$

Then

$$\boldsymbol{e}_{2} = \boldsymbol{a}_{2} - (\boldsymbol{q}_{1}^{T}\boldsymbol{a}_{2})\boldsymbol{q}_{1} = \begin{bmatrix} 0\\1\\0 \end{bmatrix} - (-2/3) \begin{bmatrix} 1/3\\-2/3\\2/3 \end{bmatrix} = \begin{bmatrix} 2/9\\5/9\\4/9 \end{bmatrix}, \quad \boldsymbol{q}_{2} = \begin{bmatrix} 2/\sqrt{45}\\5/\sqrt{45}\\4/\sqrt{45} \end{bmatrix}$$

and

$$\mathbf{e}_{3} = \mathbf{a}_{3} - (\mathbf{q}_{1}^{T} \mathbf{a}_{3}) \mathbf{q}_{1} - (\mathbf{q}_{2}^{T} \mathbf{a}_{3}) \mathbf{q}_{2} = \begin{bmatrix} 0\\0\\1 \end{bmatrix} - (2/3) \begin{bmatrix} 1/3\\-2/3\\2/3 \end{bmatrix} - (4/\sqrt{45}) \begin{bmatrix} 2/\sqrt{45}\\5/\sqrt{45}\\4/\sqrt{45} \end{bmatrix}$$
$$= \begin{bmatrix} -2/5\\0\\1/5 \end{bmatrix}, \quad \mathbf{q}_{3} = \begin{bmatrix} -2/\sqrt{5}\\0\\1/\sqrt{5} \end{bmatrix}$$

We could check that the q's are pairwise orthogonal and each have length 1. We get

$$Q = \begin{bmatrix} 1/3 & 2/\sqrt{45} & -2/\sqrt{5} \\ -2/3 & 5/\sqrt{45} & 0 \\ 2/3 & 4/\sqrt{45} & 1/\sqrt{5} \end{bmatrix} , \qquad R = \begin{bmatrix} 1 & -2/3 & 2/3 \\ 0 & 5/\sqrt{45} & 4/\sqrt{45} \\ 0 & 0 & 1/\sqrt{5} \end{bmatrix} .$$