

## Math 314/814

### Topics since the second exam

**Note:** The final exam covers all three of our topics sheets for the semester.

#### Application: Markov chains.

In many situations we wish to study a characteristic (or characteristics) of a population, which changes over time. Often the rule for how the quantities change may be linear; our goal is to understand what the long term behavior of the situation is.

Initially, the characteristic of the population (think: favorite food, political affiliation, choice of hair color) is distributed among some collection of values; we represent this *initial state* as a vector  $\vec{v}_0$  giving the fraction of the whole population which takes each value. (The entries of  $\vec{v}_0$  sum to 1.) As time progresses, with each fixed time interval the distribution of the population changes by multiplication by a *transition matrix*  $A$ , whose  $(i, j)$  entry  $a_{i,j}$  records what fraction of the population having the  $i$ -th characteristic chooses to switch to the  $j$ -th characteristic. Since every person/object in the population ends up with some characteristic, each column of  $A$  (which describes how the  $i$ -th characteristic gets redistributed) must sum to 1. After the tick of the clock, the distribution of our initial population, given by  $\vec{v}_0$ , changes to  $\vec{v}_1 = A\vec{v}_0$ . After  $n$  ticks of the clock, the population distribution is given by  $\vec{v}_n = A^n\vec{v}_0$ .

The main questions to answer are: does the population distribution stabilize over time? And if so, what does it stabilize to? A stable distribution  $\vec{v}$  is one which is unchanged as time progresses:  $A\vec{v} = \vec{v}$ . This can be determined by reinterpreting stability as  $(A - I)\vec{v} = \vec{0}$ , i.e.,  $\vec{v}$  lies in the nullspace of the matrix  $A - I$ . Which we can compute! Our solution should also have all entries non-negative (to reflect that its entries represent parts of a whole) and add up to 1. Moreover, under very mild assumptions (e.g., no entry of  $A$  is 0) every initial state  $\vec{v}_0$ , under repeated multiplication by  $A$ , will converge to the exact same stable distribution. Which we can compute by the method above!

#### Eigenvalues and eigenvectors.

For  $A$  an  $n \times n$  matrix,  $v$  is an *eigenvector* (e-vector, for short) for  $A$  if  $v \neq 0$  and  $Av = \lambda v$  for some (real or complex, depending on the context) number  $\lambda$ .  $\lambda$  is called the associated *eigenvalue* for  $A$ . A matrix which has an eigenvector has *lots* of them; if  $v$  is an eigenvector, then so is  $2v$ ,  $3v$ , etc. On the other hand, a matrix does not have lots of eigenvalues:

If  $\lambda$  is an e-value for  $A$ , then  $(\lambda I - A)v = 0$  for some non-zero vector  $v$ . So  $\text{null}(\lambda I - A) \neq \{0\}$ , so  $\det(\lambda I - A) = 0$ . But  $\det(tI - A) = \chi_A(t)$ , thought of as a function of  $t$ , is a polynomial of degree  $n$ , so has at most  $n$  roots. So  $A$  has at most  $n$  different eigenvalues.

$\chi_A(t) = \det(tI - A)$  is called the *characteristic polynomial* of  $A$ .

$\text{null}(\lambda I - A) = E_\lambda(A)$  (ignoring 0) the collection of all e-vectors for  $A$  with e-value  $\lambda$ . it is called the *eigenspace* (or e-space) for  $A$  corresponding to  $\lambda$ . An *eigensystem* for a (square) matrix  $A$  is a list of all of its e-values, along with their corresponding e-spaces.

One somewhat simple case: if  $A$  is (upper or lower) triangular, then the e-values for  $A$  are exactly the diagonal entries of  $A$ , since  $tI - A$  is also triangular, so its determinant is the product of its diagonal entries.

We call  $\dim(\text{null}(\lambda I - A))$  the *geometric multiplicity* of  $\lambda$ , and the number of times  $\lambda$  is a root of  $\chi_A(t)$  (= number of times  $(t - \lambda)$  is a factor) =  $m(\lambda)$  = the algebraic multiplicity of  $\lambda$ .

Some basic facts:

The number of real eigenvalues for an  $n \times n$  matrix is  $\leq n$ .

counting multiplicity and complex roots the number of eigenvalues =  $n$ .

For every e-value  $\lambda$ ,  $1 \leq$  the geometric multiplicity  $\leq m(\lambda)$ .  
(non-zero) e-vectors having all different e-values are linearly independent.

### Similarity and diagonalization.

The matrix  $A = \begin{pmatrix} 3 & 2 \\ 3 & 4 \end{pmatrix}$  has e-values 1 and 6 (Check!) with corresponding e-vectors  $(1, -1)$  and  $(2, 3)$ . This then means that

$$\begin{pmatrix} 3 & 2 \\ 3 & 4 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix} = \begin{pmatrix} 1 & 2 \\ -1 & 3 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 6 \end{pmatrix}, \text{ which we write } AP = PD,$$

where  $P$  is the matrix whose columns are our e-vectors, and  $D$  is a diagonal matrix. Written slightly differently, this says  $A = PDP^{-1}$ .

We say two matrices  $A$  and  $B$  are *similar* if there is an invertible matrix  $P$  so that  $AP = PB$ . (Equivalently,  $P^{-1}AP = B$ , or  $A = PBP^{-1}$ .) A matrix  $A$  is *diagonalizable* if it is similar to a diagonal matrix.

We write  $A \sim B$  if  $A$  is similar to  $B$ , i.e.,  $P^{-1}AP = B$ . We can check:

$A \sim A$ ; if  $A \sim B$  then  $B \sim A$ ; if  $A \sim B$  and  $B \sim C$ , then  $A \sim C$ . (We say that “ $\sim$ ” is an *equivalence relation*.)

Why do we care about similarity? We can check that if  $A = PBP^{-1}$ , then  $A^n = PB^nP^{-1}$ . If  $B^n$  is quick to calculate (e.g., if  $B$  is diagonal;  $B^n$  is then also diagonal, and its diagonal entries are the powers of  $B$ 's diagonal entries), this means  $A^n$  is also fairly quick to calculate!

Also, if  $A$  and  $B$  are similar, then they have the same characteristic polynomial, so they have the same eigenvalues. They do, however, have different eigenvectors; in fact, if  $AP = PB$  and  $Bv = \lambda v$ , then  $A(Pv) = \lambda(Pv)$ , i.e., the e-vectors of  $A$  are  $P$  times the e-vectors of  $B$ . Similar matrices also have the same determinant, rank, and nullity.

These facts in turn tell us when a matrix can be diagonalized. Since for a diagonal matrix  $D$ , each of the standard basis vectors  $e_i$  is an e-vector,  $R^n$  has a basis consisting of e-vectors for  $D$ . If  $A$  is similar to  $D$ , via  $P$ , then each of  $Pe_i$  =  $i$ th column of  $P$  is an e-vector. But since  $P$  is invertible, its columns form a basis for  $R^n$ , as well. SO there is a basis consisting of e-vectors of  $A$ . On the other hand, such a basis guarantees that  $A$  is diagonalizable (just run the above argument in reverse...), so we find that:

(The Diagonalization Theorem) An  $n \times n$  matrix  $A$  is diagonalizable if and only if there is basis of  $R^n$  consisting of eigenvectors of  $A$ .

And one way to guarantee that such a basis exists: If  $A$  is  $n \times n$  and has  $n$  distinct eigenvalues, then choosing an e-vector for each will always yield a linear independent collection of vectors (so, since there are  $n$  of them, you get a basis for  $R^n$ ). So:

If  $A$  is  $n \times n$  and has  $n$  distinct (real) eigenvalues,  $A$  is diagonalizable. In fact, the dimensions of all of the eigenspaces for  $A$  (for real eigenvalues  $\lambda$ ) add up to  $n$  if and only if  $A$  is diagonalizable.

### Length and inner product.

“Norm” means length! In  $\mathbb{R}^n$  this is computed as  $\|x\| = \|(x_1, \dots, x_n)\| = (x_1^2 + \dots + x_n^2)^{1/2}$

Basic facts:  $\|x\| \geq 0$ , and  $\|x\| = 0$  iff  $x = \vec{0}$ ,

$\|cu\| = |c| \cdot \|u\|$ , and  $\|u + v\| \leq \|u\| + \|v\|$  (triangle inequality)

unit vector: the norm of  $u/\|u\|$  is 1;  $u/\|u\|$  is the *unit vector* in the direction of  $u$ .

Inner product:

idea: assign a number to a pair of vectors (think: angle between them?)

In  $\mathbb{R}^n$ , we use the *dot product*:  $v = (v_1, \dots, v_n)$ ,  $w = (w_1, \dots, w_n)$

$$v \bullet w = \langle v, w \rangle = v_1 w_1 + \cdots + v_n w_n = v^T w$$

Basic facts:

$$\langle v, v \rangle = \|v\|^2 \text{ (so } \langle v, v \rangle \geq 0, \text{ and equals 0 iff } v = \vec{0})$$

$$\langle v, w \rangle = \langle w, v \rangle; \langle cv, w \rangle = \langle v, cw \rangle = c \langle v, w \rangle \quad \langle v_1 + v_2, w \rangle = \langle v_1, w \rangle + \langle v_2, w \rangle$$

### Orthogonality.

Two vectors are *orthogonal* if their angle is  $\pi/2$ , i.e.,  $\langle v, w \rangle = 0$ . Notation:  $v \perp w$ . (Also say they are *perpendicular*.)

A collection of vectors  $\{v_1, \dots, v_k\}$  is an *orthogonal set* if  $v_i \perp v_j$  for every  $i \neq j$ . If all of the vectors in an orthogonal set are non-zero, then they are linearly independent.

An *orthogonal basis* for a subspace  $W$  is a basis for  $W$  that is also an orthogonal set. If we have an orthogonal basis  $v_1, \dots, v_k$  for  $W$ , then determining the coordinates for a vector  $w \in W$  is quick:  $w = \sum a_i v_i$  for  $a_i = \langle w, v_i \rangle / \|v_i\|^2$ .

A collection of vectors  $\{v_1, \dots, v_k\}$  is an *orthonormal set* (we write “o.n. set”) if they are an orthogonal set and  $\|v_i\| = 1$  for every  $i$ . An *orthonormal basis* (o.n. basis) is a basis that is also an orthonormal set. For an o.n. basis for  $W$ , the coordinates of  $w \in W$  are even shorter:  $w = \sum a_i v_i$  for  $a_i = \langle w, v_i \rangle$ .

### Orthogonal Complements.

This notion of orthogonal vectors can even be used to reinterpret some of our dearly-held results about systems of linear equations, where all of this stuff began.

Starting with  $Ax = 0$ , this can be interpreted as saying that  $\langle \text{every row of } A, x \rangle = 0$ , i.e.,  $x$  is orthogonal to every row of  $A$ . This in turn implies that  $x$  is orthogonal to every linear combination of rows of  $A$ , i.e.,  $x$  is orthogonal to every vector in the row space of  $A$ .

This leads us to introduce a new concept: the **orthogonal complement** of a subspace  $W$  in a vector space  $V$ , denoted  $W^\perp$ , is the collection of vectors  $v$  with  $v \perp w$  for **every** vector  $w \in W$ . It is not hard to see that these vectors form a subspace of  $V$ ; the sum of two vectors orthogonal to  $w$ , for example, is orthogonal to  $w$ , so the sum of two vectors in  $W^\perp$  is also in  $W^\perp$ . The same is true for scalar multiples.

Some basic facts:

For every subspace  $W$ ,  $W \cap W^\perp = \{0\}$  (since anything in both is orthogonal to *itself*, and only the 0-vector has that property).

Finally,  $(W^\perp)^\perp = W$ ; this is because  $W$  is contained in  $(W^\perp)^\perp$  (a vector in  $W$  is orthogonal to every vector that is orthogonal to things in  $W$ ), and the dimensions of the two spaces are the same.

The importance that this has to systems of equations stems from the following facts:

$$\text{null}(A) = \text{row}(A)^\perp \quad \text{row}(A) = \text{null}(A)^\perp \quad \text{col}(A) = \text{null}(A^T)^\perp$$

This provides us with yet another (quicker?) way to decide if a system of equations  $A\vec{x} = \vec{b}$  is consistent, or rather, for *which*  $\vec{b}$  is it consistent;  $\vec{b}$  must lie in  $\text{col}(A)$ , i.e., in  $\text{null}(A^T)^\perp$ . So it must be  $\perp$  to a basis for  $\text{null}(A^T)$ . So we can compute a basis for  $\text{null}(A^T)$ ,  $v_1, \dots, v_k$ , and use this to check for consistency:  $A\vec{x} = \vec{b}$  is consistent  $\Leftrightarrow \langle \vec{b}, v_i \rangle = 0$  for every  $v_i$ .

And to compute a basis for  $W^\perp$ : start with a basis for  $W$ , writing them as the columns of a matrix  $A$ , so  $W = \text{col}(A)$ , then  $W^\perp = \text{col}(A)^\perp = \text{row}(A^T)^\perp = \text{null}(A^T)$ , which we know how to compute a basis for!

Or even better: start with a basis for  $W$ , writing them as the columns of a matrix  $A$ . The row reduce the supraugmented matrix  $(A|I) \rightarrow (R|E)$  with  $R$  in REF or RREF. Then the transposes  $V_1, \dots, v_k$  of the rows of  $E$  that stand opposite the all-0 rows of  $R$  form a basis for  $\text{null}(A^T) = W^\perp$ ! This is because  $R = EA$ , so  $R^T = A^T E^T$ , which implies that  $A^T v_i = \vec{0}$  for every  $i$ . But  $E$  is

invertible, so  $E^T$  is invertible, so the  $v_i$  are linearly independent. But!  $k =$  thenumber of  $\vec{0}$ -rows of  $R = (\# \text{ of rows of } R) - (\# \text{ of non-}\vec{0} \text{ rows of } R = (\# \text{ rows of } A) - (\text{row rank of } A) = (\# \text{ columns of } A^T) - (\text{rank of } A^T) = \text{nullity of } A^T$ , so  $v_1, \dots, v_k$  are in  $\text{null}(A^T)$ , are linearly independent, and there are as many of them as there is for a basis for  $\text{null}(A^T)$ , so they form a basis for  $\text{null}(A^T)$  !

### Orthogonal Projections.

Any vector  $v \in V$  can be written, uniquely, as  $v = w + w^\perp$ , for  $w \in W$  and  $w^\perp \in W^\perp$  ; the uniqueness comes from the result above about intersections. That it can be written that way at all comes from orthogonal projections.

We've seen that if  $w_1, \dots, w_k$  is an orthogonal basis for a subspace  $W$  of  $\mathbb{R}^n$ , and  $w \in W$ , then  $w = \frac{\langle w_1, w \rangle}{\langle w_1, w_1 \rangle} w_1 + \dots + \frac{\langle w_k, w \rangle}{\langle w_{k-1}, w_{k-1} \rangle} w_{k-1} + \frac{\langle w_k, w \rangle}{\langle w_k, w_k \rangle} w_k$

On the other hand, if  $v \in V$ , we can define the orthogonal projection

$$\text{proj}_W(v) = \frac{\langle w_1, v \rangle}{\langle w_1, w_1 \rangle} w_1 + \dots + \frac{\langle w_k, v \rangle}{\langle w_k, w_k \rangle} w_k$$

of  $v$  into  $W$ . This vector is in  $W$ , and we can show that  $v - \text{proj}_W(v)$  is orthogonal to all of the  $w_i$ , so it is orthogonal to every linear combination, i.e., it is orthogonal to every vector in  $W$ . So  $v - \text{proj}_W(v) = w' \in W^\perp$

In the case that the  $w_i$  are not just orthogonal but also *orthnormal*, we can simplify this somewhat:  $\text{proj}_W(v) = \langle w_1, v \rangle w_1 + \dots + \langle w_n, v \rangle w_n = (w_1 w_1^T + \dots + w_n w_n^T) v = P v$ , where  $P = (w_1 w_1^T + \dots + w_n w_n^T)$  is the **projection matrix** giving us orthogonal projection.

For any subspace  $W \subseteq \mathbb{R}^n$ ,  $\dim(W) + \dim(W^\perp) = n = \dim(\mathbb{R}^n)$ . Even more, a basis for  $W$  and a basis for  $W^\perp$  together form a basis for  $\mathbb{R}^n$ .

All that we need now is a method for building orthogonal bases for subspaces! (See also the formulation for the orthogonal projection which requires only a basis for  $W$ , later in these notes.)

### Gram-Schmidt Orthogonalization.

Given a basis  $v_1, \dots, v_n$  for a subspace  $W$ , we can build an orthogonal basis for  $W$  by, essentially, repeatedly subtracting from  $w_i$  its orthogonal projection onto the span of the orthogonal vectors we have built up to that point.

To do so we repeatedly use the formula

$$(*) \text{proj}_{W_i}(v) = \frac{\langle w_1, v \rangle}{\langle w_1, w_1 \rangle} w_1 + \dots + \frac{\langle w_i, v \rangle}{\langle w_i, w_i \rangle} w_i$$

for the projection of a vectors onto the span  $W_i$  of a collection of orthogonal vectors. Gram-Schmidt orthogonalization consists of repeatedly using this formula to replace a collection of vectors with ones that are orthogonal to one another, **without changing their span**. Starting with a collection  $\{v_1, \dots, v_n\}$  of vectors in  $V$ ,

$$\text{let } w_1 = v_1, \text{ then let } w_2 = v_2 - \frac{\langle w_1, v_2 \rangle}{\langle w_1, w_1 \rangle} w_1 .$$

Then  $w_1$  and  $w_2$  are orthogonal, and since  $w_2$  is a linear combination of  $w_1 = v_1$  and  $v_2$ , while the above equation can also be rewritten to give  $v_2$  as a lineaar combination of  $w_1$  and  $w_2$ , the span is unchanged. Continuing,

let  $w_3 = v_3 - \frac{\langle w_1, v_3 \rangle}{\langle w_1, w_1 \rangle} w_1 - \frac{\langle w_2, v_3 \rangle}{\langle w_2, w_2 \rangle} w_2$  ; then since  $w_1$  and  $w_2$  are orthogonal, it is not hard to check that  $w_3$  is orthogonal to **both** of them, and using the same argument, the span is unchanged (in this case,  $\text{span}\{w_1, w_2, w_3\} = \text{span}\{w_1, w_2, v_3\} = \text{span}\{v_1, v_2, v_3\}$ ).

Continuing this, we let  $w_k = v_k - \frac{\langle w_1, v_k \rangle}{\langle w_1, w_1 \rangle} w_1 - \dots - \frac{\langle w_{k-1}, v_k \rangle}{\langle w_{k-1}, w_{k-1} \rangle} w_{k-1}$

Doing this all the way to  $n$  will replace  $v_1, \dots, v_n$  with orthogonal vectors  $w_1, \dots, w_n$ , without changing the span.

Once we know how to build an orthogonal basis for a subspace  $W$ , we know how to compute the orthogonal projection of a vector onto  $W$ ; we use the formula (\*) above. This in turn allows to compute the decomposition of any vector  $\vec{v} \in \mathbb{R}^n$  as  $\vec{v} = \vec{w} + \vec{w}'$  with  $\vec{w} \in W$  and  $\vec{w}' \in W^\perp$ ;  $\vec{w} = \text{proj}_W(\vec{v})$  and  $\vec{w}' = \vec{v} - \vec{w}$ .

This in turn gives us the tools to establish some basic facts:

$(W^\perp)^\perp = W$ , since if  $\vec{w} \in W$ , then  $\vec{w} \perp \vec{v}$  for every  $\vec{v} \in W^\perp$ , so  $w \in (W^\perp)^\perp$ , while if  $\vec{v} \in (W^\perp)^\perp$ , then writing  $\vec{v} = \vec{w} + \vec{w}'$  as above, we have  $\vec{v} - \vec{w} \in (W^\perp)^\perp$ , so  $0 = \langle \vec{v} - \vec{w}, \vec{w}' \rangle = \langle \vec{v} - \vec{w}, \vec{v} - \vec{w} \rangle = \|\vec{v} - \vec{w}\|^2$ , so  $\vec{v} - \vec{w} = \vec{0}$ , so  $\vec{v} = \vec{w} \in W$ .

If  $W \subseteq \mathbb{R}^n$  is a subspace, then  $\dim(W) + \dim(W^\perp) = n$ ; this is because we can express  $W = \text{col}(A)$  for some matrix  $A$  (having columns a spanning set for  $W$ ), and then  $W^\perp = \text{null}(A^T)$ , so  $\dim(W) + \dim(W^\perp) = \text{rank}(A) + \text{nullity}(A^T) = \text{rowrank}(A) + \text{nullity}(A^T) = \text{rank}(A^T) + \text{nullity}(A^T) = (\# \text{ of pivots for } A^T) + (\# \text{ free variables for } A^T) = \# \text{ of columns of } A^T = \# \text{ of rows of } A = n$ .

Even more, any basis for  $W$ , together with a basis for  $W^\perp$ , forms a basis for  $\mathbb{R}^n$ . This is because such a collection of vectors will form  $n$  vectors in  $\mathbb{R}^n$  and will be linearly independent. This is because if we express  $\vec{0}$  as a linear combination of them, we can rearrange terms so that a linear combination of the  $W$ -vectors equals a linear combination of the  $W^\perp$ -vectors. This vector lies in  $W \cap W^\perp = \{\vec{0}\}$ , so since each basis is linearly independent, both sets of coefficients are 0.

### Best approximations.

In the real world, the coefficients and target vector of a system of linear equations are only known up to some (measurement) error. But if the rank of the matrix is too small (e.g., we have more variables than equations), small changes in values can easily lead to an inconsistent system. In other words, our target,  $\vec{b}$  might end up lying close to, but not in, the column space  $\text{col}(A)$ , of our coefficient matrix. The appropriate solution, then, is to find the value of  $A\vec{x}$ , closest to  $\vec{b}$ , and treat  $\vec{x}$  as our “solution” to the inconsistent system  $A\vec{x} = \vec{b}$ .

How? Minimize  $\|A\vec{x} - \vec{b}\|^2$ , i.e., minimize  $\vec{w} - \vec{b}$  for  $\vec{w} \in \text{col}(A)$ . If we use an orthonormal basis  $\{\vec{w}_1, \dots, \vec{w}_k\}$  for  $\text{col}(A)$ , then  $\langle \sum x_i \vec{w}_i - \vec{b}, \sum x_i \vec{w}_i - \vec{b} \rangle = \langle \vec{b}, \vec{b} \rangle + \sum (x_i^2 - 2x_i \langle \vec{w}_i, \vec{b} \rangle)$  is minimized when (the gradient of this function of the  $x_i$  is 0, i.e.)  $x_i = \langle \vec{w}_i, \vec{b} \rangle$  for each  $i$ , so the vector  $\vec{w}$  closest to  $\vec{b}$  is  $\sum \langle \vec{w}_i, \vec{b} \rangle \vec{w}_i = \text{proj}_{\text{col}(A)}(\vec{b})$ , i.e., the orthogonal projection of  $\vec{b}$  to the column space of  $A$ .

But! we don't need to build an orthogonal basis for  $\text{col}(A)$  in order to compute this;  $\vec{w} = \text{proj}_{\text{col}(A)}(\vec{b})$  is the (unique) vector  $\vec{w} \in \text{col}(A)$  such that  $\vec{w} - \vec{b} \in (\text{col}(A))^\perp = \text{null}(A^T)$ , so we need to find  $\vec{w} = A\vec{x}$  so that  $A^T(A\vec{x} - \vec{b}) = \vec{0}$ , i.e.,  $(A^T A)\vec{x} = A^T \vec{b}$ .

This linear system is consistent (we know that the needed  $A\vec{x}$  exists); solving the system for  $\vec{x}$  gives us the vector  $A\vec{x} = \text{proj}_{\text{col}(A)}(\vec{b})$ , and so gives us a method for computing the orthogonal projection onto any subspace (that we have a spanning set for), without needing to compute an orthogonal basis for it first.  $A\vec{x} = \vec{w}$  is also the closest vector to  $\vec{b}$  for which  $A\vec{x} = \vec{w}$  is consistent;  $\vec{x}$  is called the *least squares solution* to the inconsistent system  $A\vec{x} = \vec{b}$ .

Note: if  $A^T A$  is invertible (need:  $r(A) = \text{number of columns of } A$ ), then we can write  $\vec{x} = (A^T A)^{-1}(A^T \vec{b})$ ;  $A\vec{x} = A(A^T A)^{-1}(A^T \vec{b})$ . This gives us a general formula for the orthogonal projection onto a subspace  $W$ ;  $\text{proj}_W(v) = A(A^T A)^{-1}(A^T \vec{v})$ , where the columns of  $A$  form a basis for  $W$ .

### Regression Lines.

We can apply this technology to produce a method for finding the “best fit” line to a collection of data. Suppose we have a collection  $(x_1, y_1), \dots, (x_n, y_n)$  of data points, and we wish to find the line  $L(x) = y = ax + b$  that best fits the data. Typically, this means that we want, on

average, that the deviation between  $y_i$  and  $L(x_i)$  to be as small as possible. In practice, what we minimize is the distance between the “value vector”,  $[y_1, \dots, y_n]^T$  and the “predicted vector”  $[ax_1 + b, \dots, ax_n + b]^T$ . Our unknowns are  $a, b$ , and our predicted vector can be expressed as a matrix product,

$$\begin{bmatrix} ax_1 + b \\ \vdots \\ ax_n + b \end{bmatrix} = \begin{bmatrix} x_1 & 1 \\ \vdots & \vdots \\ x_n & 1 \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = A \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \vec{y}$$

So we want the vector  $[a, b]^T$  so that  $A[a, b]^T$  is closest to  $\vec{y}$ . But this is precisely the situation we just worked through; the slope ( $a$ ) and intercept ( $b$ ) of the best-fitting line are the solution to the system

$A^T A \begin{bmatrix} a \\ b \end{bmatrix} = A^T \vec{y}$ , which works out to  $\begin{bmatrix} \Sigma x_i^2 & \Sigma x_i \\ \Sigma x_i & n \end{bmatrix} \begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} \Sigma x_i y_i \\ \Sigma y_i \end{bmatrix}$  (although we need not remember that....). The  $2 \times 2$  matrix  $A^T A$  is invertible, unless all of the  $x_i$  are equal to one another.

We can do this sort of thing more generally, too. We can find the best-fitting quadratic  $Q(x) = y = ax^2 + bx + c$ , or cubic  $C(x) = y = ax^3 + bx^2 + cx + d$ , or any polynomial, using the same basic approach. Let's illustrate this with a quadratic. As with linear regression, we wish to make the sum of the terms  $[y_i - (ax_i^2 + bx_i + c)]^2$  as small as possible, which means that we wish to make

$$A \begin{bmatrix} a \\ b \\ c \end{bmatrix} \text{ as close to } \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} = \vec{y} \text{ as we can, where now } A = \begin{bmatrix} x_1^2 & x_1 & 1 \\ \vdots & \vdots & \vdots \\ x_n^2 & x_n & 1 \end{bmatrix}.$$

This, again, has solution  $\begin{bmatrix} a \\ b \\ c \end{bmatrix} = (A^T A)^{-1} A^T \vec{y}$ .  $A^T A$  is invertible so long as at least three of the  $x_i$  are distinct. This last fact follows from a fact about the Vandermonde determinant, which is the determinant of the matrix

$$\begin{bmatrix} x_1^{n-1} & \dots & x_1 & 1 \\ \vdots & & \vdots & \vdots \\ x_n^{n-1} & \dots & x_n & 1 \end{bmatrix},$$

and which equals the product of all of the differences  $x_i - x_j$  taken over pairs  $i < j$ . The determinant is therefore non-zero if all of the  $x_i$  are distinct, which means that the last  $k + 1$  columns (which are what we use for a degree  $k$  polynomial fitting) are linearly independent if at least  $k + 1$  of the  $x_i$  are distinct.