PY410 / 505
Computational Physics 1

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Next up : Linear algebra

- Covered in Chapter 4 of Garcia and Chapter 2 of Numerical Recipes

- Huge number of applications!
  - Complex circuit diagrams
  - Coupled oscillators
  - General solution of fitting arbitrary curves

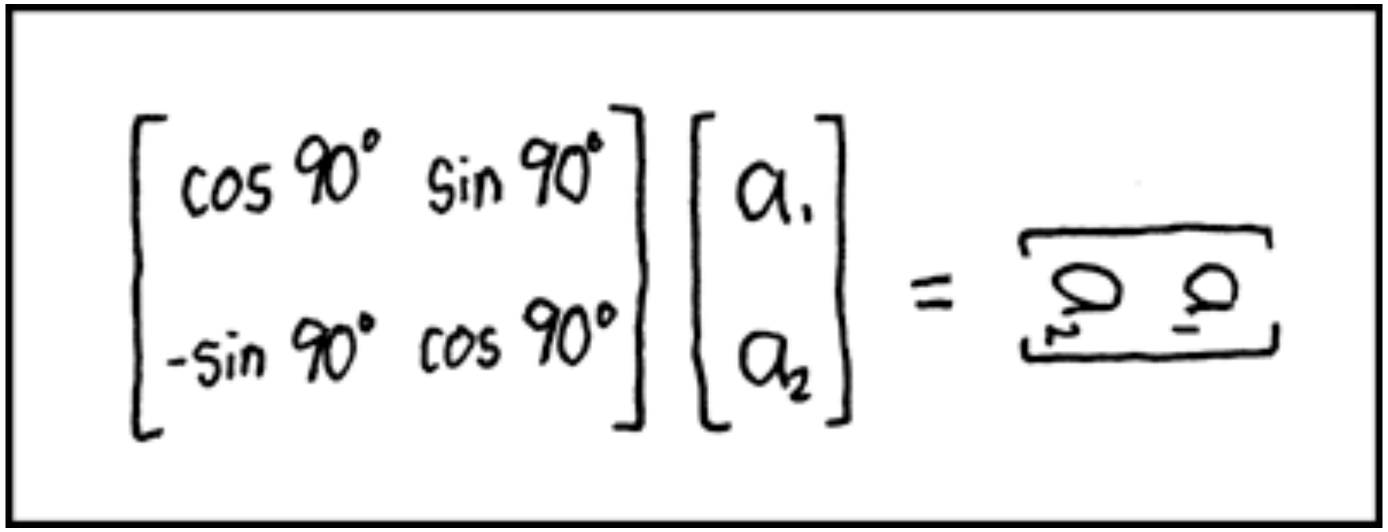
- We'll learn how to :
  - Solve linear equations
  - Compute eigenvalues
  - Apply these to various applications

Linear Algebra

- You should all be familiar with the basics of linear algebra

  - Vectors $\mathbf{A}\mathbf{x} = \mathbf{b}\,,$
  - Matrices
  - Solving matrix equations
  - Gaussian (or Gauss-Jordan) elimination
    - http://en.wikipedia.org/wiki/Gaussian_elimination

http://xkcd.com/184/



- We'll go over the computational issues here

Linear Algebra

- Recall Cramer's rule :
  - http://en.wikipedia.org/wiki/Cramer's_rule

- If we have the determinant of a matrix A :

$$|\mathbf{A}| = \sum_{i=1}^{n} (-1)^{i+j} A_{ij} \, |\mathbf{R}_{ij}| \ ,$$

  - where R_{ij} is the "residual matrix" or "minor" of A, removing row i and column j
- Then the inverse of the matrix is :

$$A_{ij}^{-1} = (-1)^{i+j} \frac{|\mathbf{R}_{ji}|}{|\mathbf{A}|} \ .$$

- This is a recursive rule

Linear Algebra

- Computing this “brute force” way is okay for small n, but problematic for large n (>10)
- Scales as n factorial (n!)

- To see this, consider an expansion of the determinant :

$$|\mathbf{A}| = \sum_P (-)^P A_{1p_1} A_{2p_2} \ldots A_{np_n} \ ,$$

- Here, P runs over the n! permutations of the indices
- 20! = 2.43x10^{18} .... yipes! (which is “yipes, factorial”)

- OK, well, scratch that idea.
  - What else ya got, Sal?

Linear Algebra

- Medium sized matrices ($n \sim 10\text{-}10^3$)
  - Gaussian elimination, LU-decomposition, and Householder method

- Larger matrices ($n > 10^3$)
  - Storage becomes a problem
  - Cannot practically do this for arbitrary matrices
  - However, most matrices are “sparse” with lots of zeroes in practical applications
  - Can, however, store and solve these fairly well

Linear Algebra

- Linear algebra is the raison d'être for numpy.
  - Let's just use it.
- Most of the scipy algorithms for linear algebra are from LAPACK. (Linear Algebra Package)
  - http://www.netlib.org/lapack/
- Other options:
  - BLAS (Basic Linear Algebra Subprograms)
    - http://en.wikipedia.org/wiki/Basic_Linear_Algebra_Subprograms
  - LAPACK
  - BOOST Basic Linear Algebra Library
    - http://www.boost.org/doc/libs/1_54_0/libs/numeric/ublas/doc/index.htm
  - matlab (the "mat" in "matlab" stands for "matrix")
    - http://www.mathworks.com/products/matlab/

Linear Algebra

- Game plan:
  - Use numpy software.
  - Go over algorithms that are used internally
  - Check into use cases

Linear Algebra

- So if you recall the Gaussian Elimination, we have a matrix equation :

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

- Or, written out for the case of n=3:

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} \ ,$$

$$\begin{pmatrix} a_{00}x_0 + a_{01}x_1 + a_{02}x_2 \\ a_{10}x_0 + a_{11}x_1 + a_{12}x_2 \\ a_{20}x_0 + a_{21}x_1 + a_{22}x_2 \end{pmatrix} = \begin{pmatrix} b_0 \\ b_1 \\ b_2 \end{pmatrix} \ .$$

Linear Algebra

- We take linear combinations of the rows to convert the matrix into "reduced row echelon form" :
  - Multiply first equation by a(10)/a(00) and subtract from second:

$$a_{10}x_0 + a_{11}x_1 + a_{12}x_2 - (a_{10}/a_{00})(a_{00}x_0 + a_{01}x_1 + a_{02}x_2) = b_1 - (a_{10}/a_{00})b_0 \; .$$

  - Then x0 is eliminated from the second equation:

$$(a_{11} - a_{10}a_{01}/a_{00})x_1 + (a_{12} - a_{10}a_{02}/a_{00})x_2 = b_1 - (a_{10}/a_{00})b_0 \; ,$$

  - which can be written as:

$$a'_{11}x_1 + a'_{12}x_2 = b'_1 \; .$$

  - Repeat until you run out of rows
  - Example:

$$\left[\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 1 & 1 & -1 & 1 \\ 3 & 11 & 5 & 35 \end{array}\right] \rightarrow \left[\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 2 & 2 & 8 \end{array}\right] \rightarrow \left[\begin{array}{ccc|c} 1 & 3 & 1 & 9 \\ 0 & -2 & -2 & -8 \\ 0 & 0 & 0 & 0 \end{array}\right] \rightarrow \left[\begin{array}{ccc|c} 1 & 0 & -2 & -3 \\ 0 & 1 & 1 & 4 \\ 0 & 0 & 0 & 0 \end{array}\right]$$

Linear Algebra

- Can also think about this in terms of an "augmented" matrix where you add the vector b as another column:

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & b_0 \\ a_{10} & a_{11} & a_{12} & b_1 \\ a_{20} & a_{21} & a_{22} & b_2 \end{pmatrix}$$

- You eliminate each row iteratively, reducing the dimension by one each time:

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} & b_0 \\ \frac{a_{10}-a_{00}a_{10}}{a_{00}} & a_{11}-\frac{a_{01}a_{10}}{a_{00}} & a_{12}-\frac{a_{02}a_{10}}{a_{00}} & b_1 - b_0 a_{10}/a_{00} \\ a_{20}-\frac{a_{00}a_{20}}{a_{00}} & a_{21}-\frac{a_{01}a_{20}}{a_{00}} & a_{22}-\frac{a_{02}a_{20}}{a_{00}} & b_2 - b_0 a_{20}/a_{00} \end{pmatrix}$$

$$\equiv \begin{pmatrix} a'_{00} & a'_{01} & a'_{02} & b'_0 \\ 0 & a'_{11} & a'_{12} & b'_1 \\ 0 & a'_{21} & a'_{22} & b'_2 \end{pmatrix}$$

$$\begin{pmatrix} a'_{00} & a'_{01} & a'_{02} & b'_0 \\ 0 & a'_{11} & a'_{12} & b'_1 \\ 0 & a'_{21}-a'_{11}a'_{21}/a'_{11} & a'_{22}-a'_{12}a'_{21}/a'_{11} & b'_2 - b'_1 a'_{21}/a'_{11} \end{pmatrix}$$

$$\equiv \begin{pmatrix} a''_{00} & a''_{01} & a''_{02} & b''_0 \\ 0 & a''_{11} & a''_{12} & b''_1 \\ 0 & 0 & a''_{22} & b''_2 \end{pmatrix}$$

Linear Algebra

- To solve for the actual equation, we then use "back substitution", starting at the last row
  - For instance

$$x_2 = \frac{b''_2}{a''_{22}} \; .$$

  - Then we use the second equation

$$x_1 = \frac{1}{a''_{11}} \left[b''_1 - a''_{12} x_2 \right] \; .$$

  - And finally

$$x_0 = \frac{1}{a''_{00}} \left[b''_0 - a''_{01} x_1 - a''_{02} x_2 \right] \; .$$

Linear Algebra

- Gaussian elimination is is $O(n^3)$ operations
  - n^2 matrix elements, and $O(n)$ row operations on each
- Back-substitution is $O(n^2)$ operations
- So the total is $O(n^3) + O(n^2) \sim O(n^3)$ for large n
- Much better than $O(n!) >> O(n^3)$
- Easy to extend to arbitrarily large n's
  - But, as we mentioned earlier, storage becomes a problem

Linear Algebra

- You can see one problem already
- If any of the rows have a zero as the first element, then you divide by zero and get an exception

- So, need to make sure this doesn't happen by "partial pivoting" :
  - Before performing the ith row operation, search for the element a_{ki} (k=i,...n-1) with the largest magnitude
  - If k != i, interchange rows i and k of the augmented matrix, and interchange x_i <---> x_k
  - Perform as usual
- Will not fail for small a_i's, also stable to roundoff errors

- Note : in "full" pivoting you swap rows AND columns

Linear Algebra

- Another variation is Gauss-Jordan elimination
  - Does not require the backsubstitution step
  - Replaces A by the inverse "in place", avoiding memory copy
- So, we have another augmented equation (again in n=3):

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} \begin{pmatrix} x_0 & a_{00}^{-1} & a_{01}^{-1} & a_{02}^{-1} \\ x_1 & a_{10}^{-1} & a_{11}^{-1} & a_{12}^{-1} \\ x_2 & a_{20}^{-1} & a_{21}^{-1} & a_{22}^{-1} \end{pmatrix} = \begin{pmatrix} b_0 & 1 & 0 & 0 \\ b_1 & 0 & 1 & 0 \\ b_2 & 0 & 0 & 1 \end{pmatrix}$$

- This is a way of stating :

$$\mathbf{A}\mathbf{x} = \mathbf{b}\,, \qquad \text{and} \qquad \mathbf{A}\mathbf{A}^{-1} = \mathbf{1}\,.$$

Linear Algebra

- Algorithm :
  - Start with zeroth row, divide by a(00) and subtract
  - Subtract all zeroth column entries (as in Gaussian elimination)
  - For row i=1,...n-1, divide by diagonal element a(ii) and eliminate elements in column i other than the diagonal by subtracting a(ij) times the ith row elements from the jth row
    - Gaussian elimination : subtracts only those below diagonal
    - Gauss-Jordan : subtracts ALL elements where i != j
  - Simultaneously perform on the augmented (b 1) matrix on the RHS

Linear Algebra

- In the end we get :

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} \text{b0} & a_{00}^{-1} & a_{01}^{-1} & a_{02}^{-1} \\ \text{b1} & a_{10}^{-1} & a_{11}^{-1} & a_{12}^{-1} \\ \text{b2} & a_{20}^{-1} & a_{21}^{-1} & a_{22}^{-1} \end{pmatrix} = \begin{pmatrix} x_0 & a_{00}^{-1} & a_{01}^{-1} & a_{02}^{-1} \\ x_1 & a_{10}^{-1} & a_{11}^{-1} & a_{12}^{-1} \\ x_2 & a_{20}^{-1} & a_{21}^{-1} & a_{22}^{-1} \end{pmatrix}$$

- A is replaced by a unit matix
- b is reduced to input vector x
- Unit matrix on RHS is replace by inverse A^{-1}

- Can also implement pivoting in this algorithm to make sure we have numeric stability

Linear Algebra

- Another variation is “LU decomposition” (“lower-upper”)
- Reduce A to an L*U product: $\mathbf{A}\mathbf{x} = \mathbf{b}$,

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} = \begin{pmatrix} \alpha_{00} & 0 & 0 \\ \alpha_{10} & \alpha_{11} & 0 \\ \alpha_{20} & \alpha_{21} & \alpha_{22} \end{pmatrix} \begin{pmatrix} \beta_{00} & \beta_{01} & \beta_{02} \\ 0 & \beta_{11} & \beta_{12} \\ 0 & 0 & \beta_{22} \end{pmatrix}$$

- Then solve the problem in two steps :
  - Solve $\mathbf{L}\mathbf{y} = \mathbf{b}$ with forward substitution:

$$y_0 = \frac{b_0}{\alpha_{00}} , \qquad y_i = \frac{1}{\alpha_{ii}} \left[b_i - \sum_{j=0}^{i-1} \alpha_{ij} y_j \right] , \qquad i = 1, 2, \ldots, n-1 .$$

  - Solve $\mathbf{U}\mathbf{x} = \mathbf{y}$, since $\mathbf{A}\mathbf{x} = \mathbf{L}(\mathbf{U}\mathbf{x}) = \mathbf{L}\mathbf{y} = \mathbf{b}$, with backward substitution :

$$x_{n-1} = \frac{y_{n-1}}{\beta_{n-1,n-1}} , \qquad x_i = \frac{1}{\beta_{ii}} \left[y_i - \sum_{j=i+1}^{n-1} \beta_{ij} x_j \right] , \qquad i = n-2, \ldots, 0 .$$

Linear Algebra

- Factoring the matrix A = LU can be done with "Crout's Algorithm" :
  - Set alpha(ii) = 1 for i=0,...n-1
  - for each j = 0,...n-1 :

    for i = 0,...j

    compute $$\beta_{ij} = a_{ij} - \sum_{k=0}^{i-1} \alpha_{ik}\beta_{kj} \;.$$

    for j = j+1,...n-1

    compute $$\alpha_{ij} = \frac{1}{\beta_{jj}}\left[a_{ij} - \sum_{k=0}^{j-1} \alpha_{ik}\beta_{jk}\right] \;.$$

- Replaces A by LU "in place":

$$\begin{pmatrix} a_{00} & a_{01} & a_{02} \\ a_{10} & a_{11} & a_{12} \\ a_{20} & a_{21} & a_{22} \end{pmatrix} \longrightarrow \begin{pmatrix} \beta_{00} & \beta_{01} & \beta_{02} \\ \alpha_{10} & \beta_{11} & \beta_{12} \\ \alpha_{20} & \alpha_{21} & \beta_{22} \end{pmatrix}$$

The RH matrix is NOT a matrix! It is a storage unit in the computer!

Linear Algebra

- Simple special case : Tridiagonal matrices

- If you have a problem such as :

$$\mathbf{M} = \begin{pmatrix} 2-c & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2-c & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2-c & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2-c & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2-c \end{pmatrix} ,$$

- This matrix is sparse!
  – Can solve in O(n) operations
- Equations are:

$$M_i^- u_{i-1} + M_i^0 u_i + M_i^+ u_{i+1} = b_i \ , \qquad i = 1, \ldots, n-1 \ .$$

- Can show that (recursively):

$$\alpha_{i-1} = -\frac{M_i^-}{M_i^0 + \alpha_i M_i^+} \ , \qquad \beta_{i-1} = \frac{b_i - \beta_i M_i^+}{M_i^0 + \alpha_i M_i^+} \ .$$

Linear Algebra

- Can start from the right boundary value for i=n-2,...0

$$u_n = \alpha_{n-1} u_{n-1} + \beta_{n-1} \qquad \text{if} \qquad \alpha_{n-1} = 0 \,, \quad \beta_{n-1} = u_n \ ,$$

- and then solve from the left boundary value for i=1,...n-1

$$u_{i+1} = \alpha_i u_i + \beta_i \ ,$$

- So we "sweep twice" and obtain O(n) operations

Linear Algebra

- Examples:
  - Polynomial fits (again)
  - Circuit diagrams
  - Boundary value problems

Recall : General fitting of curves

- This is a matrix equation, so we define the “design matrix” :

$$A_{ij} = \frac{Y_j(x_i)}{\sigma_i}$$

$$\mathbf{A} = \begin{bmatrix} Y_1(x_1)/\sigma_1 & Y_2(x_1)/\sigma_1 & \dots \\ Y_1(x_2)/\sigma_2 & Y_2(x_2)/\sigma_2 & \dots \\ \dots & \dots & \dots \end{bmatrix}$$

- Then our chi2 minimization becomes :

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

- so :

$$\vec{a} = (\mathbf{A}^T\mathbf{A})^{-1}\mathbf{A}^T\vec{b}$$

Recall : General fitting of curves

- If we define the “correlation matrix” :

$$\mathbf{C} = (\mathbf{A}^T\mathbf{A})^{-1}$$

- Then the uncertainty on a_j is :

$$\sigma_{a_j} = \sqrt{C_{jj}}$$

Recall : General fitting of curves

- As a first example, let's look at polynomial fits

$$y = \sum_{k=0}^{m-1} a_k x^k \ .$$

- Slight generalization of the linear fit we did previously
- General solution is to minimize the chi2 :

$$\chi^2(\vec{a}) \equiv \sum_{i=0}^{n-1} \left(\frac{y_i - y(x;\vec{a})}{\sigma_i} \right)^2$$

- In this case :

$$\chi^2(\vec{a}) = \sum_{i=0}^{n-1} \left(\frac{y_i - \sum_{j=0}^{M} a_j x^j}{\sigma_i} \right)^2$$

Recall : General fitting of curves

- Our design matrix is therefore :

$$A_{ij} = x_i^j / \sigma_i$$

- Caveat : This oftentimes is ill-formed, so don't go too crazy here. Typically we do quadratic, cubic, quartic, but above that it strains credibility.

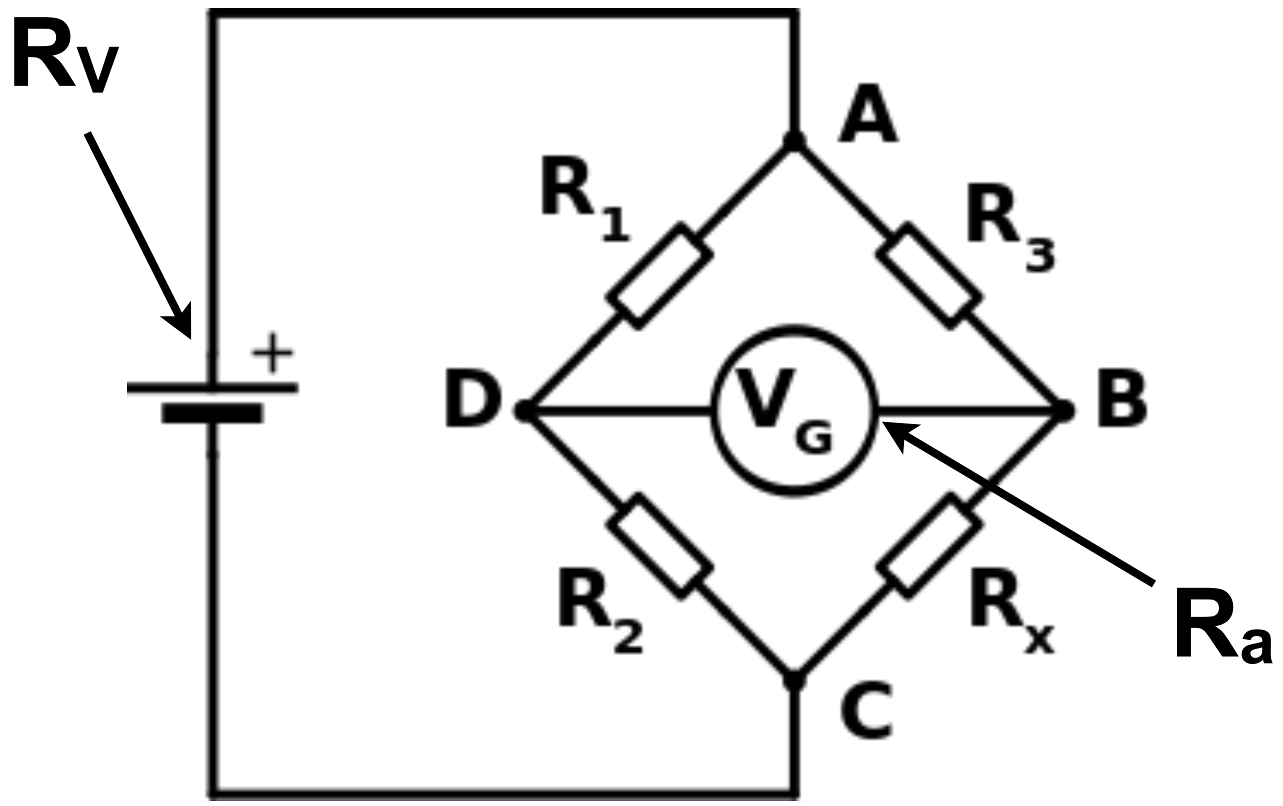
Polynomial fits

- Can finally generalize our formalism to arbitrary functional fits

- Example : quadratic fit for our CO2 data!

Linear Algebra

- Example :
  - Kirchoff's Law for a Wheatstone bridge :
  - http://en.wikipedia.org/wiki/Wheatstone_bridge



Solve for Rx given R1,R2,R2, i and V

- This is a matrix equation: $\mathbf{R}\mathbf{i} = \mathbf{v}$,

$$\begin{pmatrix} R_1 + R_v & R_2 & R_v \\ R_1 + R_a & -R_a & -R_3 \\ R_x + R_a & -R_2 - R_x - R_a & R_x \end{pmatrix} \begin{pmatrix} i_1 \\ i_2 \\ i_3 \end{pmatrix} = \begin{pmatrix} v \\ 0 \\ 0 \end{pmatrix}$$

Linear Algebra

- Try to “zero” the potential at V_G:

$$V_G = \left(\frac{R_x}{R_3 + R_x} - \frac{R_2}{R_1 + R_2} \right) V_s$$

Linear Algebra

- Example : boundary value problems
  - Consider :

$$\frac{\mathrm{d}^2 u}{\mathrm{d}x^2} = -\frac{\pi^2}{4}(u+1) \,,$$

  - with Dirichlet boundary conditions u(0) = 0 and u(1)=1
  - We can discretize this :

$$\frac{2u_i - u_{i+1} - u_{i-1}}{h^2} = \frac{\pi^2}{4}(u_i + 1) \,, \qquad i = 1, \ldots, N-1$$

  - This is therefore a sparse matrix equation with c = h^2 pi^2/4:

$$\mathbf{M} = \begin{pmatrix} 2-c & -1 & 0 & \cdots & 0 & 0 \\ -1 & 2-c & -1 & \cdots & 0 & 0 \\ 0 & -1 & 2-c & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 2-c & -1 \\ 0 & 0 & 0 & \cdots & -1 & 2-c \end{pmatrix} , \qquad \mathbf{x} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \\ \vdots \\ u_{N-2} \\ u_{N-1} \end{pmatrix} , \qquad \mathbf{b} = \begin{pmatrix} u_0 + c \\ c \\ c \\ \vdots \\ c \\ u_N + c \end{pmatrix} ,$$

Hands on!

Linear Algebra

- Today : Eigenvalues and eigenvectors, more hands on

- See Chapter 11 of Numerical Recipes

- In this case, even they recommend using packaged software for eigenvalues and eigenvectors, but let’s get the general gist here

Linear Algebra

- Example : normal modes of a harmonic oscillator between n objects

$$\mathcal{L} = \frac{1}{2}\sum_{j,k}^{n} M_{jk}\dot{q}_j\dot{q}_k - \frac{1}{2}\sum_{j,k}^{n} A_{jk}q_jq_k \ ,$$

- “Normal mode” is the mode of the system where all of the coordinates oscillate with some frequency omega:

$$q_j(t) = x_j e^{i\omega t} \ , \qquad \sum_{j=1}^{n}\left[A_{jk} - M_{jk}\omega^2\right] x_j = 0 \ , \qquad (\mathbf{A} - \mathbf{M}\omega^2)\mathbf{x} = 0 \ .$$

- Homogeneous matrix equation has solutions for omega for which the determinant is zero:

$$\det\left|\mathbf{A} - \mathbf{M}\omega^2\right| = 0 \ .$$

Eigenvalues and Eigenvectors

- This is an instance of a general class of eigenvalue and eigenvector problems
- So, if A is an nxn matrix, x is a column vector (the "right" eigenvector), lambda is a number (the "eigenvalue"), and :

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

- Then the equation is satisfied when :

$$|\mathbf{A} - \lambda\mathbf{1}| = \sum_{k=0}^{n} a_k \lambda^k = 0 \; ,$$

- This is an n-th degree polynomial in lambda that depends on the matrix elements
- N-degree polynomial ==> n different eigenvalues, so we need to solve for them

Eigenvalues and Eigenvectors

- Example :

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

- The eigenvalue equation and eigenvalues are :

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

$$(1-\lambda)(2-\lambda)-1 = \lambda^2-3\lambda+1 = 0 \quad \Rightarrow \quad \lambda_0 = \frac{3+\sqrt{5}}{2}, \quad \lambda_1 = \frac{3-\sqrt{5}}{2}.$$

- We solve for the eigenvectors :

$$\begin{pmatrix} 1 & 1 \\ 2 & 1 \end{pmatrix} \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} = (1 \pm \sqrt{2}) \begin{pmatrix} x_0 \\ x_1 \end{pmatrix} \quad \mathbf{x}^{(0)} = \begin{pmatrix} \sqrt{\frac{1}{3}} \\ \sqrt{\frac{2}{3}} \end{pmatrix}, \quad \mathbf{x}^{(1)} = \begin{pmatrix} \sqrt{\frac{1}{3}} \\ -\sqrt{\frac{2}{3}} \end{pmatrix}.$$

Eigenvalues and Eigenvectors

- Also consider :

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

- So we have:

$$(1-\lambda)^2 + 1 = \lambda^2 - 2\lambda + 2 = 0$$

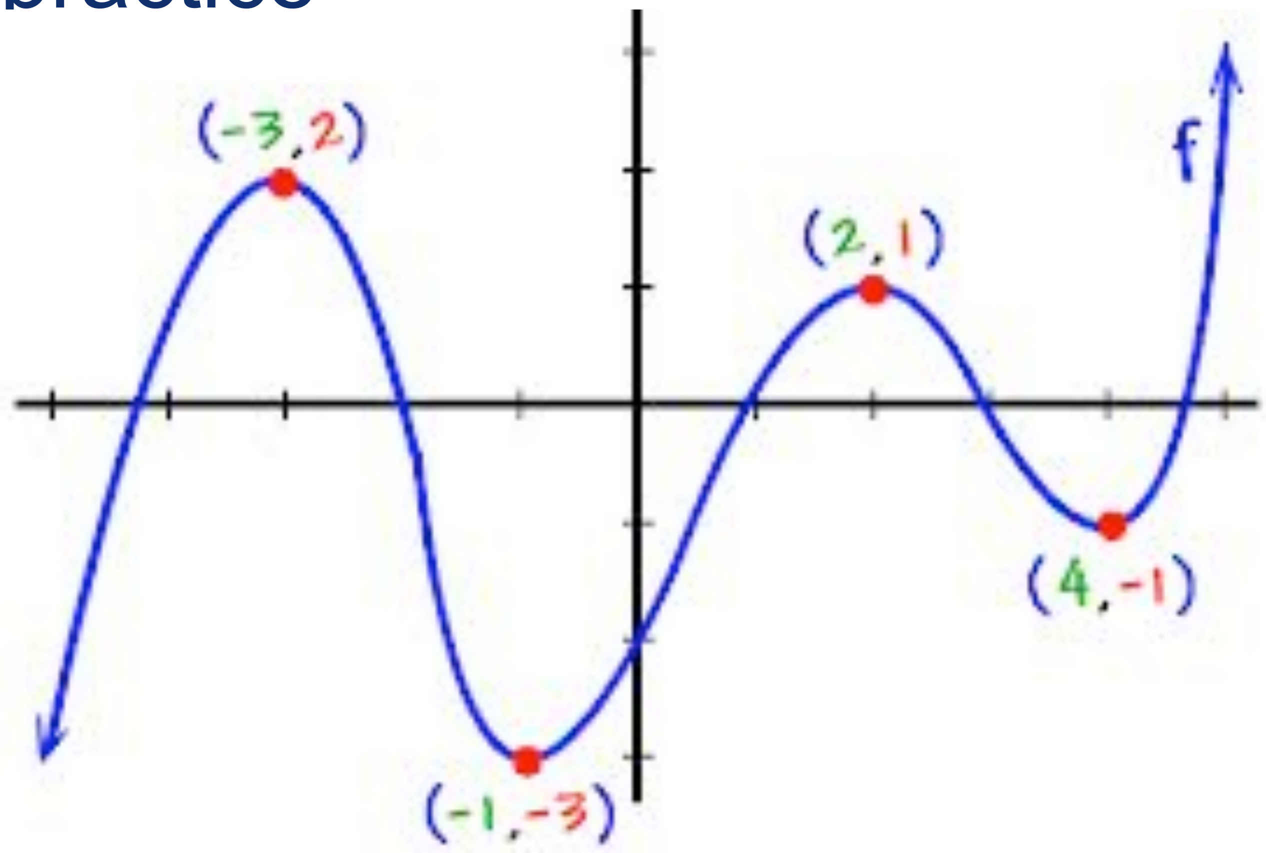
- And thus the eigenvalues are complex :

$$\lambda_0 = 1 + i \ , \quad \lambda_1 = 1 - i \ , \qquad \text{where} \qquad i = \sqrt{-1} \ .$$

Eigenvalues and Eigenvectors

- “Hey Sal! I know what we can do!” you say. “We can just find the roots of the characteristic polynomial with our root-finding methods!”

- “Excellent idea in principle, my clever students,” I say. “But unfortunately, it’s hard in practice”
  - Need to know roughly where the roots are ahead of time
  - You don’t get the eigenvectors this way either



- So, we’ll look at ways to do both!

Eigenvalues and Eigenvectors

- First, define “left” eigenvectors:

$$\mathbf{y}\mathbf{A} = \lambda\mathbf{y} \ ,$$

- In this case, y is a row vector.
- This implies : $\mathbf{A}^{\mathrm{T}}\mathbf{y} = \lambda\mathbf{y} \ ,$

- Since : $\left|\mathbf{A}^{\mathrm{T}} - \lambda\mathbf{1}\right| = \left|\mathbf{A} - \lambda\mathbf{1}\right| \ ,$

  then the left and right eigenvalues are the same
- However the left and right eigenvectors are not necessarily the same
- Left eigenvector 0, though, is orthogonal to right eigenvector 1, etc

Eigenvalues and Eigenvectors

- If we consider a complex matrix A, we can define the Hermitian conjugate :

$$\left(\mathbf{A}^{\dagger}\right)_{ij} = a^{*}_{ji} \ ,$$

  - This is also referred to as the "conjugate transpose"
  - If the a_{ij} are real, this is just the transpose
- Define a "normal" matrix if the conjugate transpose commutes with the matrix:

$$\mathbf{N} \cdot \mathbf{N}^{\dagger} = \mathbf{N}^{\dagger} \cdot \mathbf{N} \ .$$

- Note that normal matrices have the same left and right eigenvector sets

Eigenvalues and Eigenvectors

- A Hermitian matrix (or self-adjoint matrix) is defined when

$$\mathbf{H}^{\dagger} = \mathbf{H} \ ,$$

- When the elements are real, this is called a “symmetric” matrix:

$$\mathbf{S}^{\mathrm{T}} = \mathbf{S} \ ,$$

- These special matrices have :
  - n real eigenvalues
  - eigenvectors are orthogonal
  - the set of eigenvectors is “complete” (spans the n-dim space)

Eigenvalues and Eigenvectors

- Computation of eigenvalues/eigenvectors for symmetric or Hermitian matrices depends on a nice property
- If we consider the matrices formed by the right and left eigenvectors X and Y:

$$\mathbf{X} = \begin{pmatrix} \sqrt{\frac{1}{3}} & \sqrt{\frac{1}{3}} \\ \sqrt{\frac{2}{3}} & -\sqrt{\frac{2}{3}} \end{pmatrix} , \qquad \mathbf{Y} = \begin{pmatrix} \sqrt{\frac{2}{3}} & \sqrt{\frac{1}{3}} \\ \sqrt{\frac{2}{3}} & -\sqrt{\frac{1}{3}} \end{pmatrix} = \frac{2\sqrt{2}}{3}\mathbf{X}^{-1} .$$

- In general : $\mathbf{Y} \propto \mathbf{X}^{-1}$

- Can choose the normalization appropriately so that

$$\mathbf{Y} = \mathbf{X}^{-1}$$

Eigenvalues and Eigenvectors

- How does this help us?

$$
\begin{aligned}
\mathbf{Y} \cdot \mathbf{A} \cdot \mathbf{X} &= \mathbf{X}^{-1} \cdot \mathbf{A} \cdot \mathbf{X} \\
&= \mathbf{X}^{-1} \cdot \lambda \cdot \mathbf{X} \\
&= \lambda
\end{aligned}
$$

- Can exploit this fact to compute the eigenvalues!

Eigenvalues and Eigenvectors

- This is a similarity transformation!

$$\mathbf{A} \quad \rightarrow \quad \mathbf{Z}^{-1} \cdot \mathbf{A} \cdot \mathbf{Z}$$

- The interesting bit is that symmetry transformations leave the eigenvalues unchanged:

$$\begin{aligned} \det \left| \mathbf{Z}^{-1} \cdot \mathbf{A} \cdot \mathbf{Z} - \lambda \mathbf{1} \right| &= \det \left| \mathbf{Z}^{-1} \cdot (\mathbf{A} - \lambda \mathbf{1}) \cdot \mathbf{Z} \right| \\ &= \det \left| \mathbf{Z} \right| \; \det \left| \mathbf{A} - \lambda \mathbf{1} \right| \; \det \left| \mathbf{Z}^{-1} \right| \\ &= \det \left| \mathbf{A} - \lambda \mathbf{1} \right| \end{aligned}$$

- So, we can solve this easier problem instead

Eigenvalues and Eigenvectors

- Let X be the matrix of eigenvectors
  - If the matrix A is real and symmetric, then the eigenvectors are real and orthonormal, and :

$$\mathbf{X}^{-1} = \mathbf{X}^{\mathrm{T}}$$

  - If the matrix A is is Hermitian, the matrix of eigenvectors is unitary :

$$\mathbf{X}^{-1} = \mathbf{X}^{\dagger}$$

Eigenvalues and Eigenvectors

- Generalized eigenvalue problem : solve

$$\mathbf{A} \cdot \mathbf{x} = \lambda \mathbf{B} \cdot \mathbf{x}$$

- Strategy : Successively apply similarity transformations until the matrix is “almost” diagonal
  - Either diagonal, block diagonal, or tridiagonal and also easy to solve

- Nonsymmetric matrices will not, in general, have similarity matrices with real components
  - So, cannot use real similarity matrix
  - But! “Almost” can : will reduce to block-diagonal with two-by-two blocks replacing the complex eigenvalues
  - Think $\begin{pmatrix} \cos\theta & \sin\theta \\ -\sin\theta & \cos\theta \end{pmatrix}$

Eigenvalues and Eigenvectors

- Can then repeatedly apply similarity transformations until we can solve the problem "easily" :

$$\begin{aligned} \mathbf{A} \quad &\rightarrow \quad \mathbf{P}_1^{-1} \cdot \mathbf{A} \cdot \mathbf{P}_1 \quad \rightarrow \quad \mathbf{P}_2^{-1} \cdot \mathbf{P}_1^{-1} \cdot \mathbf{A} \cdot \mathbf{P}_1 \cdot \mathbf{P}_2 \\ &\rightarrow \quad \mathbf{P}_3^{-1} \cdot \mathbf{P}_2^{-1} \cdot \mathbf{P}_1^{-1} \cdot \mathbf{A} \cdot \mathbf{P}_1 \cdot \mathbf{P}_2 \cdot \mathbf{P}_3 \quad \rightarrow \quad \text{etc.} \end{aligned}$$

- If we end up in completely diagonal form, then the eigenvectors are just the columns of the total transformation:

$$\mathbf{X}_R = \mathbf{P}_1 \cdot \mathbf{P}_2 \cdot \mathbf{P}_3 \cdot \ldots$$

- Sometimes just want eigenvalues, in which case can stop when we reduce to triangular form
  - Then eigenvalues are the diagonal elements!

Eigenvalues and Eigenvectors

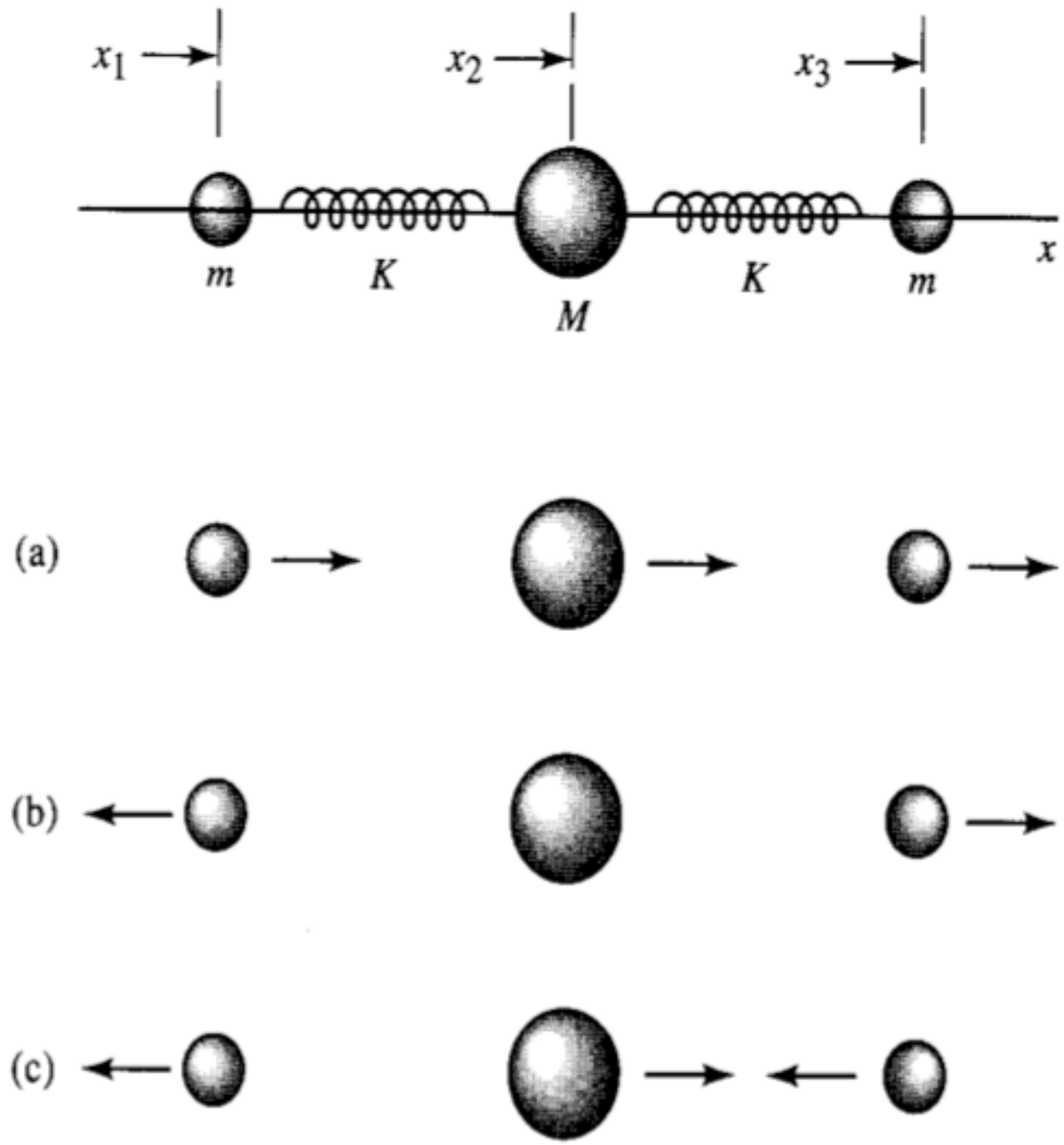
- One strategy we will look at :
  - Reduce to tridiagonal form by the Householder algorithm (Chapter 11 Section 2 of Numerical Recipes)
  - Solve the tridiagonal matrix problem using a QL algorithm with implicit shifts (Chapter 11 Section 3 of Numerical Recipes)
    - Q = orthogonal
    - L = lower triangular matrix

- These are basically “uninteresting” to go through the gory details, because they’re mostly just math tricks

- Instead, let’s just focus on an application

Eigenvalues and Eigenvectors

- Consider a linear triatomic molecule
  - Fowles and Cassiday, Chapter 11, Section 4
  - Taylor, Chapter 11, Section 6
- Approximate by masses on springs



Eigenvalues and Eigenvectors

- Lagrangian for the general case is :

$$L = \frac{1}{2}m_1\dot{x}_1^2 + \frac{1}{2}m_2\dot{x}_2^2 + \frac{1}{2}m_3\dot{x}_3^2 - \frac{1}{2}\left[k_{12}(x_1 - x_2)^2 + k_{23}(x_2 - x_3)^2\right]$$

- The equations of motion are

$$m_1\ddot{x}_1 = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_1}\right) = \frac{\partial L}{\partial x_1} = -k_{12}x_1 + k_{12}x_2$$

$$m_2\ddot{x}_2 = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_2}\right) = \frac{\partial L}{\partial x_2} = k_{12}x_1 - (k_{12} + k_{23})\,x_2 + k_{23}x_3$$

$$m_3\ddot{x}_3 = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{x}_3}\right) = \frac{\partial L}{\partial x_3} = -k_{23}x_3 + k_{23}x_2$$

- For our specific problem, we have

$$m_1 = m_3, m_2 = 2m_1, k_{12} = k_{23} = K$$

Eigenvalues and Eigenvectors

- Can be written as a matrix equation:

$$\mathbf{M}\ddot{\mathbf{q}} = -\mathbf{K}\mathbf{q}$$

- with normal modes of the form :

$$\mathbf{q}(t) = \mathbf{a}\cos(\omega t - \delta)$$

- The normal mode frequencies are eigenvalues of the generalized eigenvalue equation:

$$\mathbf{K}\mathbf{a} = \omega^2\mathbf{M}\mathbf{a}$$

Eigenvalues and Eigenvectors

- The eigenvalues are therefore:

$$\omega_1^2 = 0\,, \qquad \omega_2^2 = \frac{K}{m}\,, \qquad \omega_3^2 = \frac{K}{m}\left(1 + \frac{2m}{M}\right)$$

- And the eigenvectors are :

$$\mathbf{a}_1 = a_{11}\begin{pmatrix}1\\1\\1\end{pmatrix}\,, \qquad \mathbf{a}_2 = a_{12}\begin{pmatrix}1\\0\\-1\end{pmatrix}\,, \qquad \mathbf{a}_3 = a_{13}\begin{pmatrix}1\\-\frac{2m}{M}\\1\end{pmatrix}\,,$$

Eigenvalues and Eigenvectors

- “triatomic” python notebook