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Boyd: 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 $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$, i.e. $x = f(x)$.

or equivalently

Problem (find zero)

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

We also assume

- ▶ f is nonexpansive, i.e. $\|f(x) - f(y)\| \leq \|x - y\|$
- ▶ n is large \rightarrow matrix-free
- ▶ ∇f is unknown \rightarrow no Newton
- ▶ cost of evaluation of f is high \rightarrow no line search
- ▶ noisy problem \rightarrow no finite difference derivatives

Fixed point iteration

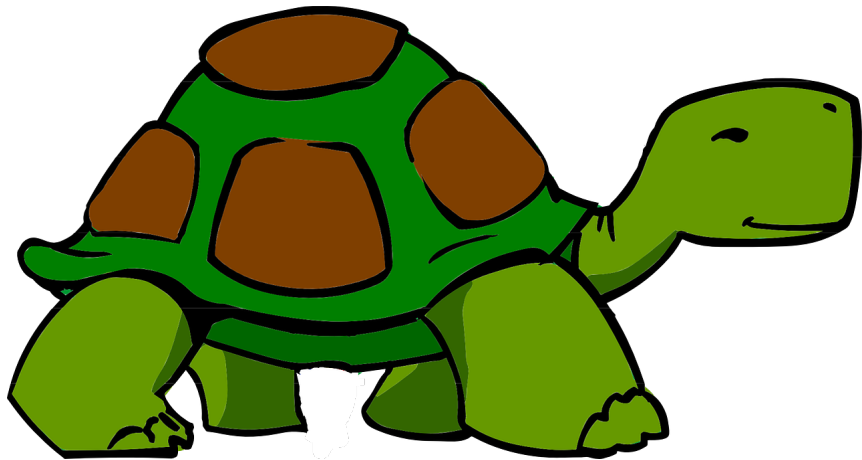
To keep things simple we try

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

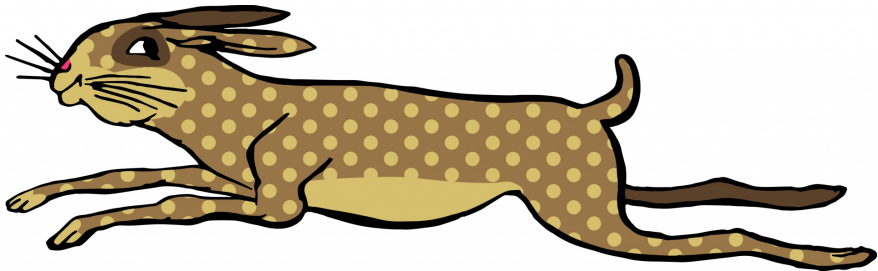
for $k = 0, 1, \dots$ **do**
| Set $x_{k+1} = f(x_k)$.
end

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 $f: \mathbb{R}^n \rightarrow \mathbb{R}^n$.

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

 Set $f_k = f(x_k)$.

 Choose $\alpha = \alpha^k \in \mathbb{R}^k$ 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 $g = \text{Id} - f$ we have the ansatz

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

```
for  $k = 0, 1, \dots$  do  
    Set  $f_k = f(x_k)$ .  
    Set  $g_k = x_k - f_k$ .  
    Choose  $\alpha \in \mathbb{R}^k$  such that  $\sum_i \alpha_i = 1$  and such that  $\alpha$   
        minimises  $\|\sum_i \alpha_i g_i\|_2$ .  
    Set  $x_{k+1} = \sum_i \alpha_i f_i$ .  
end
```

Algorithm 3: AA-II

Rewriting AA-II

Setting

$$\alpha = \begin{bmatrix} \gamma_0 \\ \gamma_1 - \gamma_0 \\ \vdots \\ \gamma_k - \gamma_{k-1} \\ 1 - \gamma_k \end{bmatrix} \text{ and } Y_k = \begin{bmatrix} g_1 - g_0 & \cdots & g_k - g_{k-1} \end{bmatrix} \in \mathbb{R}^{n \times k}$$

one obtains the least squares problem

$$\min_{\substack{\alpha \in \mathbb{R}^{k+1} \\ \sum_i \alpha_i = 1}} \left\| \sum_i \alpha_i g_i \right\| = \min_{\gamma \in \mathbb{R}^k} \|g_k - Y_k \gamma\|$$

which is solved by

$$\gamma = \gamma^k = \left(Y_k^\top Y_k \right)^{-1} Y_k^\top g_k.$$

If we now set

$$S_k = \begin{bmatrix} x_1 - x_0 & \cdots & x_k - x_{k-1} \end{bmatrix} \in \mathbb{R}^{n \times k}$$

we see that

$$\begin{aligned} S_k - Y_k &= \begin{bmatrix} x_1 - x_0 - g_0 + g_1 & \cdots & x_k - x_{k-1} - g_k + g_{k-1} \end{bmatrix} \\ &= \begin{bmatrix} f_1 - f_0 & \cdots & f_k - f_{k-1} \end{bmatrix} \end{aligned}$$

and hence

$$\begin{aligned}x_{k+1} &= \sum_i \alpha_i f(x_i) \\&= f_k - (S_k - Y_k) \gamma \\&\quad \swarrow f_k = x_k - g_k \text{ and } \gamma = (Y_k^\top Y_k)^{-1} Y_k^\top \\&= x_k - \underbrace{\left(\text{Id} + (S_k - Y_k) (Y_k^\top Y_k)^{-1} Y_k^\top \right)}_{=H_k} g_k \\&= x_k - H_k g_k.\end{aligned}$$

We thus have the reformulation

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

Set $x_1 = f(x_0)$.

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

 Set $g_k = g(x_k)$.

 Construct S_k from x_0, \dots, x_k and Y_k from g_0, \dots, g_k .

 Set $H_k = \text{Id} + (S_k - Y_k)(Y_k^\top Y_k)^{-1} Y_k^\top$.

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

end

Algorithm 4: AA-II (reformulated)

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

Proposition (Approximate inverse Jacobian)

H_k minimises $\|H_k - \text{Id}\|_F$ under the multisecant condition $H_k S_k = Y_k$.

From Broydens method we know that it is a good idea to approximate the Jacobian rather than its inverse.

Definition (Approximate Jacobian)

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

Analogously to AA-II we have

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

This yields the AA-I algorithm

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

Set $x_1 = f(x_0)$

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

 Set $g_k = g(x_k)$.

 Construct S_k from x_0, \dots, x_k and Y_k from g_0, \dots, g_k .

 Set $B_k = \text{Id} + (Y_k - S_k)(S_k^\top S_k)^{-1} S_k^\top$.

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

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

end

Algorithm 5: AA-I

Luckily for us we can save some computations by using the rank-1 update formula

Proposition (Rank-1 update for B_k)

We have

$$B_{k+1} = B_k + \frac{(y_k - B_k s_k) \hat{s}_k^\top}{\hat{s}_k^\top s_k}$$

where $y_k = g_{k+1} - g_k$, $B_0 = \text{Id}$ and

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

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

From the Sherman-Morrison formula it then follows that

Proposition (Rank-1 update for H_k)

We have

$$H_{k+1} = H_k + \frac{(s_k - H_k y_k) \hat{s}_k^\top H_k}{\hat{s}_k^\top H_k y_k}$$

where $y_k = g_{k+1} - g_k$, $H_0 = \text{Id}$ and

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

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

Taking everything together we obtain

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

Set $H_0 = \text{Id}$ and $x_1 = f(x_0)$.

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

$$\hat{s}_{k-1} = s_{k-1} - \sum_{i=0}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i.$$

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

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

end

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

Powell-type regularisation

Note that B_k may be singular. To fix this set

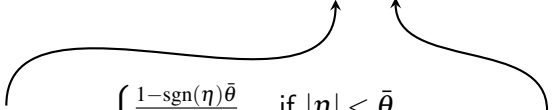
$$\tilde{y}_k = \theta_k y_k + (1 - \theta_k) B_k s_k$$

or equivalently

$$\tilde{y}_k = \theta_k y_k + (1 - \theta_k) B_k s_k$$

where

with

$$\theta_k = \phi_{\bar{\theta}}(\eta_k)$$

$$\phi_{\bar{\theta}}(\eta) = \begin{cases} \frac{1 - \text{sgn}(\eta)\bar{\theta}}{1 - \eta} & \text{if } |\eta| < \bar{\theta} \\ 1 & \text{else} \end{cases} \quad \text{and} \quad \eta_k = \frac{\hat{s}_k^\top H_k y_k}{\|\hat{s}_k\|^2}$$

One can obtain

Lemma (Powell-type regularisation)

Let $s_k \in \mathbb{R}^n$, $B_0 = \text{Id}$, and inductively

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

with \hat{s}_k and \tilde{y}_k defined as before. If this is well-defined then $|\det(B_k)| \geq \theta^k > 0$ and B_k is invertible.

Proof.

See [1, Lemma 2].



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

Set $H_0 = \text{Id}$ and $x_1 = f(x_0)$.

for $k = 0, 1, \dots$ **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 $\hat{s}_{k-1} = s_{k-1} - \sum_{i=0}^{k-2} \frac{\hat{s}_i^\top s_{k-1}}{\|\hat{s}_i\|^2} s_i$.

Set $\eta_{k-1} = \frac{\hat{s}_{k-1}^\top H_{k-1} y_{k-1}}{\|\hat{s}_{k-1}\|^2}$, $\theta_{k-1} = \phi_{\bar{\theta}}(\eta_{k-1})$ and

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

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

end

Algorithm 7: AA-I with Powell-like-regularisation

Restarting iteration

Note that

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

is ill-defined iff $\|\hat{s}_k\|^2 = \hat{s}_k^\top s_k = 0$, i.e. $\hat{s}_k = 0$. This occurs in algorithm 7 for $k > n$ as then $\hat{s}_k = 0$ by linear dependence. If we restart the algorithm with x_k as the new starting point if $k = m + 1$ for some $m \in \mathbb{N}$ or $\|\hat{s}_{k-1}\| < \tau \|s_{k-1}\|$ for some $\tau \in (0, 1)$ then

$$g_k \neq 0 \implies s_k = -B_k g_k \neq 0 \implies \hat{s}_k \neq 0.$$

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

Set $H_0 = \text{Id}$, $x_1 = f(x_0)$ 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 $H_{k-1} = \text{Id}$.

end

Set $\eta_{k-1} = \frac{\hat{s}_{k-1}^\top H_{k-1} y_{k-1}}{\|\hat{s}_{k-1}\|^2}$, $\theta_{k-1} = \phi_{\bar{\theta}}(\eta_{k-1})$ and

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

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

end

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

Lemma (Restarting iteration)

If we additionally choose m_k by the rule above we have

$$\|B_k\| \leq 3 \left(\frac{1 + \bar{\theta} + \tau}{\tau} \right)^m - 2.$$

Proof.

See [1, Lemma 3].



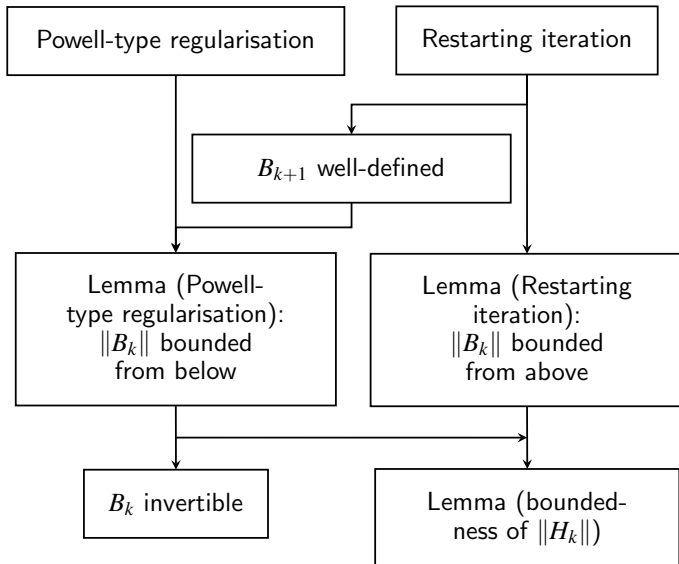
Lemma (bound on $\|H_k\|_2$)

In algorithm 8 we have that

$$\|H_k\|_2 \leq \frac{1}{\bar{\theta}^m} \left(3 \left(\frac{1 + \bar{\theta} + \tau}{\tau} \right)^m - 2 \right)^{n-1}.$$

Proof.

This follows from Lemma (Restarting iteration) and Lemma (Powell-type regularisation). □



Safeguarding steps

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

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

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

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

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

for $k = 0, 1, \dots$ **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 $H_{k-1} = \text{Id}$.

end

 Set $\eta_{k-1} = \frac{\hat{s}_{k-1}^\top H_{k-1} y_{k-1}}{\|\hat{s}_{k-1}\|^2}$, $\theta_{k-1} = \phi_{\bar{\theta}}(\eta_{k-1})$ and $\tilde{y}_{k-1} = \theta_{k-1} y_{k-1} - (1 - \theta_{k-1}) g_{k-1}$.

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

end

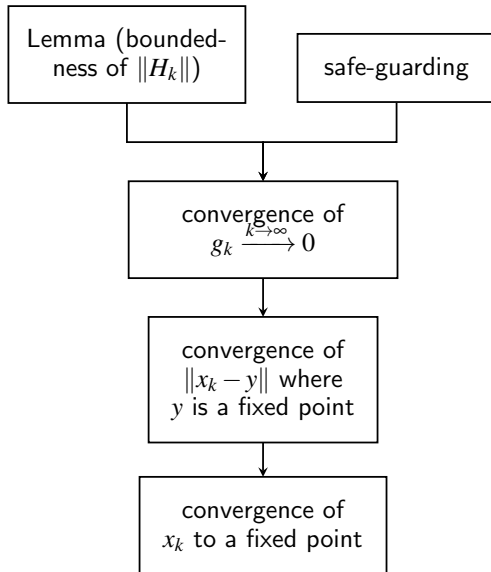
end

Algorithm 9: AA-I with Powell-like-regularisation, Restarting and Safeguarding

Convergence result

Theorem (Convergence)

Let x_k be generated by algorithm 9 then $x_k \xrightarrow{k \rightarrow \infty} x$ and $f(x) = x$ is a fixed point.



Proof, part 1.

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

Algorithm 10: The two cases for x_{k+1} .

Proof, part 1 (cont.)

Let y be a fixed point. We distinguish

case (1) $k \in K_{AA}$ then

$$\begin{aligned}\|x_{k+1} - y\| &\leq \|x_k - y\| + \|H_k g_k\| \\ &\leq \|x_k - y\| + c_1 \|g_k\| \\ &\leq \|x_k - y\| + c_2 (k+1)^{-(1+\varepsilon)}\end{aligned}\tag{1}$$

case (2) $k \in K_{KM}$ then (motivate this)

$$\|x_{k+1} - y\|^2 \leq \|x_k - y\|^2 - \alpha(1-\alpha)\|g_k\|^2 \leq \|x_k - y\|^2\tag{2}$$

Hence in any case

$$\begin{aligned}\|x_k - y\| &\leq \|x_0 - y\| + \sum_{l=0}^{k-1} \|x_{l+1} - x_l\| \\ &\leq \|x_0 - y\| + c_2 \sum_k (k+1)^{-(1+\varepsilon)} = c_3 < \infty.\end{aligned}$$

Proof, part 1 (cont.)

It then follows that

$$\begin{aligned} a_{k+1} &= \|x_{k+1} - y\|^2 \\ &\stackrel{(1),(2)}{\leq} \underbrace{\|x_k - y\|^2}_{=a_k} + \underbrace{c_2^2(k+1)^{-2(1+\varepsilon)} + 2c_2 \underbrace{\|x_k - y\|}_{\leq c_3} (k+1)^{-(1+\varepsilon)}}_{=b_k} \\ &= a_k + b_k \end{aligned} \tag{3}$$

and hence

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

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

$$a_{n_j} \xrightarrow{j \rightarrow \infty} \liminf_k a_k = \underline{a}$$
$$a_{N_j} \xrightarrow{j \rightarrow \infty} \limsup_k a_k = \bar{a}$$

Then it follows that

$$\bar{a} - \underline{a} \xleftarrow{n_j \rightarrow \infty} \bar{a} - a_{n_j} \xleftarrow{N_j \rightarrow \infty} a_{N_j} - a_{n_j} = \sum_{k=n_j}^{N_j-1} a_{k+1} - a_k \leq \sum_{k=n_j}^{\infty} b_k \xrightarrow{n_j \rightarrow \infty} 0$$

so

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

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

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

$$\|g(y_1)\| = \lim_j \|g(x_{k_j})\| = 0$$

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

$$\|y_1\| \xleftarrow{j \rightarrow \infty} \|x_{k_j}\|^2 = \|x_k - y\|^2 + \|y\|^2 + 2y^\top x_{k_j} \xrightarrow{j \rightarrow \infty} b^2 + \|y\|^2 + 2y^\top y_1$$

and analogously for y_2 . Thus

$$\|y_i\| = b^2 + \|y\|^2 + 2y^\top y_i$$

which implies

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

Proof, part 3 (cont.)

It then follows from $y \in \{y_i\}_i$ 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 solution must be a fixed point of f .

Elastic net regression

Our aim is to minimise

$$F: \mathbb{R}^{1000} \rightarrow \mathbb{R}, \quad x \mapsto \frac{1}{2} \|Ax - b\|^2 + \mu \left(\frac{1}{4} \|x\|^2 + \frac{1}{2} \|x\|_1 \right)$$

with $A \in \mathbb{R}^{500 \times 1000}$, $b \in \mathbb{R}^{500}$ and some $\mu \in \mathbb{R}$. From the Iterative Shrinkage-Thresholding Algorithm one obtains

$$f: \mathbb{R}^{1000} \rightarrow \mathbb{R}^{1000}, \quad x \mapsto S_{\alpha\mu/2} \left(x - \alpha \left(A^\top (Ax - b) + \frac{\mu}{2} x \right) \right)$$

with shrinkage operator

$$S_\kappa(x) = (\operatorname{sgn}(x_i)(|x_i| - \kappa)_+)_i$$

and some $\alpha \in \mathbb{R}$.

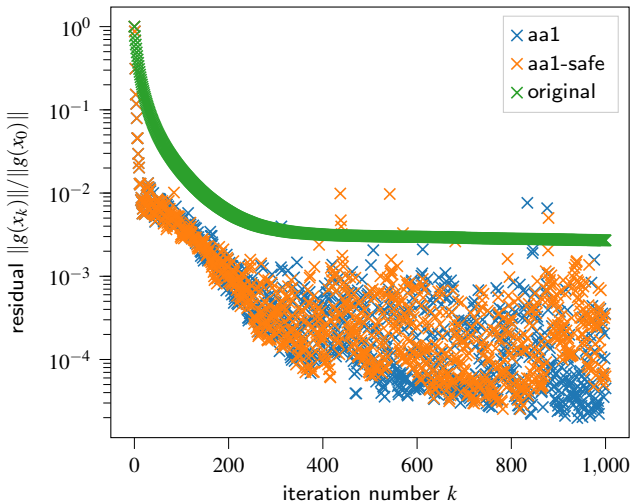


Figure: Residual norms for the elastic net regression problem.

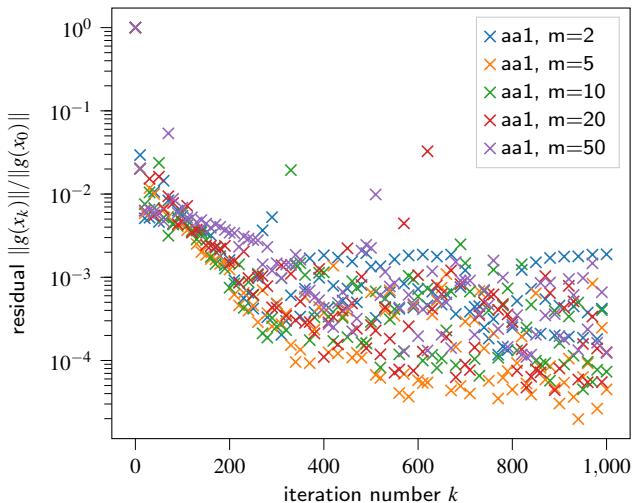


Figure: Residual norms for the elastic net regression problem.

Markov decision process

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

$$f: \mathbb{R}^{1000} \rightarrow \mathbb{R}^{1000}, \quad x \mapsto \left(\max_a R(s, a) + \gamma \sum_{s'} P(s, a, s') x_{s'} \right)_s$$

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

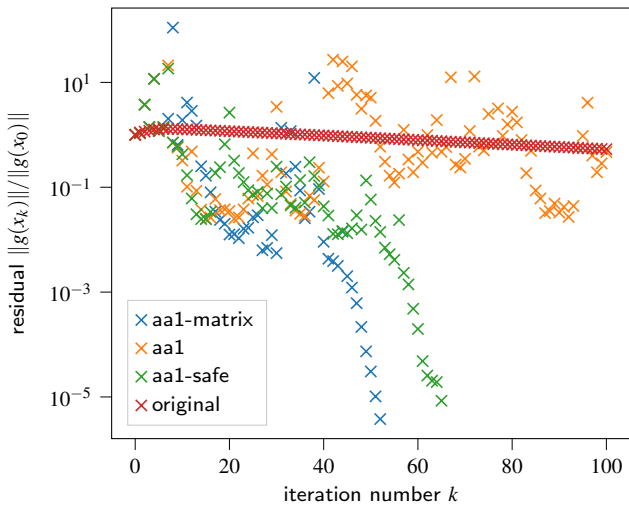


Figure: Residual norms for the elastic net regression problem.

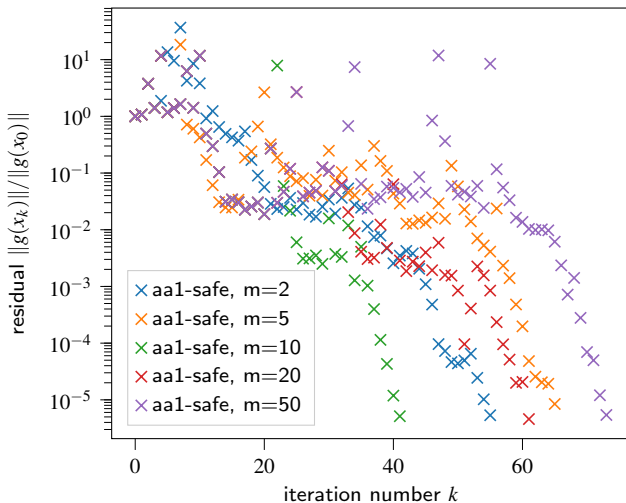


Figure: Residual norms for the elastic net regression problem.

Summary

- ▶ aim is to find a fixed point of f where
 - ▶ the dimension is large
 - ▶ f is expensive to evaluate, noisy and the gradient is a mystery
- ▶ 3 modifications to the AA-I algorithm yield well-definedness and convergence for non-expansive problems
 - ▶ Powell-type regularisation
 - ▶ Restarting iteration
 - ▶ Safeguarding steps
- ▶

Sources I

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Thank you for your attention.