Math 298
Fundamental Concepts in Computational and Applied Mathematics

Class 2

Recap

- Beware catastrophic cancellation – know limits of precision
- Ask about conditioning of a problem
- Choose stable algorithms so as to not introduce any more loss of precision than is necessary
- Conditioning is fundamentally a characteristic of the problem, while stability is related to algorithms

Discussion of Bailey's paper

- Climate modeling
  - *"almost all numerical variation occurred in one inner product loop ... and in a similar operation in a large conjugate gradient calculation"*
- N–Body atomic system simulations
  - *"solve the generalized eigenvalue problem $(\hat{H} - E\hat{S})C = 0$, where the matrices $\hat{H}$ and $\hat{S}$ are large ... and very nearly degenerate"*
- Computational Geometry and Grid Generation
  - *"small numerical errors in the computation of the point nearest to a given point on a line intersecting two planes can result in the computed point being so far from either plane as to rule out the solution being correct for a reasonable perturbation of the original problem"*

Dense Linear Algebra

- Basic Linear Algebra
  - dot products, saxpy, matvec
  - Solve $Ax = b$
  - Solve $Ax = \lambda x$
- We cannot solve anything except linear systems
- Various standard methods.
  - LU
  - Cholesky
  - QR
  - SVD
- Your choice will depend on the application and time constraints

Some useful facts

- Define the condition number of a matrix A by:
  - $\kappa(A) = ||A|| \cdot ||A^{-1}||$
- Best possible error bound for solving a system of linear equations can be given by
  - $$\frac{||x - \hat{x}||_\infty}{||x||_\infty} \leq 4\mu\kappa_\infty(A)$$
- Problems for which $\mu\kappa_\infty(A) \approx 1$ are considered ill-conditioned
- Gaussian elimination always produces solutions with relatively small residuals (minor caveats)

Stable/Unstable?
Well conditioned/Ill conditioned?

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

Comparison of algorithms

Algorithm	Work	Advantages	Disadvantages
LU	$\mathcal{O}(n^3)$	Simple	Unstable
LU w/PP	$\mathcal{O}(n^3)$	(Usually) stable Depends on growth factor ρ	Growth factor; pivoting will change structure
LU w/FP	$\mathcal{O}(n^3)$	Stable	More work than PP
QR	$\mathcal{O}(n^3)$	Stable	Twice the work of LU
SVD	$\mathcal{O}(n^3)$	Stable	More than twice the work

LU with partial pivoting

- Can show that LU/PP generates exact solution to a perturbed problem (A + E) x = b, such that

$$||E||_\infty \leq 8n^3\rho||A||_\infty\mu$$

- The growth factor ρ can grow exponentially, but in practice is usually or order 10

- Consider the residual, b - Ax:

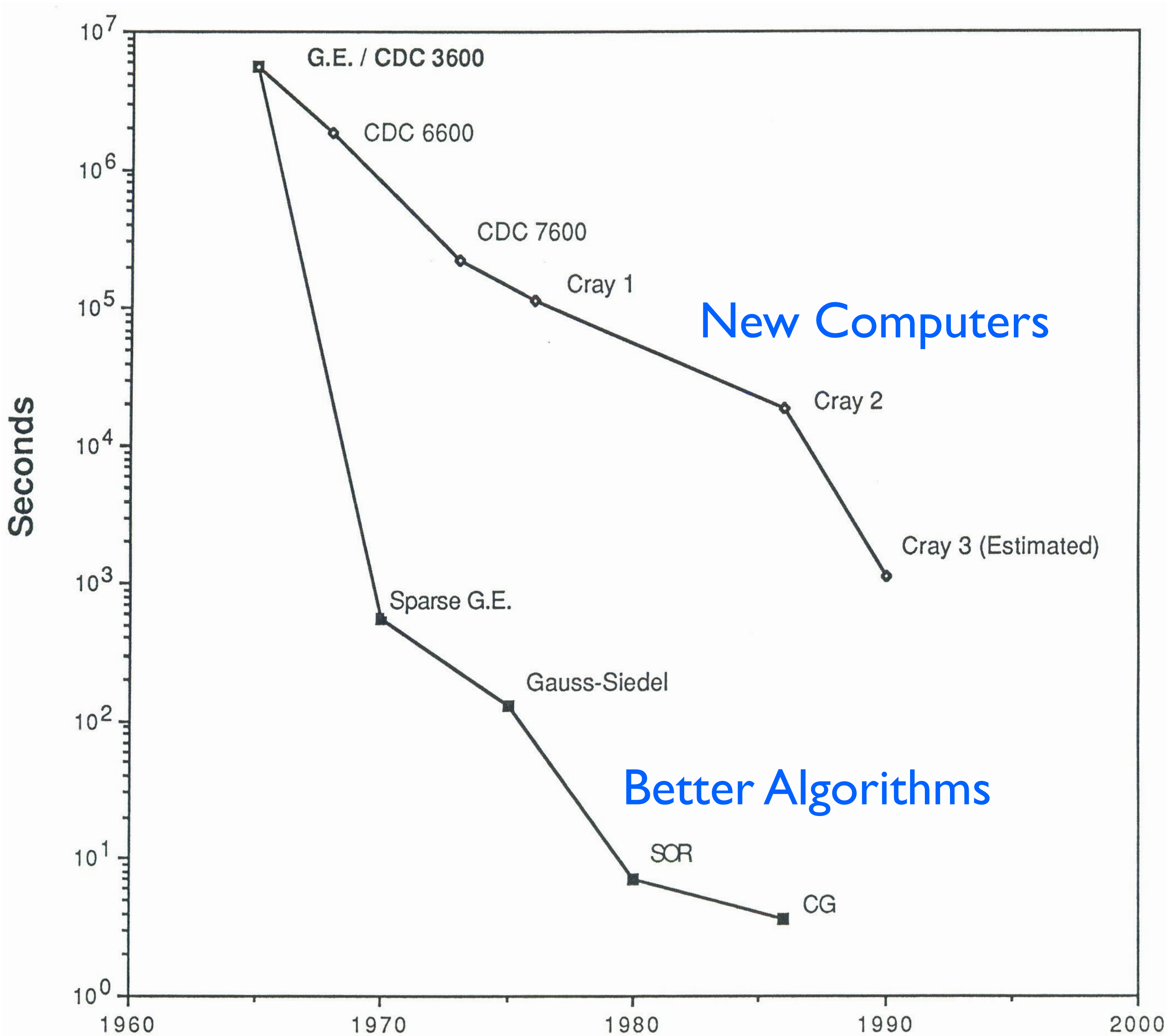
$$\begin{aligned} ||b - Ax||_\infty &= ||Ex||_\infty \\ &\leq 8n^3\rho||A||_\infty\mu||x||_\infty \\ &\approx \mu||A||_\infty||x||_\infty \end{aligned}$$

MODEL PROBLEM

- POISSON'S EQUATION
  - Steady state heat flow
  - Electrostatics
  - Simple diffusion
  - Simple fluid flow

- 3-Dimensional Geometry
- 30,000 Nodes

J.C. Meza, Presentation at SNL, 1989



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