Physics 505
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# 1 Functions of matrices

Given an $n \times n$ matrix, $A$, we often need to calculate a function of it, such as $A^k$, $e^A$, etc. One way to do it is to "diagonalize" the matrix. This means, to find an invertible $n \times n$ matrix $P$ such that $A = P\Lambda P^{-1}$ and $\Lambda$ is a diagonal matrix. Now we can calculate:

$$A^2 = P\Lambda P^{-1}P\Lambda P^{-1} = P\Lambda^2 P^{-1}, \qquad A^3 = P\Lambda^3 P^{-1}, \cdots, A^k = P\Lambda^k P^{-1},$$

and in general, $f(A) = Pf(\Lambda)P^{-1}$. The point is that since $\Lambda$ is diagonal, $f(\Lambda)$ is easy to calculate:

$$\Lambda = \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}, \qquad f(\Lambda) = \begin{pmatrix} f(\lambda_1) & 0 & \dots & 0 \\ 0 & f(\lambda_2) & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & f(\lambda_n) \end{pmatrix}.$$

(check for $f(x) = x^k$.)

The remaining question is how to find $P$ and $\Lambda$. We can write the equation $A = P\Lambda P^{-1}$ and $AP = P\Lambda$:

$$\begin{pmatrix} A_{11} & A_{12} & \dots & A_{2n} \\ A_{21} & A_{22} & \dots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \dots & A_{nn} \end{pmatrix} \begin{pmatrix} P_{11} & P_{12} & \dots & P_{2n} \\ P_{21} & P_{22} & \dots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & \dots & P_{nn} \end{pmatrix} = \begin{pmatrix} P_{11} & P_{12} & \dots & P_{2n} \\ P_{21} & P_{22} & \dots & P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1} & P_{n2} & \dots & P_{nn} \end{pmatrix} \begin{pmatrix} \lambda_1 & 0 & \dots & 0 \\ 0 & \lambda_2 & & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \lambda_n \end{pmatrix}$$

$$= \begin{pmatrix} \lambda_1 P_{11} & \lambda_2 P_{12} & \dots & \lambda_n P_{2n} \\ \lambda_1 P_{21} & \lambda_2 P_{22} & \dots & \lambda_n P_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ \lambda_1 P_{n1} & \lambda_2 P_{n2} & \dots & \lambda_n P_{nn} \end{pmatrix}.$$

Let us take only the $r^{th}$ column of this equation $(r = 1, 2, \ldots, n)$ We see that:

$$\begin{pmatrix} A_{11} & A_{12} & \ldots & A_{2n} \\ A_{21} & A_{22} & \ldots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \ldots & A_{nn} \end{pmatrix} \begin{pmatrix} P_{1r} \\ P_{2r} \\ \vdots \\ P_{nr} \end{pmatrix} = \begin{pmatrix} \lambda_r P_{1r} \\ \lambda_r P_{2r} \\ \vdots \\ \lambda_r P_{nr} \end{pmatrix}.$$

This means that the vector

$$= \begin{pmatrix} P_{1r} \\ P_{2r} \\ \vdots \\ P_{nr} \end{pmatrix}$$

is an eigenvector of $A$ with eigenvalue $\lambda_r$. We can also write this equation as:

$$\begin{pmatrix} A_{11} - \lambda_r & A_{12} & \ldots & A_{2n} \\ A_{21} & A_{22} - \lambda_r & \ldots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \ldots & A_{nn} - \lambda_r \end{pmatrix} \begin{pmatrix} P_{1r} \\ P_{2r} \\ \vdots \\ P_{nr} \end{pmatrix} = 0.$$

This means that:

$$\det(A - \lambda_r I) = \det \begin{pmatrix} A_{11} - \lambda_r & A_{12} & \ldots & A_{2n} \\ A_{21} & A_{22} - \lambda_r & \ldots & A_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ A_{n1} & A_{n2} & \ldots & A_{nn} - \lambda_r \end{pmatrix} = 0.$$

If we calculate this, we will get a polynomial equation in $\lambda_r$. (Recall that $A$ is given.) This equation will have $n$ solutions. This solutions will be $\lambda_1, \ldots, \lambda_n$.

To sum up the procedure is as follows:

1. Expand the determinant $\det(A - xI)$ as a polynomial in $x$.

2. Solve $\det(A - xI) = 0$ for $x$. Genereically, you will find $n$ solutions. (We will not discuss multiple roots here.)

3. For each solution $x = \lambda_r$ find a vector $v$ such that $(A - \lambda_r I)v = 0$. The elements of such a vector can be taken as $P_{1r}, \ldots, P_{nr}$.

4. Combine all the $n$ vectors from the previous step to form the $n \times n$ matrix $P$.

5. Calculate $f(A) = Pf(\Lambda)P^{-1}$.