Filtered Anderson acceleration for nonlinear PDEs

Sara Pollock
UNIVERSITY of FLORIDA
Department of Mathematics

Joint work with:
Leo Rebholz (Clemson University),

47th Annual Spring Lecture Series
University of Arkansas
May 4-6, 2022

DMS-{2011519}

Anderson acceleration theory | **Extrapolation for eigenvalue problems**

Students

Matt Dallas

Rhea Shroff

Simon Kato

Simon Kato

Funding

NSF DMS-$\{1852876, 2011519\}$

NSF DMS-2045059(CAREER)

Outline

- Intro and algorithm
- Some questions
- Some theory
- Using theoretical advances to improve performance
- Examples

Fixed-point iteration

Suppose

- X is a complete normed vector (Banach) space
- $\phi : X \to X$ is Lipschitz continuous: $\|\phi(x) - \phi(y)\| \leq \kappa \|x - y\|$

Fixed-point problem: Find $x \in X$ such that $\phi(x) = x$

Fixed-point iteration: Given $x_0 \in X$, set $x_{k+1} = \phi(x_k)$

Error analysis

$$\|x_{k+1} - x\| = \|\phi(x_k) - \phi(x)\| \leq \kappa \|x_k - x\|$$

If $\kappa < 1$, there is a unique fixed-point $x \in X$, and $x_k \to x$ at linear rate κ

- If $\kappa \ll 1$, great!
- If $\kappa < 1$ but $\kappa \approx 1$, no so great!
- If $\kappa > 1$, it's not so clear, but it sometimes works

- **Goal:** Improve ***efficiency*** and ***robustness*** of the iteration
- **Idea:** Use a history of previous iterates to improve the approximation

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Anderson acceleration (D. G. Anderson, 1965)

Fixed-point iteration:

$$x_{k+1} = \phi(x_k) = x_k + w_{k+1}, \quad w_{k+1} = \phi(x_k) - x_k$$

(Anderson iteration with depth m) Set (maximal) depth $m \geq 0$

Choose x_0

Compute $w_1 = \phi(x_0) - x_0$. Set $x_1 = x_0 + w_1$

For $k = 1, 2, 3, \ldots$ Set $m_k \leq \min\{k, m\}$

- -Compute $w_{k+1} = \phi(x_k) - x_k$
- -Solve: $\gamma^{k+1} = \text{argmin} \left\| w_{k+1} - F_k \gamma^{k+1} \right\|$
- -Set damping (mixing) parameter β_k ($\beta_k = 1 \Leftrightarrow$ no damping)
- -Update $x_{k+1} = \underbrace{x_k + \beta_k w_{k+1}}_{\text{f. p. update}} - \underbrace{\left(E_k \gamma^{k+1} + \beta_k F_k \gamma^{k+1}\right)}_{\text{correction}}$

where

$$E_k := \begin{pmatrix} e_k & e_{k-1} & \cdots & e_{k-m_k+1} \end{pmatrix}, \quad e_k = x_k - x_{k-1}$$

$$F_k := \begin{pmatrix} (w_{k+1} - w_k) & (w_k - w_{k-1}) & \cdots & (w_{k-m_k+2} - w_{k-m_k+1}) \end{pmatrix}$$

- E_k, F_k each have m_k columns
- γ^{k+1} is the vector of optimization coefficients
- θ_{k+1} is the gain from the optimization problem: $\|w_{k+1} - F_k \gamma^{k+1}\| = \theta_{k+1} \|w_{k+1}\|$

Example: Anderson applied to Picard for steady NSE

Picard iteration for steady Navier-Stokes (moving lid problem)

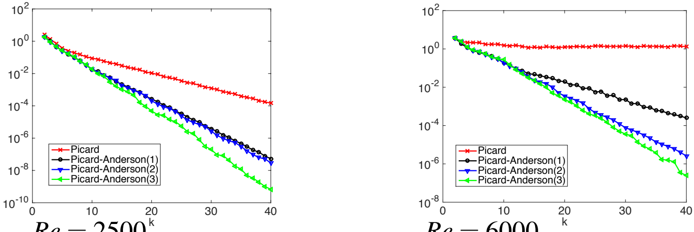
$\tilde{u}_k = \phi(u_{k-1}), \quad w_k = \tilde{u}_k - u_{k-1}$

- Choose $u_0 \in X_h$. For $k \geq 1$: Find $(\tilde{u}_k, \tilde{p}_k) \in (X_h, Q_h)$ s.t. for all $(v, q) \in (X_h, Q_h)$

$$b^*(u_{k-1}, \tilde{u}_k, v) - (\tilde{p}_k, \nabla \cdot v) + \nu(\nabla \tilde{u}_k, \nabla v) = (f, v)$$
$$(\nabla \cdot \tilde{u}_k, q) = 0$$

$$b^*(u, v, w) := (u \cdot \nabla v, w) + \frac{1}{2}((\nabla \cdot u)v, w)$$

- $(X_h, Q_h) = (\mathcal{P}_2, \mathcal{P}_1)$ Taylor-Hood elements, meshsize $h = 1/256$; 592,387 DOF. (Continuous piecewise quadratic space for velocity, continuous piecewise linear space for pressure on a triangular mesh)
- Domain: $\Omega = (0,1)^2$; no forcing $f = 0$; kinematic velocity $\nu = 1/Re$
- 'Moving lid" $u(x,1) = \langle 1, 0 \rangle^T$, no-slip (zero-velocity) condition on other sides

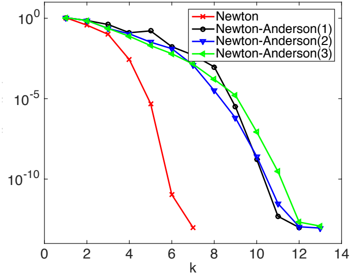


$Re = 2500$ $\qquad$ $Re = 6000$

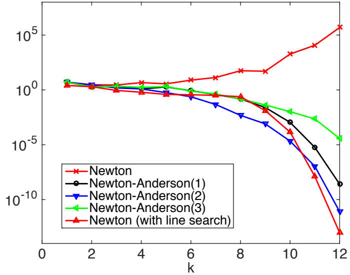
Example: Anderson applied to Newton for steady NSE

Choose $u_0 \in X_h$
For $k \geq 1$: Find $(u_k, p_k) \in (X_h, Q_h)$ satisfying for all $(v, q) \in (X_h, Q_h)$

$$b^*(u_{k-1}, u_k, v) + b^*(u_k, u_{k-1}, v) - b^*(u_{k-1}, u_{k-1}, v) - (p_k, \nabla \cdot v) + \nu(\nabla u_k, \nabla v) = (f, v)$$
$$(\nabla \cdot u_k, q) = 0$$



$Re = 1000$



$Re = 2500$

Observe: (1) Anderson applied to Newton is *superlinear* but *subquadratic*, and (2) it is doing "something similar" to damping outsde Newton's domain of convergence.

Some history

- 1965 The "Extrapolation Method," introduced by Donald Anderson
- 1996 V. Eyert, 2009 H. Fang and Y. Saad: relation to Broyden and multisecant families of updates
- 2011 H. Walker and P. Ni: results on electronic structure computations and study of efficient and robust implementation
- 2015 A. Toth and C. T. Kelley: Local convergence theory for contractive operators
  - Convergence of Anderson(m) assuming boundedness of the optimization coefficients
  - An upper bound on the convergence rate of Anderson(1) without the boundedness assumption. **Asymptotically the converegence rate is no worse than that of the underlying fixed-point iteration**
- 2019 P., Rebholz, Xiao; 2020 Evans, P. Rebholz, Xiao, acceleration theory to establish local improvement of the convergence rate for linearly converging fixed-point iterations
- 2021 P. and Rebholz, replacement of the boundedness assumption on the optimization coefficients by filtering strategy

The method (almost) is known as Pulay mixing in computational chemistry. The literature has been quickly increasing...

Recent interests:

- Adaptive parameter selection based on recent theory
- Newton-specific theory

Some questions

1. When should we use it?
2. How should we set the damping?
3. How should we set the depth m_k?
4. Do the columns of the matrix F_k we use for the least-squares problem get more linearly dependent as iterations continue?
5. **Can we improve the iteration by selecting which previous steps to use?**

Answer key: (2) dynamically; (3) dynamically;
(4) not necessarily; (5) **Yes! Our acceleration theory leads to a filtering strategy**

Extra credit: What does the picture have to do with filtering?

One-step residual bound

Theorem (P., Rebholz, 2021 (Anderson acceleration for contractive and noncontracive iterations, IMA J. Numer. Anal.)**)**

Suppose some conditions that we are about to discuss. Then the residual $w_{k+1} = g(x_k) - x_k$ from depth m acceleration satisfies the following bound

$$\|w_{k+1}\| \leq \|w_k\| \Bigg(\theta_k ((1-\beta_{k-1}) + \kappa\beta_{k-1}) + \frac{C(\sigma, c_s)\hat{\kappa}\sqrt{1-\theta_k^2}}{2} \Big(\|w_k\| h(\theta_k) + 2 \sum_{n=k-m_{k-1}+1}^{k-1} (k-n)\|w_n\| h(\theta_n) + m_{k-1} \|w_{k-m_{k-1}}\| h(\theta_{k-m_{k-1}}) \Big) \Bigg)$$

where each $h(\theta_j) \leq C\sqrt{1-\theta_j^2} + \beta_{j-1}\theta_j$, and C depends on c_s (sufficient linear independence of columns of each F_j)

For the fixed-point algorithm with the same damping factor β_{k-1}

$$\|w_{k+1}\| \leq ((1-\beta_{k-1}) + \kappa\beta_{k-1}) \|w_k\|$$

The first order term improves by factor θ_k

Higher-order terms are introduced, and they are scaled by factor $\sqrt{1-\theta_k^2}$

First residual bound

We'll assume the fixed-point operator ϕ is continuously Fréchet differentiable

Assumption

Assume $\phi \in C^1(X)$ *has a fixed point* x^* *in* X*, and there are positive constants* κ *and* $\hat{\kappa}$ *with*

(1) $\|\phi'(x)\| \le \kappa$ *for all* $x \in X$*, and*
(2) $\|\phi'(x) - \phi'(y)\| \le \hat{\kappa}\|x - y\|$ *for all* $x, y \in X$

After some Taylor expansions and triangle inequalities... $(e_j = x_j - x_{j-1})$

$$\|w_{k+1}\| \le \|w_k - F_{k-1}\gamma^k\| \left((1-\beta_{k-1}) + \kappa\beta_{k-1}\right) + \frac{\hat{\kappa}}{2} \sum_{n=k-m_{k-1}}^{k-1} \left(\|e_{n+1}\| + \|e_n\|\right) \sum_{j=n}^{k-1} \|e_j \gamma_j^k\|$$

$$= \theta_k \|w_k\| \left((1-\beta_{k-1}) + \kappa\beta_{k-1}\right) + \frac{\hat{\kappa}}{2} \sum_{n=k-m_{k-1}}^{k-1} \left(\|e_{n+1}\| + \|e_n\|\right) \sum_{j=n}^{k-1} \|e_j \gamma_j^k\|$$

Compare: with damping factor β_{k-1} and no acceleration

$$\|w_{k+1}\| \le \|w_k\| \left((1-\beta_{k-1}) + \kappa\beta_{k-1}\right)$$

Optimization gain and coefficients: relating e_k to w_k

- Update: $x_{k+1} = \underbrace{x_k + \beta_k w_{k+1}}_{\text{f. p. update}} - \underbrace{(E_k \gamma^{k+1} + \beta_k F_k \gamma^{k+1})}_{\text{correction}}$, where

$$E_k := \begin{pmatrix} e_k & e_{k-1} & \cdots & e_{k-m_k+1} \end{pmatrix}, \quad e_k = x_k - x_{k-1}$$
$$F_k := \begin{pmatrix} (w_{k+1} - w_k) & (w_k - w_{k-1}) & \cdots & (w_{k-m_k+2} - w_{k-m_k+1}) \end{pmatrix}$$

- γ^{k+1} minimizes $\|F_k \gamma - w_{k+1}\|$

Suppose we're in a finite dimensional Hilbert space

- $\gamma^{k+1} = R_k^{-1} Q_k^T w_{k+1}$, where $F_k = Q_k R_k$ is a thin QR decomposition
- $\|(I - Q_k Q_k^T) w_{k+1}\| = \|w_{k+1} - F_k \gamma^{k+1}\| = \theta_k \|w_k\|$
- $\|Q_k^T w_{k+1}\| = \|F_k \gamma^{k+1}\| = \sqrt{1 - \theta_k^2}\|w_{k+1}\|$
- θ_{k+1} can be computed by $\sqrt{1 - (\|Q_k^T w_{k+1}\| / \|w_{k+1}\|)^2}$
- $x_{k+1} - x_k = E_k R_k^{-1} Q_k^T w_{k+1} + \beta_k (I - Q_k Q_k^T) w_{k+1}$

Bounding $\|e_j\|$ by $\|w_j\|$

- To close the first residual bound

$$\|w_{k+1}\| \leq \theta_k \|w_k\| \left((1-\beta_{k-1}) + \kappa\beta_{k-1}\right) + \frac{\hat{\kappa}}{2} \sum_{n=k-m_{k-1}}^{k-1} (\|e_{n+1}\| + \|e_n\|) \sum_{j=n}^{k-1} \|e_j \gamma_j^k\|$$

require the $\|e_j\|'s$ in terms of the $\|w_j\|$'s, where $e_j = x_j - x_{j-1}$

- From last slide

$$x_{j+1} - x_j = E_j R_j^{-1} Q_j^T w_{j+1} + \beta_j (I - Q_j Q_j^T) w_{j+1}$$
$$\|e_{j+1}\| \leq \left(\sqrt{1-\theta_{j+1}^2} \|E_j R_j^{-1}\| + \theta_{j+1}\beta_j\right) \|w_{j+1}\|$$

- $\|E_j R_j^{-1}\| \leq C$ under some conditions

Conditions:

$\|E_j R_j^{-1}\| \le C = C(\sigma, c_s)$ under the conditions:

1. There is a constant σ with $\|w_{j+1} - w_j\| \ge \sigma \|e_j\|$ is satisfied, for example, if either
   - The Lipschitz constant κ of ϕ satisfies $\kappa < 1$
   - The fixed-point operator is $\phi(x) = x + f(x)$ (used to seek a zero of f), and the smallest singular value of $f'(x)$, the Jacobian of f at x, is bounded away from zero in the vicinity of a solution

2. There is a constant $c_s > 0$ with $|\sin(f_{j,i}, \text{span}\{f_{j,1}, \ldots, f_{j,i-1}\})| \ge c_s$, where $f_{j,i}$ are the columns of F_j
   - This is easily checked and enforcing it gives a novel and efficient filtering strategy!
   - For $F = QR$, $r_{ii} = \|f_i\| \sin(f_i, \text{span}\{f_1, \ldots, f_{i-1}\})$, so $|\sin(f_i, \text{span}\{f_1, \ldots, f_{i-1}\})| = r_{ii} / \|f_i\|$
   - The "sufficient linear independence" condition (or enforcement) replaces the common assumption that the optimization coefficients are bounded

The next part looks a little fancy, but it just quantifies how much the columns of F not being orthogonal messes things up, in terms of the constant c_s

A linear algebra lemma

Bounding $\|E_j R_j^{-1}\|$ by a constant requires one more result. It's probably a known result, but we couldn't find it (we proved it by induction).

Lemma

Let $\hat{Q}\hat{R}$ be the economy QR decomposition of matrix $F \in \mathbb{R}^{n\times m}$, $n \geq m$, where F has columns $f_1, \ldots f_m$, $\hat{Q}$ has orthonormal columns $q_1, \ldots q_m$, and $\hat{R} = (r_{ij})$ is an invertible upper-triangular $m \times m$ matrix. Let $\hat{R}^{-1} = (s_{ij})$ and $\mathcal{F}_j = \text{span}\{f_1, \ldots f_j\}$.

Suppose there is a constant $0 < c_s \leq 1$ such that $|\sin(f_j, \mathcal{F}_{j-1})| \geq c_s$, $j = 2, \ldots, m$, which implies another constant $0 \leq c_t < 1$ with $|\cos(a_j, q_i)| \leq c_t$, $j = 2, \ldots, m$ and $i = 1, \ldots, j-1$. Then it holds that

$$s_{11} = \frac{1}{\|f_1\|}, \qquad s_{ii} \leq \frac{1}{\|f_i\| c_s}, \; i = 2, \ldots, m,$$

$$|s_{1j}| \leq \frac{c_t(c_t + c_s)^{j-2}}{\|f_1\| c_s^{j-1}}, \; \text{and} \qquad |s_{ij}| \leq \frac{c_t(c_t + c_s)^{j-i-1}}{\|f_i\| c_s^{j-i+1}}, \; \text{for}$$

$i = 2, \ldots, m-1$ and $j = i+1, \ldots, m$.

Bounding $\|E_j R_j^{-1}\|$

Denote $\widehat{R} = R_j$ and $S = \widehat{R}^{-1}$

- Expanding, $\|E_j\hat{R}^{-1}\| = \|\begin{pmatrix} e_j \sum_{n=1}^m s_{1n} & e_{j-1} \sum_{n=2}^m s_{2n} & \cdots & e_{j-m+1} s_{mm} \end{pmatrix}\|$
- For column 1 apply the lemma, first condition, and finite geometric sum

$$\|e_j \sum_{n=1}^m s_{1n}\| \le \|e_j\| \left| \sum_{n=1}^m s_{1n} \right| \le \frac{\|e_j\|}{\|w_{j+1} - w_j\|} \left(1 + \sum_{n=2}^m \frac{c_t (c_t + c_s)^{n-2}}{c_s^{n-1}} \right) \le \sigma^{-1} \left(\frac{c_t + c_s}{c_s} \right)^{m-1}$$

For columns $p = 2, \ldots, m = m_k$

$$\|e_{j-p+1} \sum_{n=p}^m s_{pn}\| \le \frac{1}{\sigma c_s} \left(1 + \sum_{n=p+1}^m \frac{(c_t + c_s)^{n-(p+1)}}{c_s^{n-p}} \right) \le \frac{1}{\sigma c_s} \left(\frac{c_t + c_s}{c_s} \right)^{m-p}$$

For $(c_s, c_t) \neq (1, 0)$, adding all the contributions bounds $\|E_j \hat{R}^{-1}\|$ by

$$\sigma^{-1} \left(\frac{(c_t + c_s)^{m-1}(c_t + 1) - c_s^{m-1}}{c_s^{m-1} c_t} \right) = \sigma^{-1} \left(1 + \frac{(1 + c_t) \sum_{j=1}^{m-1} \binom{m-1}{j} c_t^{j-1} c_s^{m-j-1}}{c_s^{m-1}} \right)$$

- There is no c_t in the denominator
- For $(c_s, c_t) = (1, 0)$ the bound is m/σ

One-step residual bound

Theorem (P., Rebholz, 2021 (Anderson acceleration for contractive and noncontracive iterations, IMA J. Numer. Anal.)**)**

Suppose the conditions above hold. Then the residual $w_{k+1} = g(x_k) - x_k$ from depth m acceleration satisfies the following bound

$$\|w_{k+1}\| \leq \|w_k\| \left(\theta_k((1-\beta_{k-1}) + \kappa\beta_{k-1}) + \frac{C(\sigma, c_s)\hat{\kappa}\sqrt{1-\theta_k^2}}{2} \left(\|w_k\| h(\theta_k) + 2 \sum_{n=k-m_{k-1}+1}^{k-1} (k-n)\|w_n\| h(\theta_n) + m_{k-1} \|w_{k-m_{k-1}}\| h(\theta_{k-m_{k-1}}) \right) \right)$$

where each $h(\theta_j) \leq C\sqrt{1-\theta_j^2} + \beta_{j-1}\theta_j$, and C depends on c_s (sufficient linear independence of columns of each F_j)

For the fixed-point algorithm with the same damping factor β_{k-1}

$$\|w_{k+1}\| \leq ((1-\beta_{k-1}) + \kappa\beta_{k-1})\|w_k\|$$

The first order term improves by factor θ_k

Higher-order terms are introduced, and they are scaled by factor $\sqrt{1-\theta_k^2}$

How do we use this in practice

I want	and	I should
First order term smaller	residual is large	Choose β_k based on θ_k
First order term smaller	residual is small	Choose depth m_k larger
Higher-order terms smaller	depth $m_k > 1$	Filter columns of F_k to enforce sufficient LI

Strategies:

- Dynamic choice of damping β_k, based on $\theta_k\big((1-\beta_{k-1})+\kappa\beta_{k-1}\big) \leq (1+\theta_k)/2$
- **Dynamic choice of depth m_k:** based on $\log_{10}\|w_k\|$ or based on a single switch from a small to a larger depth
- **Filtering:** discard columns of F_k for which $|r_{ii}|/\|f_i\| < c$

Filtering

Multiple depths

Relaxation

Relaxation & multiple depths

Example: p-Laplacian

Picard iteration for the p-Laplacian: $-\mathrm{div}\left((|\nabla u|^2/2)^{(p-2)/2}\nabla u\right) = c$

$p > 2$: degenerate elliptic equation. Nonlinear diffusion coefficient $\to 0$ as $|\nabla u| \to 0$

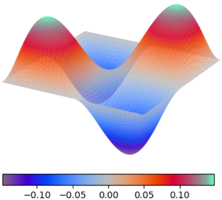
$1 < p < 2$: singular elliptic equation. Nonlinear diffusion coefficient $\to \infty$ as $|\nabla u| \to 0$

Choose $u_0 \in V_h$. For $k \geq 1$: Find $u_k \in V_h$ satisfying for all $v \in V_h$

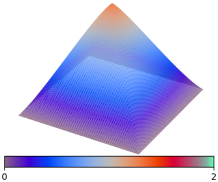
$$\int_\Omega \left(\varepsilon^2 + |\nabla u_{k-1}|^2/2\right)^{(p-2)/2} \nabla u_k \cdot \nabla v \,\mathrm{d}x = \int_\Omega cv \,\mathrm{d}x$$

$\varepsilon \geq 0$ is the *regularization*, $\varepsilon > 0$ for $1 < p < 2$

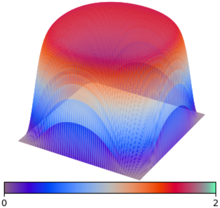
V_h : space of piecewise linear functions over a uniform left-crossed triangulation of $\Omega = (0,2) \times (0,2)$. Initial iterate: $u_0 = (x-1)(y-1)(x-2)(y-2)xy$



u_0



$p > 2$



$1 < p < 2$

Filtering for the p-Laplacian, $1 < p < 2$

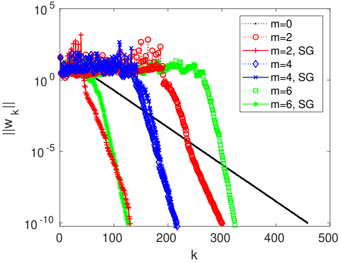
$$-\text{div}\left(\left(\varepsilon^2 + |\nabla u|^2/2\right)^{(p-2)/2}\nabla u\right) = c, \quad p = 1.06, \quad c = \pi, \quad \varepsilon = 10^{-14}$$

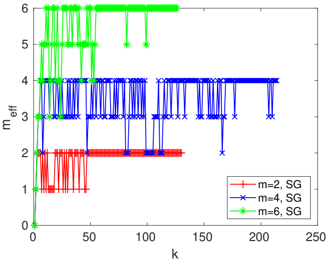
V_h : space of piecewise linear functions over a 128×128 uniform left-crossed triangulation of $\Omega = (0,2) \times (0,2)$ with $16,641$ total degrees of freedom

SG denotes "safeguarded," columns of F_k for which $r_{ii}/\|f_i\| < 0.25$ are removed.

Left: Residual histories to tolerance $\|w_k\| \leq 10^{-10}$ for constant depth with and without filtering

Right: The number of columns in F_k selected for use in each filtered iteration





Filtering can make a big difference, particularly in the *early stages*

Filtering and dynamic depth selection

$$-\text{div}\left((\varepsilon^2+|\nabla u|^2/2)^{(p-2)/2}\nabla u\right)=c,\quad p=1.06,\quad c=\pi,\quad \varepsilon=10^{-14}$$

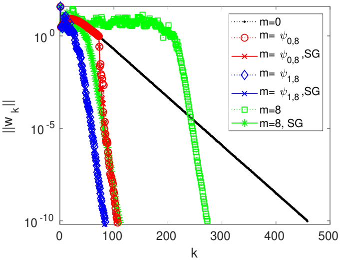
V_h : space of piecewise linear functions over a 128×128 uniform left-crossed triangulation of $\Omega=(0,2)\times(0,2)$ with $16,641$ total degrees of freedom

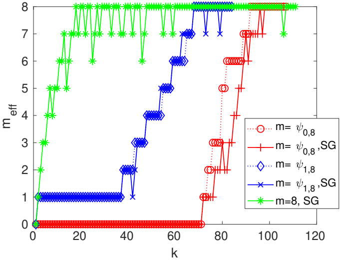
SG denotes "safeguarded," columns of F_k for which $r_{ii}/\|f_i\|<0.25$ are removed.

$\psi_{n,N}$ denotes $\min\left\{\max\{n,\lceil-\log_{10}\|w_k\|\rceil\},N\right\}$

Left: Residual histories to tolerance $\|w_k\|\le10^{-10}$ for constant and dynamic depths with and without filtering

Right: The number of columns in F_k selected for use in each filtered iteration

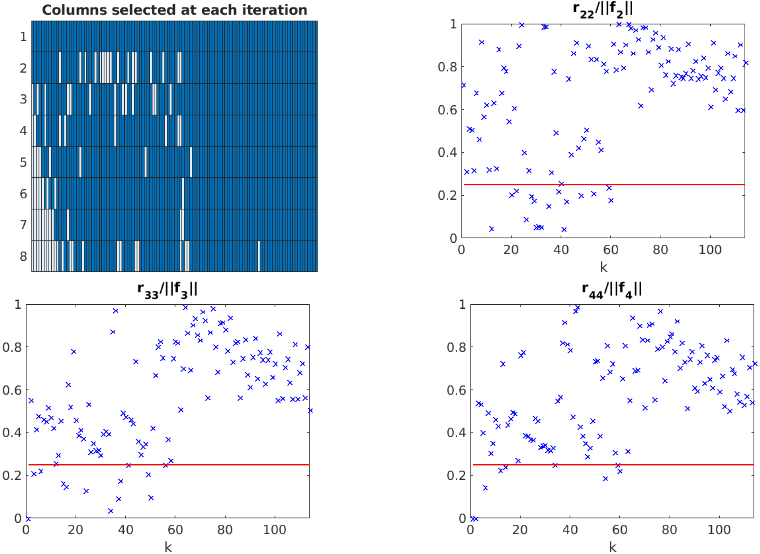




Filtering is useful for constant depths; dynamic depth selection is another way to effectively handle the *early stages*

Filtering: Which columns of F_k are used?

$$-\mathrm{div}\left((\varepsilon^2 + |\nabla u|^2/2)^{(p-2)/2}\nabla u\right) = c, \quad p = 1.06, \quad c = \pi, \quad \varepsilon = 10^{-14}$$



Results shown for $m = 8$. The columns to the left (more recent) are more often dropped!

Filtering and dynamic depth selection

$$-\text{div}\left((\varepsilon^2 + |\nabla u|^2/2)^{(p-2)/2}\nabla u\right) = c, \quad p = 1.06, \quad c = \pi, \quad \varepsilon = 10^{-14}$$

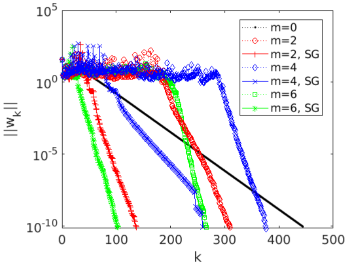
V_h : space of piecewise **quadratic** functions over a 128×128 uniform left-crossed triangulation of $\Omega = (0,2) \times (0,2)$ with $66,049$ total degrees of freedom

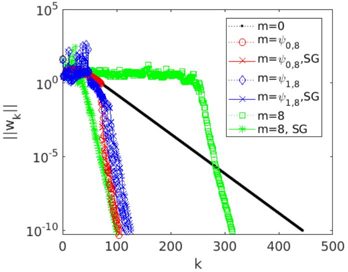
SG denotes "safeguarded," columns of F_k for which $r_{ii}/\|f_i\| < 0.45$ are removed.

$\psi_{n,N}$ denotes $\min\left\{\max\{n, \lceil -\log_{10}\|w_k\|\rceil\}, N\right\}$

Left: Residual histories to tolerance $\|w_k\| \leq 10^{-10}$ for *constant* depth with and without filtering

Right: Residual histories to tolerance $\|w_k\| \leq 10^{-10}$ for *dynamic* depth with and without filtering

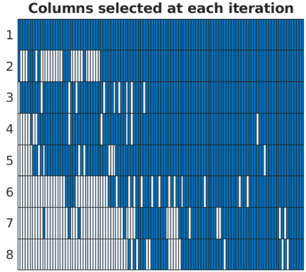


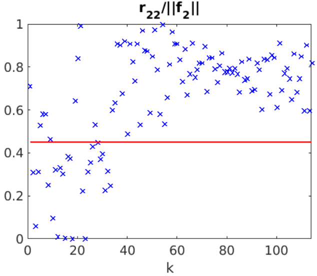


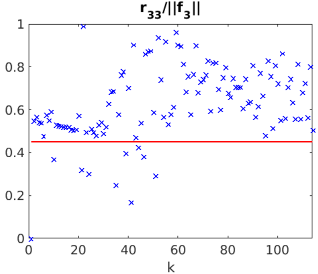
Dynamic depth selection is in this case more efficient for higher order elements

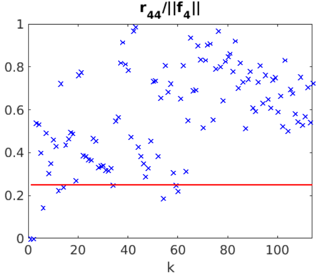
Filtering: Which columns of F_k are used?

$$-\operatorname{div}\left((\varepsilon^2 + |\nabla u|^2/2)^{(p-2)/2}\nabla u\right) = c, \quad p = 1.06, \quad c = \pi, \quad \varepsilon = 10^{-14}$$









Results shown for $m = 8$. The columns to the left (more recent) are more often dropped!

Filtering, adaptive damping and dynamic depth selection

$$-\text{div}\left((\varepsilon^2 + |\nabla u|^2/2)^{(p-2)/2}\nabla u\right) = c, \quad p = 6.0, \quad c = \pi, \quad \varepsilon = 0$$

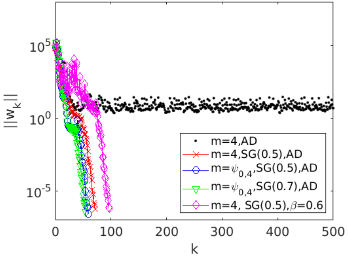
V_h : space of piecewise linear functions over a 128×128 uniform left-crossed triangulation of $\Omega = (0,2) \times (0,2)$ with $16,641$ total degrees of freedom

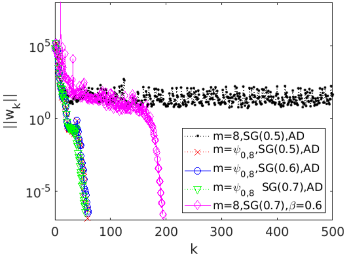
SG(s): columns of F_k for which $r_{ii}/\|f_i\| < s \in \{0.5, 0.6, 0.7\}$ are removed.

$\psi_{n,N}$ denotes $\min\left\{\max\{n, \lceil -\log_{10}\|w_k\|\rceil\}, N\right\}$

Residual histories to tolerance for constant and dynamic depths with and without filtering and adaptive damping Left: maximum depth 4. Right: maximum depth 8.

Adaptive damping (AD): $\kappa_j = \|w_{j+1} - w_j\|/\|u_k - u_{k-1}\|$. β_j chosen between $\beta_{min} = 0.1$ and $\beta_{max} = 0.6$ so that $((1-\beta_j) + \kappa_j\beta_j)\theta_{j+1} < (1+\theta_{j+1})/2$





Only *sufficiently* filtered iterations converged; adaptive damping improved convergence

A note to FEniCS users

There exist wrong ways to interface between FEniCS and SciPy's QR routines

But there are also ways that work well!

```
## ---------------------------------------------
w     = Function(V)
w1    = Function(V)
e_k   = Function(V)
w1v = as_backend_type(w1.vector()).vec()
wv = as_backend_type(w.vector()).vec()
ekv = as_backend_type(e_k.vector()).vec()
## ---------------------------------------------
```

⋮

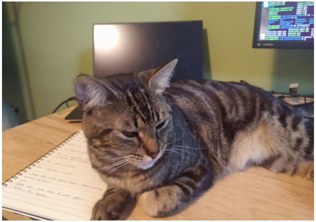
```
  ## ## -----------------------------------------
  if m_max > 0: ## -- update X_mat and F_mat
    X_mat[:,1:] = X_mat[:,:-1]
    F_mat[:,1:] = F_mat[:,:-1]
    #X_mat[:,0] = e_k.vector()
    #F_mat[:,0] = w1.vector() - w.vector();
    X_mat[:,0] = ekv.copy()
    wv.axpy(-1.0,w1v)
    F_mat[:,0] = wv.copy()
    w.vector()[:] = w1.vector()
    ## ## ----------------------------------------
```

⋮

```
    w_range, RR = la.qr_multiply(-F_mat[:,:mn],w1v,\
      overwrite_a=False,overwrite_c=False)
```

Conclusions and Outlook

- The new theoretical understanding guides the design of methods with adaptively updated filtering, algorithmic depth, and damping, to stabilize and accelerate convergence
- **If Newton is working, then use it!** If Newton is diverging, or it is “undesirable” to form a Jacobian, then applying AA to a linearly converging method *can* give Newton-like performance at low cost, *if* it is implemented well.
- Recent work includes application to non-Newtonian flows including Bingham fluids (with L. Rebholz, D. Vargun) and grade-two fluids (with L. R. Scott)
- In process: Can we put all these ideas together to create a robust globalization strategy?



Pictured: we’re working on it...

Example: Anderson applied to Picard for steady NSE (3D)

Picard iteration for steady Navier-Stokes (moving lid problem)

- Choose $u_0 \in X_h$. For $k \geq 1$: Find $(u_k, p_k) \in (X_h, Q_h)$ s.t. for all $(v, q) \in (X_h, Q_h)$

$$b^*(u_{k-1}, u_k, v) - (p_k, \nabla \cdot v) + \nu(\nabla u_k, \nabla v) = (f, v)$$
$$(\nabla \cdot u_k, q) = 0$$

$$b^*(u, v, w) := (u \cdot \nabla v, w) + \frac{1}{2}((\nabla \cdot u)v, w)$$

- $(X_h, Q_h) = (\mathcal{P}_3, \mathcal{P}_2^{disc})$ Scott-Vogelius elements, barycenter-refined tetrahedral mesh, ~ 1.3 million DOF.
- Domain: $\Omega = (0,1)^3$; no forcing $f = 0$; kinematic velocity $\nu = 1/Re$
- 'Moving lid" $u(x, y, 1) = \langle 1, 0, 0 \rangle^T$, no-slip (zero-velocity) condition on other sides
- $Re = 2500$