Recitation 1

Adam Floyd Hannon

Office Hours: MWF 9am-10am or by e-mail appointment

Topic Outline

1. a. Fourier Transform & b. Fourier Series
2. Linear Algebra Review
3. Eigenvalue/Eigenvector Problems

1. a. Fourier Transform

The 1D Fourier transform $\hat{f}(k)$ of a function $f(x)$ is defined as follows with conjugate variable $k$:

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(x) e^{-ikx} dx$$

Similarly, the inverse 1D Fourier Transform is given as:

$$f(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{f}(k) e^{ikx} dx$$

Fourier transforms are useful for things such as solving differential equations, analyzing continuous periodic functions spectrums, and examining functions with a conjugate variable dependence as will be seen in quantum mechanics.
Experimentally, Fourier transforms are used in all sorts of signal processing, such as FTIR spectroscopy (Fourier transform infrared spectroscopy) where a material sample is emitted with a broadband spectrum of infrared radiation. The amplitude of the transmitted radiation is measured as a function of time by a computer, and the time signal is converted to a spectral signal using a numerical Fourier transform algorithm. Similar techniques are used in auto-tuning frequencies in music.
A couple of important functions that you will encounter in Fourier analysis include:

Delta Function

$$\delta(x-a) = \begin{cases} \infty, & x = a \\ 0, & x \neq a \end{cases}$$

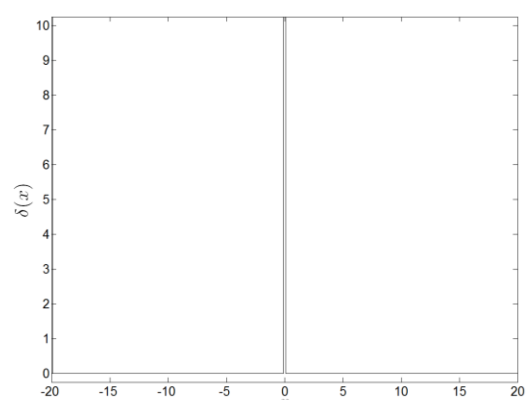


Figure 1: Plot of a delta function with $a$ = 0.

Error Function

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-u^2}\, du$$

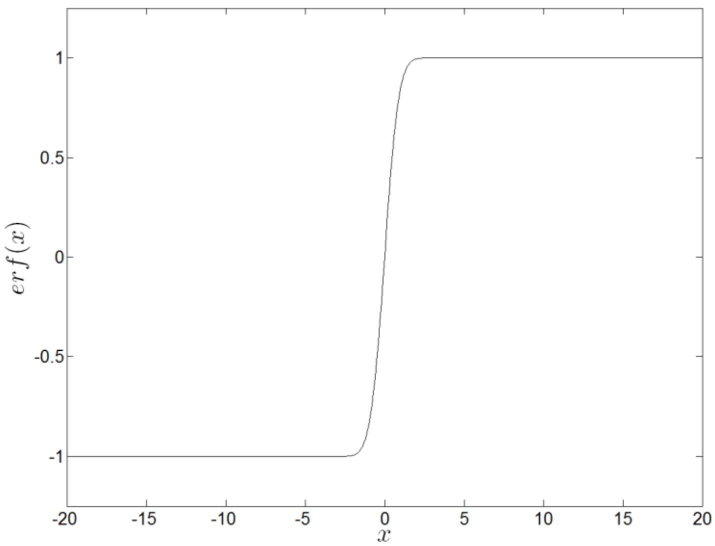


Figure 2: Plot of the error function.

e.g. 1:

What is the Fourier Transform of $f(x) = e^{-\alpha|x|}$

$$\hat{f}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\alpha|x|} e^{-ikx} dx = \frac{1}{\sqrt{2\pi}} \left( \int_{-\infty}^{0} e^{(\alpha-ik)x} dx + \int_{0}^{\infty} e^{-(\alpha+ik)x} dx \right)$$

$$= \frac{1}{(\alpha-ik)\sqrt{2\pi}} \left(e^{(\alpha-ik)x}\right)\Big|_{-\infty}^{0} - \frac{1}{(\alpha+ik)\sqrt{2\pi}} \left(e^{-(\alpha-ik)x}\right)\Big|_{0}^{\infty}$$

$$= \frac{1-0}{(\alpha-ik)\sqrt{2\pi}} - \frac{0-1}{(\alpha+ik)\sqrt{2\pi}} = \frac{(\alpha+ik)+(\alpha-ik)}{(\alpha^2+k^2)\sqrt{2\pi}} = \sqrt{\frac{2}{\pi}} \frac{a}{(\alpha^2+k^2)}$$

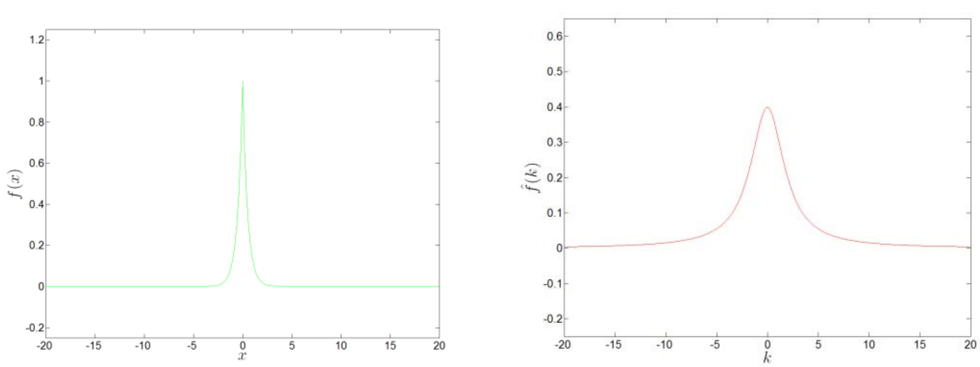


Figure 3: Left: Plot of $f(x) = e^{-\alpha|x|}$. Right: Plot of $\hat{f}(k) = \sqrt{\frac{2}{\pi}} \frac{a}{(\alpha^2+k^2)}$. $a = 2$

1. b. Fourier Series

One can show that any periodic function with period from [-$P$,$P$] or any function with a finite domain confined to an interval [-$P$,$P$] can be built up from a set of sine and cosine functions. This is known as a Fourier series where $f(x)$ is given as:

$$f(x) = a_0 + \sum_{n=1}^{\infty} \left( a_n \cos\frac{n\pi x}{P} + b_n \sin\frac{n\pi x}{P} \right)$$

The Fourier coefficients $a_0$, $a_n$, and $b_n$ are given as:

$$a_0 = \frac{1}{2P} \int_{-P}^{P} f(x) dx$$
$$a_n = \frac{1}{2P} \int_{-P}^{P} f(x) \cos\left(\frac{n\pi x}{P}\right) dx$$
$$b_n = \frac{1}{2P} \int_{-P}^{P} f(x) \sin\left(\frac{n\pi x}{P}\right) dx$$

In the context of quantum mechanics and cases we will study in the class, the Fourier series is important as it is made up of a set of orthonormal basis functions similar to the wave functions we will examine.

Sometimes the Fourier series is used in an exponential form using Euler's relationship:

$$e^{\pm i\theta} = \cos(\theta) \pm i\sin(\theta)$$

Note that the Fourier transform as discussed before is used when a function is defined by a continuous frequency domain while here for Fourier series the frequency domain is discrete in the Fourier coefficients $a_0$, $a_n$, and $b_n$.

e.g. 2.

Compare the various Fourier frequency components of

$$f(x) = 3\text{x}^2 \; \{x \in [-10{,}10]\}$$

and find the Fourier series expansion of the function.

Here $P$ = 10.

$$a_0 = \frac{1}{20} \int_{-10}^{10} 3x^2 dx = \frac{3}{20}\left(\frac{x^3}{3}\right)\Bigg|_{-10}^{10} = \frac{3}{20}\left(\frac{2000}{3}\right) = 100$$
$$a_n = \frac{1}{20} \int_{-10}^{10} 3x^2 \cos\left(\frac{n\pi x}{10}\right) dx$$
$$= \left(3x^2\left(\frac{10}{20n\pi}\right)\sin\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10} - \left(\frac{10}{20n\pi}\right)\int_{-10}^{10} 6\text{x} \sin\left(\frac{n\pi x}{10}\right) dx$$

$$= \left(3x^2\left(\frac{10}{20n\pi}\right)\sin\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10} + \left(6x\left(\frac{100}{20n^2\pi^2}\right)\cos\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10}$$

$$-\left(\frac{100}{20n^2\pi^2}\right)\int_{-10}^{10} 6\cos\left(\frac{n\pi x}{10}\right)dx$$

$$= \left(3x^2\left(\frac{10}{20n\pi}\right)\sin\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10} + \left(6x\left(\frac{100}{20n^2\pi^2}\right)\cos\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10}$$

$$-\left(\left(\frac{1000}{20n^3\pi^3}\right)6\sin\left(\frac{n\pi x}{10}\right)\right)\Bigg|_{-10}^{10}$$

$$= 0 + 120\left(\frac{5}{n^2\pi^2}\right)2\cos(n\pi) - 0 \rightarrow a_n = (-1)^n\left(\frac{1200}{n^2\pi^2}\right)$$

$$b_n = \frac{1}{10}\int_{-10}^{10} 3x^2 \sin\left(\frac{n\pi x}{10}\right)dx = 0 : \text{Odd function.}$$

$$\therefore\ f(x) = 100 + \sum_{n=1}^{\infty}(-1)^n\left(\frac{1200}{n^2\pi^2}\right)\cos\left(\frac{n\pi x}{10}\right)$$

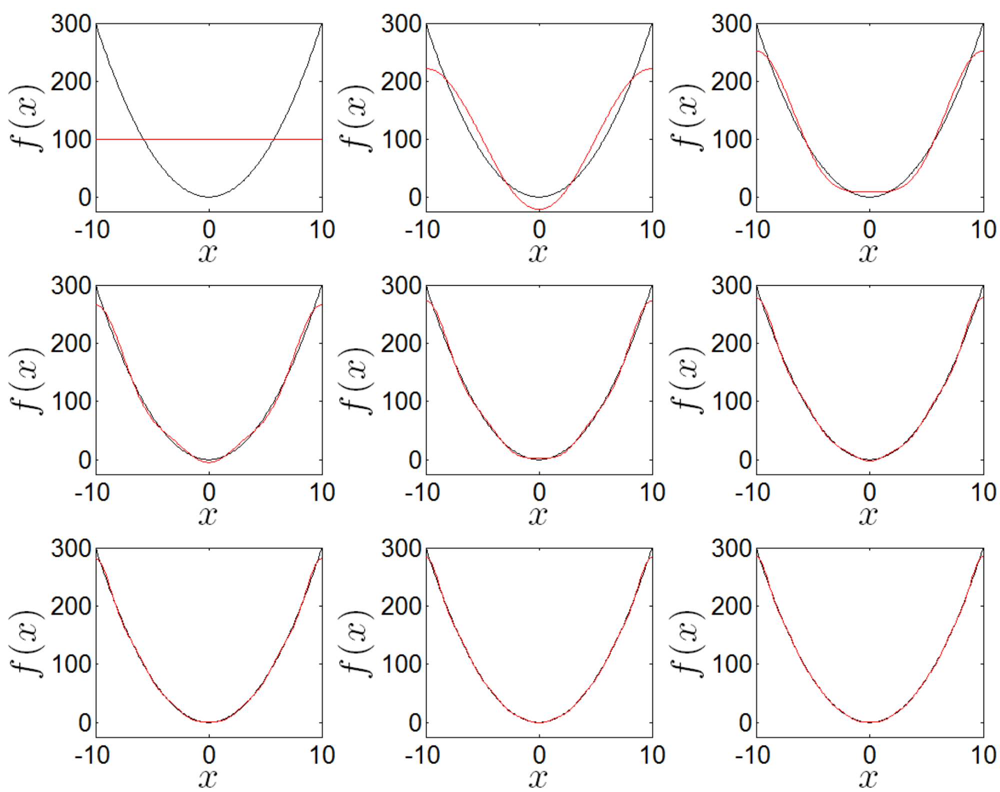

Figure 4: Comparison for the *n*th term Fourier series of $3x^2$ (red) with the function itself (black) from $n = 0$ to 8 from top left to bottom right.

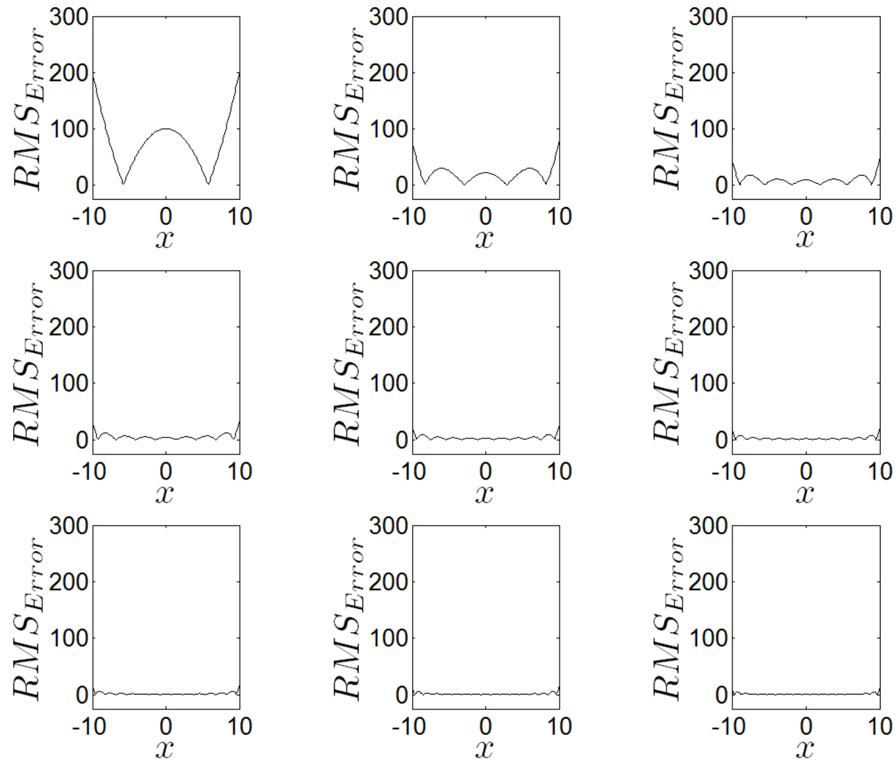


Figure 5: Root mean square difference error of $f(x) = 3x^2$ and its nth term Fourier series from $n$ = 0 to 8 from top left to bottom right.

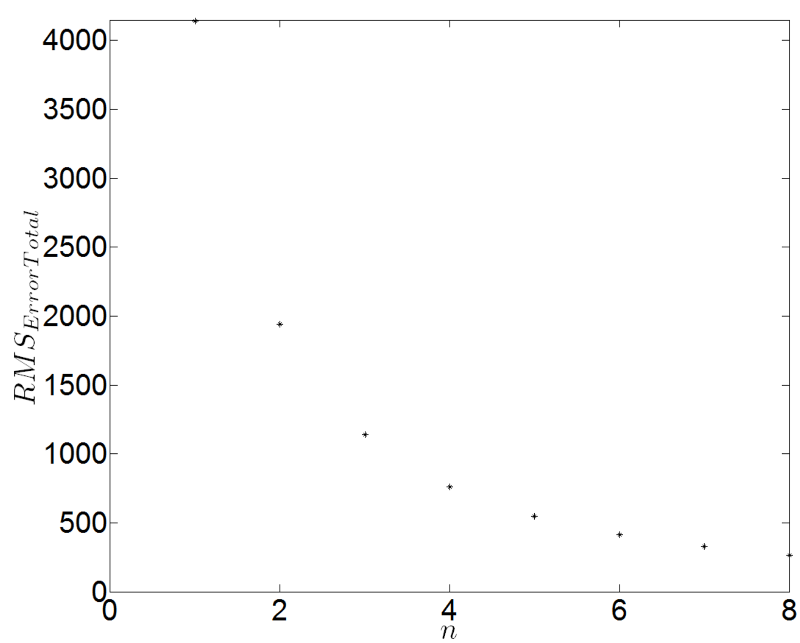


Figure 6: Total RMS difference error of $f(x) = 3x^2$ and its nth term Fourier series vs $n$.

2. Linear Algebra Review

A vector $\vec{v}$ is a set of scalar quantities with a given dimension $n$ in a space $S$.
Vectors can contain variables, functions, or numbers.
Vectors can combine in a variety of ways and have their own rules of how they combine.
Vectors can add just like scalars, adding each value in each vector location separately.
Vectors addition rules:

Commutative
$$\vec{u}+\vec{v}=\vec{v}+\vec{u}$$
Associative
$$(\vec{u}+\vec{v})+\vec{w}=\vec{v}+(\vec{u}+\vec{w})$$
Identity
$$\vec{u}+\vec{0}=\vec{u}$$

Vector scalar multiplication:
$$\alpha(\beta\vec{u})=(\alpha\beta\vec{u})$$
Distributive
$$(\alpha+\beta)\vec{u}=\alpha\vec{u}+\beta\vec{u}$$
$$\alpha(\vec{u}+\vec{v})=\alpha\vec{u}+\alpha\vec{v}$$
Identity
$$1\vec{u}=\vec{u}$$

The above rules are all that are necessary for vectors. However, for the systems we will consider, we will also need the vector dot product. We will consider a set notation to simplify the definition of the dot product.

Dot Product
$$\vec{u}=\{u_i\}=\{u_1,u_2,\cdots,u_n\}\ \&\ \vec{v}=\{v_i\}=\{v_1,v_2,\cdots,v_n\}$$
$$\vec{u}\cdot\vec{v}=\{u_i\cdot v_i\}=\{u_1\cdot v_1+u_2\cdot v_2+\cdots+u_n\cdot v_n\}$$

If $\vec{u}$ and $\vec{v}$ are complex, then the dot product is altered slightly such that one vector is the complex conjugate.
$$\vec{u}\cdot\vec{v}^*=\{u_i\cdot {v_i}^*\}=\{u_1\cdot {v_1}^*+u_2\cdot {v_2}^*+\cdots+u_n\cdot {v_n}^*\}$$

The dot product of a vector with itself defines the magnitude of the vector. If the magnitude is 1, the vector is a normal vector.
If the dot product of two different vectors is 0, then the vectors are orthogonal.
For an $n$ dimensional system, a set of $n$ orthonormal vectors $\vec{e}_i$ defines a complete basis for that system. It is possible to create a complete basis with vectors that are not all orthonormal, but for mathematical convenience we will focus on orthonormal bases.
This means any possible state $\vec{v}$ in that system can be constructed from a linear combination of these basis vectors.
$$\vec{v}=\sum_i^n c_i\vec{e}_i$$

Later we will look at a similar situation with continuous function spaces in quantum mechanics. This is analogous to the idea how one can represent a function in terms of the sum of Fourier series coefficients multiplied by sine and cosine functions.

In addition to vectors, one can construct matrices which are essentially vectors of vectors. For our purposes we will only examine *n*X*m* 2D matrices. Matrices have their own rules of addition and multiplication similar to vectors.
The following shows a schematic of an *n*X*m* matrix.

$$\begin{array}{cc} & m \text{ columns} \\ n \text{ rows} & \begin{bmatrix} a & \cdots & b \\ \vdots & \ddots & \vdots \\ c & \cdots & d \end{bmatrix} \end{array}$$

Matrix addition and scalar multiplication rules all follow the same rules as vectors.
For strict matrix multiplication, a matrix can only multiply another matrix or vector that shares the same number of elements on the side one is multiplying. This means for example a 3X2 matrix can multiply a 2X4 only from the left, while a 2X4 and 4X2 can multiply from either side. The resulting matrix will be *N*X*M* if the multiplying matrices from left to right are *N*X*n* times *n*X*M*. This will be illustrated in the following example.

e.g. 3
Matrix and vector multiplication

$$\hat{A} = \begin{bmatrix} 2 & 0 \\ 3 & 1 \end{bmatrix} \ \hat{B} = \begin{bmatrix} 5 & 4 \\ 3 & 2 \\ 1 & i \end{bmatrix} \ \vec{a} = \begin{bmatrix} i \\ 1 \end{bmatrix} \ \vec{b} = \begin{bmatrix} 5 & 0 & 2 \end{bmatrix}$$

You are given the above matrices and vectors. Calculate the following, or explain why you cannot.

$$\hat{A}\hat{B}, \hat{B}\hat{A}, \hat{A}\vec{a}, \hat{B}\vec{a}, \vec{b}\hat{B}, \vec{a} \cdot \vec{a}$$

$\hat{A}\hat{B}$ cannot be calculated since $\hat{A}$ is a 2X2 but $\hat{B}$is a 3X2.
$\hat{B}\hat{A}$ can be calculated since the inner dimension is now the same at 2.

$$\hat{B}\hat{A} = \begin{bmatrix} 5 & 4 \\ 3 & 2 \\ 1 & i \end{bmatrix} \begin{bmatrix} 2 & 0 \\ 3 & 1 \end{bmatrix} = \begin{bmatrix} 5 \cdot 2 + 4 \cdot 3 & 5 \cdot 0 + 4 \cdot 1 \\ 3 \cdot 2 + 2 \cdot 3 & 3 \cdot 0 + 2 \cdot 1 \\ 1 \cdot 2 + i \cdot 3 & 1 \cdot 0 + i \cdot 1 \end{bmatrix} = \begin{bmatrix} 22 & 4 \\ 6 & 2 \\ 2 + 3i & i \end{bmatrix}$$

$$\hat{A}\vec{a} = \begin{bmatrix} 2 & 0 \\ 3 & 1 \end{bmatrix} \begin{bmatrix} i \\ 1 \end{bmatrix} = \begin{bmatrix} 2 \cdot i + 0 \cdot 1 \\ 3 \cdot i + 1 \cdot 1 \end{bmatrix} = \begin{bmatrix} 2i \\ 1 + 3i \end{bmatrix}$$

$$\hat{B}\vec{a} = \begin{bmatrix} 5 & 4 \\ 3 & 2 \\ 1 & i \end{bmatrix} \begin{bmatrix} i \\ 1 \end{bmatrix} = \begin{bmatrix} 5 \cdot i + 4 \cdot 1 \\ 3 \cdot i + 2 \cdot 1 \\ 1 \cdot i + i \cdot 1 \end{bmatrix} = \begin{bmatrix} 4 + 5i \\ 2 + 3i \\ 2i \end{bmatrix}$$

$$\vec{b}\hat{B} = \begin{bmatrix} 5 & 0 & 2 \end{bmatrix} \begin{bmatrix} 5 & 4 \\ 3 & 2 \\ 1 & i \end{bmatrix} = \begin{bmatrix} 5 \cdot 5 + 0 \cdot 3 + 2 \cdot 1 & 5 \cdot 4 + 0 \cdot 2 + 2 \cdot i \end{bmatrix} = \begin{bmatrix} 27 & 20 + 2i \end{bmatrix}$$

$$\vec{a} \cdot \vec{a} = \begin{bmatrix} i \\ 1 \end{bmatrix} \begin{bmatrix} -i & 1 \end{bmatrix} = -i \cdot i + 1 \cdot 1 = - -1 + 1 = 2$$

3. Eigenvalue/Eigenvector Problems

Eigenvalue and eigenvector problems come up repeatedly in science engineering, especially in quantum mechanics where the time-independent Schrödinger equation is an eigenvalue equation.

For now, we will examine problems where the "operator", which we will define later, is a matrix and the "state" that is acted upon is a vector.

If a matrix $\hat{A}$ multiplies a vector $\vec{v}$ that is an eigenvector of $\hat{A}$, $\lambda$ is an eigenvalue of $\hat{A}$ if the following is true.

$$\hat{A}\vec{v} = \lambda\vec{v}$$

Thus, the effect of multiplying $\hat{A}$ onto one of its eigenvectors is the same as multiplying by a scalar value $\lambda$.
To solve for the eigenvalues, there are only 2 ways to satisfy the eigenvalue condition.
The trivial case is $\vec{v} = 0$, in which we are not interested.
The other case occurs if the determinant of $\hat{A} - \lambda\mathbf{I}$, where **I** is the identity matrix, is 0.

$$\det\left|\hat{A} - \lambda\mathbf{I}\right| = 0$$

This condition yields a polynomial equation in $\lambda$ with roots that are the eigenvalues of $\hat{A}$.
For matrices we will consider in class that are Hermitian, such that the transpose complex conjugate of the matrix equals itself, all eigenvalues will be real, although the eigenvectors may be complex.
To find the eigenvectors that each corresponds to the eigenvalues, it is necessary only to substitute each eigenvalue into the original eigenvalue equation and solve for each $\vec{v}$ for each $\lambda$. This results in *n* linearly dependent equations that can be solved to find a parameterized form of the eigenvector. This form can be normalized using the dot product of the eigenvector with itself.
e.g. 4
Pauli Spin Matrices and Vectors
The Pauli matrices are 3 2X2 matrices used when studying spin in quantum mechanics.

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

Find the eigenvalues and eigenvectors of each matrix, and show that the eigenvectors for each form an orthonormal basis set.
For $\sigma_x$

$$det\begin{vmatrix} -\lambda & 1 \\ 1 & -\lambda \end{vmatrix} = 0 = \lambda^2 - 1 \rightarrow \lambda = \begin{cases} -1 \\ 1 \end{cases}$$

For $\sigma_y$

$$det\begin{vmatrix} -\lambda & -i \\ i & -\lambda \end{vmatrix} = 0 = \lambda^2 - 1 \rightarrow \lambda = \begin{cases} -1 \\ 1 \end{cases}$$

For $\sigma_z$

$$det\begin{vmatrix} 1-\lambda & 0 \\ 0 & -1-\lambda \end{vmatrix} = 0 = (1-\lambda)(-1-\lambda) \rightarrow \lambda = \begin{cases} -1 \\ 1 \end{cases}$$

Therefore, all 3 Pauli matrices have the same two eigenvalues, -1 and 1.
For the eigenvectors:
For $\sigma_x$ for $\lambda = 1$

$$\begin{bmatrix} -1 & 1 \\ 1 & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$-a + b = 0 \;\&\; a - b = 0$$

These are the same equations, so a=b. So we can write the eigenvector as

$$\vec{v}_{x+} = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ 1 \end{bmatrix} \text{ Normalizing } \vec{v}_{x+} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ 1 \end{bmatrix}$$

For $\sigma_x$ for $\lambda = -1$

$$\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$a + b = 0$$

$$\vec{v}_{x-} = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ -1 \end{bmatrix} \text{ Normalizing } \vec{v}_{x-} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -1 \end{bmatrix}$$

For $\sigma_y$ for $\lambda = 1$

$$\begin{bmatrix} -1 & -i \\ i & -1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$-a - bi = 0 \;\&\; ai - b = 0$$

$$\vec{v}_{y+} = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ i \end{bmatrix} \text{ Normalizing } \vec{v}_{y+} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ i \end{bmatrix}$$

For $\sigma_y$ for $\lambda = -1$

$$\begin{bmatrix} 1 & -i \\ i & 1 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$a - bi = 0 \;\&\; ai + b = 0$$

$$\vec{v}_{y-} = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ -i \end{bmatrix} \text{ Normalizing } \vec{v}_{y-} = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 \\ -i \end{bmatrix}$$

For $\sigma_z$ for $\lambda = 1$

$$\begin{bmatrix} 0 & 0 \\ 0 & -2 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$0 = 0 \;\& -2b = 0$$

$$\vec{v}_{z+} = \begin{bmatrix} a \\ b \end{bmatrix} = a\begin{bmatrix} 1 \\ 0 \end{bmatrix} \text{ Normalizing } \vec{v}_{z+} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

For $\sigma_z$ for $\lambda = -1$

$$\begin{bmatrix} 2 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$$

$$2a = 0 \;\&\; 0 = 0$$

$$\vec{v}_{z-} = \begin{bmatrix} a \\ b \end{bmatrix} = b\begin{bmatrix} 0 \\ 1 \end{bmatrix} \text{ Normalizing } \vec{v}_{z-} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

To show these vectors form an orthonormal basis set, we just show their dot products are 0 since we already normalized them.

$$\vec{v}_{x+} \cdot \vec{v}_{x-} = \frac{1}{\sqrt{2}}^{2}\begin{bmatrix} 1 \\ 1 \end{bmatrix}\begin{bmatrix} 1 & -1 \end{bmatrix} = \frac{1}{2}(1 \cdot 1 + 1 \cdot -1) = 0$$

$$\vec{v}_{y+} \cdot \vec{v}_{y-} = \frac{1}{\sqrt{2}}^{2}\begin{bmatrix} 1 \\ i \end{bmatrix}\begin{bmatrix} 1 & i \end{bmatrix} = \frac{1}{2}(1 \cdot 1 + i \cdot i) = 0$$

$$\vec{v}_{z+} \cdot \vec{v}_{z-} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}\begin{bmatrix} 0 & 1 \end{bmatrix} = (1 \cdot 0 + 0 \cdot 1) = 0$$