Anderson Acceleration:
An Overview

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Anderson Acceleration


Consider a fixed-point iteration: \( x_{k+1} = g(x_k), \quad g : \mathbb{R}^n \rightarrow \mathbb{R}^n \).

\begin{align*}
\text{Anderson Acceleration} & \\
\text{Given } x_0 \text{ and } m \geq 1, \text{ set } x_1 = g(x_0). \\
\text{For } k = 1, 2, \ldots \\
\text{Set } m_k = \min\{m, k\}. \\
\text{Set } F_k = [f(x_k-m_k), \ldots, f(x_k)], \text{ where } f(x) \equiv g(x) - x. \\
\text{Solve } \min_{\alpha \in \mathbb{R}^{m_k+1}} \|F_k \alpha\|_2 \ \text{s. t. } \sum_{i=0}^{m_k} \alpha_i = 1. \\
\text{Set } x_{k+1} = \sum_{i=0}^{m_k} \alpha_i g(x_k-m_k+i). \\
\end{align*}

Can allow a damped step: \( x_{k+1} = (1 - \beta_k) \sum_{i=0}^{m_k} \alpha_i x_k-m_k+i + \beta_k \sum_{i=0}^{m_k} \alpha_i g(x_k-m_k+i). \)
Suppose $g(x) = Ax + b$ for $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$.

Then $x_{k+1} = \sum_{i=0}^{m_k} \alpha_i g(x_k - m_k + i) = g(\sum_{i=0}^{m_k} \alpha_i x_k - m_k + i)$, or

$$x_{k+1} = g(x_{min})$$

where $x_{min} = \sum_{i=0}^{m_k} \alpha_i x_k - m_k + i$ has minimal residual within the affine subspace containing $\{x_k - m_k + i\}_{i=0,...,m_k}$. 
In a broad category with . . .

▶ “charge-mixing” methods for electronic-structure computations;
Broyden (Kresse–Furthmüller 1996), C. Yang et al. (2008)

▶ methods based on quasi-Newton updating;
(2009), Haelterman et al. (2009, 2010)

▶ Krylov acceleration methods.

Essentially (or nearly) the same method has been independently described several times.

Various names: Anderson mixing, nonlinear GMRES, Krylov acceleration, DIIS or Pulay mixing, QN-ILS.
Another broad category . . .

- *vector-extrapolation* methods, especially polynomial methods: (reduced-rank, minimal-polynomial, modified minimal-polynomial);
- *vector* and *topological* $\varepsilon$-*algorithms*.


Brezinski, Redivo-Zaglia, & Saad (2018) formulate a variant of reduced-rank extrapolation (RRE) that is “similar in spirit, but not quite equivalent, to AA.”
Assume . . .

▶ \( g(x) = Ax + b \) for \( A \in \mathbb{R}^{n \times n}, \ b \in \mathbb{R}^n \).
▶ Anderson acceleration is not truncated, i.e., \( m_k = k \) for each \( k \).
▶ \((I - A)\) is nonsingular.
▶ (Unrestarted) GMRES is applied to \((I - A)x = b\) with initial point \( x_0 \).

**W–Ni (2011)**

Suppose also that, for some \( k > 0 \), \( r_{G_{MRES}}^{k-1} \neq 0 \) and \( \|r_{G_{MRES}}^{j-1}\|_2 > \|r_{G_{MRES}}^{j}\|_2 \) for \( 0 < j < k \). Then

\[
\sum_{i=0}^{k} \alpha_i x_i^{AA} = x_k^{G_{MRES}} \text{ and } x_{k+1}^{AA} = g(x_k^{G_{MRES}}).
\]

Potra & Engler (2013) extended to allow a damped step.
Consider . . .

- \( Ax = b \) for nonsingular \( A \in \mathbb{R}^n \).
- \( A = M - N \) for nonsingular \( M \in \mathbb{R}^{n \times n} \).
- Stationary iteration \( x_{k+1} = g(x_k) \equiv M^{-1}Nx_k + M^{-1}b \).

Assume . . .

- Anderson acceleration is not truncated, i.e., \( m_k = k \) for each \( k \).
- GMRES is applied to \( M^{-1}Ax = M^{-1}b \) with initial point \( x_0 \).

**Corollary**

Suppose also that, for some \( k > 0 \), \( r^\text{GMRES}_{k-1} \neq 0 \) and \( \|r^\text{GMRES}_{j-1}\|_2 > \|r^\text{GMRES}_j\|_2 \) for \( 0 < j < k \). Then

\[
\sum_{i=0}^{k} \alpha_i x_i^{\text{AA}} = x_k^{\text{GMRES}} \quad \text{and} \quad x_{k+1}^{\text{AA}} = g(x_k^{\text{GMRES}}).
\]
Successive Anderson acceleration iterates are related by
\[ x_{k+1} = x_k - B_k^{-1} f(x_k), \]  
(\textcolor{red}{\star})

where \( f(x) \equiv g(x) - x \) and \( B_k \) is the second Broyden multi-secant update of \(-I\) satisfying
\[ B_k(x_{i+1} - x_i) = f(x_{i+1}) - f(x_i), \quad k - m_k \leq i \leq k - 1. \]  
(\textcolor{red}{\star\star})

- Clarifies and extends work of Eyert (1996).

- Degroote et al. (2009) and Haelterman et al. (2009, 2010) have independently developed very similar QN-LS and QN-ILS methods using multi-secant updating.
Fang–Saad (2008) define an *Anderson family* of methods of the form (⋆), with Anderson acceleration designated the *Type II* method.

The Anderson family *Type I* method has the form (⋆), in which $B_k$ is the first Broyden multi-secant update of $-I$ satisfying (⋆⋆).

For affine $g$, W–Ni (2011) give results relating the Type I method to the Arnoldi method (FOM) analogous to those relating AA to GMRES:

$$
\sum_{i=0}^{k} \alpha_i x_i^{\text{Type I}} = x_{k}^{\text{Arnoldi}} \quad \text{and} \quad x_{k+1}^{\text{Type I}} = g(x_k^{\text{Arnoldi}}).
$$
Can this updating approach be used to exploit problem structure?
Can this updating approach be used to exploit problem structure?

Set $x_k = (\Delta x_{k-m_k}, \ldots, \Delta x_{k-1})$, $F_k = (\Delta f_{k-m_k}, \ldots, \Delta f_{k-1})$.

Suppose we want an update of $-I$ satisfying $B_k x_k = F_k$ and $B_k = B_k^T$. 

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Boutet et al. (2019, 2021a, 2021b) are exploring modified strategies in a more general multi-secant updating context.
Can this updating approach be used to exploit problem structure?

Set \( \chi_k = (\Delta x_{k-m_k}, \ldots, \Delta x_{k-1}) \), \( \mathcal{F}_k = (\Delta f_{k-m_k}, \ldots, \Delta f_{k-1}) \).

Suppose we want an update of \(-I\) satisfying \( B_k \chi_k = \mathcal{F}_k \) and \( B_k = B_k^T \).

Schnabel (1983): \( \exists B_k \) such that \( B_k \chi_k = \mathcal{F}_k \) and \( B_k = B_k^T \) \( \iff \chi_k^T \mathcal{F}_k = \mathcal{F}_k^T \chi_k \).
Can this updating approach be used to exploit problem structure?

Set \( \chi_k = (\Delta x_{k-m}, \ldots, \Delta x_{k-1}) \), \( \mathcal{F}_k = (\Delta f_{k-m}, \ldots, \Delta f_{k-1}) \).

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Boutet et al. (2019, 2021a, 2021b) are exploring modified strategies in a more general multi-secant updating context.
Assume . . .

- $g : D \to D$ for closed $D \subseteq \mathbb{R}^n$;
- $g$ is continuously differentiable on $D$;
- $\exists \kappa \in (0, 1)$ such that $\|g(y) - g(x)\| \leq \kappa \|y - x\|$ for $x, y \in D$.

This implies . . .

- $\exists! x_* \in D$ such that $x_* = g(x_*)$.
- Fixed-point iterates converge globally with $\|x_{k+1} - x_*\| \leq \kappa \|x_k - x_*\|$.
- $\|g'(x)\| \leq \kappa$ in $D$ and $I - g'(x)$ is invertible in $D$.

Chen–Kelley (2019)

Suppose also that $\exists M$ such that $\sum_{i=0}^{m_k} |\alpha_i| \leq M$ for all $k$. Then the AA residuals and iterates converge locally and $r$-linearly to $x_*$ with

$$\limsup_{k \to \infty} \|f(x_k)\|^{1/k} = \limsup_{k \to \infty} \|x_k - x_*\|^{1/k} \leq \kappa.$$
Toth–Kelley (2015) give a slightly weaker $r$-linear convergence result, assuming $g$ is Lipschitz continuously differentiable. They also ...

- show that the convergence is $q$-linear if either (a) $\| \cdot \| = \| \cdot \|_2$ and $m_k = 1$ for all $k$, or (b) $g$ is linear;
- discuss the condition $\sum_{i=0}^{m_k} |\alpha_i| \leq M$ and give strategies for enforcing it;
- discuss using norms other than $\| \cdot \|_2$ in the minimization problem for the $\alpha_i$.

Chen–Kelley (2019) consider EDIIS from Kudin et al. (2002), described as differing from AA by requiring each $\alpha_i \geq 0$.

Assuming only convexity of $D$ and contractivity of $g$ in $D$, they show global $r$-linear convergence in $D$, with

$$\|x_k - x_*\| \leq \left( \frac{\kappa^1}{(m+1)} \right)^k \|x_0 - x_*\|.$$
Convergence (cont.)

Assume . . .

- $g : \mathbb{R}^n \to \mathbb{R}^n$ is uniformly Lipschitz continuously differentiable;
- $\exists \kappa \in (0, 1)$ such that $\|g(y) - g(x)\| \leq \kappa \|y - x\|$ for $x, y \in \mathbb{R}^n$.

(Implications as before.)

Evans et al. (2020)

Suppose also that $\exists M$ and $\epsilon > 0$ such that for all $k > m$, $\sum_{i=0}^{m-1} |\alpha_i| \leq M$ and $|\alpha_m| \geq \epsilon$. Then

$$\|f(x_{k+1})\| \leq \theta_{k+1} \left[ (1 - \beta_k) + \kappa \beta_k \right] \|f(x_k)\| + \sum_{i=0}^{m} O \left( \|f(x_{k-m+i})\|^2 \right), \quad (\star \star \star)$$

where $\beta_k = \text{damping parameter}$ and $\theta_{k+1} = \| \sum_{i=0}^{m} \alpha_i f(x_{k-m+i}) \| / \|f(x_k)\|$.

Note: $\theta_{k+1} \leq 1$. 
With $\beta_k = 1$, (⋆⋆⋆) gives

$$\|f(x_{k+1})\| \leq \kappa \left\| \sum_{i=0}^{m} \alpha_i f(x_{k-m+i}) \right\| + h.o.t. \leq \kappa \|f(x_k)\| + h.o.t.$$ 

Since $f(x) = [g'(x_*) - I](x - x_*) + h.o.t$, this gives

$$\|x_{k+1} - x_*\|_* \leq (\kappa + \delta)\|x_k - x_*\|_* + h.o.t.,$$

where $\|v\|_* \equiv \|f'(x_*)v\| = \|[I - g'(x_*)]v\|$ and $\delta > 0$ is arbitrarily small.
With $\beta_k = 1$, (***) gives

$$\|f(x_{k+1})\| \leq \kappa \left\| \sum_{i=0}^{m} \alpha_i f(x_{k-m+i}) \right\| + \text{h.o.t.} \leq \kappa \|f(x_k)\| + \text{h.o.t.}$$

Since $f(x) = [g'(x_*) - I](x - x_*) + \text{h.o.t}$, this gives

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With continuous differentiability and contractivity, we have directly

$$\|x_{k+1} - x_*\| = \left\| \sum_{i=0}^{m} \alpha_i [g(x_{k-m+i}) - g(x_*)] \right\| \leq \left\| \sum_{i=0}^{m} \alpha_i g'(x_*)(x_{k-m+i} - x_*) \right\| + \text{h.o.t.}$$

$$\leq \kappa \left\| \sum_{i=0}^{m} \alpha_i x_{k-m+i} - x_* \right\| + \text{h.o.t.}$$

If $g$ is affine and AA is not truncated, then $\|x_{k+1}^{AA} - x_*\| \leq \kappa \|x_k^{GMRES} - x_*\|$. 
Convergence (cont.)

With $\beta_k = 1$, ($\star\star\star$) gives

$$\|f(x_{k+1})\| \leq \kappa \|\sum_{i=0}^{m} \alpha_i f(x_{k-m+i})\| + \text{h.o.t.} \leq \kappa \|f(x_k)\| + \text{h.o.t.}$$

Since $f(x) = [g'(x_*) - I](x - x_*) + \text{h.o.t}$, this gives

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With continuous differentiability and contractivity, we have directly

$$\|x_{k+1} - x_*\| = \|\sum_{i=0}^{m} \alpha_i [g(x_{k-m+i}) - g(x_*)]\| \leq \|\sum_{i=0}^{m} \alpha_i g'(x_*)(x_{k-m+i} - x_*)\| + \text{h.o.t.}$$

$$\leq \kappa \|\sum_{i=0}^{m} \alpha_i x_{k-m+i} - x_*\| + \text{h.o.t.}$$

If $g$ is affine and AA is not truncated, then $\|x_{k+1}^{AA} - x_*\| \leq \kappa \|x_k^{GMRES} - x_*\|$.

Caution: All h.o.t. depend on $x_{k-m+i}$ for $i = 0, \ldots, m$. 
Wrapping up . . .

- Have outlined major theoretical properties of AA and its relationship to other algorithms.

- Promising areas of research (IMHO):
  - exploiting problem structure in AA,
  - sharpening local convergence results.

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Thank you!


