Scientific Computing: Lecture 21

- Introduction to (reminder of?) matrices
- Solving systems of equations
- Matrix objects in Numpy
- Eigenvector and value problems
- Exercise: Solve 3D linear system

CLASS NOTES

- Final Project proposals due today by midnight (use HW Box folder).
- HW09 posted later in the week
- Coming up next: Partial Differential Equations. Note: Optional for undergraduate students.

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Matrices

- Matrices are mathematical objects which are handy for representing certain types of data structures.
- Represented as a 2D grid of numbers with dimensions *m* x *n*.

$$A = \begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{pmatrix}$$

- Above is a 3 x 3 matrix, which is said to be square (m=n)

Matrix operations

- Identity matrix: $I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}$ $\quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$
- Inverse of a matrix:

$$A^{-1}A = I \qquad A^{-1} = \frac{1}{ad-bc}\begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$$

- Determinant of a matrix: $\det\begin{pmatrix} a & b \\ c & d \end{pmatrix} = (ad - bc)$
- Multiplication by a scalar: $3\begin{pmatrix} a & b \\ c & d \end{pmatrix} = \begin{pmatrix} 3a & 3b \\ 3c & 3d \end{pmatrix}$

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Systems of equations

- Consider a system of N algebraic equations with N unknown quantities.
- How do we solve for these unknowns?

$$3x - 2y = 4$$

$$5x + 1y = 10$$

- Solve for x in terms of y using eqn 1 and substitute into eqn 2. Then solve for y and use that to solve for x.
- Can represent this system as a matrix problem.

System as a matrix equation

- In equation form, this would be

$$3x - 2y = 4$$
$$5x + 1y = 10$$

$$AX = b \Rightarrow \begin{pmatrix} 3 & -2 \\ 5 & 1 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 4 \\ 10 \end{pmatrix}$$

- Now solve by multiplying inverse
- Need to be careful taking the inverse of a matrix – can lead to divide by 0, or singularities.

$$A^{-1}AX = A^{-1}b$$
$$IX = A^{-1}b$$

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Eigenvalue Problems

- Mathematically, if A is a square matrix, the eigenvector (v) and associated eigenvalues (λ) are defined by:

$$Av = \lambda v$$

- Eigenvalues are the solutions to the characteristic polynomial produced by:

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

- Many applications in science. Eigenvalues are typically parameters in a physical system: energies, natural frequencies, …
- Commonly see these methods employed in classical and quantum mechanics, acoustics, optics, ….

Numpy linalg library

- numpy.linalg as several useful tools for linear algebra.
- If A is a square matrix:
  - eig(A) – returns eigenvalues and vectors (can be complex) of A.
  - solve(A,b) – solves (returns vector X) linear system of equations

    $$AX = b \Rightarrow$$

    det(A) – returns determinant of A
  - svd(A) – returns singular value decomposition of A (way of dealing with the inverse of ill conditioned matrices)

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Matrix objects in Numpy

- 2D arrays are like matrices and have many appropriate methods (trace, transpose,…)
- A special matrix object is also supplied:
  `A = matrix(a_2D_array)`
- New features and methods
  - Proper matrix multiplication: A*A
  - Proper power of a matrix: A**2
  - trace, inverse (A.I)

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Exercises

- Exercise 1:
  - Consider the following linear system

$$-10x + 10y = 2$$
$$-10x - y + 2z = 4$$
$$2x - 10y - 8z = -3$$

  - Express the problem in a matrix format in Python and solve X x_0, y_o, z_o

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