ELEC95018 - Mathematics 2

Lecture notes

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Chapter 1

Linear Algebra 2.1: Orthogonal Subspaces, Projection, Least-squares

Begin with the picture of the four fundamental subspaces of an $m \times n$ matrix A, which we obtained in the last chapter

For picture, see lectures.

We found out quite a lot about these subspaces: their dimension, how to find bases. We've also seen how this relates to the existence and uniqueness of solutions of the central equation $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$. This innocuous matrix equation, a system of m linear equations in n unknowns, is the focus of all our efforts. In this chapter we address the problem identified earlier, when no solution exists, the system is inconsistent. So far all we've found is how to identify the problem using elimination, pivot and free variables, rank. All very nice, but still no solution... what is to be done? A burning question!

In this chapter we will develop the first of several methods of finding an approximate solution to $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ when an exact solution does not exist. But before addressing the question, we need a few more tools.

1.1 Orthogonal Subspaces

We remember **orthogonal** or perpendicular vectors. If $\underline{\mathbf{x}}$ and $\underline{\mathbf{y}}$ are orthogonal, the angle they form is $\pi/2$ and with $\underline{\mathbf{x}} + \underline{\mathbf{y}}$ they form a right-angled triangle.

For picture, see lectures.

Going by Pythagoras, this can be written as

$$|\underline{\mathbf{x}}|^2 + |\underline{\mathbf{y}}|^2 = |\underline{\mathbf{x}} + \underline{\mathbf{y}}|^2 \ .$$

Recall that this holds, even when we are in $\mathbb{R}^n$, where pictures can't be drawn so easily.

Recall also, that $|\underline{\mathbf{v}}|^2 = \underline{\mathbf{v}} \cdot \underline{\mathbf{v}}$ as vectors, but now we need to go to the more refined approach of taking the scalar product as the matrix multiplication of a row vector, a matrix with one row, and a column vector, a matrix with one column, giving

$$|\underline{\mathbf{v}}|^2 = \underline{\mathbf{v}}^T \underline{\mathbf{v}}$$

with this, we rewrite the Pythagorean relation as

$$|\underline{\mathbf{x}}|^2 + |\underline{\mathbf{y}}|^2 = |\underline{\mathbf{x}} + \underline{\mathbf{y}}|^2 \quad \Rightarrow \quad \underline{\mathbf{x}}^T\underline{\mathbf{x}} + \underline{\mathbf{y}}^T\underline{\mathbf{y}} = (\underline{\mathbf{x}} + \underline{\mathbf{y}})^T(\underline{\mathbf{x}} + \underline{\mathbf{y}}) = \underline{\mathbf{x}}^T\underline{\mathbf{x}} + \underline{\mathbf{y}}^T\underline{\mathbf{x}} + \underline{\mathbf{x}}^T\underline{\mathbf{y}} + \underline{\mathbf{y}}^T\underline{\mathbf{y}}$$

and cancelling like terms and noting that $\underline{\mathbf{y}}^T\underline{\mathbf{x}} = \underline{\mathbf{x}}^T\underline{\mathbf{y}}$, given that the dot product is also commutative, we obtain

$$2\underline{\mathbf{x}}^T\underline{\mathbf{y}} = 0 \quad \Rightarrow \underline{\mathbf{x}}^T\underline{\mathbf{y}} = 0$$

as the other condition expressing the orthogonality of two vectors. We need to decide what we do with the zero vector. It makes no sense to talk about the angle between the zero vector and another vector $\underline{\mathbf{x}}$, but it is obvious that $\underline{\mathbf{x}}^T\underline{\mathbf{0}} = \mathbf{0}$ for any vector $\underline{\mathbf{x}}$. For constistency, we go with the algebraic definition and say that the zero vector is orthogonal to all vectors.

So how can we define orthogonality between two subspaces? We say that two subspaces U, V are **orthogonal subspaces** if every vector in U is orthogonal to every vector in V, formally

$$\forall \underline{\mathbf{u}} \in U, \underline{\mathbf{v}} \in V, \quad \underline{\mathbf{u}}^T \underline{\mathbf{v}} = 0 \, .$$

Consider a wall in the room you're in and a floor: they are planes in $\mathbb{R}^3$. If the origin is in the edge where floor meets wall, then we can extend these to infinity and think of them as subspaces. It's obvious that the floor and wall meet at $90°$, but are they orthogonal subspaces?

No, because we can get many diagonal vectors in the wall, which will not be orthogonal to any vectors in the floor. Or even worse, think of a vector in the line where the two intersect: these are in both subspaces, and a vector can never be orthogonal to itself...unless it's the zero vector. So we immediately see that for two subspaces to be orthogonal they must have only the zero vector in their intersection:

$$U \cap V = \{\underline{\mathbf{0}}\} \, .$$

In the $xy-$plane $\mathbb{R}^2$, lines through the origin are subspaces, and their intersection is the origin, $\underline{\mathbf{0}}$, but that alone isn't enough to make them orthogonal subspaces, they must still form the right angle where they meet.

In $\mathbb{R}^3$ if we take the infinitely extended wall again and an infitnite line in the floor which intersects the wall at the origin, then the two subspaces can be orthogonal, but again, the angle needs to be a right angle.

So we turn to the four fundamental subspaces: they are two pairs of orthogonal subspaces. If A is $m \times n$, then the row space $C(A^T)$ and nullspace $N(A)$ are orthogonal subspaces of $\mathbb{R}^n$. To see this, first consider that *any* vector in the row space is a linear combination of rows of A: We take the m rows of A as $\underline{\mathbf{r}}_1^T, \underline{\mathbf{r}}_2^T, \ldots, \underline{\mathbf{r}}_m^T$, so A can be written in terms of its rows as

$$A = \begin{pmatrix} \underline{\mathbf{r}}_1^T \\ \underline{\mathbf{r}}_2^T \\ \underline{\mathbf{r}}_3^T \\ \vdots \\ \vdots \\ \underline{\mathbf{r}}_m^T \end{pmatrix} \Longrightarrow A^T = (\underline{\mathbf{r}}_1, \underline{\mathbf{r}}_2, \underline{\mathbf{r}}_3, \ldots \underline{\mathbf{r}}_m)$$

We note that in A, the rows are $\underline{\mathbf{r}}_i^T$: a row vector is always the transpose of a column vector, the default. So A^T has columns $\underline{\mathbf{r}}_1, \underline{\mathbf{r}}_2, \underline{\mathbf{r}}_3, \ldots \underline{\mathbf{r}}_m$. Careful with this!

Thus, an element in the row space of A, expressed as an element of the column space of A^T will be

$$\underline{\mathbf{a}} = a_1 \underline{\mathbf{r}}_1 + a_2 \underline{\mathbf{r}}_2 + \ldots + a_m \underline{\mathbf{r}}_m \in C(A^T)$$

and as rows these are

$$\underline{\mathbf{a}}^T = a_1 \underline{\mathbf{r}}_1^T + a_2 \underline{\mathbf{r}}_2^T + \ldots + a_m \underline{\mathbf{r}}_m^T$$

Now consider a vector $\underline{\mathbf{x}}$ in the nullspace, it must satisfy $A\underline{\mathbf{x}} = \underline{\mathbf{0}}$. If we write A in terms of its rows, this looks as follows:

$$A\underline{\mathbf{x}} = \begin{pmatrix} \underline{\mathbf{r}}_1^T \\ \underline{\mathbf{r}}_2 \\ \underline{\mathbf{r}}_3 \\ \vdots \\ \vdots \\ \underline{\mathbf{r}}_m \end{pmatrix} \underline{\mathbf{x}} = \underline{\mathbf{0}}$$

Each row of A, multiplied by $\underline{\mathbf{x}}$ gives a zero-entry in the zero vector, so the above is the same as

$$\begin{gathered} \underline{\mathbf{r}}_1^T \underline{\mathbf{x}} = 0 \\ \underline{\mathbf{r}}_2^T \underline{\mathbf{x}} = 0 \\ \underline{\mathbf{r}}_3^T \underline{\mathbf{x}} = 0 \\ \vdots \\ \vdots \\ \underline{\mathbf{r}}_m^T \underline{\mathbf{x}} = 0 \end{gathered}$$

Each of these equations says that $\underline{\mathbf{x}}$ is orthogonal to a row of A, so $\underline{\mathbf{x}}$ is orthogonal to every row of A. So for any vector $\underline{\mathbf{a}}$ in the row space, we have

$$\underline{\mathbf{a}}^T\underline{\mathbf{x}} = (a_1\underline{\mathbf{r}}_1^T + a_2\underline{\mathbf{r}}_2^T + \ldots + a_m\underline{\mathbf{r}}_m^T)\underline{\mathbf{x}} = a_1\underline{\mathbf{r}}_1^T\underline{\mathbf{x}} + a_2\underline{\mathbf{r}}_2^T\underline{\mathbf{x}} + \ldots + a_m\underline{\mathbf{r}}_m^T\underline{\mathbf{x}} = 0 + 0 + \ldots + 0 = 0$$

so $\underline{\mathbf{x}}$ is orthogonal to every vector in the row space. As $\underline{\mathbf{x}}$ is any vector in the nullspace, we have the result.

The same argument holds for column space $C(A)$ and left-nullspace $N(A^T)$, which are orthogonal subspaces of $\mathbb{R}^m$, as they are the row space and nullspace of A^T.

We note that the two pairs of orthogonal subspaces occupy they whole of $\mathbb{R}^n$ and $\mathbb{R}^m$ in the sense that the whole of the parent space is included. Row space and nullspace intersect only in the zero vector and their dimensions r and $n-r$ add up to the dimension of the parent space $\mathbb{R}^n$.

We can turn this around. Consider $\mathbb{R}^3$ and two lines through the origin, meeting there with a right angle: they are orthogonal subspaces, but can they be the nullspace and row space of a matrix? No, because their dimensions, both $= 1$, would have to add up to the whole of $\mathbb{R}^3$, so we'd need a plane, 2-D, and a line, 1-D, for them to be row and nullspace: two lines don't cover the whole space.

Example 1.1. *Show that nullspace and row space of*

$$A = \begin{pmatrix} 1 & 2 & 5 \\ 2 & 4 & 10 \end{pmatrix}$$

are orthogonal subspaces of $\mathbb{R}^3$*.*

The matrix clearly has rank 1, no need for work here, so the row space is all multiples of the first row:

$$C(A^T) = k\begin{pmatrix} 1 \\ 2 \\ 5 \end{pmatrix}$$

and dim$C(A^T) = 1 =$rank(A). We can immediately deduce that dim$N(A) = n - r = 3 - 1 = 2$, so it's a plane. If every vector in this plane is orthogonal to the vectors in the 1-D row space, then this is the plane orthogonal to $(1, 2, 5)^T$, which will give us the cartesian equation, but we would like the nullspace in terms of the special solutions of $A\underline{\mathbf{x}} = \underline{\mathbf{0}}$. One row operation gives

$$A \sim \begin{pmatrix} 1 & 2 & 5 \\ 0 & 0 & 0 \end{pmatrix}$$

so that $A\underline{\mathbf{x}} = \underline{\mathbf{0}} \Rightarrow \mathbf{x_1} + \mathbf{2x_2} + \mathbf{5x_3} = \mathbf{0}$ and letting x_2, x_3 be the free variables, the special solutions are

$$\begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} -5 \\ 0 \\ 1 \end{pmatrix}$$

and their linear combinations form the nullspace. Taking

$$\begin{pmatrix} -2 \\ 1 \\ 0 \end{pmatrix}^T \begin{pmatrix} 1 \\ 2 \\ 5 \end{pmatrix} = 0 \quad \text{and} \quad \begin{pmatrix} -5 \\ 0 \\ 1 \end{pmatrix}^T \begin{pmatrix} 1 \\ 2 \\ 5 \end{pmatrix} = 0$$

we see that every vector in the row space is orthogonal to every vector in the nullspace, as expected. In fact, the nullspace contains all the vectors orthogonal to the row space and vice-versa.

The two subspaces somehow "add up" to the whole of $\mathbb{R}^n$, they are called **orthogonal complements**:

dim$N(A)$+dim$C(A^T) =$dim$\mathbb{R}^n = n$ and dim$N(A^T)$+dim$C(A) =$dim$\mathbb{R}^m = m$.

This, together with the orthogonality of the subspaces is one of the fundamental results in Linear Algebra.

1.2 The matrix A^TA; Projection revisited

We now return to the problem of $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ when there is no solution, but we would still like to "solve" the equation: we want to find the best possible approximation. Say for example we have a "tall" matrix: more rows than columns, $m > n$. An example might be many measurements of the postion of a satellite, hundreds of them: large m. These give us m equations to estimate the n parameters determining the trajectory, where n is much smaller, say around 6 or less. The problem is that the measurements include noise, inaccuracies, and we would like to separate the noise from the essential information.

One approach might be to throw away equations until the matrix is square. But: (a) this does not guarantee a solution exists, and (b) we might be throwing away equations representing more accurate measurements than the ones we're keeping. So this won't do. To develop the more subtle approach, first a few tools.

1.2.1 Properties of A^TA

A matrix that turns up repeatedly is A^TA. We already know this matrix is square, $n \times n$ and symmetric . Is it invertible? If not, what is it's nullspace?

Consider the problematic equation

$$A\underline{\mathbf{x}} = \underline{\mathbf{b}}$$

and multiply by A^T to get the better equation

$$A^TA\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$$

where we have changed $\underline{\mathbf{x}}$ to $\hat{\underline{\mathbf{x}}}$ because they are not the same. There is no $\underline{\mathbf{x}}$, so we will need to find $\hat{\underline{\mathbf{x}}}$ so that, somehow, the error in the approximation is as small as possible.

In the "better" equation, when is A^TA invertible?

Example 1.2. *Take $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$:*

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \end{pmatrix}$$

Here A is 3×2 and has rank 2, full column rank. Then

$$A^TA = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 5 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 5 \end{pmatrix} = \begin{pmatrix} 3 & 8 \\ 8 & 30 \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{c}}_1^T\underline{\mathbf{c}}_1 & \underline{\mathbf{c}}_1^T\underline{\mathbf{c}}_2 \\ \underline{\mathbf{c}}_2^T\underline{\mathbf{c}}_1 & \underline{\mathbf{c}}_2^T\underline{\mathbf{c}}_2 \end{pmatrix}$$

where $\underline{\mathbf{c}}_i$ are the columns of A. This is invertible. What if we have

$$A^TA = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 2 & 2 \end{pmatrix} \begin{pmatrix} 1 & 2 \\ 1 & 2 \\ 1 & 2 \end{pmatrix} = \begin{pmatrix} 3 & 6 \\ 6 & 12 \end{pmatrix} ?$$

This is not invertible, because $\underline{\mathbf{c}}_2$ is a multiple of $\underline{\mathbf{c}}_1$: we have $\underline{\mathbf{c}}_2 = k\underline{\mathbf{c}}_1$, in this case with $k = 2$. When this happens, then

$$A^TA = \begin{pmatrix} \underline{\mathbf{c}}_1^T\underline{\mathbf{c}}_1 & \underline{\mathbf{c}}_1^Tk\underline{\mathbf{c}}_1 \\ k\underline{\mathbf{c}}_1^T\underline{\mathbf{c}}_1 & k\underline{\mathbf{c}}_1^Tk\underline{\mathbf{c}}_1 \end{pmatrix}$$

and we see that here the second column is the same multiple of the first column. So invertibility of A^TA depends on A having independent columns, which is equivalent to $N(A) = \underline{\mathbf{0}}$. An invertible matrix has $N(A) = \underline{\mathbf{0}}$, so we have

$$N(A^TA) = N(A) \quad \text{and} \quad \text{rank}\,(A^TA) = \text{rank}\,(A)\,.$$

Let's prove this. Suppose $A^TA\underline{\mathbf{x}} = \underline{\mathbf{0}}$. If A^TA is invertible, then $\underline{\mathbf{x}} = \underline{\mathbf{0}}$ must be the only solution here. We multiply both sides with $\underline{\mathbf{x}}^T$, giving

$$\underline{\mathbf{x}}^TA^TA\underline{\mathbf{x}} = \underline{\mathbf{x}}^T\underline{\mathbf{0}} = \mathbf{0} \Rightarrow (\mathbf{A}\underline{\mathbf{x}})^{\mathbf{T}}\mathbf{A}\underline{\mathbf{x}} = \mathbf{0}$$

We recognize the expression on the left as the magnitude of the vector $A\underline{\mathbf{x}}$, so now

$$|A\underline{\mathbf{x}}| = 0$$

But only one vector has magnitude zero, so

$$A\underline{\mathbf{x}} = \underline{\mathbf{0}} \,.$$

If A has independent columns, full column rank, then the nullspace is the zero vector, and the only solution to this last equation is $\underline{\mathbf{x}} = \underline{\mathbf{0}}$. We have deduced that if A has independent columns, then the only solution to

$$A^T A\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

is $\underline{\mathbf{x}} = \underline{\mathbf{0}}$. For a square matrix, this implies invertibility, so $A^T A$ is invertible.

1.2.2 Projection in 1D

From a previous chapter we recall the projection of one vector onto another

For picture, see lectures.

This time we are interested in the point given by $\underline{\mathbf{p}}$, the projection of $\underline{\mathbf{b}}$ onto $\underline{\mathbf{a}}$, for a specific purpose: this is the point on $\underline{\mathbf{a}}$ *nearest* to $\underline{\mathbf{b}}$. Our objective is to obtain $\underline{\mathbf{b}}$, but this is not available, we can only get to points on $\underline{\mathbf{a}}$, so we take the nearest point on $\underline{\mathbf{a}}$ as an approximation, and $\underline{\mathbf{e}} \neq \underline{\mathbf{0}}$ is the resulting error.

Recall that the projection is obtained as $\underline{\mathbf{p}} = \lambda\underline{\mathbf{a}}$ with

$$\lambda = \frac{\underline{\mathbf{a}} \cdot \underline{\mathbf{b}}}{\underline{\mathbf{a}} \cdot \underline{\mathbf{a}}} = \frac{\underline{\mathbf{a}}^T\underline{\mathbf{b}}}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}$$

adapting to the notation of matrix multiplication. Hence

$$\underline{\mathbf{p}} = \frac{\underline{\mathbf{a}}^T\underline{\mathbf{b}}}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}\underline{\mathbf{a}} = \frac{(\underline{\mathbf{a}}^T\underline{\mathbf{b}})\underline{\mathbf{a}}}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}$$

Consider the numerator, it's a scalar multiplying a vector, so we can write

$$(\underline{\mathbf{a}}^T\underline{\mathbf{b}})\underline{\mathbf{a}} = \underline{\mathbf{a}}(\underline{\mathbf{a}}^T\underline{\mathbf{b}}) \,.$$

This last expression can also, validly, be seen as the multiplication of three matrices: $(n \times 1)[(1 \times n)(n \times 1)]$. Given the associative property we can rewrite once more as

$$\underline{\mathbf{a}}(\underline{\mathbf{a}}^T\underline{\mathbf{b}}) = (\underline{\mathbf{a}}\underline{\mathbf{a}}^T)\underline{\mathbf{b}}$$

where the last result is $[(n \times 1)(1 \times n)](n \times 1)$. This finally gives

$$\underline{\mathbf{p}} = \frac{\underline{\mathbf{a}}\underline{\mathbf{a}}^T}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}\underline{\mathbf{b}} = P\underline{\mathbf{b}}$$

where P is the matrix

$$P = \frac{\underline{\mathbf{a}}\underline{\mathbf{a}}^T}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}$$

more precisely, the $n \times n$ matrix $\underline{\mathbf{a}}\underline{\mathbf{a}}^T$, multiplied by the scalar $(\underline{\mathbf{a}}^T\underline{\mathbf{a}})^{-1}$. It is the **projection matrix**, entirely dependent on $\underline{\mathbf{a}}$, which when multiplying a vector, gives the projection of that vector onto $\underline{\mathbf{a}}$.

Consider the projection matrix P. If $\underline{\mathbf{p}} = P\underline{\mathbf{b}}$, then $\underline{\mathbf{p}}$ is in the column space of P, since $P\underline{\mathbf{b}}$ is a combination of the columns of P. We also know that any such vector $\underline{\mathbf{p}}$ lies on a line through $\underline{\mathbf{a}}$, so the column space of P is 1-dimensional and P has rank one. (In fact, it's not difficult to see that any matrix which is the product of a row$\times$column has rank 1.) It's also obvious that P is symmetric, recall our observation of $A^T A$.

What happens if we project twice onto $\underline{\mathbf{a}}$? The first time we go from $\underline{\mathbf{b}}$ to $\underline{\mathbf{p}}$, but the second time, nothing happens, given that we're already on the line through $\underline{\mathbf{a}}$. So

$$P^2\underline{\mathbf{b}} = P(P\underline{\mathbf{b}}) = P\underline{\mathbf{p}} = \underline{\mathbf{p}} = P\underline{\mathbf{b}} \,.$$

Hence we can conclude that

$$P^2 = P \,.$$

1.2.3 Projection in 2D and higher

We return to our problem $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ which has no solution. To find the closest thing to a solution, we consider that $A\underline{\mathbf{x}}$ is in the column space of $C(A)$, and look for $\underline{\mathbf{p}}$, the closest vector in $C(A)$ to $\underline{\mathbf{b}}$, noting how projection can fulfil that role. We then solve $A\hat{\underline{\mathbf{x}}} = \underline{\mathbf{p}}$ where $\underline{\mathbf{p}}$ is the projection of $\underline{\mathbf{b}}$ onto the column space of A. Say the column space is a plane in $\mathbb{R}^3$:

For picture, see lecture.

Then $\underline{\mathbf{p}}$ is the nearest point to $\underline{\mathbf{b}}$ in the plane, and the error is $\underline{\mathbf{e}} = \underline{\mathbf{b}} - \underline{\mathbf{p}}$, orthogonal to the plane. Let the column space have basis $\underline{\mathbf{a}}_1$, $\underline{\mathbf{a}}_2$ where

$$A = (\underline{\mathbf{a}}_1 \underline{\mathbf{a}}_2) \, .$$

Note that we are making the assumption of independent columns here, which we have used earlier. Then

$$\underline{\mathbf{p}} = x_1 \underline{\mathbf{a}}_1 + x_2 \underline{\mathbf{a}}_2$$

is in the plane. We then prefer to write

$$\underline{\mathbf{p}} = A\hat{\underline{\mathbf{x}}}$$

and we seek $\hat{\underline{\mathbf{x}}}$. A key observation is that

$$\underline{\mathbf{e}} = \underline{\mathbf{b}} - \underline{\mathbf{p}} = \underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}$$

is perpendicular to the plane, and if $\underline{\mathbf{p}}$ is in the column space, the error $\underline{\mathbf{e}}$ must be in $N(A^T)$, the subspace orthogonal to the column space! But this is easily established in 2D. Given $\underline{\mathbf{e}} = \underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}$ is perpendicular to the plane, it is perpendicular to both basis vectors of that plane, so

$$\underline{\mathbf{a}}_1^T(\underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}) = 0 \quad \text{and} \quad \underline{\mathbf{a}}_2^T(\underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}) = 0$$

or, in matrix form,

$$\begin{pmatrix} \underline{\mathbf{a}}_1^T \\ \underline{\mathbf{a}}_2^T \end{pmatrix}(\underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}) = \underline{\mathbf{0}} \quad \Rightarrow \quad \mathbf{A^T}(\underline{\mathbf{b}} - \mathbf{A}\hat{\underline{\mathbf{x}}}) = \underline{\mathbf{0}}$$

confirming that $\underline{\mathbf{e}} = \underline{\mathbf{b}} - A\hat{\underline{\mathbf{x}}}$ is in the nullspace of A^T. We rewrite this as

$$\boxed{A^T A\hat{\underline{\mathbf{x}}} \; = \; A^T\underline{\mathbf{b}}}$$

a key equation, with solution

$$\hat{\underline{\mathbf{x}}} \; = \; (A^T A)^{-1} A^T \underline{\mathbf{b}}$$

and our first step to finding this is to observe that

$$\underline{\mathbf{p}} = A\hat{\underline{\mathbf{x}}} \; = \; A(A^T A)^{-1} A^T \underline{\mathbf{b}} \; = \; P\underline{\mathbf{b}} \, .$$

(Recall, the 1-D projection matrix $P = \dfrac{\mathbf{a}\mathbf{a}^T}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}}$: when projecting in higher than 1D, we can't divide by $\underline{\mathbf{a}}^T\underline{\mathbf{a}}$ and instead multiply by $(A^T A)^{-1}$!)

So the projection matrix is $P = A(A^T A)^{-1} A^T$. Careful here, we might use the associative property and use $(AB)^{-1} = B^{-1}A^{-1}$ to write

$$P = A[A^{-1}(A^T)^{-1}]A^T = I$$

which would be nonsense. What went wrong? The problem is that $A^T A$ is invertible, under the right conditions, but A and A^T aren't, not being square matrices. If A were square and invertible, then $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ would have the unique solution $\underline{\mathbf{x}} = A^{-1}\underline{\mathbf{b}}$ and we wouldn't be here. In that case P would indeed be the identity matrix, because $\underline{\mathbf{b}}$ would be in the column space of A and there is no need for projection.

We saw that in 1D, the projection matrix had two properties:

(i) P is symmetric, and (ii) $P^2 = P$.

This is not hard to confirm here:

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

so P is symmetric, and we have used the property that the transpose of the inverse is the inverse of the transpose. Similarly

$$P^2 = [A(A^TA)^{-1}A^T][A(A^TA)^{-1}A^T] = A(A^TA)^{-1}(A^TA)(A^TA)^{-1}A^T = A(I)(A^TA)^{-1}A^T = A(A^TA)^{-1}A^T = P$$

The gist ist that $P = A(A^TA)^{-1}A^T$ projects $\underline{\mathbf{b}}$ to the nearest point in $C(A)$. There are two extreme cases to cosider:

(i) If $\underline{\mathbf{b}}$ is in the column space, then $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ for some $\underline{\mathbf{x}}$ and $P\underline{\mathbf{b}} = A(A^TA)^{-1}A^T(A\underline{\mathbf{x}}) = A\underline{\mathbf{x}} = \underline{\mathbf{b}}$.
(ii) if $\underline{\mathbf{b}}$ is perpendicular to the column space then it is in $N(A^T)$, the subspace orthogonal to $C(A)$, so $A^T\underline{\mathbf{b}} = \underline{\mathbf{0}}$ and hence $P\underline{\mathbf{b}} = A(A^TA)^{-1}A^T\underline{\mathbf{b}} = \underline{\mathbf{0}}$.

Most vectors will be in neither subspace, but have components in both. Projection picks out the component of $\underline{\mathbf{b}}$ that is in $C(A)$ and eliminates the component in $N(A^T)$.

This can be seen geometrically:

for picture, see lectures

Given that $\underline{\mathbf{p}} + \underline{\mathbf{e}} = \underline{\mathbf{b}}$ and $\underline{\mathbf{p}} = P\underline{\mathbf{b}}$, we can see the error vector as $\underline{\mathbf{e}} =$ projection of $\underline{\mathbf{b}}$ onto $N(A^T)$ and $\underline{\mathbf{e}} = (I - P)\underline{\mathbf{b}}$.

1.3 Application: Least-squares method or Linear Regression

Suppose we have a lot of points in the $ab-$plane, and we would like to fit them to the nearest line with equation $b = C + Da$ This corresponds to having many observations of a satellite and fitting these to obtain some parameters of the trajectory. The line has just the two parameters C, D. Suppose the points (observations) are $(1,1)$, $(2,2)$ and $(3,2)$, clearly not on a line.

For picture, see lectures.

Example 1.3. *Find the line of best fit through the points* $(1,1)$, $(2,2)$ *and* $(3,2)$*, using the method of least squares.*

We want to find the line that minimizes the total distance between $b-$coordinates on the line and the $b-$coordinates of the measured points. So the line would satisfy $b(t) = C + Da$ and if it went through the points, we would have

$$\begin{array}{rrl} C+ & D & = 1 \\ C+ & 2D & = 2 \\ C+ & 3D & = 2 \end{array}$$

Obviously, this overdetermined system has no solution. In matrix form we have $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$, with $\underline{\mathbf{x}} = (C, D)^T$, the unknown parameters:

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} C \\ D \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix},$$

and we note that A has independent columns, which we need. Can you think of what it would mean if we had some dependent columns and how to resolve this?

To find the best fit solution, we solve $A^TA\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$: where $\hat{\underline{\mathbf{x}}} = (\hat{C}\ ,\ \hat{D})^T$ will be our "best" approximations to the impossible C, D. The error in the approximation is the sum of the errors in each point, which are, in turn, given by the difference in $b-$coordinates between the given points and the line. In each case, the error has magnitude (squared) $|\underline{\mathbf{e}}_i|^2 = |\underline{\mathbf{b}}_i - \underline{\mathbf{p}}_i| = |A\underline{\mathbf{x}}_i - \underline{\mathbf{b}}_i|^2$. We would like to minimize the sum of these errors, giving the name of the process as **least squares method**; we are working backwards from a set of points to finding a line, hence the name **linear regression**; both refer to the same process.

For picture, see lectures.

Statisticians would seek to remove outliers which are "clear" errors: values so far away from most points that we can safely disregard them, e.g. add the point $(0,5)$ to the picture: huge error. How to choose the outliers is another story, and we will assume for now that there aren't any!

Let p_1, p_2 and p_3 be the $b-$coordinates on the line, then

$$\begin{array}{rrl} C+ & D & = p_1 \\ C+ & 2D & = p_2 \\ C+ & 3D & = p_3 \end{array}$$

For a solution to exist, we require $\underline{\mathbf{p}} = (p_1, p_2, p_3)^T \in C(A)$. To find $\hat{\underline{\mathbf{x}}} = (\hat{C}\ ,\ \hat{D})^T$, the key equation is $A^T A\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$. In any situation of error estimation, noise elimination, fitting parameters, this is the first equation to use. So

$$A^T A\hat{\underline{\mathbf{x}}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}\begin{pmatrix} \hat{C} \\ \hat{D} \end{pmatrix} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix} = A^T\underline{\mathbf{b}} \quad \Rightarrow \quad \begin{pmatrix} 3 & 6 \\ 6 & 14 \end{pmatrix}\begin{pmatrix} \hat{C} \\ \hat{D} \end{pmatrix} = \begin{pmatrix} 5 \\ 11 \end{pmatrix}$$

We already know that $A^T A$ is invertible, given that A has independent columns. We can solve the last matrix equation for $\hat{C}\ ,\ \hat{D}$, this system is also called the **normal equations**. The solution is $\hat{C} = 2/3$ and $\hat{D} = 1/2$. Hence the best line is

$$b = \frac{1}{2}a + \frac{2}{3},$$

which looks very much like the one we drew. So $p_1 = 7/6$, a little above $b_1 = 1$, $p_2 = 5/3$, a little below $b_2 = 2$, and $p_3 = 13/6$, a little above $b_3 = 2$. Recall that we began with the idea of visualizing $\underline{\mathbf{p}}$ as the vector "nearest" $\underline{\mathbf{b}}$ so that $A\hat{\underline{\mathbf{x}}} = \underline{\mathbf{p}}$ has a solution. In that sense we now have three points on the line $y = \frac{1}{2}x + \frac{2}{3}$:

$$(1, 7/6)\,, \quad (2, 5/3)\,, \quad \text{and} \quad (3, 13/6)$$

'near'

$$(1, 2)\,, \quad (2, 2)\,, \quad \text{and} \quad (3, 2)$$

where nearness has been quanfied as mimimizing the sum of the squares of the errors.

The errors are $e_1 = 1 - 7/6 = -1/6$, $e_2 = 2 - 5/3 = 1/3$ and $e_3 = 2 - 13/6 = -1/6$.

We observe

$$\begin{pmatrix} 1 \\ 2 \\ 2 \end{pmatrix} = \underline{\mathbf{b}} = \underline{\mathbf{p}} + \underline{\mathbf{e}} = \begin{pmatrix} \frac{7}{6} \\ \frac{5}{3} \\ \frac{13}{6} \end{pmatrix} + \begin{pmatrix} -\frac{1}{6} \\ \frac{1}{3} \\ -\frac{1}{6} \end{pmatrix}$$

and that, as expected, $\underline{\mathbf{p}}$ is in the column space of A, where the parameters $\hat{C}, \hat{D}$ of the line give the solution $A\hat{\underline{\mathbf{x}}} = \underline{\mathbf{p}}$:

$$\begin{pmatrix} 1 & 1 \\ 1 & 2 \\ 1 & 3 \end{pmatrix}\hat{\underline{\mathbf{x}}} = \frac{2}{3}\begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} + \frac{1}{2}\begin{pmatrix} 1 \\ 2 \\ 3 \end{pmatrix} = \begin{pmatrix} \frac{7}{6} \\ \frac{5}{3} \\ \frac{13}{6} \end{pmatrix}.$$

Similarly, we confirm that, as expected, $\underline{\mathbf{e}}$ is in the nullspace of A^T:

$$A^T\underline{\mathbf{e}} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & 2 & 3 \end{pmatrix}\begin{pmatrix} -\frac{1}{6} \\ \frac{1}{3} \\ -\frac{1}{6} \end{pmatrix} = \underline{\mathbf{0}}\,.$$

If we throw a ball, we expect the trajectory to be a parabola or very nearly one, so if we have measurements of the position of a ball at different times along its trajectory, we should not try to fit a line through these, but a parabola.

Example 1.4. *Find the quadratic of best fit to the points* $(x, y) = (-1, 1)(0, 3), (1, 4), (2, 0)$, *where* $y(x)$ *is the trajectory of an object thrown at an acute angle to the horizontal, subject to gravity.*

Begin by formulating the problem: we require parameters a, b, c for the parabolic curve $y = ax^2 + bx + c$ satisfying:

at $(-1, 1)$: $1 = a - b + c$,
at $(0, 3)$: $3 = 0a + 0b + c$,
at $(1, 4)$: $4 = a + b + c$,
at $(2, 0)$: $0 = 4a + 2b + c$.

or in matrix notation, taking $\underline{\mathbf{x}} = (a, b, c)^T$, we are attempting to solve

$$A\underline{\mathbf{x}} = \begin{pmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \end{pmatrix} \underline{\mathbf{x}} = \begin{pmatrix} 1 \\ 3 \\ 4 \\ 0 \end{pmatrix} = \underline{\mathbf{b}}$$

which has no solution. Verify: DIY.

Again we begin by solving $A^T A\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$, where $\hat{\underline{\mathbf{x}}} = (\hat{a}, \hat{b}, \hat{c})$ gives the parameters of the quadratic best fit.

$$A^T A\hat{\underline{\mathbf{x}}} = \begin{pmatrix} 1 & 0 & 1 & 4 \\ -1 & 0 & 1 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \end{pmatrix} \hat{\underline{\mathbf{x}}} = \begin{pmatrix} 1 & 0 & 1 & 4 \\ -1 & 0 & 1 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 3 \\ 4 \\ 0 \end{pmatrix} = A^T\underline{\mathbf{b}}$$

which simplifies to

$$\begin{pmatrix} 18 & 8 & 6 \\ 8 & 6 & 2 \\ 6 & 2 & 4 \end{pmatrix} \hat{\underline{\mathbf{x}}} = \begin{pmatrix} 5 \\ 3 \\ 8 \end{pmatrix}$$

The last matrix is $A^T A$ and is invertible as long as the columns of A are independent, easy to verify. Inverting we obtain

$$\hat{\underline{\mathbf{x}}} = (A^T A)^{-1}(A^T\underline{\mathbf{b}}) = \frac{1}{20} \begin{pmatrix} 5 & -5 & -5 \\ -5 & 9 & 3 \\ -5 & 3 & 11 \end{pmatrix} \begin{pmatrix} 5 \\ 3 \\ 8 \end{pmatrix} = \begin{pmatrix} -1.5 \\ 1.3 \\ 3.6 \end{pmatrix}$$

so the quadratic has equation

$$y = -1.5x^2 + 1.3x + 3.6 \, .$$

Check the points here, we obtain

$$(-1, 0.8), (0, 3.6), (1, 3.4), (2, 0.2)$$

"near"

$$(-1, 1), (0, 3), (1, 4), (2, 0) \, ,$$

easily visualized:

Hence the projection of $\underline{\mathbf{b}}$ onto the column space $C(A)$ is $\underline{\mathbf{p}} = (0.8, 3.6, 3.4, 0.2)^T$ giving the error vector as

$$\underline{\mathbf{e}} = \underline{\mathbf{b}} - \underline{\mathbf{p}} = \begin{pmatrix} 1 \\ 3 \\ 4 \\ 0 \end{pmatrix} - \begin{pmatrix} 0.8 \\ 3.6 \\ 3.4 \\ 0.2 \end{pmatrix} = \begin{pmatrix} 0.2 \\ -0.6 \\ 0.6 \\ -0.2 \end{pmatrix}$$

We can confirm that $\underline{\mathbf{p}}$ is in the column space of A, where the parameters of the parabola gives the desired combination of the columns of A:

$$\begin{pmatrix} 1 & -1 & 1 \\ 0 & 0 & 1 \\ 1 & 1 & 1 \\ 4 & 2 & 1 \end{pmatrix} \hat{\underline{\mathbf{x}}} = -1.5 \begin{pmatrix} 1 \\ 0 \\ 1 \\ 4 \end{pmatrix} + 1.3 \begin{pmatrix} -1 \\ 0 \\ 1 \\ 2 \end{pmatrix} + 3.6 \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 0.8 \\ 3.6 \\ 3.4 \\ 0.2 \end{pmatrix} = \underline{\mathbf{p}}$$

Similarly, we confirm that $\underline{\mathbf{e}}$ is in the left nullspace $N(A^T)$ calculating

$$A^T\underline{\mathbf{e}} = \begin{pmatrix} 1 & 0 & 1 & 4 \\ -1 & 0 & 1 & 2 \\ 1 & 1 & 1 & 1 \end{pmatrix} \begin{pmatrix} 0.2 \\ -0.6 \\ 0.6 \\ -0.2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Exercise: Minimize the least squares using partial differentiation. Write the error as a function of three variables, a, b, c as follows. For each point (x, y), calculate the square of the error: $(ax^2 + bx + c - y)^2$.

So for $(1, 4)$ the error squared is $[a(1)^2 + b(1) + c - 4]^4$, for $(-1, 1)$, the error squared is $[a(-1)^2 + b(-1) + c - 1]^2$ and so on. Adding the squares of the four errors gives you a function, call it $E(a, b, c)$. Obtain the minimum of this function by taking the three partial derivatives w.r.t a, b, c, and setting them equal to zero.

Chapter 2

Linear Algebra 2.2: Orthogonality and QR

2.1 Orthonormal vectors and orthogonal matrices

Recall the notion of a set of orthonormal vectors $\underline{\mathbf{q}}_1, \underline{\mathbf{q}}_2, \ldots \underline{\mathbf{q}}_n$: each vector is a unit vector and distinct vectors are orthogonal, or perpendicular. The vectors $\underline{\mathbf{i}}, \underline{\mathbf{j}}, \underline{\mathbf{k}}$ are one such obvious set, and a good way to write this is in terms of matrix multiplication. If

$$\underline{\mathbf{q}}_i^T \underline{\mathbf{q}}_j = \begin{cases} 1\,, & i = j \\ 0\,, & i \neq j \end{cases} \quad \text{for} \quad 1 \leq i, j \leq n$$

then the vectors $\underline{\mathbf{q}}_1, \underline{\mathbf{q}}_2, \ldots \underline{\mathbf{q}}_n$ form an **orthonormal** set. Recall that the default vector $\underline{\mathbf{q}} \in \mathbb{R}^n$ is a column vector, and we defined the inner product of two vectors as the product of a row vector $\underline{\mathbf{q}}^T$, a matrix with one row, and a column vector $\underline{\mathbf{q}}$, a matrix with one column, giving a scalar, which we call $|\underline{\mathbf{q}}|^2$.

If the n orthonormal vectors are in $\mathbb{R}^n$, then they form a basis: it's not hard to show that orthonormal vectors are independent, left as an exercise. This is an orthonormal basis. Form them into a matrix Q, whose columns are orthonormal vectors:

$$Q = \begin{pmatrix} & & & \\ \underline{\mathbf{q}}_1 & \underline{\mathbf{q}}_2 & \cdots & \underline{\mathbf{q}}_n \\ & & & \end{pmatrix}$$

and consider $Q^T Q$ (this is a product we have met before, and will meet again). The rows of Q^T are the orthonormal vectors as row vectors $\underline{\mathbf{q}}_i^T$:

$$Q^T Q = \begin{pmatrix} \underline{\mathbf{q}}_1^T \\ \underline{\mathbf{q}}_2^T \\ \vdots \\ \underline{\mathbf{q}}_n^T \end{pmatrix} \begin{pmatrix} & & & \\ \underline{\mathbf{q}}_1 & \underline{\mathbf{q}}_2 & \cdots & \underline{\mathbf{q}}_n \\ & & & \end{pmatrix}$$

For once we think of matrix multiplication AB in terms of inner product of a row of A with a column of B, so we get

$$Q^T Q = \begin{pmatrix} \underline{\mathbf{q}}_1^T \underline{\mathbf{q}}_1 & \underline{\mathbf{q}}_1^T \underline{\mathbf{q}}_2 & \cdots & \underline{\mathbf{q}}_1^T \underline{\mathbf{q}}_n \\ \underline{\mathbf{q}}_2^T \underline{\mathbf{q}}_1 & \underline{\mathbf{q}}_2^T \underline{\mathbf{q}}_2 & \cdots & \underline{\mathbf{q}}_2^T \underline{\mathbf{q}}_n \\ \vdots & \vdots & \vdots & \vdots \\ \underline{\mathbf{q}}_n^T \underline{\mathbf{q}}_1 & \underline{\mathbf{q}}_n^T \underline{\mathbf{q}}_2 & \cdots & \underline{\mathbf{q}}_n^T \underline{\mathbf{q}}_n \end{pmatrix} = \begin{pmatrix} 1 & 0 & \ldots & 0 \\ 0 & 1 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 \end{pmatrix} = I_n$$

the identity. So Q^T and Q are inverse matrices. This shows the two definitions of a matrix of this form: (i) A square matrix Q is said to be an **orthogonal matrix** if its columns are a set of orthonormal vectors; (ii) A square matrix Q is said to be an **orthogonal matrix** if $Q^T = Q^{-1}$. Some authors use one definition, some the other, they are equivalent.

Example 2.1. *(a) Recall permutation matrices? Here is one:*

$$Q_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 1 \end{pmatrix}$$

This matrix when multiplying A on the left gives Q_1A, which swaps rows 2 and 3 of A. It is obviously orthogonal, as we recognize its columns as $\underline{\mathbf{i}}, \underline{\mathbf{k}}, \underline{\mathbf{j}}$.

(b) The rotation matrix

$$Q_2 = \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix}$$

is also orthogonal. Check: DIY.

(c) The matrix

$$Q_3 = \begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}$$

is almost orthogonal. Its columns are orthogonal vectors, but they are not normalized, unit vectors. Hence normalization gives the orthogonal matrix

$$Q_3' = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ -\frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \end{pmatrix}.$$

What happens if Q is not square? It can still satisfy some of the properties seen above. Consider

$$Q = \begin{pmatrix} 2 & -3 \\ 3 & 6 \\ 6 & -2 \end{pmatrix}$$

and compute

$$Q^TQ = \begin{pmatrix} 2 & 3 & 6 \\ -3 & 6 & -2 \end{pmatrix} \begin{pmatrix} 2 & -3 \\ 3 & 6 \\ 6 & -2 \end{pmatrix} = \begin{pmatrix} 49 & 0 \\ 0 & 49 \end{pmatrix} = 49I_2$$

so the columns of Q 'are orthogonal and if we normalize them, taking

$$Q = \frac{1}{7}\begin{pmatrix} 2 & -3 \\ 3 & 6 \\ 6 & -2 \end{pmatrix}$$

then the columns form an orthonormal set and $Q^TQ = I_2$. But we note that QQ^T is not the identity, even though this is true for an orthogonal matrix Q. Our new Q has some properties of an orthogonal matrix, but is missing the key property of being square: an orthogonal matrix has a full set of independent columns, they are an orthonormal basis! So an obvious question to ask is: how can we get a full set? We'd like a third orthonormal vector.*Woher nehmen und nicht stehlen?*

One approach is to spot it: the integers $2, 3, 6$ will work, if we get the right order and sign. We need the third column

$$\frac{1}{7}\begin{pmatrix} 6 \\ 2 \\ -3 \end{pmatrix}$$

giving an orthonormal basis of columns in an orthogonal matrix:

$$Q = \frac{1}{7}\begin{pmatrix} 2 & -3 & 6 \\ 3 & 6 & 2 \\ 6 & -2 & -3 \end{pmatrix}$$

with $Q^TQ = QQ^T = I_3$. Check: DIY.

2.1.1 Orthogonal matrix and Projection

Recall how a projection works: we would like to project onto the column space of a matrix, as we did, for example, in the least-squares algorithm. Recall: a system of linear equations $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ has no solution, but we can find the nearest point to $\underline{\mathbf{b}}$ in the column space of A, so that $A^TA\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$ does have a solution.

The matrix that projected onto $C(A)$ was a projection matrix $P = A(A^TA)^{-1}A^T$. Now consider the projection matrix for an orthogonal matrix Q:

$$P = Q(Q^TQ)^{-1}Q^T = Q(I_n)Q^T = QQ^T = I_n$$

Previously, we had to solve $A^TA\hat{\underline{\mathbf{x}}} = A^T\underline{\mathbf{b}}$, but now we have $Q^TQ\hat{\underline{\mathbf{x}}} = \hat{\underline{\mathbf{x}}} = Q^T\underline{\mathbf{b}}$, so each entry is obtained with a single inner product: $\hat{\underline{\mathbf{x}}}_i = \underline{\mathbf{q}}_i^T\underline{\mathbf{b}}$.

The point is that orthogonal matrices are excellent and one thing we need to look at is the question:

How can we obtain an orthonormal basis?

We can't rely on the trick of just spotting a solution, as in the last example. To help us with this, we use the Gram-Schmidt Orthonormalization procedure, or just

2.2 Gram-Schmidt Process

We begin with a set of independent vectors in $\mathbb{R}^n$. If there are n of these, they form a basis, but the process also works with less than a full set.

Begin with any two independent vectors, $\underline{\mathbf{a}}\,\underline{\mathbf{b}}$.

For picture, see lectures.

We've seen this construction: the projection of $\underline{\mathbf{b}}$ onto $\underline{\mathbf{a}}$, which we called $\lambda\underline{\mathbf{a}}$ uses the perpendicular vector $\underline{\mathbf{x}}_2$ in the construction:

$$\lambda\underline{\mathbf{a}} + \underline{\mathbf{x}}_2 = \underline{\mathbf{b}} \quad \text{with} \quad \lambda = \frac{\underline{\mathbf{a}}^T\underline{\mathbf{b}}}{\underline{\mathbf{a}}^T\underline{\mathbf{a}}} \Longrightarrow \underline{\mathbf{x}}_2 = \underline{\mathbf{b}} - \lambda\underline{\mathbf{a}}$$

and $\underline{\mathbf{x}}_2$ is orthogonal to $\underline{\mathbf{a}}$.

We can think of $\underline{\mathbf{b}}$ as having two components with respect to $\underline{\mathbf{a}}$: a parallel and an orthogonal component:

$$\lambda\underline{\mathbf{a}} + \underline{\mathbf{x}}_2 = \underline{\mathbf{b}}$$

where $\lambda\underline{\mathbf{a}}$ is parallel to $\underline{\mathbf{a}}$ and $\underline{\mathbf{x}}_2$ is orthogonal to $\underline{\mathbf{a}}$. To obtain the orthogonal component, we subtracted the parallel component, the projection $\lambda\underline{\mathbf{a}}$, from $\underline{\mathbf{b}}$, giving $\underline{\mathbf{b}} - \lambda\underline{\mathbf{a}}$, the orthogonal component.

For picture, see lectures.

We can do this for more than two vectors. Take $\underline{\mathbf{c}}$, independent of $\underline{\mathbf{a}}$ and $\underline{\mathbf{b}}$: the third vector $\underline{\mathbf{c}}$ will have components in the direction of $\underline{\mathbf{a}}$ and in the direction of $\underline{\mathbf{b}}$: the projections of $\underline{\mathbf{c}}$ onto $\underline{\mathbf{a}}$, resp. $\underline{\mathbf{b}}$, or the components of $\underline{\mathbf{c}}$ along $\underline{\mathbf{a}}$, resp. $\underline{\mathbf{b}}$. Subtract them both from $\underline{\mathbf{c}}$ and you get a new vector, orthogonal to both $\underline{\mathbf{a}}$ and $\underline{\mathbf{b}}$!

So here's the algorithm for three vectors. Let $\underline{\mathbf{x}}_1 = \underline{\mathbf{a}}$. Then $\underline{\mathbf{x}}_2 = \underline{\mathbf{b}} - \lambda\underline{\mathbf{a}}$, orthogonal to $\underline{\mathbf{x}}_1$. Then take

$$\underline{\mathbf{x}}_3 = \underline{\mathbf{c}} \quad - \underbrace{\left(\frac{\underline{\mathbf{x}}_1^T\underline{\mathbf{c}}}{\underline{\mathbf{x}}_1^T\underline{\mathbf{x}}_1}\right)\underline{\mathbf{x}}_1}_{\text{component of } \underline{\mathbf{c}} \text{ along } \underline{\mathbf{x}}_1} - \underbrace{\left(\frac{\underline{\mathbf{x}}_2^T\underline{\mathbf{c}}}{\underline{\mathbf{x}}_2^T\underline{\mathbf{x}}_2}\right)\underline{\mathbf{x}}_2}_{\text{component of } \underline{\mathbf{c}} \text{ along } \underline{\mathbf{x}}_2}$$

By construction, $\underline{\mathbf{x}}_3$ will be orthogonal to both $\underline{\mathbf{x}}_1$ and $\underline{\mathbf{x}}_2$, easily shown by direct substitution, i.e. left as exercise! And so on. Take a fourth independent vector and subtract its components along the previous three, giving $\underline{\mathbf{x}}_4$, orthogonal to the previous three.

That was the part due to Gram: to take a set of independent vectors and obtain an orthogonal set from these. The last is the easy part, due to Schmidt: normalize them, make them into unit vectors:

$$\underline{\mathbf{q}}_i = \frac{1}{|\underline{\mathbf{x}}_i|}\underline{\mathbf{x}}_i \quad \text{for} \quad i = 1 \ldots n$$

giving an orthonormal basis for $\mathbb{R}^n$.

Example 2.2. *Consider the basis of* $\mathbb{R}^3$

$$\underline{\mathbf{v}}_1 = \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}, \underline{\mathbf{v}}_2 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \underline{\mathbf{v}}_3 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix}.$$

Obtain an orthonormal basis by implementing the Gram-Schmidt process.

(i) $\underline{\mathbf{x}}_1 = \underline{\mathbf{v}}_1 = \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}$.

(ii) $\underline{\mathbf{x}}_2 = \underline{\mathbf{v}}_2 - \frac{\underline{\mathbf{x}}_1^T \underline{\mathbf{v}}_2}{\underline{\mathbf{x}}_1^T \underline{\mathbf{x}}_1} \underline{\mathbf{x}}_1 = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} - \frac{3}{5} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} = \frac{1}{5} \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix}$.

At this point we use common-sense rather than implementing the algorithm blindly. Both

$$\frac{1}{5} \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix}$$

are orthogonal to $\underline{\mathbf{x}}_1$. We get rid of the fraction and choose $\underline{\mathbf{x}}_2 = \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix}$, simplifying later calculations.

(iii) $\underline{\mathbf{x}}_3 = \underline{\mathbf{v}}_3 - \frac{\underline{\mathbf{x}}_2^T \underline{\mathbf{v}}_3}{\underline{\mathbf{x}}_2^T \underline{\mathbf{x}}_2} \underline{\mathbf{x}}_2 - \frac{\underline{\mathbf{x}}_1^T \underline{\mathbf{v}}_3}{\underline{\mathbf{x}}_1^T \underline{\mathbf{x}}_1} \underline{\mathbf{x}}_1 = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} - \frac{15}{30} \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix} - \frac{5}{5} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}$.

It is easy to check that $\underline{\mathbf{x}}_1$, $\underline{\mathbf{x}}_2$, $\underline{\mathbf{x}}_3$ form an orthogonal basis for $\mathbb{R}^3$. However, it is not yet orthonormal. To get an orthonormal basis, we need to divide each vector by its length:

$$\underline{\mathbf{q}}_1 = \frac{1}{\|\underline{\mathbf{x}}_1\|} \underline{\mathbf{x}}_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}.$$

$$\underline{\mathbf{q}}_2 = \frac{1}{\|\underline{\mathbf{x}}_2\|} \underline{\mathbf{x}}_2 = \frac{1}{\sqrt{30}} \begin{bmatrix} 2 \\ -1 \\ 5 \end{bmatrix}.$$

$$\underline{\mathbf{q}}_3 = \frac{1}{\|\underline{\mathbf{x}}_3\|} \underline{\mathbf{x}}_3 = \frac{1}{\sqrt{6}} \begin{bmatrix} -2 \\ 1 \\ 1 \end{bmatrix}.$$

And then, $\underline{\mathbf{q}}_1$, $\underline{\mathbf{q}}_2$, $\underline{\mathbf{q}}_3$ form an orthonormal basis for $\mathbb{R}^3$.

Note: we could have picked any of the three to be $\underline{\mathbf{x}}_1$. After that we could have picked any of the remaining two to obtain $\underline{\mathbf{x}}_2$: lots of possible different answers, all valid.

2.3 QR-factorization

What did we do in Gram-Schmidt? We began with a set of three independent vectors $\underline{\mathbf{a}}_1, \underline{\mathbf{a}}_2, \underline{\mathbf{a}}_3$ in $\mathbb{R}^3$ - or n vectors in $\mathbb{R}^n$. We constructed a new set of vectors as linear combinations of those three. If we form $\underline{\mathbf{a}}_1, \underline{\mathbf{a}}_2, \underline{\mathbf{a}}_3$ into a matrix A, and from the orthonormal vectors, we form the orthogonal matrix Q. Given the relations between the columns of A and Q, we can write these as a matrix product:

$$A = QR$$

and finding R turns out to be remarkably easy.

First, consider that

- $\underline{\mathbf{q}}_1$ is a linear combination of $\underline{\mathbf{a}}_1$, trivially.
- $\underline{\mathbf{q}}_2$ is a linear combination of $\underline{\mathbf{a}}_1, \underline{\mathbf{a}}_2$, which implies that
- $\underline{\mathbf{a}}_1, \underline{\mathbf{a}}_2$ are linear combinations of $\underline{\mathbf{q}}_1, \underline{\mathbf{q}}_2$, and therefore, crucially:
- $\underline{\mathbf{q}}_3$ which is orthogonal to $\underline{\mathbf{q}}_1$ and $\underline{\mathbf{q}}_2$, is therefore **also** orthogonal to $\underline{\mathbf{a}}_1$ and $\underline{\mathbf{a}}_2$

Therefore, at any step of the algorithm, the newly generated $\underline{\mathbf{q}}_i$ is not only orthogonal to all the previous $\underline{\mathbf{q}}_{r<i}$, but also to the columns of A used in their construction: all $\underline{\mathbf{a}}_{r<i}$!

Now use $Q^{-1} = Q^T$ and write

$$R = Q^T A = \begin{pmatrix} \underline{\mathbf{q}}_1^T \\ \underline{\mathbf{q}}_2^T \\ \underline{\mathbf{q}}_3^T \end{pmatrix} \begin{pmatrix} \underline{\mathbf{a}}_1 \, \underline{\mathbf{a}}_2 \, \underline{\mathbf{a}}_3 \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_1 & \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_2 & \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_3 \\ \underline{\mathbf{q}}_2^T\underline{\mathbf{a}}_1 & \underline{\mathbf{q}}_2^T\underline{\mathbf{a}}_2 & \underline{\mathbf{q}}_2^T\underline{\mathbf{a}}_3 \\ \underline{\mathbf{q}}_3^T\underline{\mathbf{a}}_1 & \underline{\mathbf{q}}_3^T\underline{\mathbf{a}}_2 & \underline{\mathbf{q}}_3^T\underline{\mathbf{a}}_3 \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_1 & \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_2 & \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_3 \\ 0 & \underline{\mathbf{q}}_2^T\underline{\mathbf{a}}_2 & \underline{\mathbf{q}}_2^T\underline{\mathbf{a}}_3 \\ 0 & 0 & \underline{\mathbf{q}}_3^T\underline{\mathbf{a}}_3 \end{pmatrix}$$

where the matrix R is upper-triangular because the entries below the diagonal have the product of $\underline{\mathbf{q}}_i$ with columns of A, where $\underline{\mathbf{a}}_{r<i}$, i.e. orthogonality holds.

Example 2.3. *Finish the previous example by obtaining the $QR-$factorization for A, where*

$$A = \begin{pmatrix} 1 & 1 & 1 \\ 2 & 1 & 2 \\ 0 & 1 & 3 \end{pmatrix}.$$

We note that A has as columns the three vectors $\underline{\mathbf{v}}_1, \underline{\mathbf{v}}_2, \underline{\mathbf{v}}_3$ so that Q will have as columns, the orthonormal set we obtained:

$$Q = \begin{pmatrix} \frac{1}{\sqrt{5}} & \frac{2}{\sqrt{30}} & -\frac{2}{\sqrt{6}} \\ \frac{2}{\sqrt{5}} & -\frac{1}{\sqrt{30}} & \frac{1}{\sqrt{6}} \\ 0 & \frac{5}{\sqrt{30}} & \frac{1}{\sqrt{6}} \end{pmatrix} = \frac{1}{\sqrt{30}} \begin{pmatrix} \sqrt{6} & 2 & -2\sqrt{5} \\ 2\sqrt{6} & -1 & \sqrt{5} \\ 0 & 5 & \sqrt{5} \end{pmatrix}.$$

The entries of R are easily computed.

$$\underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_1 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}^T \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix} = \sqrt{5}\,, \quad \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_2 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}^T \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} = \frac{3}{5}\sqrt{5} \quad \underline{\mathbf{q}}_1^T\underline{\mathbf{a}}_3 = \frac{1}{\sqrt{5}} \begin{bmatrix} 1 \\ 2 \\ 0 \end{bmatrix}^T \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} = \sqrt{5} \quad etc.$$

giving

$$R = \begin{pmatrix} \sqrt{5} & \frac{3}{5}\sqrt{5} & \sqrt{5} \\ 0 & \frac{1}{5}\sqrt{30} & \frac{1}{2}\sqrt{30} \\ 0 & 0 & \frac{1}{2}\sqrt{6} \end{pmatrix}$$

Now multiply to confirm $A = QR$.

The interesting aspect here is that even though having orthogonal Q is useful, it turns out that *any* $m \times n$ matrix A with independent columns can be factorized into $A = QR$, but Q will not always be square, it will be $m \times n$, though R is indeed $n \times n$, square. The columns of Q will be orthonormal, and it doesn't matter if there isn't a full set of these, we still have $Q^TQ = I$: we may not have an invertible Q, but can still proceed with the next step. (Note that A must be square or "tall": $m \geq n$; if there are more columns than rows, we can't have independent columns.)

Example 2.4. *Given the 3×2 "tall" matrix*

$$A = \begin{pmatrix} 2 & 1 \\ 3 & 12 \\ 6 & 10 \end{pmatrix},$$

obtain the $QR-$factorization.

Before we calculate, what are we expecting? A is 3×2, so Q will be 3×2 and R will be 2×2. Now take $\underline{\mathbf{x}}_1 = \begin{pmatrix} 2 \\ 3 \\ 6 \end{pmatrix} = \underline{\mathbf{c}}_1$, the first column of A. Then if $\underline{\mathbf{c}}_2$ is the second column,

$$\underline{\mathbf{x}}_2 = \underline{\mathbf{c}}_2 - \frac{\underline{\mathbf{q}}_1^T \underline{\mathbf{c}}_2}{\underline{\mathbf{q}}_1^T \underline{\mathbf{q}}_1} \underline{\mathbf{q}}_1 = \begin{pmatrix} 1 \\ 12 \\ 10 \end{pmatrix} - \frac{2+36+60}{4+9+36} \begin{pmatrix} 2 \\ 3 \\ 6 \end{pmatrix} = \begin{pmatrix} -3 \\ 6 \\ -2 \end{pmatrix}$$

and after normalization our first matrix is

$$Q = \frac{1}{7} \begin{pmatrix} 2 & -3 \\ 3 & 6 \\ 6 & -2 \end{pmatrix}$$

where we have already seen how $Q^T Q = I_2$. With

$$Q^T A = Q^T (QR) = R \Longrightarrow \begin{pmatrix} \underline{\mathbf{q}}_1^T \\ \underline{\mathbf{q}}_2^T \end{pmatrix} \begin{pmatrix} \underline{\mathbf{c}}_1 \ \underline{\mathbf{c}}_2 \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{q}}_1^T \underline{\mathbf{c}} 1 & \underline{\mathbf{q}}_1^T \underline{\mathbf{c}}_2 \\ 0 & \underline{\mathbf{q}}_2^T \underline{\mathbf{c}}_2 \end{pmatrix} = \begin{pmatrix} 7 & 14 \\ 0 & 7 \end{pmatrix} = R \, .$$

Finish by multiplying to confirm that $A = QR$.

Recall how we the method of least-squares relied on a matrix A with independent columns:

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

Now, with $QR-$ factorization we can write

$$A^T A = (QR)^T QR = (R^T Q^T)(QR) = R^T (Q^T Q) R = R^T R$$

as $Q^T Q = I$, and need to solve

$$R^T R \hat{\underline{\mathbf{x}}} = R^T Q^T \underline{\mathbf{b}} \, ,$$

and now reason as follows: given that A has independent columns, we have established earlier that $A^T A$ is invertible, and therefore $R^T R = A^T A$ is also invertible, and hence R^T is invertible. Thus, we can multiply by $(R^T)^{-1}$ and get

$$R \hat{\underline{\mathbf{x}}} = Q^T \underline{\mathbf{b}} \, .$$

Finally, as R is upper triangular, this is ready for back-substitution: very fast. There is a computational cost in obtaining Q and R, but it is less than the previous approach.

2.4 QR-algorithm

The most important application of the $QR-$factorization is in its application as a core part of the $QR-$algorithm, beyond the scope of this short course. Finding the eigenvalues (see next chapter) of large matrices, in order of magnitude is extremely useful. Often, all we need are the largest eigenvalues: they determine a great deal of the behaviour of a system. To find these, we use an algorithm which repeatedly employs Gram-Schmidt to obtain the $QR-$factorization of successive matrices, where the diagonal elements of R iteratively converge on the eigenvalues, in order of magnitude. The interested reader will find a very good example here:

Chapter 3

Linear Algebra 2.3: Eigenvalues, Eigenvectors and Diagonalization

3.1 Motivation

Recall that our usual $A\underline{\mathbf{x}} = \underline{\mathbf{b}}$ can also be thought of as a matrix acting on a vector $\underline{\mathbf{x}}$ to produce another vector $\underline{\mathbf{b}}$. Everything we do in this chapter and a lot of what follows hinges on the question

What about when $\underline{\mathbf{b}}$ is parallel to $\underline{\mathbf{x}}$?

We begin with a simple example in $\mathbb{R}^2$. Let

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

and think of multiplication by A as a transformation of the plane $\mathbb{R}^2$. Every vector $\underline{\mathbf{x}} \in \mathbb{R}^2$ is mapped to another vector, by multiplication with A. It turns out that points $\underline{\mathbf{x}}$ on the main diagonal $y = x$ stay on that diagonal but their distance to the origin is multiplied by 3: $A\underline{\mathbf{x}} = 3\underline{\mathbf{x}}$, for $\underline{\mathbf{x}} = k(1,1)^T$:

$$A\underline{\mathbf{x}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} k \\ k \end{pmatrix} = \begin{pmatrix} 2k+k \\ k+2k \end{pmatrix} = 3 \begin{pmatrix} k \\ k \end{pmatrix} = 3\underline{\mathbf{x}} \,.$$

Similary, points on the other diagonal, $y = -x$ stay put entirely; $A\underline{\mathbf{x}} = \underline{\mathbf{x}}$, for $\underline{\mathbf{x}} = k(1,-1)^T$:

$$A\underline{\mathbf{x}} = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \begin{pmatrix} k \\ -k \end{pmatrix} = \begin{pmatrix} 2k-k \\ k-2k \end{pmatrix} = \begin{pmatrix} k \\ -k \end{pmatrix} = \underline{\mathbf{x}} \,.$$

For picture, see lectures.

This is the type of behaviour we're interested in. In both cases $\underline{\mathbf{b}}$ is parallel to $\underline{\mathbf{x}}$, in the second case identical to $\underline{\mathbf{x}}$. In general, given a square matrix A, we would like to know which non-zero vectors $\underline{\mathbf{x}}$ and scalars λ satisfy

$$A\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}} \,.$$

We only consider non-zero $\underline{\mathbf{x}}$, given that $A\underline{\mathbf{0}} = \lambda\underline{\mathbf{0}}$ for any A and any λ, so not very interesting.

3.2 Introduction and Examples

The central equation is called the **eigenvalue equation**. For a square matrix A, if

$$A\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}} \,,$$

the vectors $\underline{\mathbf{x}} \neq \underline{\mathbf{0}}$ which satisfy this equation are called the **eigenvectors** of A, with corresponding **eigenvalues** λ.

An obvious one is the identity matrix I, because we can say $I\underline{\mathbf{x}} = 1\underline{\mathbf{x}}$ for any $\underline{\mathbf{x}}$, so the identity matrix has all vectors as eigenvectors, with eigenvalue $\lambda = 1$.

Similarly, consider

Example 3.1.

$$A = \begin{pmatrix} 3 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

and recall

$$\underline{\mathbf{i}} = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \quad \underline{\mathbf{j}} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \text{and} \quad \underline{\mathbf{k}} = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}$$

then obviously $A\underline{\mathbf{i}} = 3\underline{\mathbf{i}}, A\underline{\mathbf{j}} = 2\underline{\mathbf{j}}$, and $A\underline{\mathbf{k}} = 4\underline{\mathbf{k}}$, so the vectors $\underline{\mathbf{i}}, \underline{\mathbf{j}}, \underline{\mathbf{k}}$ are the eigenvectors of the A with corresponding eigenvalues $3, 2, 4$, respectively.

We make the obvious and general observation, gleaned from the first example. Every point on the diagonals $y = \pm x$ was mapped by A to another or the same point on its diagnoal. So if $\underline{\mathbf{x}}$ is an eigenvector, so is any non-zero multiple $k\underline{\mathbf{x}}$:

$$A(k\underline{\mathbf{x}}) = \lambda(k\underline{\mathbf{x}}) \Rightarrow k(A\underline{\mathbf{x}}) = k(\lambda\underline{\mathbf{x}}) \Rightarrow A\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}}\,.$$

We have already seen some of these at work.

Example 3.2. *Consider a projection matrix P which projects onto a plane, the column space $C(A)$ of some matrix A, where $P = A(A^TA)^{-1}A^T$.*

Then

$$P\underline{\mathbf{x}} = \underline{\mathbf{b}}$$

is in that plane. So if $\underline{\mathbf{x}}$ is already in that plane, we get

$$P\underline{\mathbf{x}} = \underline{\mathbf{x}}$$

so any $\underline{\mathbf{x}}$ in that plane is an eigenvector for P, with eigenvalue $\lambda = 1$. We sometimes refer to such a space as an **eigenspace** of the matrix, with the corresponding eigenvalue $\lambda = 1$. No surprise: it is the column space, so it makes sense to claim it's a subspace.

We also recall that if $\underline{\mathbf{x}} \in N(A)$, an element of the nullspace of A, then we recall that the column space and nullspace are orthogonal subspaces: any vector in one is perpendicular to any vector in the other. So $\underline{\mathbf{x}}$ is perpendicular to the plane and

$$P\underline{\mathbf{x}} = \underline{\mathbf{0}} = \mathbf{0}\underline{\mathbf{x}}$$

We conclude that any vector in the nullspace is also an eigenvector for P. with eigenvalue zero. Both nullspace and column space of A are eigenspaces of P.

Example 3.3. *Or consider a permutation matrix*

$$B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

which swaps the two rows if multiplying any other matrix.

So if we multiply

$$\underline{\mathbf{x}}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

we swap the rows and get $\underline{\mathbf{x}}_1$ back. In other words

$$B\underline{\mathbf{x}}_1 = \underline{\mathbf{x}}_1$$

and $\underline{\mathbf{x}}_1$ is an eigenvector of B, with eigenvalue $\lambda = 1$. Similarly, if we multiply

$$\underline{\mathbf{x}}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

we swap the rows and get $-\underline{\mathbf{x}}_2$. So

$$B\underline{\mathbf{x}}_2 = -\underline{\mathbf{x}}_2$$

and $\underline{\mathbf{x}}_2$ is another eigenvector of B, with eigenvalue $\lambda = -1$.

These are the same eigenvectors as in our first example

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}.$$

Compare:

$$B = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \Rightarrow \begin{cases} \lambda = 1 & \underline{\mathbf{x}}_1 = (1,\ 1)^T \\ \lambda = -1 & \underline{\mathbf{x}}_2 = (1,\ -1)^T \end{cases}$$

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \Rightarrow \begin{cases} \lambda = 3 & \underline{\mathbf{x}}_1 = (1,\ 1)^T \\ \lambda = 1 & \underline{\mathbf{x}}_2 = (1,\ -1)^T \end{cases}$$

We note that $A = B + 2I$ and going from B to A we have also added 2 to the eigenvalues! To see this, consider

$$A\underline{\mathbf{x}} = (B + 2I)\underline{\mathbf{x}} = B\underline{\mathbf{x}} + 2I\underline{\mathbf{x}} = B\underline{\mathbf{x}} + 2\underline{\mathbf{x}}$$

If the eigenvalues of B are λ then

$$A\underline{\mathbf{x}} = B\underline{\mathbf{x}} + 2\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}} + 2\underline{\mathbf{x}} = (\lambda + 2)\underline{\mathbf{x}}$$

so A has the same eigenvectors as B, with eigenvalues increased by 2, as seen.

3.3 Solving the Eigenvalue Equation

We've seen a few obvious examples and the very first one just given, but we don't yet have a systematic way of finding the eigenvalues and eigenvectors.

From

$$A\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}} \Rightarrow A\underline{\mathbf{x}} - \lambda\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

we would like to factor out the $\underline{\mathbf{x}}$ and to do so we recognize that $I\underline{\mathbf{x}} = \underline{\mathbf{x}}$ so that

$$A\underline{\mathbf{x}} - \lambda I\underline{\mathbf{x}} = \underline{\mathbf{0}} \Rightarrow (\mathbf{A} - \lambda\mathbf{I})\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

Recall that we want $\underline{\mathbf{x}} \neq \underline{\mathbf{0}}$ and in general we remember that

$$M\underline{\mathbf{x}} = \underline{\mathbf{0}} \quad \text{has} \begin{cases} \text{only the zero solution,} & \text{if } \det(M) \neq 0 \\ \text{infinitely many solutions,} & \text{if } \det(M) = 0 \end{cases}$$

In other words, for non-zero solutions $\underline{\mathbf{x}}$ to exist, we require

$$\det(A - \lambda I) = 0\,,$$

the matrix $A - \lambda I$ needs to be singular.

Note that the last equation, when we expand the determinant, will be a function

$$P_A(\lambda) = \det(A - \lambda I)$$

is called the **characteristic polynomial** of the matrix A, and the equation

$$\det(A - \lambda I) = 0$$

is called the **characteristic equation**. For $n \times n$ matrix A, this is a polynomial equation of degree n, with at most n solutions, real or complex conjugates, distinct or repeated. These are the eigenvalues.

This gives the algorithm: to find the eigenvalues and eigenvectors of a matrix A,

- find all scalars λ that are zeros of the charasteristic equation

$$P_A(\lambda) = \text{det}(A - \lambda I) = 0$$

to find the eigenvalues.

- for each such λ find a non-zero solution of the equation

$$(A - \lambda I)\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

to derive the corresponding eigenvectors.

Example 3.4. *Find eigenvalues and eigenvectors of the matrix*

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

Begin with the characteristic equation:

$$A - \lambda I \;=\; \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix} \;-\; \lambda \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \;=\; \begin{pmatrix} 2-\lambda & 1 \\ 1 & 2-\lambda \end{pmatrix} \Longrightarrow \det(A - \lambda I) \;=\; (2-\lambda)(2-\lambda) - 1 = 0$$

with solutions $\lambda = 3, 1$, as expected.

To find the eigenvectors, we solve

$$(A - \lambda I)\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

for each eigenvalue. Begin with $\lambda = 3$, then

$$A - 3I = \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix} \underline{\mathbf{x}} = \underline{\mathbf{0}}\,,$$

is a system with a free variable. We expect this: as the matrix $A - \lambda I$ is singular then the linear system $(A - \lambda I)\underline{\mathbf{x}} = \underline{\mathbf{0}}$ has infinitely many solutions. In this case, if $\underline{\mathbf{x}} = (x, y)^T$, then both rows have $x - y = 0 \Rightarrow x = y$ and we have the first eigenvector

$$\underline{\mathbf{x}}_1 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

as claimed. For $\lambda = 1$, we get

$$A - I = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \underline{\mathbf{x}} = \underline{\mathbf{0}}\,,$$

and both rows give $x = -y$ and the eigenvector is

$$\underline{\mathbf{x}}_2 = \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

In both cases, any non-zero multiple of $\underline{\mathbf{x}}_i$ would work, we choose a simple one.

Example 3.5. *Consider a rotation by $\pi/2$, with matrix*

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

and find its eigenvalues and eigenvectors.

Here's something entirely new: $\text{det}(R - \lambda I) = \text{det}\begin{pmatrix} -\lambda & -1 \\ 1 & -\lambda \end{pmatrix} = \lambda^2 + 1 = 0 \Rightarrow \lambda = \pm i$

We haven't seen complex eigenvalues before, but as solutions of a real polynomial, we expect that possibility. Now we lose the idea of a transformation of the plane. There will be no real vectors $\underline{\mathbf{x}}$ satisfying

$$R\underline{\mathbf{x}} = \pm i\underline{\mathbf{x}}\,.$$

But that also makes sense: If multiplication by R is a rotation in the plane, then all points other than the origin will rotate, by $\pi/2$. None will stay on a line, which would be multiplication by a constant. There are *no* real vectors satisfying $R\underline{\mathbf{x}} = \pm i\underline{\mathbf{x}}$. But if we accept vectors with complex components, that's perfectly fine. So for $\lambda = i$ we have

$$R - iI = \begin{pmatrix} -i & -1 \\ 1 & -i \end{pmatrix} \Rightarrow \begin{pmatrix} -i & -1 \\ 1 & -i \end{pmatrix} \underline{\mathbf{x}} = \underline{\mathbf{0}}$$

gives two equations $-ix - y = 0$ and $x - iy = 0$. Where's the free variable? Multiply the first by i and get the second, to see. So a solution would be $y = 1 \Rightarrow x = i$ and the first eigenvector is

$$\underline{\mathbf{x}}_1 = \begin{pmatrix} i \\ 1 \end{pmatrix} .$$

Similarly, for $\lambda = -i$, we get

$$(R + iI)\underline{\mathbf{x}} = \begin{pmatrix} i & -1 \\ 1 & i \end{pmatrix} \underline{\mathbf{x}} = \underline{\mathbf{0}}$$

gives $ix - y = 0$ and $x + iy = 0$, with a solution $x = 1 \Rightarrow y = i$ so the second eigenvector is

$$\underline{\mathbf{x}}_2 = \begin{pmatrix} 1 \\ i \end{pmatrix} .$$

Note: we will see later that symmetric matrices always have real eigenvalues. R is **anti-symmetric** which is defined as $R^T = -R$, and such matrices have purely imaginary eigenvalues.

Example 3.6. *Another interesting property of eigenvalues can be seen here Calculate the eigenvalues of the general* 2×2 *matrix.*

$$A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} .$$

Begin with

$\det(A - \lambda I) = (a - \lambda)(d - \lambda) - bc = 0 \Rightarrow \lambda^2 - (a + d)\lambda + ad - bc = 0$.

We know that in a quadratic equation, the negative of the linear coefficient is the sum of the roots, while the constant is the product:

$$a + d = \lambda_1 + \lambda_2 \quad \text{and} \quad ad - bc = \lambda_1\lambda_2$$

Here, $a + d$ is the sum of the diagonal elements of A, also called the **trace** of A, or $Tr(A)$. And we recognize $ad - bc$ as the determinant. It can be shown that for a general $n \times n$ matrix, this holds as well:

$$Tr(A) = \sum_{i=1}^{n} a_{ii} = \sum_{i=1}^{n} \lambda_i \quad \text{and} \quad \prod_{i=1}^{n} \lambda_i = \det(A) .$$

where $\prod_{i=1}^{n} x_i$ means the product $x_1 x_2 x_3 \cdots x_n$, similar to $\sum_{i=1}^{n}$.

It's easy enough to show that:

- $\mathrm{Tr}(A + B) = \mathrm{Tr}(A) + \mathrm{Tr}(B)$, $\mathrm{Tr}(A - B) = \mathrm{Tr}(A) - \mathrm{Tr}(B)$
- $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$, $\mathrm{Tr}(ABC) = \mathrm{Tr}(BCA) = \mathrm{Tr}(CAB)$
- $\mathrm{Tr}(A^T) = \mathrm{Tr}(A)$

Left as exercise.

Example 3.7. *Find the eigenvalues and eigenvectors of*

$$A = \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix}$$

Left as exercise. Note that A is symmetric, so expect real eigenvalues.

3.4 Diagonalization

Assume that the $n \times n$ matrix A has n independent eigenvectors $\underline{\mathbf{x}}_1, \ldots \underline{\mathbf{x}}_n$, with eigenvalues $\lambda_1, \ldots, \lambda_n$. Let the matrix S have the eigenvectors as columns. Then S has the form

$$S = \left(\ \underline{\mathbf{x}}_1, \underline{\mathbf{x}}_2, \ldots, \underline{\mathbf{x}}_n \ \right) \ .$$

Now consider $AS =$

$$A \left(\ \underline{\mathbf{x}}_1, \underline{\mathbf{x}}_2, \ldots, \underline{\mathbf{x}}_n \ \right) = \left(\ A\underline{\mathbf{x}}_1, A\underline{\mathbf{x}}_2, \ldots, A\underline{\mathbf{x}}_n \ \right) = \left(\ \lambda_1\underline{\mathbf{x}}_1, \lambda_2\underline{\mathbf{x}}_2, \ldots, \lambda_n\underline{\mathbf{x}}_n \ \right) = \left(\ \underline{\mathbf{x}}_1, \underline{\mathbf{x}}_2, \ldots, \underline{\mathbf{x}}_n \ \right) \begin{pmatrix} \lambda_1 & 0 & 0 & \ldots & 0 \\ 0 & \lambda_2 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \ldots & \lambda_n \end{pmatrix}$$

The last product is $A\Lambda$ where Λ is the $n \times n$ diagonal matrix, with eigenvalues on the diagonal, in the same order as eigenvectors in S:

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & 0 & \ldots & 0 \\ 0 & \lambda_2 & 0 & \ldots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \lambda_n \end{pmatrix}$$

As S has n independent columns, it is invertible and we can write

$$A = S\Lambda S^{-1} \quad \text{or} \quad \Lambda = S^{-1}AS \ .$$

This is the **diagonalization** of A and is available for most matrices. Write down a random matrix, there is a very high likelihood that the matrix has n independent eigenvectors so that S and S^{-1} exist. If A has n distinct eigenvalues, then this is always true. Degenerate cases occur when A has repeated eigenvalues. In that case a full set of eigenvectors may or may not exist. For example

$$A = \begin{pmatrix} 2 & 3 \\ 0 & 2 \end{pmatrix}$$

has the repeated eigenvalue $\lambda = 2$, trivially. When we try to find eigenvectors we get

$$A - \lambda I = \begin{pmatrix} 0 & 3 \\ 0 & 0 \end{pmatrix} \Rightarrow (A - 2I)\underline{\mathbf{x}} = \underline{\mathbf{0}}$$

has only one solution vector $\underline{\mathbf{x}} = k(1,0)^T$. On the other hand,

$$A = \begin{pmatrix} 2 & 0 \\ 0 & 2 \end{pmatrix}$$

also has the repeated eigenvalue $\lambda = 2$, but solving $(A - 2I)\underline{\mathbf{x}} = \underline{\mathbf{0}}$ gives two independent eigenvectors $\underline{\mathbf{x}}_1 = k(1,0)^T$ and $\underline{\mathbf{x}}_2 = k(0,1)^T$.

In the case of repeated eigenvalues, if λ is a root repeated k times as a solution of the characteristic equation, we say it has **algebraic multiplicity** k. The number of independent eigenvectors corresponding to that eigenvalue is its **geometric multiplicity** which may be less than k, as in the case above where $\lambda = 2$ has algebraic multiplicity 2 and geometric multiplicity 1.

Example 3.8. *Having found the eigenvalues and eigenvectors of*

$$A = \begin{pmatrix} 1 & 1 & 3 \\ 1 & 1 & -3 \\ 3 & -3 & -3 \end{pmatrix}$$

earlier, now obtain a diagonal matrix Λ and an invertible matrix S, so that $A = SAS^{-1}$.

Left as exercise. You do not need to compute S^{-1}, but may notice that the eigenvectors are orthogonal which would simplify the next step.

3.5 Powers of matrices and the exponential matrix

The simplest use of diagonalization is in obtaining powers of a matrix in a manageable form. Let $A = S\Lambda S^{-1}$. Then

$$A^2 = (S\Lambda S^{-1})(S\Lambda S^{-1}) = S\Lambda(S^{-1}S)\Lambda S^{-1} = S\Lambda^2 S^{-1}$$

where

$$\Lambda^2 = \begin{pmatrix} \lambda_1^2 & 0 & 0 & \dots & 0 \\ 0 & \lambda_2^2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & \lambda_n^2 \end{pmatrix}$$

and, similarly, $A^k = S\Lambda^k S^{-1}$.

Now consider the following. We define the **matrix exponential** e^A as an infinite series, as follows:

$e^A = I + A + \frac{1}{2}A^2 + \frac{1}{3!}A^3 + \ldots + \frac{1}{n!}A^n + \ldots$ and use the diagonalization to write it as

$$e^A = SIS^{-1} + S\Lambda S^{-1} + \frac{1}{2}S\Lambda^2 S^{-1} + \frac{1}{3!}S\Lambda^3 S^{-1} + \ldots \;= S\left(I + \Lambda + \frac{1}{2}\Lambda^2 + \frac{1}{3!}\Lambda^3 + \ldots\right)S^{-1}$$

$$= S\begin{pmatrix} 1+\lambda_1+\frac{1}{2}\lambda_1^2+\frac{1}{3!}\lambda_1^3+\ldots & 0 & 0 & \dots & 0 \\ 0 & 1+\lambda_2+\frac{1}{2}\lambda_2^2+\ldots & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & 1+\lambda_n+\frac{1}{2}\lambda_n^2+\ldots \end{pmatrix} S^{-1}$$

$$= S\begin{pmatrix} e^{\lambda_1} & 0 & 0 & \dots & 0 \\ 0 & e^{\lambda_2} & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \dots & e^{\lambda_n} \end{pmatrix} S^{-1}$$

The last matrix is denoted e^Λ and thus we can easily represent

$$e^A = Se^\Lambda S^{-1}$$

and as each of the exponential series on the diagonal in e^Λ converges, this guarantees convergence of the infinite series of matrices in e^A. The matrix exponential has many applications: we look at an important one in the next section: systems of coupled ODEs.

3.6 Coupled First-Order ODEs

The matrix exponential can be applied to systems of coupled first-order equations and in systems control we often come across such equations:

$$\dot{\mathbf{x}}(t) = A\mathbf{x}(t) + B\mathbf{u}(t), \qquad \mathbf{x}(t_0) = \mathbf{x}_0 \tag{3.1}$$

with solution

$$\mathbf{x}(t) = e^{A(t-t_0)}\mathbf{x}_0 + \int_{t_0}^{t} e^{A(t-\tau)}B\mathbf{u}(\tau)d\tau\,. \qquad (**)$$

The equation represents a *state space* model, where $\mathbf{x}(t)$ can be a vector of state variables $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ with coupled ODEs describing their behaviour, so that A is an $n \times n$ matrix. We illustrate with a simple example, the 2×2 case. We have two state variables, $x_1(t)$ and $x_2(t)$, and two coupled first-order eqautions:

$$\dot{x_1} = ax_1 + bx_2 + u_1(t)$$
$$\dot{x_2} = cx_1 + dx_2 + u_2(t)$$

For the first attempt to solve the system, we set $u \equiv 0$ to further simplify and write

$$\dot{\underline{\mathbf{x}}} = \begin{pmatrix} \dot{x_1} \\ \dot{x_2} \end{pmatrix} = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = A\underline{\mathbf{x}}$$

If A can be diagonalized, the solution is simple. If no diagonalization is available, solutions may take more work! Assume we can diagonalize. This does not require A to be symmetric, only for A to have a full set of n, here two, independent eigenvectors. In the general case, we will have an invertible matrix S and a diagonal matrix Λ such that

$$A = S\Lambda S^{-1} \quad \text{and} \quad \Lambda = S^{-1}AS$$

Now consider a new vector of variables $\underline{\mathbf{y}}(t) = \begin{pmatrix} y_1(t) \\ y_2(t) \end{pmatrix}$ satisfying $\dot{\underline{\mathbf{y}}} = \Lambda\underline{\mathbf{y}}$.

Then consider the substitution $\underline{\mathbf{x}} = S\underline{\mathbf{y}}$ and proceed:

$$\dot{\underline{\mathbf{x}}} = S\dot{\underline{\mathbf{y}}} = S(\Lambda\underline{\mathbf{y}}) = S(S^{-1}AS)\underline{\mathbf{y}} = A(S\underline{\mathbf{y}}) = A\underline{\mathbf{x}}\,.$$

We see that $\underline{\mathbf{x}} = S\underline{\mathbf{y}}$ is the solution of our coupled system of equations! All that is required is to find the eigenvalues and eigenvectors of A.

Example 3.9. *Solve the system* $\dot{\underline{\mathbf{x}}} = A\underline{\mathbf{x}}$ *where* $A = \begin{pmatrix} 1 & 1 \\ 4 & 1 \end{pmatrix}$. *and* $x_1(0) = x_2(0) = 1$.

This is not an exercise in finding eigenvalues/vectors. Check for yourself that they are $\lambda_{1,2} = 3, -1$ with corresponding eigenvectors $\underline{\mathbf{a_1}} = (1,2)^T$ and $\underline{\mathbf{a_2}} = (1,-2)^T$. Hence

$$S = \begin{pmatrix} 1 & 1 \\ 2 & -2 \end{pmatrix}, \qquad \Lambda = \begin{pmatrix} 3 & 0 \\ 0 & -1 \end{pmatrix}$$

and we can immediately solve

$$\dot{\underline{\mathbf{y}}} = \Lambda\underline{\mathbf{y}} \Rightarrow \begin{array}{rcl} \dot{y_1} &=& 3y_1 \\ \dot{y_2} &=& -y_2 \end{array} \Rightarrow \underline{\mathbf{y}} = \begin{array}{rcl} y_1 &=& c_1e^{3t} \\ y_2 &=& c_2e^{-t} \end{array}$$

Now we have the solution

$$\underline{\mathbf{x}} = S\underline{\mathbf{y}} = \begin{pmatrix} 1 & 1 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} c_1e^{3t} \\ c_2e^{-t} \end{pmatrix} = \begin{pmatrix} c_1e^{3t} + c_2e^{-t} \\ 2c_1e^{3t} - 2c_2e^{-t} \end{pmatrix}$$

or, better:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix} c_1e^{3t} + \begin{pmatrix} 1 \\ -2 \end{pmatrix} c_2e^{-t}$$

Note how eigenvectors and eigenvalues appear in the solution:

$$\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \underline{\mathbf{a_1}}c_1e^{\lambda_1 t} + \underline{\mathbf{a_2}}c_2e^{\lambda_2 t}\,.$$

The arbitrary constants of integration $c_{1,2}$ are determined using the initial conditions:

$$x_1(0) = 1 \Rightarrow 1 = c_1 + c_2\,, \quad x_2(0) = 1 \Rightarrow 1 = 2c_1 - 2c_2\,,$$

two equations in two unknowns, which we solve for $c_1 = 3/4$ and $c_2 = 1/4$. Finally we have solutions

$$x_1(t) = \frac{3}{4}e^{3t} + \frac{1}{4}e^{-t}\,, \quad x_2(t) = \frac{3}{2}e^{3t} - \frac{1}{2}e^{-t}\,.$$

That was the homogenous case, involving only the state variables and their derivatives, but no terms $u(t)$, functions only of the independent variable t. For the inhomogenous case, we take a slightly different approach. We have the coupled system of equations

$$\dot{\underline{\mathbf{x}}}(t) = A\underline{\mathbf{x}}(t) + \underline{\mathbf{u}}(t)\,. \qquad (*)$$

Assume A can be diagonalized, so that $S^{-1}AS = \Lambda$. As before $\underline{\mathbf{x}} = S\underline{\mathbf{y}}$, but we begin with $\underline{\mathbf{y}} = S^{-1}\underline{\mathbf{x}}$ and $\underline{\mathbf{h}}(t) = S^{-1}\underline{\mathbf{u}}$. Multiplying (*) on the left by S^{-1} gives

$$S^{-1}\dot{\underline{\mathbf{x}}} = S^{-1}A\underline{\mathbf{x}} + S^{-1}\underline{\mathbf{u}}$$

$$\Rightarrow \underline{\dot{\mathbf{y}}} = S^{-1}A(SS^{-1})\underline{\mathbf{x}} + \underline{\mathbf{h}} = \Lambda(S^{-1}\underline{\mathbf{x}}) + \underline{\mathbf{h}} = \Lambda\underline{\mathbf{y}} + \underline{\mathbf{h}}\,.$$

Again, we have a decoupled system: $\underline{\dot{\mathbf{y}}} = \Lambda\underline{\mathbf{y}} + \underline{\mathbf{h}}$ with the two linear equations $\dot{y}_i - \lambda_i y = h_i(t)$ with $i = 1, 2$. The integrating factors are $e^{-\lambda_i t}$ giving the solution

$$\frac{d}{dt}\left(ye^{-\lambda_i t}\right) = h_i e^{-\lambda_i t} \Rightarrow ye^{-\lambda_i t} = \int h_i e^{-\lambda_i t}\, dt + c_i \Rightarrow y_i = c_i e^{\lambda_i t} + e^{\lambda_i t}\int h_i e^{-\lambda_i t}\, dt$$

and we note how the solution includes the solution of the homogenous equation and an integral involving $h(t)$, recall complementary function and particular integral. Finally we return to $\underline{\mathbf{x}} = S\underline{\mathbf{y}}$, multiplying the solution by S, as before.

In general, if we have a vector of n functions $\underline{\mathbf{x}}(t)$ satisfying n coupled first order ODEs, we can write

$$\frac{d\underline{\mathbf{x}}}{dt} = A\underline{\mathbf{x}}$$

with a vector of n initial conditions $\underline{\mathbf{x}}(0)$, and proceed as above, as long as A can be diagonalized, using the substitution $\underline{\mathbf{x}} = S\underline{\mathbf{y}}$ to decouple the system:

$S\frac{d\underline{\mathbf{y}}}{dt} = \frac{d\underline{\mathbf{x}}}{dt} = A\underline{\mathbf{x}} = AS\underline{\mathbf{y}} \Rightarrow \frac{d\underline{\mathbf{y}}}{dt} = S^{-1}AS\underline{\mathbf{y}} = \Lambda\underline{\mathbf{y}}$ with solution vector

$$\underline{\mathbf{y}}(t) = \begin{pmatrix} \underline{\mathbf{y}}_1 \\ \underline{\mathbf{y}}_2 \\ \vdots \\ \underline{\mathbf{y}}_n \end{pmatrix} = \begin{pmatrix} y_1(0)e^{\lambda_1 t} \\ y_2(0)e^{\lambda_2 t} \\ \vdots \\ y_n(0)e^{\lambda_n t} \end{pmatrix} = e^{\Lambda t}\underline{\mathbf{y}}(0)$$

where the exponential matrix $e^{\Lambda t}$ has diagonal elements $e^{\lambda_i t}$. The initial conditions give $\underline{\mathbf{y}}(0) = S^{-1}\underline{\mathbf{x}}(0)$ and the decoupling gives the solution

$$\underline{\mathbf{x}}(t) = S\underline{\mathbf{y}} = Se^{\Lambda t}S^{-1}\underline{\mathbf{x}}(0) = e^{At}\underline{\mathbf{x}}(0)\ ,$$

used extensively in Signals and Systems as well as Control Theory. Note that this matches the definition for $n = 1$, where the "matrix" is 1×1, a scalar, and the system reduces to a single first-order linear ODE, as seen in year one:

$$\frac{dx}{dt} = ax \Rightarrow x(t) = x(0)e^{at}\ .$$

The expression at the beginning of this section is a more general version, and you will see it in other modules. For reference, the derivation (loosely) is as follows: begin with

$$\dot{x} - Ax = Bu(t)$$

and obtain the integrating factor $e^{-\int A\ dt} = e^{-At}$ to rewrite the ODE as

$$\frac{d}{dt}\left(e^{-At}x\right) = e^{-At}Bu(t) \Longrightarrow e^{-At}x = \int e^{-At}Bu(t)\ dt + C \Longrightarrow x(t) = e^{At}\left(C + \int e^{-At}Bu(t)dt\right)$$

Next, recognize that t is a dummy variable of integration and can be replaced by any other variable, here τ, provided we set t as the upper limit:

$$x(t) = e^{At}\left(C + \int^{t} e^{-A\tau}Bu(\tau)d\tau\right)$$

Now introduce a lower limit and absorbing it in the constant C, which becomes C_1:

$$x(t) = e^{At}\left(C_1 + \int_{t_0}^{t} e^{-A\tau}Bu(\tau)d\tau\right)$$

Now we include e^{At} inside the integral (which is harmless since the integration is with respect to τ). Now write $e^{At}C_1 = \left(e^{At}e^{-At_0}\right)\left(e^{At_0}C_1\right) = e^{A(t-t_0)}C_2$:

$$x(t) = e^{A(t-t_0)}C_2 + \int_{t_0}^{t} e^{A(t-\tau)}Bu(\tau)d\tau$$

Setting $t = t_0$ gives $C_2 = x(t_0) = x_0$:

$$x(t) = e^{A(t-t_0)}x_0 + \int_{t_0}^{t} e^{A(t-\tau)}Bu(\tau)d\tau$$

Finally, the last equation remains valid when $x(t)$, usually called the state, and $u(t)$, usually called the input, are vector signals and A and B are matrices with compatible dimensions, assuming diagonalization of A, of course.

Chapter 4

Linear Algebra 2.4: Symmetric Matrices and the SVD

4.1 Symmetric Matrices and the Spectral Theorem

We've claimed that real symmetric matrices have real eigenvalues. It turns out that in this case, eigenvectors corresponding to distinct eigenvalues are orthogonal and we can always find a full set of orthogonal eigenvectors: symmetric matrices make life easy! This result is normally known as the Spectral Theorem.

We prove that all eigenvalues are real. We begin with

$$A\underline{\mathbf{x}} = \lambda\underline{\mathbf{x}}$$

and take the complex conjugate of every term:

$$\bar{A}\bar{\underline{\mathbf{x}}} = \bar{\lambda}\bar{\underline{\mathbf{x}}}$$

Given that A has real entries, we have

$$A\bar{\underline{\mathbf{x}}} = \bar{\lambda}\bar{\underline{\mathbf{x}}}$$

and take the transpose:

$$(A\bar{\underline{\mathbf{x}}})^T = (\bar{\lambda}\bar{\underline{\mathbf{x}}})^T \Rightarrow \bar{\underline{\mathbf{x}}}^T A^T = \bar{\underline{\mathbf{x}}}^T\bar{\lambda} \Rightarrow \bar{\underline{\mathbf{x}}}^T A = \bar{\underline{\mathbf{x}}}^T\bar{\lambda}$$

as A is symmetric. Now multiply the last equation on the right by $\underline{\mathbf{x}}$ to get

$$(\bar{\underline{\mathbf{x}}}^T A)\underline{\mathbf{x}} = (\bar{\underline{\mathbf{x}}}^T\bar{\lambda})\underline{\mathbf{x}} \qquad (*)$$

and multiply the eigenvalue equation on the left by $\bar{\underline{\mathbf{x}}}^T$

$$\bar{\underline{\mathbf{x}}}^T(A\underline{\mathbf{x}}) = \bar{\underline{\mathbf{x}}}^T(\lambda\underline{\mathbf{x}}) \qquad (**)$$

Given that matrix multiplication is associative, the lhs of both $(*)$ and $(**)$ are the same, so the rhs is also equal:

$$\bar{\underline{\mathbf{x}}}^T(\lambda\underline{\mathbf{x}}) = (\bar{\underline{\mathbf{x}}}^T\bar{\lambda})\underline{\mathbf{x}} \Rightarrow \lambda(\bar{\underline{\mathbf{x}}}^T\underline{\mathbf{x}}) = \bar{\lambda}(\bar{\underline{\mathbf{x}}}^T\underline{\mathbf{x}}) \Rightarrow \lambda = \bar{\lambda}$$

We were able to cancel $\bar{\underline{\mathbf{x}}}^T\underline{\mathbf{x}} = |\underline{\mathbf{x}}|^2 \neq 0$ because

$$\bar{\underline{\mathbf{x}}}^T\underline{\mathbf{x}} = \bar{x_1}x_1 + \bar{x_2}\underline{\mathbf{x}}_2 + \ldots + \bar{x_n}x_n = |x_1|^2 + |x_2|^2 + |x_3|^2 + \ldots |x_n|^2$$

and the last expression is never zero unless all entries of $\underline{\mathbf{x}}$ are zero, but then $\underline{\mathbf{x}} = \underline{\mathbf{0}}$, which is not possible for an eigenvector.

We have shown part of the **Spectral Theorem**:

Theorem 4.1. *Let A be a real $n \times n$ symmetric matrix. Then A has real eigenvalues and n orthogonal eigenvectors.*

The spectral theoerm guarantees that we get n orthogonal eigenvectors, but obtaining them requires extra work when an eigenvalue is repeated. Eigenvectors corresponding to distinct eigenvalues are automatically orthogonal, left as an exercise. Eigenvectors corresponding to a repeated eigenvalue need to be *made* orthogonal. If an eigenvalue has algebraic multiplicity two, we need two orthogonal eigenvectors. To do so, obtain two independent eigenvectors satisfying

$$(A - \lambda I)\underline{\mathbf{x}} = \underline{\mathbf{0}}\,,$$

in other words, find a basis for the Nullspace of $A - \lambda I$. Then use projection to find an orthogonal basis, as seen previously. When an eigenvalue has algebraic multiplicity greater than two, use Gram-Schmidt.

We say that a symmetric matrix is *orthogonally diagonalizable:* in the sense that we can obtain S from the orthonormal eigenvectors of A, so that S is an orthogonal matrix, and

$$A = S\Lambda S^T\,.$$

Example 4.1. *We find the orthogonal diagonalization of*

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

This matrix, as seen previously, has eigenvalues and corresponding eigenvectors

$$\lambda_1 = 1\,, \underline{\mathbf{x}}_1 = \begin{pmatrix} 1 \\ -1 \end{pmatrix} \quad \text{and} \quad \lambda_2 = 3\,, \underline{\mathbf{x}}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Note that A is symmetric, and the eigenvectors corresponding to distinct eigenvalues are automatically orthogonal. We normalize them:

$$\hat{x}_1 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}\,, \quad \text{and} \quad \hat{x}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}\,, \Longrightarrow S = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix} \quad \text{and} \quad \Lambda = \begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}$$

and the orthogonal diagonalization is

$$A = S\Lambda S^T = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}\frac{1}{\sqrt{2}}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ -1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 3 \end{pmatrix}\begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}$$

Exercise. Obtain the orthogonal diagonalization of $A = \begin{pmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{pmatrix}$.

4.2 The DFT Matrix

We have seen how some matrices can have complex entries. To deal with such matrices we need to define a new notion of magnitude/length. For a vector $\underline{\mathbf{x}}$ with complex entries we define

$$|\underline{\mathbf{x}}| = \bar{\underline{\mathbf{x}}}^T\underline{\mathbf{x}}$$

so if

$$\underline{\mathbf{x}} = \begin{pmatrix} 1 \\ i \end{pmatrix} \Rightarrow |\underline{\mathbf{x}}| = (1,\ -i)\begin{pmatrix} 1 \\ i \end{pmatrix} = 1 - i^2 = 2$$

and $|\underline{\mathbf{x}}| = 0 \Leftrightarrow \underline{\mathbf{x}} = \underline{\mathbf{0}}$. Note that this covers both cases: complex and real vectors, given that $\bar{\underline{\mathbf{x}}} = \underline{\mathbf{x}}$ for a real vector.

Similarly, we define the complex analogue of a symmetric matrix. A matrix A is called **Hermitian** if

$$A^H = \bar{A}^T = A\,.$$

For example

$$A = \begin{pmatrix} 1 & 1-i \\ 1+i & 2 \end{pmatrix}$$

is Hermitian. With this definition, a real symmetric matrix is just a special case of the more general complex Hermitian matrix. The notation A^H is sometimes used for $\bar{A}^T$, called the **Hermitian transpose.**

Similarly, two vectors $\underline{\mathbf{q}}_i, \underline{\mathbf{q}}_j$ are orthonormal if

$$\underline{\mathbf{q}}_i^H \underline{\mathbf{q}}_j \;=\; \bar{\underline{\mathbf{q}}}_i^{\,T} \underline{\mathbf{q}}_j = \begin{cases} 1\,, & i = j\,, \\ 0\,, & i \neq j\,. \end{cases}$$

If we have an orthonormal set, we can form the matrix Q:

$$Q = \begin{pmatrix} \underline{\mathbf{q}}_1 \, \underline{\mathbf{q}}_2 \cdots \underline{\mathbf{q}}_n \end{pmatrix}$$

and multiply by the transpose of the complex conjugate:

$$Q^H Q \;=\; \bar{Q}^T Q = \begin{pmatrix} \bar{\underline{\mathbf{q}}}_1^T \\ \bar{\underline{\mathbf{q}}}_2^T \\ \vdots \\ \bar{\underline{\mathbf{q}}}_n^T \end{pmatrix} \begin{pmatrix} \underline{\mathbf{q}}_1 \, \underline{\mathbf{q}}_2 \cdots \underline{\mathbf{q}}_n \end{pmatrix} \begin{pmatrix} \bar{\underline{\mathbf{q}}}_1^T \underline{\mathbf{q}}_1 & \bar{\underline{\mathbf{q}}}_1^T \underline{\mathbf{q}}_2 & \cdots & \bar{\underline{\mathbf{q}}}_1^T \underline{\mathbf{q}}_n \\ \bar{\underline{\mathbf{q}}}_2^T \underline{\mathbf{q}}_1 & \bar{\underline{\mathbf{q}}}_2^T \underline{\mathbf{q}}_2 & \cdots & \bar{\underline{\mathbf{q}}}_2^T \underline{\mathbf{q}}_n \\ \vdots & \vdots & & \vdots \\ \bar{\underline{\mathbf{q}}}_n^T \underline{\mathbf{q}}_1 & \bar{\underline{\mathbf{q}}}_n^T \underline{\mathbf{q}}_2 & \cdots & \bar{\underline{\mathbf{q}}}_n^T \underline{\mathbf{q}}_n \end{pmatrix} \;=\; I_n$$

An invertible complex matrix satisfying $\bar{Q}^T Q = I_n$ is called **unitary** which reduces to orthogonal matrix when entries are real.

An extremely useful unitary matrix is the **DFT matrix**, also called **Fourier matrix**, used in the Discrete Fourier Transform (DFT) and in the closely allied Fast Fourier Transform (FFT) algorithm.

Let ω be a complex number satisfying $\omega^n = 1$, so that $1, \omega, \omega^2, \omega^3, \ldots \omega^{n-1}$ are the n^{th} roots of unity, and define

$$F_n = \frac{1}{\sqrt{n}} \begin{pmatrix} 1 & 1 & 1 & 1 & \ldots & 1 \\ 1 & \omega & \omega^2 & \omega^3 & \ldots & \omega^{n-1} \\ 1 & \omega^2 & \omega^4 & \omega^6 & \ldots & \omega^{2(n-1)} \\ 1 & \omega^3 & \omega^6 & \omega^9 & \ldots & \omega^{3(n-1)} \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 1 & \omega^{n-1} & \omega^{2(n-1)} & \omega^{3(n-1)} & \ldots & \omega^{(n-1)(n-1)} \end{pmatrix}$$

It's not hard to see that $(F_n)_{ij} = \omega^{ij}$, for $0 \leq i, j \leq n-1$. Note: this is standard in Electronic Engineering. In Mathematics, indices $1 \leq i, j \leq n$ are used, for the same matrix.

For example, if $n = 4$, then $\omega = i$, $\omega^2 = -1$, $\omega^3 = -i$, and $\omega^4 = 1$, giving

$$F_4 = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & i & -1 & -i \\ 1 & -1 & 1 & -1 \\ 1 & -i & -1 & i \end{pmatrix}$$

and it's not hard to see that the columns are orthonormal vectors and that F_4 is in fact unitary. Check: DIY. Multiply out $\bar{F}_4^T F_4$.

4.3 Positive-definite Matrices

Not all matrices can be diagonalized, as we have seen. Symmetric/Hermitian matrices are good for lots of reasons, but the fact that they are always diagonalizable, and orthogonally diagonalizable, is especially useful. Even more useful are positive-definite matrices, which we can think of as symmetric++.

A **positive-definite** matrix is a symmetric matrix whose eigenvalues are all positive. It has all the useful properties of a symmetric matrix, and a few more, as we will see.

There are several characterictics equivalent to having positive eigenvalues. Here is one: a symmetric matrix A is positive definite if

$$\underline{\mathbf{x}}^T A \underline{\mathbf{x}} > 0$$

for every non-zero vector $\underline{\mathbf{x}}$. The same idea extends to Hermitian, but we take $\underline{\mathbf{x}}^H$ on the left.

As A is symmetric, there exist orthogonal S and diagonal Λ so that $A = S\Lambda S^T$. Hence

$$\underline{\mathbf{x}}^T A \underline{\mathbf{x}} = \underline{\mathbf{x}}^T (S\Lambda S^T) \underline{\mathbf{x}} = (\underline{\mathbf{x}}^T S)\Lambda (S^T \underline{\mathbf{x}}) = (S^T \underline{\mathbf{x}})^T \Lambda (S^T \underline{\mathbf{x}})$$

Let $(y_1, y_2, \ldots y_n) = \underline{\mathbf{y}} = S^T \underline{\mathbf{x}}$, then

$$\underline{\mathbf{x}}^T A \underline{\mathbf{x}} = \underline{\mathbf{y}}^T \Lambda \underline{\mathbf{y}} = \lambda_1 y_1^2 + \lambda_2 y_2^2 + \ldots + \lambda_n y_n^2 > 0$$

given that all $\lambda_i > 0$. The expression could be zero if $\underline{\mathbf{y}} = \underline{\mathbf{0}}$, but $\underline{\mathbf{y}} = S^T \underline{\mathbf{x}}$ and as S^T is invertible, and $\underline{\mathbf{x}} \neq \underline{\mathbf{0}}$, this possibility is excluded.

Recall how useful the matrix $A^T A$ has been, even for non-square A. We already know it's symmetric, and as long as A has full column rank, i.e. independent columns, we also know that $A^T A$ is invertible, and both properties have been useful. Now consider

$$\underline{\mathbf{x}}^T (A^T A) \underline{\mathbf{x}} = (\underline{\mathbf{x}}^T A^T)(A \underline{\mathbf{x}}) = (A \underline{\mathbf{x}})^T (A \underline{\mathbf{x}})$$

and let $\underline{\mathbf{y}} = A \underline{\mathbf{x}}$ .Then

$$\underline{\mathbf{x}}^T (A^T A) \underline{\mathbf{x}} = \underline{\mathbf{y}}^T \underline{\mathbf{y}} = |\underline{\mathbf{y}}|^2 > 0\,.$$

Could this be zero? Only if $\underline{\mathbf{y}} = A \underline{\mathbf{x}} = \underline{\mathbf{0}}$. This could happen if $\underline{\mathbf{x}} = \underline{\mathbf{0}}$, but we have excluded that. Another possibility would be a non-zero $\underline{\mathbf{x}} \in N(A)$, but recall that a matrix with independent columns has only the zero vector in the nullspace! Hence $\underline{\mathbf{y}} \neq \underline{\mathbf{0}}$ for any non-zero $\underline{\mathbf{x}}$. So

$$\underline{\mathbf{x}}^T (A^T A) \underline{\mathbf{x}} > 0 \quad \text{for every} \quad \underline{\mathbf{x}} \neq \underline{\mathbf{0}}$$

and hence $A^T A$ is a positive definite matrix.

If, on the other hand, A has some column dependency, then we know that $A^T A$ will not be invertible. It also means that A has at least one zero eigenvalue. In that case, we have

$$\underline{\mathbf{x}}^T (A^T A) \underline{\mathbf{x}} \;\geq\; 0$$

and $A^T A$ is called **positive semi-definite**.

4.4 The Singular Value Decomposition

That sets up all the tools we need to move to the **Singular Value Decomposition**, so useful it has its own acronym: SVD. Arguably, the most important result in applied Linear Algebar, the SVD is the "best" decomposition yet. LU and QR have their limitations: for a start, there's no diagonal matrix. If a matrix is square it might be diagonalizable, or it might not, only *if* it has n distinct eigenvalues, do we get a diagonal matrix in $S\Lambda S^{-1}$, and only **if** the matrix is symmetric do we get $S\Lambda S^T$ with orthogonal S. That's a lot of ifs. The SVD is available for **any** matrix, including non-square.

Given any $m \times n$ matrix A, the Singular Value Decomposition of A is

$$A = U \Sigma V^T$$

where U and V are orthogonal matrices (unitary, if complex numbers involved) and Σ is diagonal, though not necessarily square. Here diagonal is more general than we've seen before: Σ will be $m \times n$ and will have zero-entries everywhere except on the main diagonal, where $i = j$.

The first thing to note is sizes. If A is $m \times n$ then

$$\underbrace{A}_{m\times n} = \underbrace{U}_{m\times m}\ \underbrace{\Sigma}_{m\times n}\ \underbrace{V^T}_{n\times n}$$

Let the rank of A be r. Then we write

$$\Sigma = \begin{pmatrix} \sigma_1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sigma_r & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix}$$

where $(\Sigma)_{ii} = \sigma_i \neq 0$ for $i = 1 \dots r$, called the **singular values** of A, and zero entries everywhere else. The colums of U are called **left singular vectors** and the columns of V are the **right singular vectors** Given that the rank $r \leq m, n$, there will be at least one extra row or column of zeroes, unless A is square and invertible, so that $r = m = n$, in which case Σ will also be square (and invertible, with every diagonal entry non-zero).

The first thing to note here is from the consideration of what happens if we write

$$A = (U\Sigma)V^T = \begin{pmatrix} \underline{\mathbf{u}}_1\ \underline{\mathbf{u}}_2 \dots \underline{\mathbf{u}}_r\ \underline{\mathbf{u}}_{r+1} \dots \underline{\mathbf{u}}_m \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sigma_r & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} V^T$$

The $m \times n$ matrix $U\Sigma$ has the first column $U($ first column of $\Sigma)$ as a linear combination of the columns of U with coefficients from the first column of Σ:

$$\begin{pmatrix} \underline{\mathbf{u}}_1\ \underline{\mathbf{u}}_2 \dots \underline{\mathbf{u}}_r\ \underline{\mathbf{u}}_{r+1} \dots \underline{\mathbf{u}}_m \end{pmatrix} \begin{pmatrix} \sigma_1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = \sigma_1 \underline{\mathbf{u}}_1 + 0\underline{\mathbf{u}}_2 + \dots + 0\underline{\mathbf{u}}_r$$

Similarly, the second column of $U\Sigma$ is $U($ second column of $\Sigma)$ as a linear combination of the columns of U with coefficients from the second column of Σ:

$$= 0\sigma_1 + \sigma_2\underline{\mathbf{u}}_2 + 0\underline{\mathbf{u}}_3 + \dots + 0\underline{\mathbf{u}}_r$$

and so on giving

$$A = (U\Sigma)V^T = \begin{pmatrix} \sigma_1\underline{\mathbf{u}}_1\ \sigma_2\underline{\mathbf{u}}_2 \dots \sigma_r\underline{\mathbf{u}}_r & \underbrace{\underline{\mathbf{0}} \dots \underline{\mathbf{0}}}_{n-r \text{ zero vectors}} \end{pmatrix} \begin{pmatrix} \underline{\mathbf{v}}_1^T \\ \underline{\mathbf{v}}_2^T \\ \vdots \\ \underline{\mathbf{v}}_n^T \end{pmatrix} = \sigma_1\underline{\mathbf{u}}_1\underline{\mathbf{v}}_1^T + \dots + \sigma_r\underline{\mathbf{u}}_r\underline{\mathbf{v}}_r^T$$

Each term in the last sum is a rank-1 $m \times n$ matrix, as the product of a column vector $\underline{\mathbf{u}}_i \in \mathbb{R}^m$ and a row vector $\underline{\mathbf{v}}_i^T \in \mathbb{R}^n$, weighted by σ_i. Ordering the σ_i in descending order of magnitude: $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r$ allows us to make an effective approximation of A by discarding terms with sufficiently small σ_i! This is a key part in the applications of the SVD to data compression, and other applications. If A is large and we don't want to transmit all of it, we take the largest singular values, transmit these and the vectors $\underline{\mathbf{u}}, \underline{\mathbf{v}}$, and get a good approximation.

4.4.1 SVD and fundamental subspaces

To identify the columns of U and V, we begin by writing

$$AV = (U\Sigma V^T)V = U\Sigma(V^TV) = U\Sigma$$

since V is an orthogonal matrix. Likewise

$$A^TU = (U\Sigma V^T)^TU = V\Sigma^TU^TU = V\Sigma^T$$

We return to the picture used before, taking multiplication by A as a map from $\mathbb{R}^n$ to $\mathbb{R}^m$, involving the four fundamental subspaces:

For picture, see lectures

Let $\underline{\mathbf{v}}_1, \underline{\mathbf{v}}_2, \underline{\mathbf{v}}_3, \ldots \underline{\mathbf{v}}_n \in \mathbb{R}^n$ be the columns of V, an orthonomal set of vectors. Similarly, let $\underline{\mathbf{u}}_1, \underline{\mathbf{u}}_2, \underline{\mathbf{u}}_3, \ldots \underline{\mathbf{u}}_m \in \mathbb{R}^m$ be the columns of U, another orthonomal set of vectors. We multiply

$$AV = U\Sigma \implies A\begin{pmatrix} \underline{\mathbf{v}}_1 \ \underline{\mathbf{v}}_2 \ldots \underline{\mathbf{v}}_r \ \underline{\mathbf{v}}_{r+1} \ldots \underline{\mathbf{v}}_n \end{pmatrix} = \begin{pmatrix} A\underline{\mathbf{v}}_1 \ A\underline{\mathbf{v}}_2 \ldots A\underline{\mathbf{v}}_r \ A\underline{\mathbf{v}}_{r+1} \ldots A\underline{\mathbf{v}}_n \end{pmatrix} = \begin{pmatrix} \sigma_1\underline{\mathbf{u}}_1 \ \sigma_2\underline{\mathbf{u}}_2 \ldots \sigma_r\underline{\mathbf{u}}_r \quad \underbrace{\underline{\mathbf{0}} \ldots \underline{\mathbf{0}}}_{n-r \text{ zero vectors}} \end{pmatrix}$$

as derived above.

This can be broken up by columns:

$$\begin{array}{rcl} A\underline{\mathbf{v}}_1 &=& \sigma_1\underline{\mathbf{u}}_1 \\ A\underline{\mathbf{v}}_2 &=& \sigma_2\underline{\mathbf{u}}_2 \\ \vdots & \vdots & \vdots \\ A\underline{\mathbf{v}}_r &=& \sigma_r\underline{\mathbf{u}}_r \end{array} \quad (1) \quad \text{and} \quad \begin{array}{rcl} A\underline{\mathbf{v}}_{r+1} &=& \underline{\mathbf{0}} \\ A\underline{\mathbf{v}}_{r+2} &=& \underline{\mathbf{0}} \\ \vdots & \vdots & \vdots \\ A\underline{\mathbf{v}}_n &=& \underline{\mathbf{0}} \end{array} \quad (2)$$

Similarly,

$$A^TU = V\Sigma^T \implies A^T\begin{pmatrix} \underline{\mathbf{u}}_1 \ \underline{\mathbf{u}}_2 \ldots \underline{\mathbf{u}}_r \ \underline{\mathbf{u}}_{r+1} \ldots \underline{\mathbf{u}}_m \end{pmatrix} = \begin{pmatrix} \underline{\mathbf{v}}_1 \ \underline{\mathbf{v}}_2 \ldots \underline{\mathbf{v}}_r \ \underline{\mathbf{v}}_{r+1} \ldots \underline{\mathbf{v}}_n \end{pmatrix} \begin{pmatrix} \sigma_1 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 0 & \sigma_2 & 0 & \ldots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \ldots & \sigma_r & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 & 0 \\ 0 & 0 & 0 & \ldots & 0 & 0 & 0 \end{pmatrix}$$

As with $U\Sigma$ before, the r non-zero entries in Σ^T on the right simplify this to

$$\begin{pmatrix} A^T\underline{\mathbf{u}}_1 \ A^T\underline{\mathbf{u}}_2 \ldots A^T\underline{\mathbf{u}}_r \ A^T\underline{\mathbf{u}}_{r+1} \ldots A^T\underline{\mathbf{u}}_m \end{pmatrix} = \begin{pmatrix} \sigma_1\underline{\mathbf{v}}_1 \ \sigma_2\underline{\mathbf{v}}_2 \ldots \sigma_r\underline{\mathbf{v}}_r \quad \underbrace{\underline{\mathbf{0}} \ldots \underline{\mathbf{0}}}_{m-r \text{ zero vectors}} \end{pmatrix}$$

and by columns we have

$$\begin{array}{rcl} A^T\underline{\mathbf{u}}_1 &=& \sigma_1\underline{\mathbf{v}}_1 \\ A^T\underline{\mathbf{u}}_2 &=& \sigma_2\underline{\mathbf{v}}_2 \\ \vdots & \vdots & \vdots \\ A^T\underline{\mathbf{u}}_r &=& \sigma_r\underline{\mathbf{v}}_r \end{array} \quad (3) \quad \text{and} \quad \begin{array}{rcl} A^T\underline{\mathbf{u}}_{r+1} &=& \underline{\mathbf{0}} \\ A^T\underline{\mathbf{u}}_{r+2} &=& \underline{\mathbf{0}} \\ \vdots & \vdots & \vdots \\ A^T\underline{\mathbf{u}}_m &=& \underline{\mathbf{0}} \end{array} \quad (4)$$

Recall first $N(A)$, the nullspace of A, with dimension $n-r$. Given that in (2) we have $n-r$ independent vectors satisfying $A\underline{\mathbf{v}}_i = \underline{\mathbf{0}}$, we see that $\underline{\mathbf{v}}_{r+1} \ldots \underline{\mathbf{v}}_n$ are a basis for the nullspace of A.

In (3), each expression on the left is a linear combination of the columns of A^T, so that the vectors on the right are in $C(A^T)$, the row space of A, with dimension r. We have r independent vectors $\underline{\mathbf{v}}_1 \ldots \underline{\mathbf{v}}_r$ in the row space, so they form a basis of the row space! Both of these are subspaces of $\mathbb{R}^n$, recall that they are orthogonal complements, reflected in the fact that their bases taken together, the vectors $\underline{\mathbf{v}}_1 \ldots \underline{\mathbf{v}}_n$ are an orthonormal basis of $\mathbb{R}^n$.

Similarly, in $\mathbb{R}^m$ we have $N(A^T)$ the left nullspace of A, with dimension $m-r$. In (4) we have $m-r$ independent vectors satisfying $A^T\underline{\mathbf{u}}_i = \underline{\mathbf{0}}$, so $\underline{\mathbf{u}}_{r+1} \ldots \underline{\mathbf{u}}_m$ form a basis of the left nullspace.

And finally, in (1), each expression on the left is a linear combination of the columns of A, so the vectors on the right are in $C(A)$, the column space of A, the fourth fundamental subspace, with dimension r. We have r independent vectors $\underline{\mathbf{u}}_1 \ldots \underline{\mathbf{u}}_r$ in the column space, so they form a basis. Both of these are subspaces of $\mathbb{R}^m$, recall that they are orthogonal complements, reflected in the fact that their bases taken together, the vectors $\underline{\mathbf{u}}_1 \ldots \underline{\mathbf{u}}_m$ are an orthonormal basis of $\mathbb{R}^m$.

This completes the **Fundamental Theorem of Linear Algebra**. First we had the dimensions of the four fundamental subspaces, then the fundamental subspaces as two pairs of orthogonal complements in $\mathbb{R}^n$ and $\mathbb{R}^m$. Now we complete it with bases of the four subspaces giving orthogonal matrices U and V to diagonalize A.

Only one question remains now. We wrote down a diagonal matrix Σ with the singular values σ_i, but where do these come from? It turns out that this is the easy part! Remember how useful the matrix A^T was? Consider the following

$$A^TA = (U\Sigma V^T)^T(U\Sigma V^T) = V\Sigma^TU^TU\Sigma V^T = V(\Sigma^T\Sigma)V^T$$

as U is orthogonal. A^TA and $\Sigma^T\Sigma$ are both $n \times n$, as are V and V^T. It should not be hard to see that we have

$$A^TA = V(\Sigma^T\Sigma)V^T = V \begin{pmatrix} \sigma_1^2 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \sigma_2^2 & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sigma_r^2 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} V^T$$

This is the orthogonal diagonalization of the positive semi-definite matrix A^TA and the eigenvalues are σ_i^2 and often zero. This gives us the algorithm to find V:

- Find A^TA
- Find the eigenvalues and orthonormal eigenvectors of A^TA
- Form orthonormal eigenvectors into V
- The roots of non-zero eigenvalues give the singular values.

Similarly

$$AA^T = A = (U\Sigma V^T)(U\Sigma V^T)^T = U\Sigma V^TV\Sigma^TU^T = U(\Sigma\Sigma^T)U^T$$

where all matrices this time are $m \times m$ and $\Sigma\Sigma^T$ has the same eigenvalues σ_i^2 on the diagonal. So this is the orthogonal diagonalization of AA^T with the same non-negative eigenvalues and its eigenvectors form U. Note that the r non-zero eigenvalues are the same but one version has more zero eigenvalues than the other, depending on which is larger: m or n. It makes sense to calculate the smaller of the two matrices A^TA or AA^T and obtain one set of eigenvectors using the eigenvalues, while the other set can be done with either (1) or (3), above and complete the larger set with the nullspace of the larger matrix. In practice we may not calculate all the eigenvalues anyway, looking only for the largest, dominant ones. More on this later!

Example 4.2. *Find the SVD for* $A = \begin{pmatrix} 2 & 2 & 0 \\ -1 & 1 & 0 \end{pmatrix}$.

We note that the rank is obviously 2, so expect two singular values. This is a 2×3 matrix, so we need 2×2 matrix U, 2×3 matrix Σ and 3×3 matrix V. As A^TA is 3×3 and AA^T is 2×2 we calculate that one first:

$$AA^T = \begin{pmatrix} 8 & 0 \\ 0 & 2 \end{pmatrix}$$

with eigenvalues 8 and 2, no need for calculation. The corresponding eigenvectors are $\underline{\mathbf{u}}_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}$ and $\underline{\mathbf{u}}_2 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$ forming a basis of the column space, $C(A)$, U is the 2×2 identity matrix, and the singular values are $\sigma_1 = \sqrt{8}$ and $\sigma_2 = \sqrt{2}$. We can use these to obtain $\underline{\mathbf{v}}_1$ and $\underline{\mathbf{v}}_2$:

$$\underline{\mathbf{v}}_1 = \frac{1}{\sigma_1}A^T\underline{\mathbf{u}}_1 = \frac{1}{\sqrt{8}}\begin{pmatrix} 2 & -1 \\ 2 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \quad \text{and} \quad \underline{\mathbf{v}}_2 = \frac{1}{\sigma_2}A^T\underline{\mathbf{u}}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} 2 & -1 \\ 2 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix} -1 \\ 1 \\ 0 \end{pmatrix}$$

These are a basis of the row space $C(A^T)$. In applications, it will usually not be necessary to even find the remaining nullspace vectors: here they complete the picture. We need one more, $\underline{\mathbf{v}}_3$, a basis for $N(A)$ and to find it we solve

$$A\underline{\mathbf{v}}_3 = \underline{\mathbf{0}} \Rightarrow \begin{pmatrix} 2 & 2 & 0 \\ -1 & 1 & 0 \end{pmatrix}\begin{pmatrix} x \\ y \\ z \end{pmatrix} = \underline{\mathbf{0}}$$

The first row gives $x = -y$ and the second row gives $x = y$. Hence $x = y = 0$ and we choose the free variable $z = 1$ to obtain a normalized, unit vector:

$$\underline{\mathbf{v}}_3 = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \quad \Longrightarrow \quad V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix}$$

Finally, we have the SVD of A:

$$A = \begin{pmatrix} 2 & 2 & 0 \\ -1 & 1 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} \sqrt{8} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 & 0 \\ -1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \; = \; U\Sigma V^T$$

An alternative, equivalent approach would be to begin with

$$A^T A = A = \begin{pmatrix} 5 & 3 & 0 \\ 3 & 5 & 0 \\ 0 & 0 & 0 \end{pmatrix},$$

as expected, a symmetric matrix. Solve the eigenvalue equation and find eigenvalues $8, 2, 0$, confirming that the matrix is positive semi-definite. Note the same two eigenvalues as for AA^T. So the singular values are $\sigma_1 = \sqrt{8}$ and $\sigma_2 = \sqrt{2}$. Similarly, the three eigenvectors for $A^T A$ are the three vectors $\underline{\mathbf{v}}_i$ calculated in the first instance, and then follow with $A\underline{\mathbf{v}}_{1,2} = \sigma_{1,2}\underline{\mathbf{u}}_{1,2}$ to find the two columns of U. Left as exercise!

4.5 Pseudoinverses

Recall that if we have "good" bases $\underline{\mathbf{u}}_i$ for the column space and $\underline{\mathbf{v}}_i$ for the row space of a matrix A, then multiplying by A is a map from one to the other and

$$A\underline{\mathbf{v}}_i = \sigma_i \underline{\mathbf{u}}_i$$

as we have seen. So A^{-1} must act in the opposite direction

$$A^{-1}\underline{\mathbf{u}}_i = \frac{1}{\sigma_i}\underline{\mathbf{v}}_i$$

so for A^{-1}, the $\underline{\mathbf{u}}_i$ are a basis for the row space, and the $\underline{\mathbf{v}}_i$ a basis for its column space, and the singular values here are the reciprocals of the singular values of A!

Well, all of that makes sense **if** A is invertible and A^{-1} actually exists. But if A isn't invertible, or not even square, we can use the SVD to find a workaround: the **Moore-Penrose inverse**, or just plain **pseudoinverse** of A, denoted by A^+ where

$$\underbrace{A^+}_{n\times m} = \underbrace{V}_{n\times n}\;\underbrace{\Sigma^+}_{n\times m}\;\underbrace{U^T}_{m\times m} = \begin{pmatrix} \underline{\mathbf{v}}_1 & \underline{\mathbf{v}}_2 \cdots \underline{\mathbf{v}}_r & \underline{\mathbf{v}}_{r+1} \cdots \underline{\mathbf{v}}_n \end{pmatrix} \begin{pmatrix} \frac{1}{\sigma_1} & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & \frac{1}{\sigma_2} & 0 & \dots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \frac{1}{\sigma_r} & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \\ 0 & 0 & 0 & \dots & 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} \underline{\mathbf{u}}_1 & \underline{\mathbf{u}}_2 \cdots \underline{\mathbf{u}}_r & \underline{\mathbf{u}}_{r+1} \cdots \underline{\mathbf{u}}_m \end{pmatrix}^T$$

When A is invertible, then A^+ is the same as the inverse, but when not, we can still multiply

$$AA^+ = (U\Sigma V^T)(V\Sigma^+ U^T) = U(\Sigma\Sigma^+)U^T$$

where $\Sigma\Sigma^+$ is an $m \times m$ diagonal matrix with r ones on the diagonal and $m - r$ zeroes. If A has full row rank, i.e $m = r$, we have $\Sigma\Sigma^+ = I_r = I_m$ and thus

$$AA^+ \; = \; U(\Sigma\Sigma^+)U^T = UI_mU^T = I_m$$

and A^+ is called a **right inverse** of A.

Likewise,

$$A^+A = (V\Sigma^+U^T)(U\Sigma V^T) = V\Sigma^+\Sigma V^T \, .$$

where $\Sigma^+\Sigma$ is an $n \times n$ matrix. If A has full column rank, i.e $n = r$, then $\Sigma^+\Sigma = I_r = I_n$ and

$$A^+A = V\Sigma^+\Sigma V^T = VI_nV^T = I_n$$

and A^+ is called a **left inverse** of A.

If $r < m$ and $r < n$, neither of the above holds true, but applications exist regardless of the rank. See, for example, Strang, *Introduction to Linear Algebra*.

Example 4.3. *Find the pseudoinverse of* $A = \begin{pmatrix} 2 & 2 & 0 \\ -1 & 1 & 0 \end{pmatrix}$.

We have

$$A^+ = V\Sigma^+U^T = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & -1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & \sqrt{2} \end{pmatrix} \begin{pmatrix} \frac{1}{\sqrt{8}} & 0 \\ 0 & \frac{1}{\sqrt{2}} \\ 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} \frac{1}{4} & -\frac{1}{2} \\ \frac{1}{4} & \frac{1}{2} \\ 0 & 0 \end{pmatrix}$$

and multiplying

$$AA^+ = \begin{pmatrix} 2 & 2 & 0 \\ -1 & 1 & 0 \end{pmatrix} \begin{pmatrix} \frac{1}{4} & -\frac{1}{2} \\ \frac{1}{4} & \frac{1}{2} \\ 0 & 0 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$$

because $r = m = 2$: we see that A has full row rank, and A^+ is a right inverse.

4.6 Principal Component Analysis

This is possibly the best application of the SVD and we will look at two possible uses. First, returning to the notion of SVD as giving a matrix as a sum of rank-one matrices:

$$A = \sigma_1 \underline{\mathbf{u}}_1 \underline{\mathbf{v}}_1^T + \sigma_2 \underline{\mathbf{u}}_2 \underline{\mathbf{v}}_2^T + \ldots + \sigma_r \underline{\mathbf{u}}_r \underline{\mathbf{v}}_r^T \, .$$

We can decide on an optimal value $0 < R < r$ at which to truncate the sum above and still get a good approximation of A. Extracting essential information from the SVD is called **Principal Component Analysis** or PCA.

4.6.1 PCA in Statistics

The first application is in Statistical analysis of data. Let the $m \times n$ matrix be a collection of data: n samples with m data points in each sample, for example, the exam marks of 6 students on 2 exams, Mathematics and Physics, would give a 2×6 matrix, so each column represents the marks of one students and each row the marks in one exam. We begin by subtracting from each row the mean of the marks in that row, giving marks for each exam in a normla distribution, centred at zero. This is the matrix A, e.g.

$$A = \begin{pmatrix} 3 & -4 & 7 & 1 & -4 & -3 \\ 7 & -6 & 8 & -1 & -1 & -7 \end{pmatrix}$$

We can plot these results and if students generally score similarly well or otherwise in both exams, then the data points will be clustered around a line in $\mathbb{R}^2$:

For Figure, see lectures

In Statistics, given an $m \times n$ matrix A with rows centred on zero, we form the **Sample Covariance Matrix**

$$S = \frac{1}{n-1} AA^T \, .$$

In A, each entry shows the distance to the mean. In S diagonal entries show the sum of the squared disctances of the data to the mean, so

$$S_{11} = s_1^2 = \sum_{i=1}^{n} (a_{1i} - \mu_1)^2 \, ,$$

is the sum of the squares of the distances to the mean μ_1 in the first row of A. These values s_i^2 are the **sample variances**. Variance is crucial in statistics, as seen in your parallel module. To continue with the above example, a small variance suggests most students scoring close to the mean, while a large variance means a wider spread. In a normal distribution, 68% of the data are in the interval $[\mu_i - s_i, \mu_i + s_i]$. Entries off the diagonal are the **sample covariance**, giving a measure of how correlated the marks are. If, say S_{12} is large and positive, this is strong positive correlation between the first two rows of A; if A has the marks, as above, that would show students scoring equally well in both exams. If, on the other hand, S_{12} is large and negative, this is strong negative correlation and shows students scoring well in one exam and badly in the other. If it's close to zero, then the data are uncorrelated. For the example of the marks, we have

$$S = \frac{1}{5}AA^T = \begin{pmatrix} 20 & 25 \\ 25 & 40 \end{pmatrix}$$

We see that $S_{12} = 25$, so the marks show a strong positive correlation. On the diagonal, s_1 is smaller than s_2, so there is a larger spread of marks in the second exam. Finally we come to the SVD. The eigenvalues of S are $\approx 57, 3$, so we can write

$$A \approx \sqrt{57}\underline{\mathbf{u}}_1\underline{\mathbf{v}}_1^T + \sqrt{3}\underline{\mathbf{u}}_2\underline{\mathbf{v}}_2^T$$

The eigenvector $\underline{\mathbf{u}}_1$ shows the direction of the line around which the data is clustered. The eigenvector $\underline{\mathbf{u}}_2$ is orthogonal to the line and $\sigma_2 = \sqrt{3}$ measures the spread of the marks across the line. The closer the points to the line, overall, the smaller σ_2 and the more correlated the points. The line has positive gradient, indicating postive correlation.

For a larger dimensional set of data, we will need more components than merely the first one, as in the example above, so in $\mathbb{R}^3$, the data may be not clustered near a line, but near a plane, so there would be two principal components, with their directions $\underline{\mathbf{u}}_{1,2}$ giving the plane, and the spread around the plane measured by σ_3.

4.6.2 PCA in Data Compression

Take a digital image consisting of 1400×2000 pixels, say. For transmission, this would be 3 million values for greyscale, 9 million for a colour image: a bit much, and not necessary. We take the image as a rectangular 1400×2000 matrix and compute the SVD:

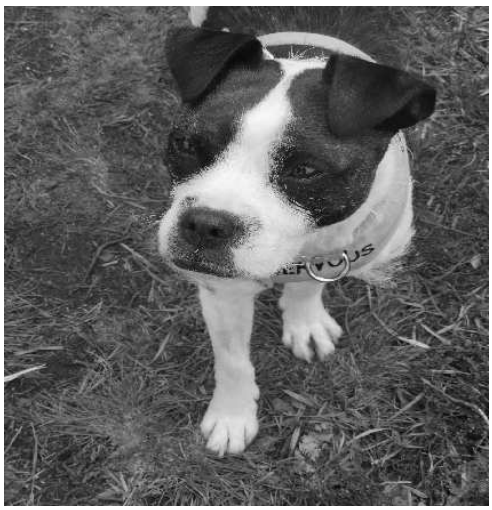
$$\underbrace{A}_{1400\times2000} = \underbrace{U}_{1400\times1400} \quad \underbrace{\Sigma}_{1400\times2000} \quad \underbrace{V^T}_{2000\times2000}$$

Using Matlab code (adapted from Brunton):

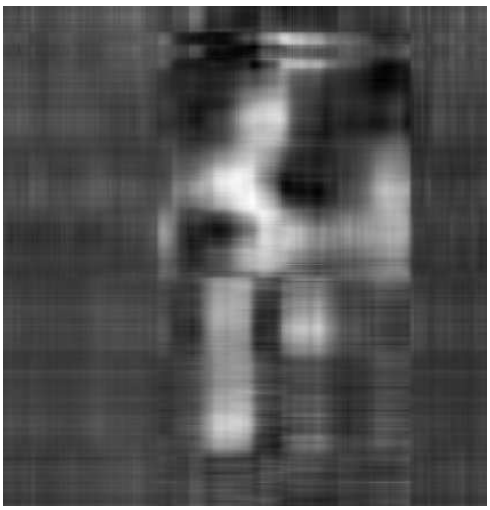
```
A=imread('ollie2.jpg');
X=double(rgb2gray(A)); % convert RBG to gray, 256 bit to double.
nx = size(X,1); ny = size(X,2);
[U,S,V] = svd(X);
figure
subplot(2,2,1)
imagesc(X), axis off,
colormap gray,
title('Original')
plotind=2;

   for r=[5 20 100] % truncation value
Xapprox = U(:,1:r)*S(1:r,1:r)*V(:,1:r)'; % approximate image
subplot(2,2,plotind), plotind = plotind + 1;
imagesc(Xapprox), axis off
title(['R=',num2str(r,'%d'), ', ', num2str(100*r*(nx+ny)/(nx*ny),'%2.2f'), '% storage']);
end
set(gcf,'Position',[100 100 550 400])
```

Original

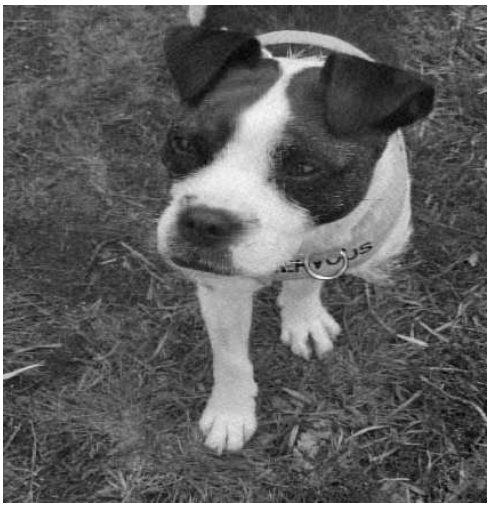


R=5, 0.32% storage



R=20, 1.28% storage

R=100, 6.40% storage



To reconstruct the matrix, it's sufficient to transmit the largest singular values and their respective singular vectors. An excellent level of reproduction is achieved with truncation at $R = 100$, where the data required to transmit is 6.4% of the original total.

THE END