Numerical Linear Algebra

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Linear Algebra deals with

Matrices = Boxes of Numbers

$$\begin{pmatrix} 1 & 2 \\ 3 & 4 \\ 5 & 6 \end{pmatrix}$$

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & a_{14} \\ a_{21} & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & a_{33} & a_{34} \end{pmatrix}$$

$$\begin{pmatrix} x \\ y \\ z \end{pmatrix}$$

NUMERICAL Linear Algebra

Errors in matrices and algorithms

Linear system $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$
Elements accurate to three digits

$$\boldsymbol{A} = \begin{pmatrix} .1234 & 5.678 \\ 2.469 & 11.35 \end{pmatrix} \qquad \boldsymbol{b} = \begin{pmatrix} 0.000 \\ 1.200 \end{pmatrix}$$

How many accurate digits in solution $\boldsymbol{x}$?

Answer: None

NUMERICAL Linear Algebra

Matrix elements have errors
Algorithms make errors
Floating point arithmetic causes errors

Tasks in numerical linear algebra:

- Determine conditioning of problem
  How sensitive is solution to errors in input?
- Design stable algorithms
  Algorithms should not amplify errors

What can numerical linear algebra do for us?

Search Engines

Google

Netscape

YAHOO!

msn

altavista

AOL

excite

Ask Jeeves

overture

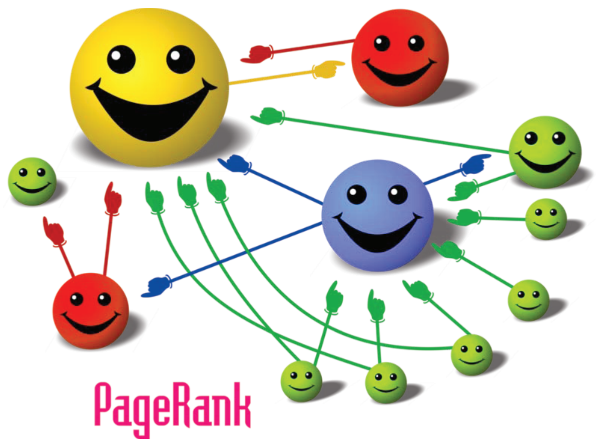
Inktomi

Quantum Physics

(Computational) Plumbing

Search Engines

Google's PageRank



PageRank $\approx$ importance of web page

High PageRank $\Longrightarrow$ web page displayed
early among search results

Computing PageRank

PageRank vector p:
one component for each web page

PageRank is an eigenvector:

$$G\,p = \lambda\,p, \qquad \lambda = 1$$

G is $n \times n$ stochastic matrix

$n =$ # web pages on the Internet

$=$ hundreds of billions

Problems

$$Gp = \lambda p, \qquad \lambda = 1$$

- Dimension of matrix G is HUGE
- How to compute an approximation for p?
- Methods must be fast.
- Methods must use little memory.
- Methods must be accurate.
- How to define accuracy?
- How to exploit the structure of the matrix G?

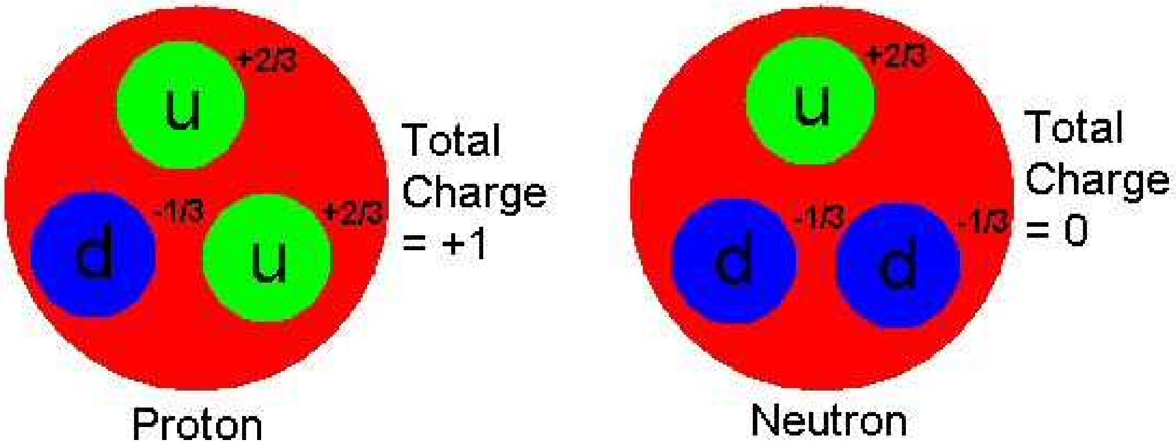
Tools

- Eigenvalues & Eigenvectors
- Jordan canonical forms
- Theory of Markov chains
- Matrix perturbation theory
- Krylov space methods

Joint work with Teresa Selee

Quantum Physics

Fermions: protons, neutrons, electrons, . . .



- Want: thermodynamic properties
  average energy, heat capacity, . . .
- How: compute partition function
- Partition function $\rightsquigarrow$ characteristic polynomial

Characteristic Polynomial

Characteristic polynomial of $n \times n$ matrix A

$$\begin{aligned} p(\lambda) &\equiv \det(A - \lambda I) \\ &= \lambda^n + c_1 \lambda^{n-1} + \cdots + c_{n-1}\lambda + c_n \end{aligned}$$

where

$$c_1 = -\operatorname{trace}(A), \qquad c_n = (-1)^n \det(A)$$

Need to compute coefficients c_i

Problems

$$\det(A - \lambda I) = \lambda^n + c_1\lambda^{n-1} + \cdots + c_{n-1}\lambda + c_n$$

- c_i are illconditioned:
  sensitive to small changes in matrix A
- c_i have widely different magnitudes:
  from extremely small to extremely large
- Numerical methods are unstable:
  unreliable and inaccurate

Tools

- Eigenvalues & Eigenvectors
- Matrix perturbation theory
- Elementary symmetric functions
- Stability & round off error analyses
- Scaling strategies against underflow & overflow
- Hybrid numerical/symbolic methods

Joint work with Dean Lee (Physics) and Rizwana Rehman

(Computational) Plumbing

Condition estimation

The basis of linear system solvers

Condition Estimation

- Linear system solution $\boldsymbol{A}\boldsymbol{x} = \boldsymbol{b}$

  If $Cy = b$ then

$$\frac{\|x - y\|}{\|y\|} \leq \|\boldsymbol{A}\| \, \|\boldsymbol{A}^{-1}\| \, \frac{\|A - C\|}{\|A\|}$$

- Condition number $\|\boldsymbol{A}\| \, \|\boldsymbol{A}^{-1}\|$

  Sensitivity of x to changes in A and b

- Want: estimate of $\|\boldsymbol{A}\| \, \|\boldsymbol{A}^{-1}\|$

Problems

Want: $\|A\|\|A^{-1}\|$ where A is $n \times n$

- n is LARGE
- Exact computation too slow: $\sim n^3$ ops
- Estimate should be
  - fast: $\sim n$ ops
  - accurate: within a factor of 10
  - matrix-free:
    only matrix vector products with A
  - transpose-free: A^T not available

Tools

- Probabilistic algorithms

  For real $n \times n$ matrix A:

$$\|A\|_F \approx \sqrt{n}\|A\boldsymbol{v}\|_2$$

  $\boldsymbol{v}$ uniformly distributed on unit n-sphere
- Multivariate statistics
- Singular value decomposition
- Krylov space methods

Joint work with Tim Kelley

How to Get Started

Courses in Numerical Linear Algebra:

- MA523: Linear Transformation & Matrix Theory
- MA580: Numerical Analysis I