Joys and pitfalls of numerical computing

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10/14/21

FWAM *Episode III — Revenge of the Si~~th~~ngular Value Decomposition*

[1]Center for Computational Mathematics, Flatiron Institute, Simons Foundation

Goals/outline

Crucial practical advice & good habits, examples, further reading

- how does accuracy improve with effort? *rate of convergence*
- finite-precision ("rounding error") considerations
- what accuracy is *reasonable* to demand? conditioning of a *problem*
- did you mess up getting such accuracy? stability of an *algorithm*

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Please ask questions*

$*$ with finite time-frequency product ☺

PS I will ask YOU questions ☺

Accuracy: how much to you need? have?

Usually care about *relative* error: $\varepsilon := \frac{\text{size of error of thing}}{\text{size of thing}} = \frac{|y_{\text{computed}} - y_{\text{true}}|}{|y_{\text{true}}|}$

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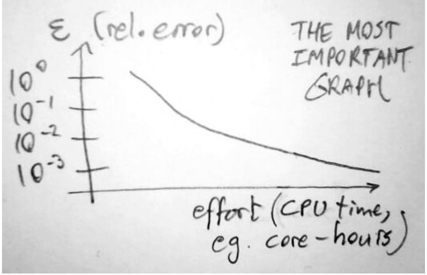
In our line of work there is really only one graph that matters:



- useful to measure and/or understand this even for simple tasks
- is crucial for larger tasks! methods differ in graph shapes (rates)

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Convergence of a computational routine/method

Often a routine has one (usually many) *convergence parameters*: "dials"

eg how many iterations you run an iterative method, resolution $h = 1/N$ in discretization, number of terms in summing a series, depth/width of a neural net, # of input data, # independent samples you average, size of box (or # particles) in a random simulation, ... and convergence parameters of any sub-functions called inside your beast

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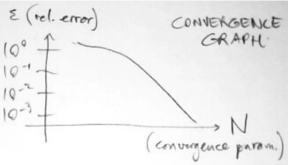

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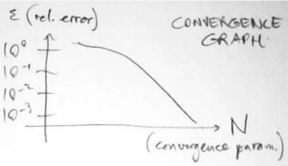

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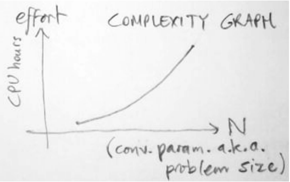

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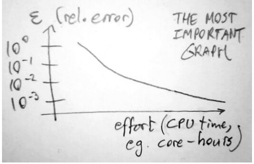

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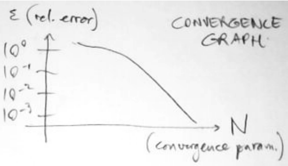

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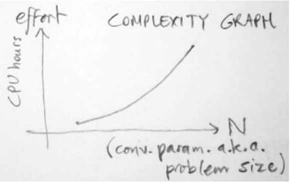

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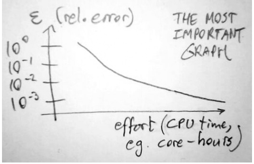

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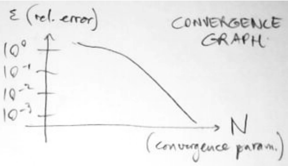

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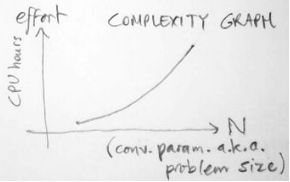

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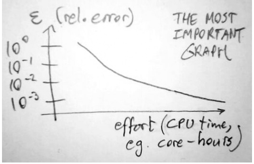

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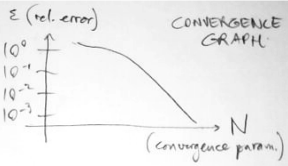

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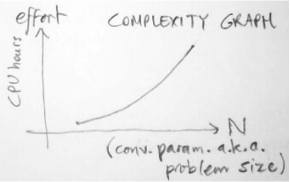

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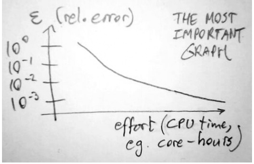

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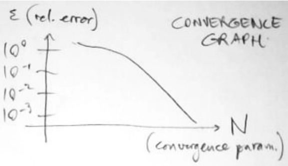

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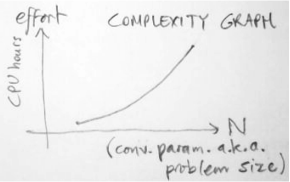

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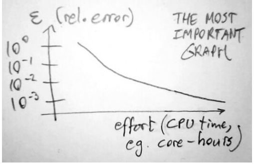

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- some useful methods do *not* converge, eg asymptotic methods

$(\sqrt{\pi}/2)\,\mathrm{erfc}(x) := \int_x^\infty e^{-t^2}dt = e^{-x^2}(1/2x - 1/4x^3 + \dots)$ please don't use $N\to\infty$ terms!

Convergence $\varepsilon(N)$: EXAMPLE I (series)

Toy example: goal compute $y := 1 + \frac{1}{4} + \frac{1}{9} + \cdots = \sum_{k=1}^{\infty} k^{-2}$

```
function y = truncsum(N)
y = 0;
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Expected accuracy $\varepsilon(N)$?

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10^2	1.63498390018489
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10^6	1.64493306684877
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Quick to experiment with your func:

- "self-convergence" to unknown y_{true} digits "freeze"

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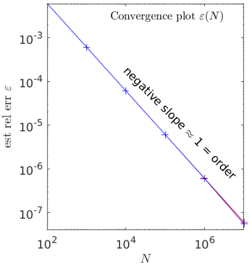
Quick to experiment with your func:

- "self-convergence" to unknown y_{true} digits "freeze"
- Rate? Use your best y as y_{true}, plot errors relative to it.

see $\varepsilon(N) \sim cN^{-1}$ 1st-order, algebraic $\rightarrow$ use loglog plot:



math: rigorous tail bnds $\varepsilon(N) \leq \int_N^{\infty} k^{-2} dk = N^{-1}$

rigor unusual; but think, read, measure the rate, compare!

- slow! accelerate? Richardson (etc) extrapolation

Convergence: EXAMPLE II (toy big PCA)

Given $M \times N$ dense matrix A big, eg $M = 40000$ genes, $N = 20000$ samples, 7 GB

Seek $\sigma_1(A) = \sqrt{\lambda_{\max}(A^T A)}$, and assoc. singular vec. $\mathbf{v}_1$ 1st cmpnt, PCA

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Simple method: power iteration on $A^T A$ takes 14 s; `svd(A)` would be ~ 1 hr

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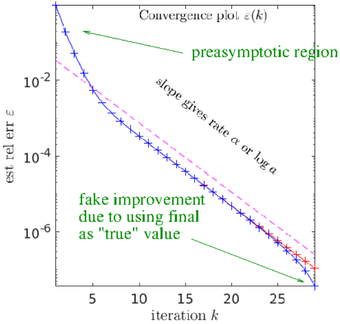

- See $\varepsilon \sim ca^k = ce^{-\alpha k}$ → use log-lin. plot. Called geometric/exponential conv.
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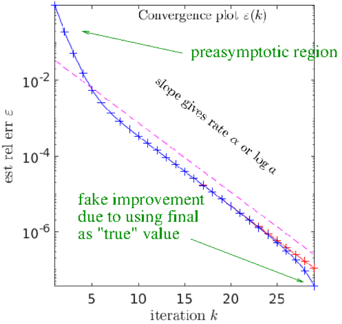

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But much better methods exist: *Randomized SVD*, Lanczos ($A^T A$)

$\rightarrow$ lesson is not "code your own methods", rather "test convergence"!

Convergence: EXAMPLE III (stochastic)

Monte Carlo: iid samples y_j drawn from a pdf p
simple task: estimate $\mu := \int yp(y)dy$?

usual estimator $\hat{\mu} = \frac{1}{N}\sum_{j=1}^{N} y_j$ sample mean

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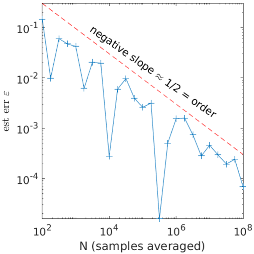
- convergence $\frac{1}{2}$-order (theory: CLT) $\rightarrow$ v. slow!
- error ε stochastic $\rightarrow$ now conv. accel. not poss.



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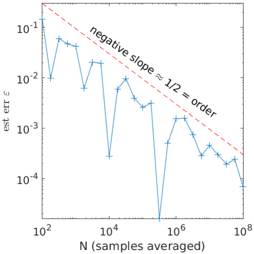

OTHER CONVERGENCE EXAMPLES

- Taylor series, poly interpolants: exponential $\varepsilon \sim e^{-\alpha N}$ if func analytic

  once you have them, integrate/differentiate *analytically*: spectral methods (Dan, Fri 11:30am)
- Newton methods (root-find in $\mathbb{R}$, or min in $\mathbb{R}^d$): $\varepsilon \sim e^{-cN^2}$ "quadratic"

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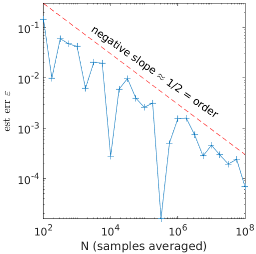

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Point isn't to memorize rates of methods: rather *measure* them (type & prefactor) by habit in any routine you use/write

Then you can pick a good N to get acceptable ε, trust results

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Floating-point representation, rounding error

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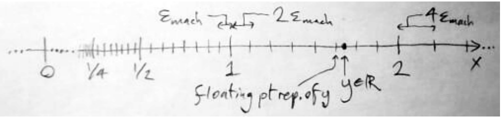

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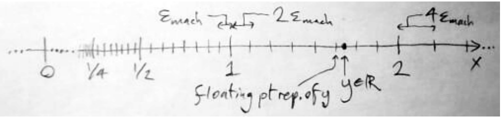

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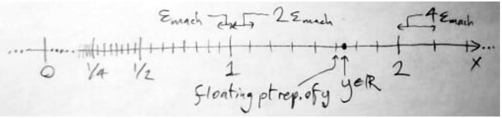

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eg, in double: `(1 + 1e-16) - 1 = ?`

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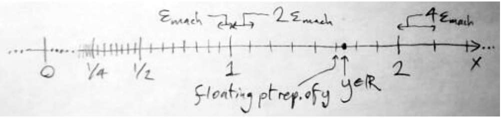

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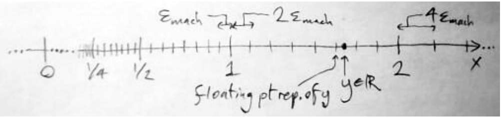

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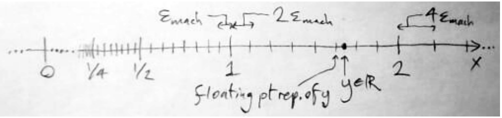

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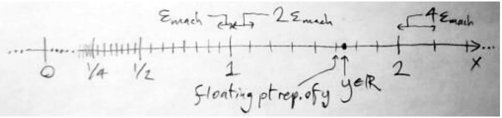

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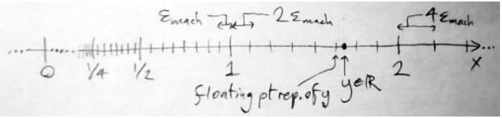

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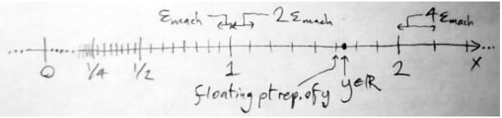

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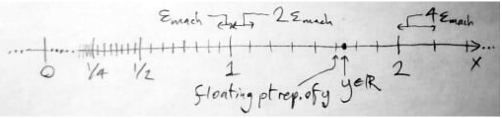

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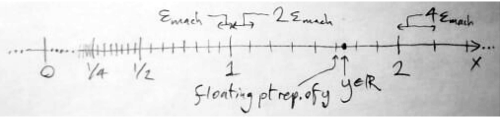

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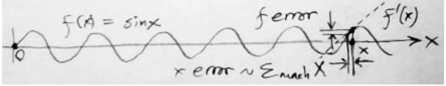

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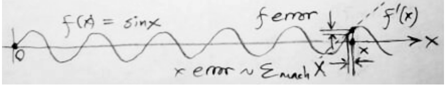

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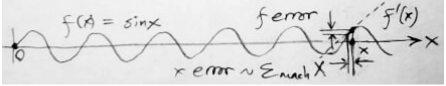

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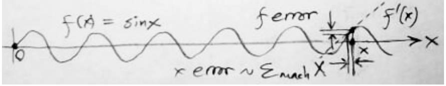

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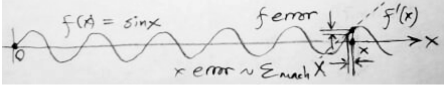

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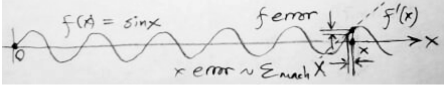

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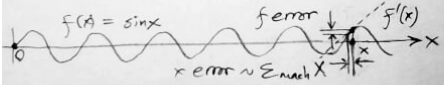

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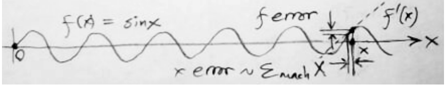

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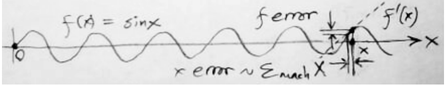

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Thus: backward stable $\Rightarrow$ rel. err. $\varepsilon = \mathcal{O}(\kappa \varepsilon_{\text{mach}})$ by rule: can't demand more!

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1) Consequences for physical simulations (nonlinear ODEs, PDEs...)

Eg, task: solve ODE

$$\begin{cases} u' = F(t,u) & \text{for } 0 \le t \le T \\ u(0) = x & \text{initial condition} \end{cases}$$

Output "$f(x)$" is final state $u(T)$

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here $\mathcal{O}$ implies some "small" const, eg $\lesssim 10^2$

Thus: backward stable $\Rightarrow$ rel. err. $\varepsilon = \mathcal{O}(\kappa\varepsilon_{\text{mach}})$ by rule: can't demand more!

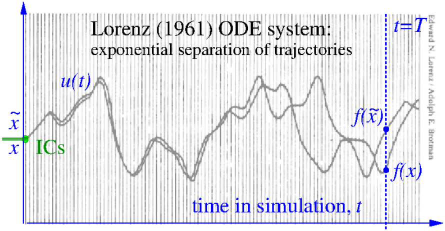
1) Consequences for physical simulations (nonlinear ODEs, PDEs. . .)

Eg, task: solve ODE

$$\begin{cases} u' = F(t,u) & \text{for } 0 \le t \le T \\ u(0) = x & \text{initial condition} \end{cases}$$

Output "$f(x)$" is final state $u(T)$

κ = sensitivity to IC



Stability of an algorithm (method) for some task

Recap: task "eval. $f(x)$" has cond. # $\kappa(x) := \left|\frac{xf'(x)}{f(x)}\right|$ indep. of any method

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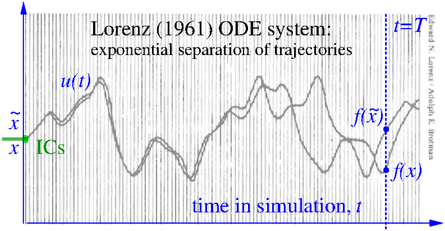

- common that $\kappa \sim e^{\lambda T}$ (Lyapunov exponent $\lambda > 0$, chaos, eg n-body sims.)
- then even stable solver must soon lose all accurate digits see: shadowing
- meaning of long-T numerics is only *statistical* (correlations, manifold, etc)

Stability of algorithms: more examples

Recap: (backward) stable if "exact answer to nearly the right question"

2) There are unstable algorithms . . . don't use them!

Eg eval. $f(x) = 1 - \cos(x)$, for $|x| \ll 1$ we all know $f(x) = x^2/2 + \mathcal{O}(x^4)$

ALWAYS FIRST ASK: Is *task* (problem) well-conditioned?

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Task is $\mathbf{f}(\mathbf{b}) =$ "$\mathbf{c}$ solving $A\mathbf{c} = \mathbf{b}$" brain hurts because $\mathbf{b}$ is input, $\mathbf{c}$ is output!

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Defn. relative residual of $\tilde{\mathbf{c}}$ is $\frac{\|A\tilde{\mathbf{c}}-\mathbf{b}\|}{\|\mathbf{b}\|}$:

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- even a stable alg doesn't mean $\tilde{\mathbf{c}}$ is close to $\mathbf{c}$ . . .

Let's demo a classic *unstable algorithm* . . .

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MATLAB demo: unstable vs stable linear solve

```
>> c = [1;2;3];                              % "true" solution column vector
>> A = ones(3,3) + 1e-14*rand(3,3)           % system matrix (precisely: ill-cond.)
A =       1.00000000000001         1.00000000000001                        1
          1.00000000000001         1.00000000000001         1.00000000000001
                         1                        1         1.00000000000001
>> b = A*c;                                  % make data (input to solver)
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Now let's do some solving. . .

```
>> ct = inv(A)*b;                     % classic pitfall, may be unstable
>> norm(A*ct-b) / norm(b)             % rel resid terrible, proving it's unstable!
                  0.046875
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      8.54650082837135e-17
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```

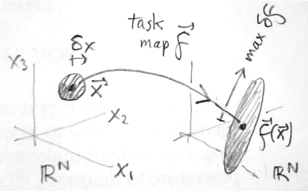
If time: here's one stable way to store a soln operator...

```
[U,S,V] = svd(A); W = diag(1./diag(S))*U';    % inv(A)=VW, need two factors
ct = V*(W*b);                                 % apply them to any RHS
norm(A*ct-b) / norm(b)                        % rel resid again O(e_mach)
      2.83455365181694e-16
```

If time: conditioning of linear systems

For vector map $\mathbf{f}(\mathbf{x})$, condition number is

$$\kappa(\mathbf{x}) := \lim_{\delta x \to 0} \sup_{\|\delta \mathbf{x}\| \le \delta \mathbf{x}} \frac{\|\delta \mathbf{f}\| / \|\mathbf{f}\|}{\|\delta \mathbf{x}\| / \|\mathbf{x}\|}$$



- Lin. solve task: can show $\kappa(\mathbf{b}) \le \kappa(A) := \|A\|\,\|A^{-1}\| = \frac{\sigma_1(A)}{\sigma_N(A)}$ or ∞

Consequence for how accurate solution $\tilde{\mathbf{c}}$ is? Let $\varepsilon = \frac{\|\tilde{\mathbf{c}} - \mathbf{c}\|}{\|\mathbf{c}\|}$ rel. soln. err.

Now recall: stable solver (best you can demand) has $\varepsilon = \mathcal{O}(\kappa \varepsilon_{\text{mach}})$

if A ill-cond, natural that $\mathbf{c}$ floppy in certain directions, since residual small

- Idea useful in inverse problems: replace $\varepsilon_{\text{mach}}$ by meas. err; reverse above pic!

Idea to sample *all* $\mathbf{c}$ consistent w/ small residual $\to$ Bayes Inv. Prob. (Bob, Fri 9:10am)

Recap

- Convergence rates (type & prefactor) key to *measure* and understand
- Finite-precision $\varepsilon_{\text{mach}}$ can be amplified by catastrophic cancellation
- Before methods, first understand condition # of your *problem*

  condition number of problem combines with $\varepsilon_{\text{mach}}$ to limit accuracy of *any* method
- Stable methods: solve exactly some $\varepsilon_{\text{mach}}$-perturbation of problem

  "(un)stable" vs "ill-conditioned" have precise definitions: learn and use!

  check for unstable method and avoid
- For linear systems: "stable" $\Leftrightarrow$ finds relative residual $\mathcal{O}(\varepsilon_{\text{mach}})$

References for today material

- *Numerical Methods*. Anne Greenbaum & Tim Chartier. book (2012)
- *Numerical Linear Algebra*. Trefethen & Bau. book (1997)

Convergence acceleration and all-round fun:

- *The SIAM 100-Digit Challenge*. book (2004)

Randomized SVD, PCA, and big matrix factorizations:

- Halko, Martinsson & Tropp. *SIAM Rev.* **53**(2) 217–288 (2011)
- Martinsson's slides at `http://users.oden.utexas.edu/~pgm`

I will host slides at `https://users.flatironinstitute.org/~ahb`
(also see: 2019 FWAM on interpolation & quadrature; Burns on PDE)

Starting new Sci. Comput. Seminar & Concepts, 9:45am Tues, 3rd fl.

(fortnightly from 10/26, see Indico)

THANK-YOU!

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