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M\crNA
Manchester Numerical Analysis

Multiprecision Inverse Computation

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Numerical Linear Algebra Group Meeting
3 April 2019

Newton-Schulz Method

For $A \in \mathbb{R}^{m \times n}$ we have the following iterative scheme for computing A^+:

- $X_{k+1} = (2I - X_k A)X_k$, $X_0 = \alpha A^T$.
- Denoting $E_k = I - X_k A$, we have that $E_{k+1} = E_k^2 = \cdots = E_0^{2^{k+1}}$ and so require $\|I - \alpha A^T A\|_2 < 1$ for convergence.
- Require $0 < \alpha < 2/\|A\|_2^2$.
- For all results shown we use $\alpha = 1/(\|A\|_1 \|A\|_\infty)$.

Newton-Schulz Method

Convergence test: Define

$$\text{res}_L = \frac{\|I - X_k A\|_\infty}{\|X_k\|_\infty \|A\|_\infty}.$$

We assume convergence when $\text{res}_L < \epsilon$, the machine epsilon of the precision in which we are working.

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- If $\kappa_2(A) = 10^8$, we require at least 53 iterations.

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Expensive!

Increasing Precision

- Given a sequence of increasing precisions, we perform the iteration in a given precision until we obtain convergence and then increase the precision.
- That is $\text{res}_L < \epsilon_p$, with ϵ_p the machine epsilon of the relevant precision.
- For all experiments shown, we use **fp16** $\rightarrow$ **fp32** $\rightarrow$ **fp64**.

Simulating fp16

- We use the newly released `chop` from Higham & Pranesh (2019) to simulate IEEE half precision in MATLAB.
- **`https://github.com/higham/chop`**
- Perform each scalar operation in **fp64** or **fp32** and round to **fp16**.

Computing $AB = \sum_{k=1}^{n} A(:,k)B(k,:)$, we call `chop` only $\mathcal{O}(n)$ times.

Numerical Results

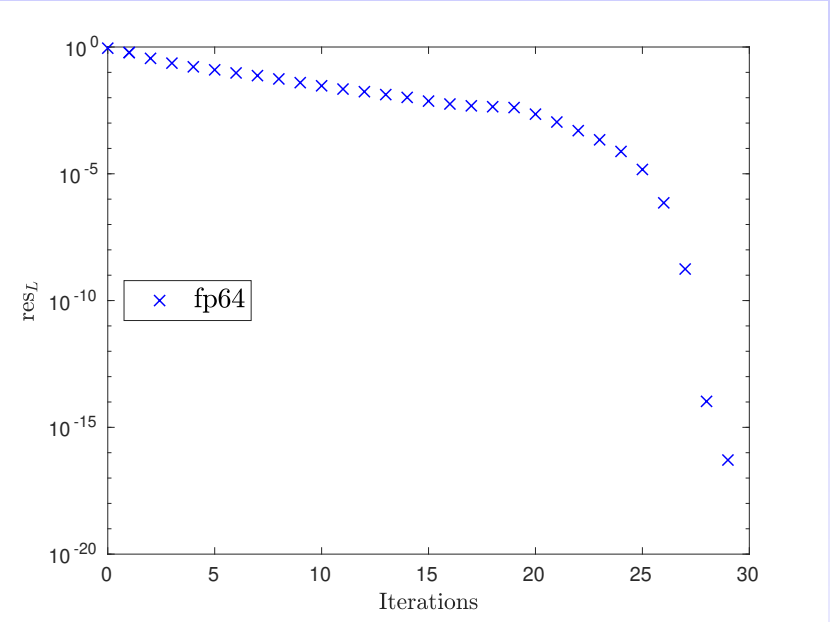

Figure 1: **fp64** implementation.

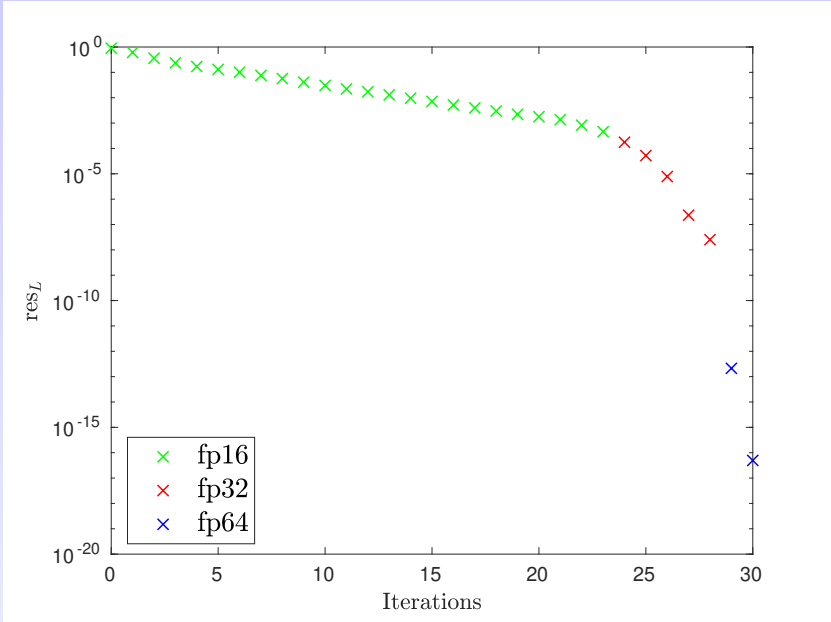

Figure 2: Increasing precision implementation.

In both we have A sampled from $\mathcal{N}(0,1)$ and $n = 100$. Here $\kappa_2(A) \approx 7e+02$.

Numerical Results

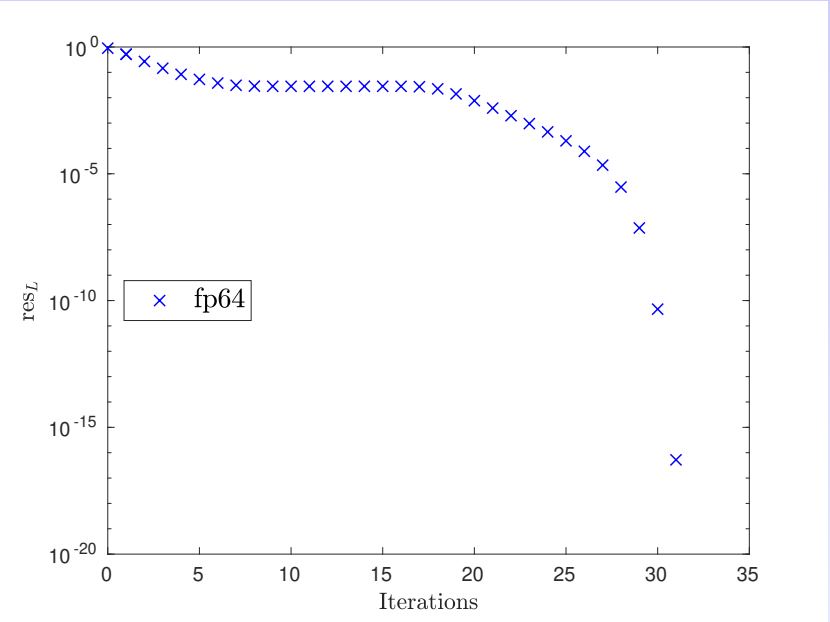

Figure 3: **fp64** implementation.

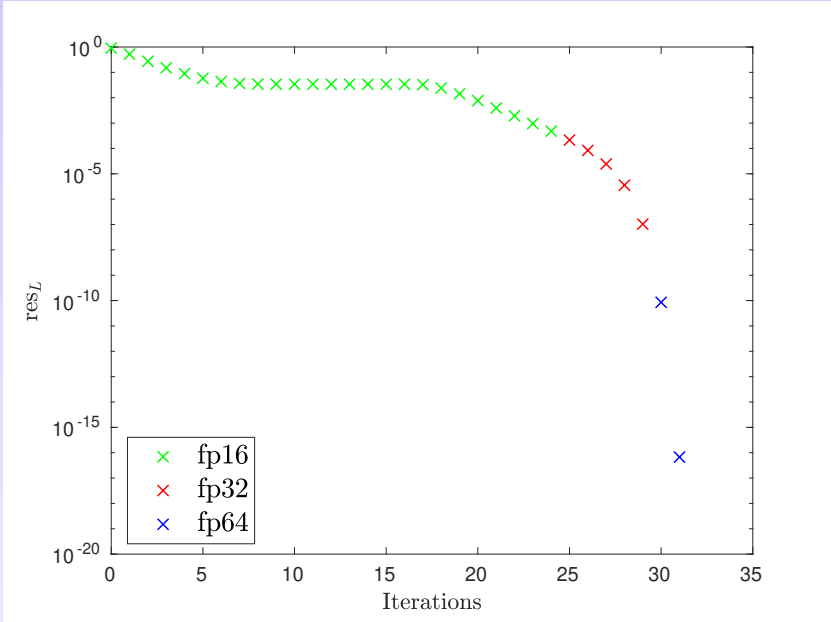

Figure 4: Increasing precision implementation.

Here A is from `gallery('randsvd')` with $n = 100$ and $\kappa_2(A) = 1e+03$.

Acceleration

Pan & Schreiber (1991) introduce two forms of acceleration.

- **Scaling:** Compute α at each iteration so that we now have $X_{k+1} = \alpha_{k+1}(2I - X_k A)X_k$.
- **Cubic polynomials:** For $\rho > 0$ and $T_k = X_k A$, compute $X_{k+1} = (1/\rho)(T_k^2 - (2+\rho)T_k + (1+2\rho)I)X_k$.

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We compute $\delta = \|T_k - T_k^2\|_F$ and $\bar{\delta} = \delta/n$. If $\text{trace}(T_k) < n - 1/2$ then:

- If $\delta > 1/4$ and $\bar{\delta} < 1/4$, we accelerate by scaling.
- If $\delta < 1/4$ we accelerate with cubic polynomials.
- Here $\rho = 1/2 - \sqrt{1/4 - \delta}$, $\bar{\rho} = 1/2 - \sqrt{1/4 - \bar{\delta}}$ and $\alpha_{k+1} = 2/(1 + (2 - \bar{\rho})\bar{\rho})$.

Preconditioning the iteration

Computing LU factors in low precision, we can then compute $\tilde{A} = U^{-1}L^{-1}A$.

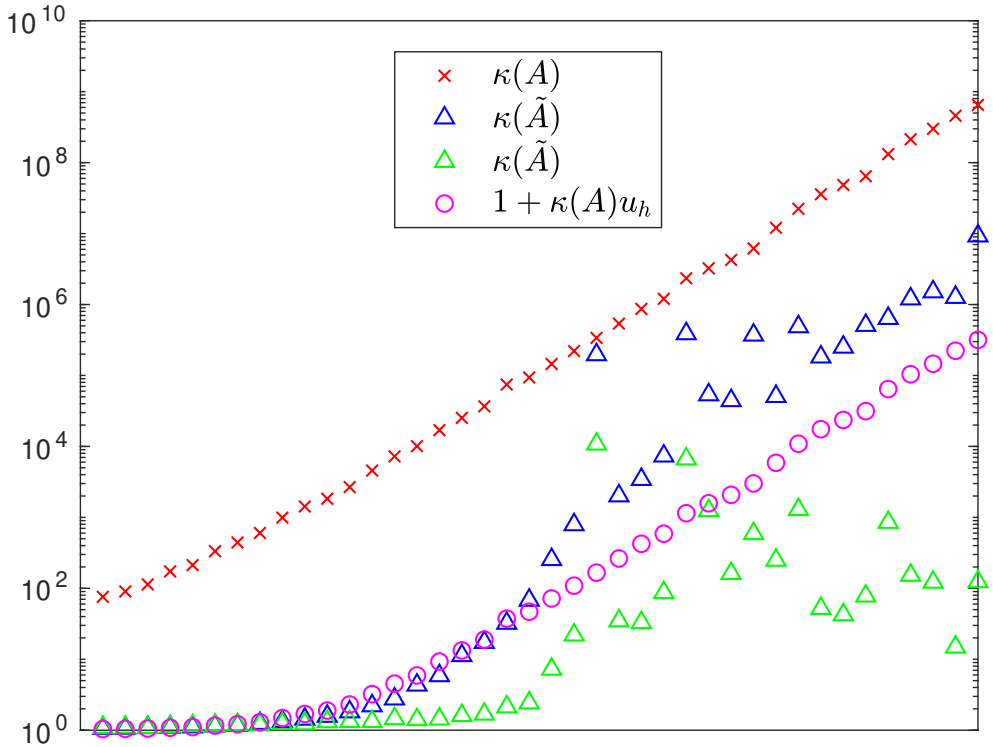
We don't form these inverses explicitly, but instead compute $\tilde{A}$ by a set of triangular solves.

Higham & Carson (2017) verify the relation

$$\kappa_\infty(\tilde{A}) \approx 1 + \kappa_\infty(A)u.$$

Preconditioning the Iteration

- Must compute the solves in **fp64** to recover a solution accurate to **fp64**.
- How does this mixture of precisions affect the approximation?



Improved Iteration

LU factors computed in **fp16**, triangular solves computed in **fp64**.

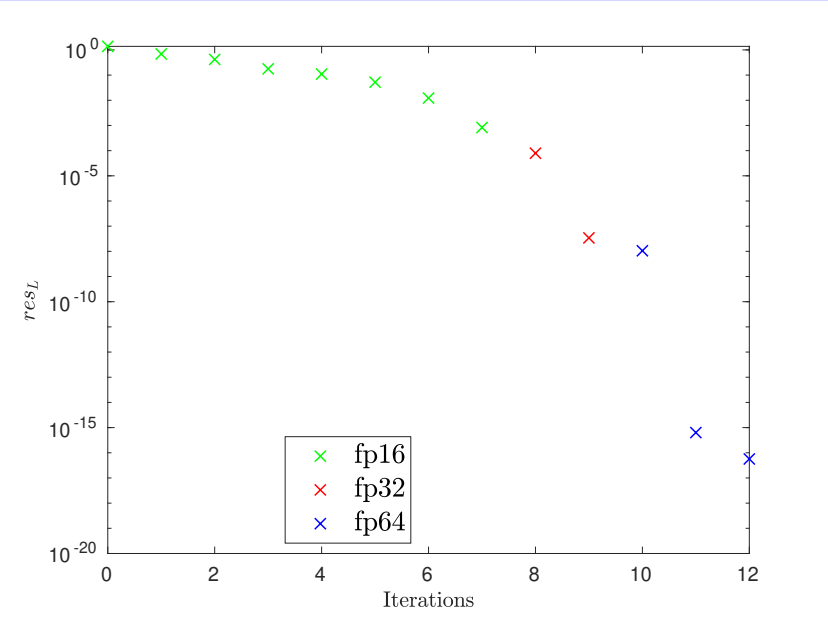


Figure 6: A sampled from $\mathcal{N}(0,1)$ with $\kappa_2(A) \approx 1e+03$.

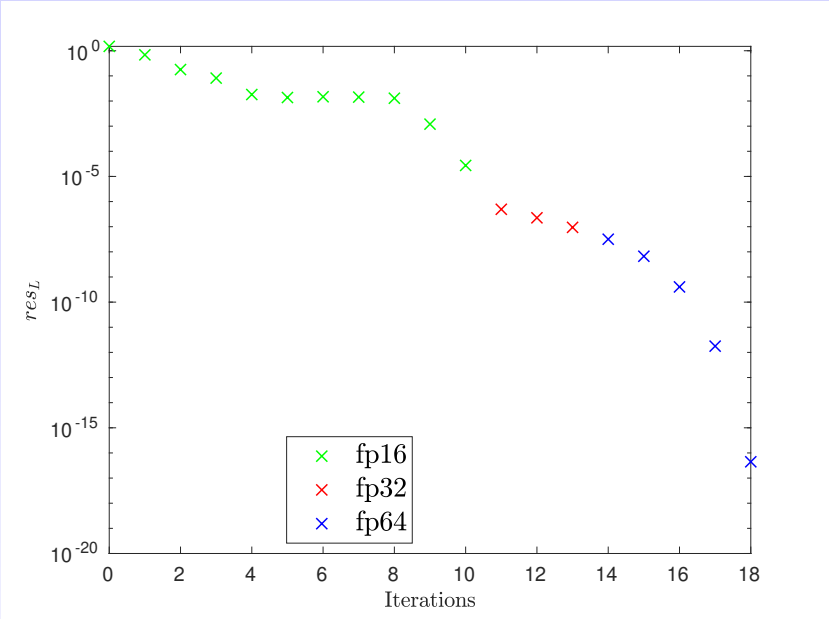


Figure 7: $\kappa_2(A) = 1e+08$ with one small singular value.

Iterative Refinement

Higham & Carson (2017, 2018) present results from iterative refinement in three precisions (u_f, u, u_r).

Algorithm 1 Iterative refinement in three precisions.

1: Compute LU factors $A = \hat{L}\hat{U}$ in precision u_f.
2: Solve $Ax_0 = b$ in precision u_f using the LU factors and store at precision u.
3: **for** $i = 0 : \infty$ **do**
4: Compute $r_i = b - Ax_i$ in precision u_r
5: and round to precision u.
6: Solve $\tilde{A}d_i = \hat{U}^{-1}\hat{L}^{-1}r_i$ at precision u by GMRES.
7: $x_{i+1} = x_i + d_i$ at precision u.
8: **end for**

Alternative Preconditioning

- Instead of the LU factors, we precondition the GMRES solves with B, a low precision approximation to A^{-1} obtained iteratively.

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- Instead of the LU factors, we precondition the GMRES solves with B, a low precision approximation to A^{-1} obtained iteratively.
- We compare results of these variants of iterative refinement:

	$\kappa_2(A)$	$\kappa_\infty(A)$	LU cost	B cost
1	$1e+04$	$9e+04$	$2(17)$	$2(4)$
2	$1e+06$	$7.4e+06$	$3(185)$	$2(75)$
3	$1e+09$	$2.01e+10$	$-(-)$	$9(45)$

- We show total number of iterative refinement steps and GMRES iterations, shown in parentheses, required.
- 1 and 2 above are the default of `gallery('randsvd')` and 3 contains one small singular value.

Alternative Preconditioning

- Obtaining B much more expensive than LU factors.
- As seen earlier, we need to precondition the Newton-Schulz iteration to obtain convergence. We must also compute relevant triangular solves, done in **fp32** here.
- Try more values of (u_f, u, u_r).

Questions?

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