Project presentation of

Zhang, et al.: Globally Convergent Type-I Anderson Acceleration for Non-Smooth Fixed-Point Iterations

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The problem setting

Problem (find fixed point)

Find a fixed point $x \in \mathbb{R}^n$ *of* $f : \mathbb{R}^n \to \mathbb{R}^n$*, i.e.* $x = f(x)$*.*

or equivalently

Problem (find zero)

Find a zero $x \in \mathbb{R}^n$ *of* $g = \mathrm{Id} - f$*, i.e.* $0 = g(x)$*.*

We also assume

- f has a fixed point.
- f is non-expansive, i.e. $\|f(x) - f(y)\| \leq \|x - y\|$.
- ∇f is unknown $\to$no Newton
- noisy problem $\to$no finite difference derivatives
- cost of evaluating f is high $\to$no line search
- n is large $\to$matrix-free

Fixed point iteration

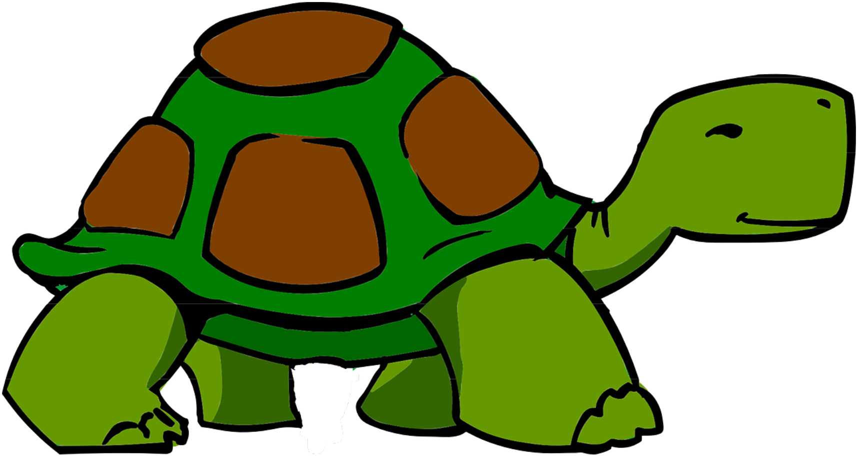
To keep things simple we try

Input : Initial value $x_0 \in \mathbb{R}^n$ and function $f\colon \mathbb{R}^n \to \mathbb{R}^n$.

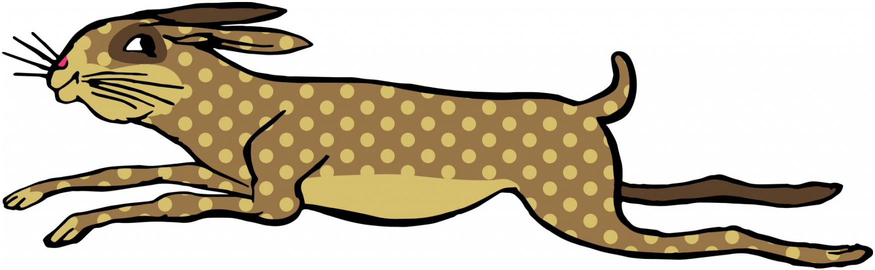
for $k = 0, 1, \ldots$ **do**
  Set $x_{k+1} = f(x_k)$.
end

Algorithm 1: Fixed point iteration (original)

This works, but ...



We want to be like...



General AA

We may as well use the information gained from previous evaluations. In the following we assume for simplicity that our memory is unlimited. If we form a weighted average we get

Input : $x_0 \in \mathbb{R}^n$ and $f \colon \mathbb{R}^n \to \mathbb{R}^n$.

for $k = 0, 1, \ldots$ **do**

  Set $f_k = f(x_k)$.
  Choose $\alpha = \alpha^k \in \mathbb{R}^{k+1}$ such that $\sum_i \alpha_i = 1$.
  Set $x_{k+1} = \sum_i \alpha_i f_i$.

end

Algorithm 2: General AA (Anderson Acceleration)

AA-II

Since finding a fixed point of f is equivalent to finding a zero of $g = \mathrm{Id} - f$ the following seems like a good idea

Input : $x_0 \in \mathbb{R}^n$ and $f : \mathbb{R}^n \to \mathbb{R}^n$.

for $k = 0, 1, \ldots$ **do**

   Set $f_k = f(x_k)$.

   Set $g_k = x_k - f_k$.

   Choose $\alpha \in \mathbb{R}^{k+1}$ such that $\sum_i \alpha_i = 1$ and such that α minimises $\|\sum_i \alpha_i g_i\|_2$.

   Set $x_{k+1} = \sum_i \alpha_i f_i$.

end

Algorithm 3: AA-II

AA-II (reformulated)

One can show that this can be brought into the form of a quasi-Newton-like method

Input : $x_0 \in \mathbb{R}^n$ and $f\colon \mathbb{R}^n \to \mathbb{R}^n$.

Set $x_1 = f(x_0)$.
for $k = 0, 1, \ldots$ **do**
    Set $g_k = g(x_k)$.
    Construct $S_k = \begin{bmatrix} x_1 - x_0 & \cdots & x_k - x_{k-1} \end{bmatrix} \in \mathbb{R}^{n \times k}$ and $Y_k = \begin{bmatrix} g_1 - g_0 & \cdots & g_k - g_{k-1} \end{bmatrix} \in \mathbb{R}^{n \times k}$.
    Set $H_k = \mathrm{Id} + (S_k - Y_k)\left(Y_k^\top Y_k\right)^{-1} Y_k^\top \in \mathbb{R}^{n \times n}$.
    Set $x_{k+1} = x_k - H_k g_k$.
end

Algorithm 4: AA-II (reformulated)

AA-I

This is the form of a quasi-Newton-like method so one could expect H_k to be an approximate inverse of $\nabla f(x_k)$. Indeed one can show

Proposition (Approximate inverse Jacobian)

H_k minimises $\|H_k - \mathrm{Id}\|_F$ under the multi-secant condition $H_k S_k = Y_k$.

Proof.

See [1]. ☐

The good Broyden method approximates the Jacobian rather than its inverse and tends to yield better results. This motivates

Definition (Approximate Jacobian)

Let B_k be minimiser of $\|B_k - \mathrm{Id}\|_F$ under the condition $B_k Y_k = S_k$.

One can show that

$$B_k = \mathrm{Id} + (Y_k - S_k)\left(S_k^\top S_k\right)^{-1} S_k^\top .$$

This yields the AA-I algorithm

Input : $x_0 \in \mathbb{R}^n$ and $f \colon \mathbb{R}^n \to \mathbb{R}^n$.

Set $x_1 = f(x_0)$
for $k = 0, 1, \ldots$ **do**
  Set $g_k = g(x_k)$.
  Construct S_k from $x_0, \ldots, x_k$ and Y_k from $g_0, \ldots, g_k$.
  Set $B_k = \mathrm{Id} + (Y_k - S_k)\left(S_k^\top S_k\right)^{-1} S_k^\top \in \mathbb{R}^{n \times n}$.
  Set $H_k = B_k^{-1}$.
  Set $x_{k+1} = x_k - H_k g_k$.
end

Algorithm 5: AA-I

But this algorithm has some problems

- computational efficiency: the approach is not matrix-free
  $\rightarrow$rank-1 update for B_k and later H_k
- well-definedness of H_k: B_k might not be well-defined or singular
  $\rightarrow$Powell-type regularisation, restarting iteration
- memory usage: though infinite memory is nice to have it is not very realistic $\rightarrow$restarting iteration
- convergence: the algorithm does not necessarily converge
  $\rightarrow$safeguarding steps

Computational efficiency: Rank-1 update for B_k

One can show

Proposition (Rank-1 update for B_k)

We have

$$B_k = B_{k-1} + \frac{(y_{k-1} - B_{k-1} s_{k-1})\hat{s}_{k-1}^\top}{\hat{s}_{k-1}^\top s_{k-1}}$$

where $y_{k-1} = g_k - g_{k-1}$, $B_0 = \mathrm{Id}$ *and*

$$\hat{s}_{k-1} = s_{k-1} - \sum_{j=0}^{k-2} \frac{\hat{s}_j^\top s_{k-1}}{\|\hat{s}_j\|^2} \hat{s}_j$$

is the Gram-Schmidt orthogonalisation of $s_{k-1} = x_k - x_{k-1}$.

Proof.

See [1]. $\square$

Input : $x_0 \in \mathbb{R}^n$ and $f\colon \mathbb{R}^n \to \mathbb{R}^n$.

Set $B_0 = \mathrm{Id}$ and $x_1 = f(x_0)$.
for $k = 0, 1, \ldots$ **do**
  Set $g_k = g(x_k)$.
  Set $s_{k-1} = x_k - x_{k-1}$, $y_{k-1} = g_k - g_{k-1}$ and
  $\hat{s}_{k-1} = s_{k-1} - \sum_{i=0}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.
  Set $B_k = B_{k-1} + \frac{(y_{k-1} - B_{k-1}s_{k-1})\hat{s}_{k-1}^\top}{\hat{s}_{k-1}^\top s_{k-1}}$.
  Set $H_k = B_k^{-1}$.
  Set $x_{k+1} = x_k - H_k g_k$.
end

Algorithm 6: AA-I (rank-1 update)

Well-definedness of H_k: Powell-type regularisation

To fix the singularity of B_k we use Powell-type regularisation.

s **Input :** $x^0 \in \mathbb{R}^n$, $f\colon \mathbb{R}^n \to \mathbb{R}^n$ and $\bar{\theta} \in (0,1)$.

Set $B_0 = \mathrm{Id}$ and $x_1 = f(x_0)$.
for $k = 0, 1, \ldots$ **do**
    Set $g_k = g(x_k)$, $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$.
    Set $\hat{s}_{k-1} = s_{k-1} - \sum_{i=0}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.
    Choose θ_{k-1} in dependence of $\bar{\theta}$.
    Set $\tilde{y}_{k-1} = \theta_{k-1} y_{k-1} - (1-\theta_{k-1}) g_{k-1}$.
    Set $B_k = B_{k-1} + \frac{(\tilde{y}_{k-1} - B_{k-1} s_{k-1}) \hat{s}_{k-1}^\top}{\hat{s}_{k-1}^\top s_{k-1}}$.
    Set $H_k = B_k^{-1}$.
    Set $x_{k+1} = x_k - H_k g_k$.
end

Algorithm 7: AA-I with Powell-type regularisation

Well-definedness of H_k, memory usage: Restarting iteration

If $\hat{s}_k = 0$ the update

$$B_k = B_{k-1} + \frac{(\tilde{y}_{k-1} - B_{k-1} s_{k-1})\hat{s}_{k-1}^\top}{\hat{s}_{k-1}^\top s_{k-1}}$$

is ill-defined. This occurs in algorithm 7 e.g. for $k > n$ as then $\hat{s}_k = 0$ by linear dependence. Hence we restart the algorithm with x_k as the new starting point if

- $k = m + 1$ for some fixed $m \in \mathbb{N}$ or
- $\|\hat{s}_{k-1}\| < \tau \|s_{k-1}\|$ for some fixed $\tau \in (0, 1)$.

It can be shown that B_k is then well-defined.

Input : $x^0 \in \mathbb{R}^n$, $f\colon \mathbb{R}^n \to \mathbb{R}^n$, $m \in \mathbb{N}$ and $\bar{\theta}, \tau \in (0,1)$

Set $B_0 = \mathrm{Id}$, $x_1 = f(x_0)$ and $m_0 = 0$.

for $k = 0, 1, \dots$ **do**

 Set $g_k = g(x_k)$, $m_k = m_{k-1} + 1$, $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$.

 Set $\hat{s}_{k-1} = s_{k-1} - \sum_{i=k-m_k}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.

 if $m_k = m + 1$ *or* $\|\hat{s}_{k-1}\| < \tau \|s_{k-1}\|$ **then**

  Set $m_k = 0$, $\hat{s}_{k-1} = s_{k-1}$ and $B_{k-1} = \mathrm{Id}$.

 end

 Choose θ_{k-1} in dependence of $\bar{\theta}$.

 Set $\tilde{y}_{k-1} = \theta_{k-1} y_{k-1} - (1 - \theta_{k-1}) g_{k-1}$.

 Set $B_k = B_{k-1} + \frac{(\tilde{y}_{k-1} - B_{k-1} s_{k-1}) \hat{s}_{k-1}^\top}{\hat{s}_{k-1}^\top s_{k-1}}$.

 Set $H_k = B_k^{-1}$.

 Set $x_{k+1} = x_k - H_k g_k$.

end

Algorithm 8: AA-I with Powell-type regularisation and Restarting

One can then show

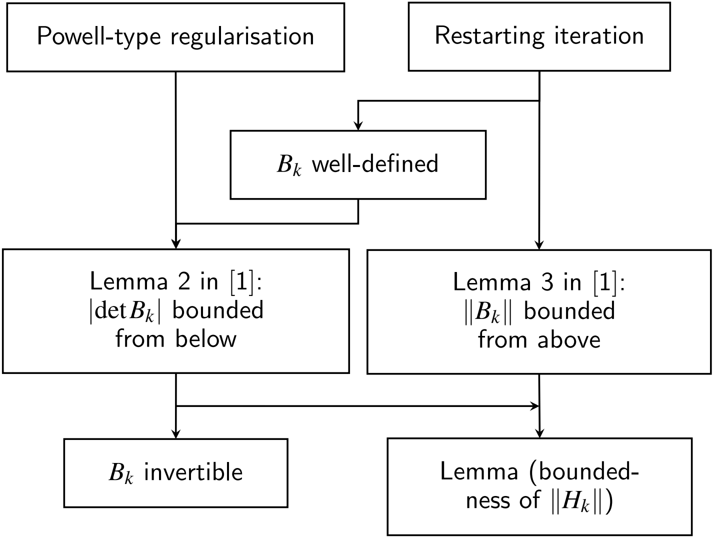
Lemma (bound on $\|H_k\|_2$)

In algorithm 8 we have that H_k is well-defined and there exists a constant $c_1 = c_1(m, n, \bar{\theta}, \tau) > 0$ such that

$$\|H_k\|_2 \leq c_1 \,.$$

Proof.

See [1, Corollary 4]. □


Powell-type regularisation
Restarting iteration
B_k well-defined
Lemma 2 in [1]: $|\det B_k|$ bounded from below
Lemma 3 in [1]: $\|B_k\|$ bounded from above
B_k invertible
Lemma (boundedness of $\|H_k\|$)

Computational efficiency: Rank-1 update for H_k

From the Sherman-Morrison formula one can obtain

Proposition (Rank-1 update for H_k)

We have

$$H_k = H_{k-1} + \frac{(s_{k-1} - H_{k-1} y_{k-1}) \hat{s}_{k-1}^\top H_{k-1}}{\hat{s}_{k-1}^\top H_{k-1} y_{k-1}}$$

Input : $x^0 \in \mathbb{R}^n$, $f\colon \mathbb{R}^n \to \mathbb{R}^n$, $\boldsymbol{m} \in \mathbb{N}$ and $\bar{\theta}, \boldsymbol{\tau} \in (0,1)$

Set $H_0 = \mathrm{Id}$, $x_1 = f(x_0)$ and $\boldsymbol{m_0 = 0}$.

for $k = 0, 1, \ldots$ **do**

Set $g_k = g(x_k)$, $m_k = m_{k-1} + 1$, $s_{k-1} = x_k - x_{k-1}$ and $y_{k-1} = g_k - g_{k-1}$.

Set $\hat{s}_{k-1} = s_{k-1} - \sum_{i=k-m_k}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.

if $m_k = m+1$ *or* $\|\hat{s}_{k-1}\| < \tau \|s_{k-1}\|$ **then**

Set $m_k = 0$, $\hat{s}_{k-1} = s_{k-1}$ and $H_{k-1} = \mathrm{Id}$.

end

Choose θ_{k-1} in dependence of $\bar{\theta}$.

Set $\tilde{y}_{k-1} = \theta_{k-1} y_{k-1} - (1 - \theta_{k-1}) g_{k-1}$.

Set $H_k = H_{k-1} + \frac{(s_{k-1} - H_{k-1}\tilde{y}_{k-1})\hat{s}_{k-1}^\top H_{k-1}}{\hat{s}_{k-1}^\top H_{k-1}\tilde{y}_{k-1}}$.

Set $x_{k+1} = x_k - H_k g_k$.

end

Algorithm 9: AA-I with Powell-type regularisation and Restarting

Convergence: Safeguarding steps

To guarantee the decrease in $\|g_k\|$ one can interleave the AA-I steps with Krasnosel'skii-Mann (KM) steps which are given by

$$x_{k+1} = (1-\alpha)x_k + \alpha f_k$$

for some fixed $\alpha \in (0,1)$.

Input : $x^0 \in \mathbb{R}^n$, $f\colon \mathbb{R}^n \to \mathbb{R}^n$, $m \in \mathbb{N}$, $\bar{\theta}, \tau, \alpha \in (0,1)$ and safe-guarding constants $D, \varepsilon > 0$

Set $H_0 = \mathrm{Id}$, $x_1 = \tilde{x}_1 = f(x_0)$, $m_0 = n_{AA} = 0$ and $\bar{U} = \|g_0\|_2$.

for $k = 0, 1, \ldots$ **do**

Set $g_k = g(x_k)$, $m_k = m_{k-1} + 1$, $s_{k-1} = \tilde{x}_k - x_{k-1}$ and $y_{k-1} = g(\tilde{x}_k) - g_{k-1}$.

Set $\hat{s}_{k-1} = s_{k-1} - \sum_{i=k-m_k}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.

if $m_k = m+1$ *or* $\|\hat{s}_{k-1}\| < \tau \|s_{k-1}\|$ **then**

Set $m_k = 0$, $\hat{s}_{k-1} = s_{k-1}$ and $H_{k-1} = \mathrm{Id}$.

end

Choose θ_{k-1} in dependence of $\bar{\theta}$.

Set $\tilde{y}_{k-1} = \theta_{k-1} y_{k-1} - (1 - \theta_{k-1}) g_{k-1}$.

Set $H_k = H_{k-1} + \frac{(s_{k-1} - H_{k-1}\tilde{y}_{k-1})\hat{s}_{k-1}^\top H_{k-1}}{\hat{s}_{k-1}^\top H_{k-1}\tilde{y}_{k-1}}$ and $\tilde{x}_{k+1} = x_k - H_k g_k$.

if $\|g_k\| \leq D\bar{U}(n_{AA}+1)^{-(1+\varepsilon)}$ **then**

Set $x_{k+1} = \tilde{x}_{k+1}$ and $n_{AA} = n_{AA} + 1$.

else

Set $x_{k+1} = (1-\alpha)x_k + \alpha f_k$.

end

end

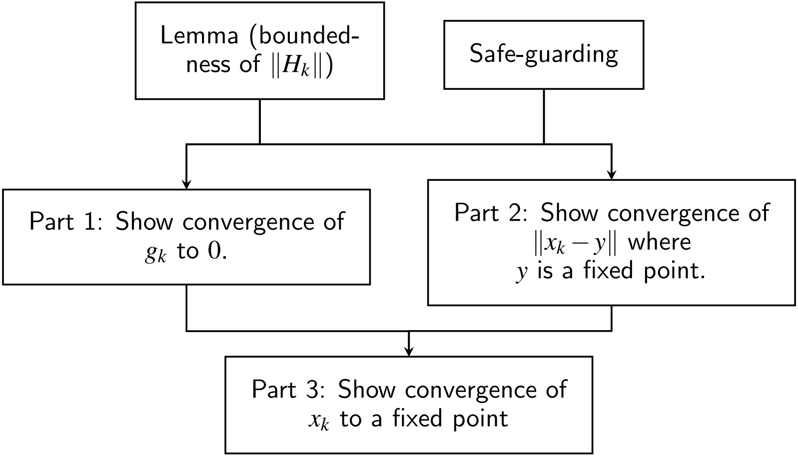
Algorithm 10: AA-I with Powell-type regularisation, restarting and safeguarding

Convergence result

Theorem (Convergence)

Let x_k be generated by algorithm 10 then x_k converges to a fixed point of f.

Proof, strategy.



Proof, part 1.

The proof follows [1, Theorem 6]. We partition $\mathbb{N} = K_{AA} \sqcup K_{KM}$ where $K_{AA} = \{k_0, k_1, \ldots\}$ denote the indices k where the algorithm chose an AA-step (a) and $K_{KM} = \{l_0, l_1, \ldots\}$ where the algorithm chose a KM-step (b).

if $\|g_k\| \leq D\bar{U}(n_{AA}+1)^{-(1+\varepsilon)}$ **then**
  Set $x_{k+1} = \tilde{x}_{k+1}$ and $n_{AA} = n_{AA}+1$. (a)
else
  Set $x_{k+1} = (1-\alpha)x_k + \alpha f_k$. (b)
end

Algorithm 11: The two cases for x_{k+1}.

Proof, part 1 (cont.).

Let y be a fixed point. We distinguish

case (a) $k_i \in K_{AA}$ then

$$\begin{aligned} \|x_{k_i+1} - y\| &\leq \|x_{k_i} - y\| + \|H_{k_i} g_{k_i}\| \\ &\leq \|x_{k_i} - y\| + c_1 \|g_k\| \\ &\leq \|x_{k_i} - y\| + c_2 (i+1)^{-(1+\varepsilon)} \end{aligned} \tag{1}$$

case (b) $l_i \in K_{KM}$ then one can show (see [1, Theorem 6])

$$\|x_{l_i+1} - y\|^2 \leq \|x_{l_i} - y\|^2 - \alpha(1-\alpha)\|g_{l_i}\|^2 \tag{2}$$

where one uses the non-expansiveness of f and the fact that y is a fixed point.

Hence in any case

$$\|x_k - y\| \leq \|x_0 - y\| + c_2 \sum_i (i+1)^{-(1+\varepsilon)} = c_3 < \infty .$$

Proof, part 1 (cont.).

It then follows that

$$
\begin{aligned}
a_{k_i+1} &= \|x_{k_i+1} - y\|^2 \overset{(1),(2)}{\leq} \left(\|x_{k_i} - y\| + c_2(i+1)^{-(1+\varepsilon)}\right)^2 \\
&\leq \underbrace{\|x_{k_i} - y\|^2}_{=a_{k_i}} + \underbrace{c_2^2(i+1)^{-2(1+\varepsilon)} + 2c_2 \overbrace{\|x_{k_i} - y\|}^{\leq c_3}(i+1)^{-(1+\varepsilon)}}_{=b_{k_i}} \qquad (3) \\
&= a_{k_i} + b_{k_i}
\end{aligned}
$$

and hence

$$
\alpha(1-\alpha)\sum_i \|g_{l_i}\|^2 \overset{(2)}{\leq} \sum_i a_{l_i} - a_{l_i+1} \overset{(3)}{\leq} a_0 + \sum_k b_k < \infty
$$

We therefore have $\lim_i \|g_{l_i}\| = 0$. It also follows from $\|g_{k_i}\| \leq D\bar{U}(i+1)^{-(1+\varepsilon)}$ that $\lim_i \|g_{k_i}\| = 0$. Thus indeed $\lim_k \|g_k\| = 0$.

Proof, part 2.

Let now n_j and $N_j \geq n_j$ be such that

$$a_{n_j} \xrightarrow{j\to\infty} \liminf_k a_k = \underline{a}$$

$$a_{N_j} \xrightarrow{j\to\infty} \limsup_k a_k = \overline{a}$$

Then it follows that

$$\overline{a} - \underline{a} \xleftarrow{n_j\to\infty} \overline{a} - a_{n_j} \xleftarrow{N_j\to\infty} a_{N_j} - a_{n_j} = \sum_{k=n_j}^{N_j-1} a_{k+1} - a_k \overset{(3)}{\leq} \sum_{k=n_j}^{\infty} b_k \xrightarrow{n_j\to\infty} 0$$

so

$$\limsup_k a_k = \overline{a} \leq \underline{a} = \liminf_k a_k$$

and thus $a_k = \|x_k - y\|$ converges to some a.

Proof, part 3.

Let k_j and l_j be convergent subsequences of x_k convergent against y_1 and y_2 respectively. Since by continuity of g

$$\|g(y_1)\| = \lim_j \|g(x_{k_j})\| \overset{\text{part 1}}{=} 0$$

we have that y_1 is a fixed point and y_2 too. Now by part 2

$$\|y_1\|^2 \xleftarrow{j\to\infty} \|x_{k_j}\|^2 = \|x_{k_j} - y\|^2 - \|y\|^2 + 2y^\top x_{k_j} \xrightarrow{j\to\infty} a - \|y\|^2 + 2y^\top y_1$$

and analogously for y_2. Thus

$$\|y_i\|^2 = a - \|y\|^2 + 2y^\top y_i$$

which implies

$$2y^\top (y_1 - y_2) = \|y_1\|^2 - \|y_2\|^2 .$$

Proof, part 3 (cont.).

It then follows from

$$2y^\top(y_1 - y_2) = \|y_1\|^2 - \|y_2\|^2$$

with $y = y_i$ that

$$y_1^\top(y_1 - y_2) = y_2^\top(y_1 - y_2)$$

and further

$$(y_1 - y_2)^\top(y_1 - y_2) = 0$$

and thus $y_1 = y_2$. We have shown that two convergent subsequences have the same limit and hence x_k is convergent and the limit must be a fixed point of f.

Elastic net regression

The aim is to find a fixed point of

$$f\colon \mathbb{R}^{1000} \to \mathbb{R}^{1000}, \quad x \mapsto S_{\alpha\mu/2}\Big(x - \alpha\Big(A^\top(Ax-b) + \frac{\mu}{2}x\Big)\Big)$$

with shrinkage operator

$$S_\kappa(x) = \big(\operatorname{sgn}(x_i)(|x_i| - \kappa)_+\big)_{i=1}^{1000}$$

and $A \in \mathbb{R}^{500\times 1000}$, $b \in \mathbb{R}^{500}$ and some $\alpha, \mu \in \mathbb{R}$ as in [1].

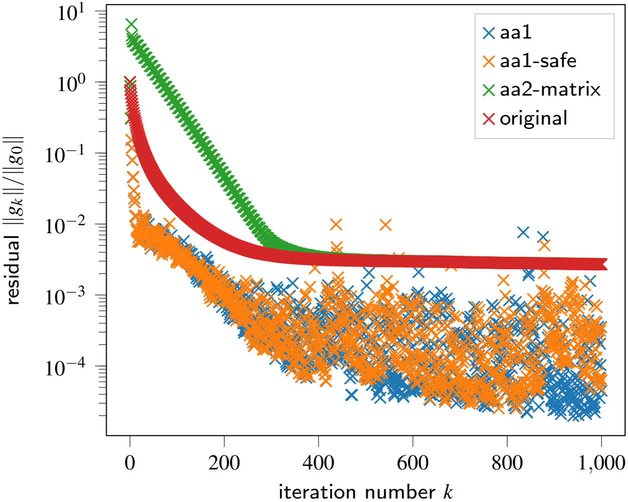


Figure: Residual norms for the elastic net regression problem.

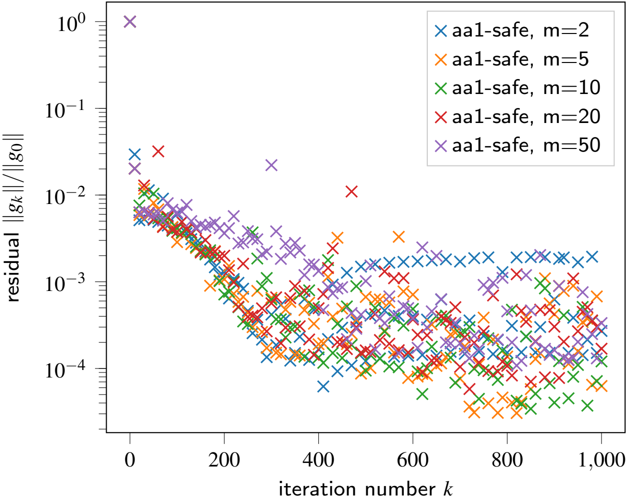


Figure: Residual norms for the elastic net regression problem.

Markov decision process

Our aim is to find a fixed point of the Bellman operator

$$f\colon \mathbb{R}^{1000} \to \mathbb{R}^{1000}, \quad x \mapsto \left(\max_a \left(R_{sa} + \gamma \sum_{s'} P_{sas'} x_{s'} \right) \right)_{s=1}^{1000}$$

with some $R \in \mathbb{R}^{300\times 200}$, $P \in \mathbb{R}^{300\times 200\times 300}$, $\gamma \in \mathbb{R}$ as in [1].

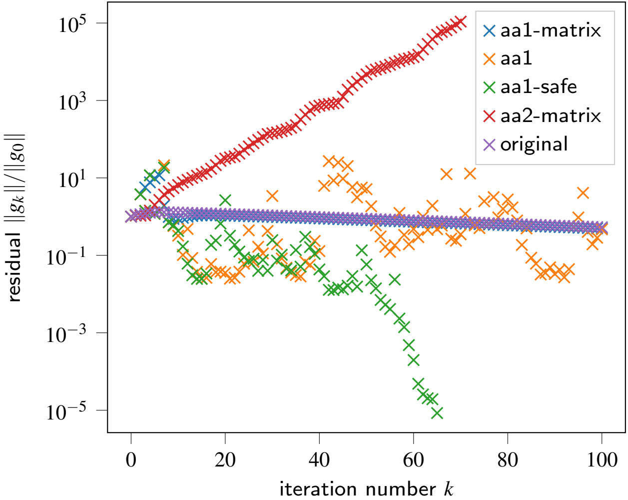


Figure: Residual norms for the Markov decision process problem.

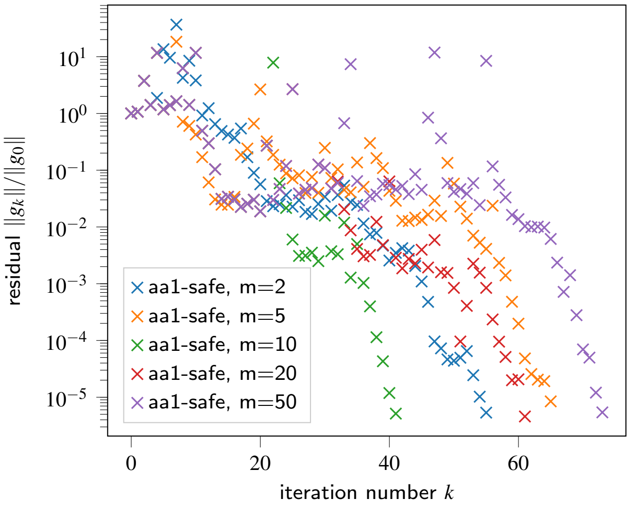


Figure: Residual norms for the Markov decision process problem.

Summary

- The aim is to find a fixed point of a non-expansive f where
  - the dimension is large
  - f is expensive to evaluate, noisy and the gradient is a mystery
- The main idea is to generalise the fixed point iteration with $x_{k+1} = \sum_i \alpha_i f_i$ for some clever choice of $\alpha = \alpha^k \in \mathbb{R}^{k+1}$.
- Modifications of the AA-I algorithm:
  - Powell-type regularisation $\rightarrow$well-definedness
  - Restarting iteration $\rightarrow$well-definedness, limited memory
  - Safeguarding steps $\rightarrow$convergence
  - Rank-1 update for H_k $\rightarrow$matrix-free
- Convergence result
- Numerical experiments: AA-I with the modifications often outperforms the fixed point iteration.

Main source

[1] J. Zhang, B. O'Donoghue, and S. Boyd, "Globally convergent type-I Anderson acceleration for nonsmooth fixed-point iterations," *SIAM J. Optim.*, vol. 30, no. 4, pp. 3170–3197, 2020, ISSN: 1052-6234. DOI: 10.1137/18M1232772. [Online]. Available: https://doi-org.ludwig.lub.lu.se/10.1137/18M1232772.

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Thank you for your attention.