Trace

This document is a more in-depth discussion of trace, which I hinted at in class. Some of it requires material from later in the course, so you can refer back to this when they are introduced. The second example computes the matrix of a reflection in 3D, which I did not have time to do in lecture.

Definition. Let $A = [a_{ij}]_{i,j}$ be an $n \times n$ matrix, then the *trace* of A is the sum of its diagonal elements $a_{11} + a_{22} + \cdots + a_{n,n}$. It is denoted by $\mathrm{Tr}(A)$.

Example.

1. The trace of the identity matrix I_n is n.
2. In $\mathbb{R}^2$, the projection onto the line parallel to $\left[\begin{smallmatrix} w_1 \\ w_2 \end{smallmatrix}\right]$ has matrix

$$\frac{1}{w_1^2 + w_2^2} \begin{pmatrix} w_1^2 & w_1 w_2 \\ w_1 w_2 & w_2^2 \end{pmatrix}$$

   Its trace is $\frac{1}{w_1^2+w_2^2}(w_1^2 + w_2^2) = 1$.

I have said that matrices are avatars of linear transformations used for computation. The matrix of a linear transformation depends on the coordinate system chosen: a good choice sometimes drastically simplifies the problem. However, there are some "geometric properties" of a linear transformation which should not depend on the coordinate. One such example is the determinant, which measures how much a linear transformation scales the volume. There is a purely algebraic definition of the determinant of a matrix, and the statement that it is a geometric property is that

$$\det(A) = \det(PAP^{-1}) \qquad \text{for all invertible matrices } P$$

The trace is also one such geometric property, or equivalently,

$$\mathrm{Tr}(A) = \mathrm{Tr}(PAP^{-1}) \qquad \text{for all invertible matrices } P$$

In fact, more is true: for all $n \times n$ matrices A and B.

$$\boxed{\mathrm{Tr}(AB) = \mathrm{Tr}(BA)}$$

The geometric interpretation is a lot more subtle, and not really clear. One explanation I like is

Theorem. Trace is the derivative of the determinant: if ϵ is small, and A is an $n \times n$ matrix, then

$$\det(I_n + \epsilon A) = 1 + \epsilon\,\mathrm{Tr}(A) + (\text{small error term})$$

Now let's consider orthogonal projection and reflection. Given a line L in $\mathbb{R}^n$, we can choose coordinates so that L is the x_1-axis, then $L^\perp$ is the (hyper)plane containing the other coordinates (this is a change of basis). In these coordinates, the matrices are easy to write down:

$$[\mathrm{proj}_L] = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}, \quad [\mathrm{proj}_{L^\perp}] = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}, \quad [\mathrm{ref}_{L^\perp}] = \begin{pmatrix} -1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix}$$

Essentially, proj_L only keeps the first coordinate, $\mathrm{proj}_{L^\perp}$ keeps everything except for the first coordinate, and $\mathrm{ref}_{L^\perp}$ changes the sign of the first coordinate. We can compute that

$$\mathrm{Tr}(\mathrm{proj}_L) = 1, \quad \mathrm{Tr}(\mathrm{proj}_{L^\perp}) = n - 1, \quad \mathrm{Tr}(\mathrm{ref}_{L^\perp}) = n - 2$$

This must hold for the matrices of the operators in *every* coordinate system. More generally, the trace of an orthogonal projection operator is equal to the dimension of its image.

Example. We will compute the reflection across the plane $P : 2x - y + z = 0$ in $\mathbb{R}^3$.

The first step is to find a vector $\vec{w}$ perpendicular to P. We can take $\vec{w} = \left[\begin{smallmatrix} 2 \\ -1 \\ 1 \end{smallmatrix}\right]$ (recall that $\vec{v}_1 \cdot \vec{v}_2 = 0$ is equivalent to $\vec{v}_1$ and $\vec{v}_2$ are perpendicular). Let L be the line parallel to $\vec{w}$, then $P = L^{\perp}$.

Now, we can use the reflection formula

$$\mathrm{ref}_P(\vec{v}) = \vec{v} - 2\mathrm{proj}_L(\vec{v})$$

In particular,

$$\mathrm{ref}_P(\vec{e}_1) = \mathrm{ref}_P\left(\left[\begin{smallmatrix} 1 \\ 0 \\ 0 \end{smallmatrix}\right]\right) = \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} - 2\left(\frac{\left[\begin{smallmatrix} 2 \\ -1 \\ 1 \end{smallmatrix}\right] \cdot \left[\begin{smallmatrix} 1 \\ 0 \\ 0 \end{smallmatrix}\right]}{\left\|\left[\begin{smallmatrix} 2 \\ -1 \\ 1 \end{smallmatrix}\right]\right\|^2}\right) \begin{bmatrix} 2 \\ -1 \\ 1 \end{bmatrix} = \frac{1}{3}\begin{bmatrix} -1 \\ 2 \\ -2 \end{bmatrix}$$

Similarly, we can compute

$$\mathrm{ref}_P(\vec{e}_2) = \frac{1}{3}\begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix}, \quad \mathrm{ref}_P(\vec{e}_3) = \frac{1}{3}\begin{bmatrix} -2 \\ 1 \\ 2 \end{bmatrix}$$

So finally,

$$[\mathrm{ref}_P] = \frac{1}{3}\begin{bmatrix} -1 & 2 & -2 \\ 2 & 2 & 1 \\ -2 & 1 & 2 \end{bmatrix}$$

Its trace is $\frac{1}{3}(-1 + 2 + 2) = 1$, which is equal to $n - 2$. Moreover, you can check that $[\mathrm{ref}_P]\vec{w} = -\vec{w}$, so the answer passes a few checks.

We end with a connection with quantum mechanics.

Theorem. There does not exist $n \times n$ matrices A and B and non-zero scalar λ such that

$$AB - BA = \lambda I_n$$

Proof. The traces of the two sides are not equal.

$$\mathrm{Tr}(AB - BA) = \mathrm{Tr}(AB) - \mathrm{Tr}(BA) = 0, \quad \mathrm{Tr}(\lambda I_n) = n\lambda \neq 0$$ □

In classical quantum mechanics, a particle is described by a state vector, which is just a function on $\mathbb{R}$ (satisfying certain decay conditions at infinity). Its position $\hat{x}$ and momentum $\hat{p}$ are operators (linear transformation from a space to itself) on functions: if $\psi(x)$ is the state of a particle, then

$$(\hat{x}(\psi))(x) = x\psi(x), \quad (\hat{p}(\psi))(x) = -i\hbar\psi'(x)$$

The more usual notation in physics is $\hat{x}|\psi\rangle$ and $\hat{p}|\psi\rangle$. It is linear in the sense of the second definition of a linear transformation:

$$\hat{x}(\psi + \varphi) = \hat{x}(\psi) + \hat{x}(\varphi), \text{ etc.}$$

Observe that

$$((\hat{x}\hat{p} - \hat{p}\hat{x})\psi)(x) = x(-i\hbar\psi'(x)) + i\hbar(x\psi(x))' = i\hbar\psi(x)$$

This is the relation underlying the Heisenberg uncertainty principle. This contradicts the theorem, so the trace cannot be well-defined for the two operators. On general infinite dimensional spaces, the operators for which trace can be defined are very important. Fredholm theory features prominently in their study.

The above definitions of $\hat{x}$ and $\hat{p}$ are essentially due to Schrödinger. Heisenberg formulated quantum mechanics in terms of infinite matrices A and B such that $AB - BA = i\hbar$. It is a theorem in functional analysis that any space carrying two operators satisfying this relation must be the same as Schrödinger's space, "up to relabelling the coordinates", so both points of view are equivalent.