Connecting Quasi-Newton with Extrapolation:

Black-box, Memory Efficient and Line-search Free Acceleration via Stabilized Anderson Mixing

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Overview

1. Motivation and Problem Statement
2. Acceleration: connecting quasi-Newton with extrapolation
   - Good news and bad news
3. A generic stabilization scheme
   - Stabilization of AA-I
   - Stabilization of AA-II
   - Global convergence: solvable settings
   - A browse through effect of stabilization
4. Applications
   - Conic optimization + SCS 2.x
   - Prox-affine optimization + A2DR
5. Beyond convexity

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Fixed-point problems

- We consider solving a fixed-point (FP) problem $v = F(v)$, where $F : \mathbb{R}^n \to \mathbb{R}^n$ is potentially non-smooth.

[1] $\|v\|_H = \sqrt{v^T H v}$ for some PD matrix H

Fixed-point problems

- We consider solving a fixed-point (FP) problem $v = F(v)$, where $F : \mathbb{R}^n \to \mathbb{R}^n$ is potentially non-smooth.
- **Assumption**: F is **non-expansive** in l_2 (or H-norm[1]), *i.e.*,

$$\|F(v) - F(w)\|_2 \leq \|v - w\|_2 \text{ for any } v,\ w \in \mathbb{R}^n$$

  or **contractive** in an arbitrary norm $\|\cdot\|$.
- Simplest solution: averaged iteration, a.k.a. Krasnosel'skiĭ-Mann (KM) iteration

$$v^{k+1} = F_\alpha(v^k) = (1-\alpha)v^k + \alpha F(v^k),\ \alpha \in (0,1).$$

- Convergence is robust, but sublinear in theory and slow in practice: can we **(safely)** do better?

[1] $\|v\|_H = \sqrt{v^T H v}$ for some PD matrix H

Why non-smooth non-expansive fixed-point problems?

Many (potentially complicated) algorithms in optimization and beyond can be reformulated as **"black-box" fixed-point** problems.

Examples:

- (Any) convex optimization with no strong convexity
  - $\text{minimize}_{x \in C}\ f(x)$, C is convex, f is convex and L-strongly smooth.

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  - Optimality $\Leftrightarrow$ $x = F(x),\ F(x) := \Pi_C\left(x - \frac{1}{L}\nabla f(x)\right)$.
  - Projection is non-differentiable and non-expansive, but non-contractive without strong convexity.

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Examples:

- Discounted Markov decision processes (MDP)
  - Value iteration: $v^{k+1} = Tv^k$, where T is the Bellman operator:

$$(Tv)_s = \max_{a=1,\ldots,A} R(s,a) + \gamma \sum\nolimits_{s'=1}^{S} P(s,a,s')v_{s'}.$$

  - Optimality $\Leftrightarrow$ $v = Tv$.
  - Contractive in l_∞, but still non-differentiable due to max.

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Examples:

- Nash equilibrium in a multiplayer game $\Leftrightarrow$ monotone inclusion problem $\Leftrightarrow$ non-smooth non-expansive fixed-point problem.

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Algorithm 1 Extrapolation framework

Input: initial point x_0, fixed-point mapping $F : \mathbb{R}^n \to \mathbb{R}^n$.
for $k = 0, 1, \ldots$ **do**
  Choose m_k (*e.g.*, $m_k = \min\{m, k\}$ for some integer $m \geq 0$).
  Select weights α_j^k based on the last m_k iterations, with $\sum_{j=0}^{m_k} \alpha_j^k = 1$.
  $v^{k+1} = \sum_{j=0}^{m_k} \alpha_j^k F(v^{k-m_k+j})$.

Such a framework subsumes many different algorithms, among which one of the most natural and popular method is Anderson acceleration (1965):

$$\text{minimize} \quad \| \sum_{j=0}^{m_k} \alpha_j G(v^{k-m_k+j}) \|_2^2 \quad \text{subject to} \quad \sum_{j=0}^{m_k} \alpha_j = 1,$$

where $G(v) := v - F(v)$ is the residual.

Literature comments

- Also known as **Type-II Anderson acceleration** (AA-II), Anderson/Pulay mixing, Pulay's direct inversion iterative subspace (DIIS), nonlinear GMRES, minimal polynomial extrapolation (MPE), reduced rank extrapolation (RRE), etc.

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  - MLE, matrix completion, K-means, computer vision and deep learning.

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- Widely used in computational quantum chemistry and material sciences, and recently introduced to optimization applications
  - MLE, matrix completion, K-means, computer vision and deep learning.
- Equivalent to **multi-secant quasi-Newton** methods (see below) – development separated from the main-stream, connection established very recently in Fang and Saad 2009.
  - Extrapolation: good for intuition.
  - Quasi-Newton: good for derivations.

From extrapolation to quasi-Newton

- Recall the selection of α_j^k in AA-II (constrained least-squares):

$$\text{minimize} \quad \|\sum_{j=0}^{m_k} \alpha_j G(v^{k-m_k+j})\|_2^2 \quad \text{subject to} \quad \sum_{j=0}^{m_k} \alpha_j = 1,$$

- Reformulation: minimize $\|g^k - Y_k \gamma\|_2$
  - variable $\gamma = (\gamma_0, \ldots, \gamma_{m_k-1})$.
  - $g^i = G(v^i)$, $Y_k = [y^{k-m_k} \ \ldots \ y^{k-1}]$ with $y^i = g^{i+1} - g^i$ for each i.
  - $\alpha_0 = \gamma_0$, $\alpha_i = \gamma_i - \gamma_{i-1}$ for $1 \le i \le m_k - 1$ and $\alpha_{m_k} = 1 - \gamma_{m_k-1}$.

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  - $\alpha_0 = \gamma_0$, $\alpha_i = \gamma_i - \gamma_{i-1}$ for $1 \le i \le m_k - 1$ and $\alpha_{m_k} = 1 - \gamma_{m_k-1}$.
- $v^{k+1} = \sum_{j=0}^{m_k} \alpha_j^k F(v^{k-m_k+j}) = v^k - H_k g^k$,
  - $H_k := I + (S_k - Y_k)(Y_k^T Y_k)^{-1} Y_k^T$
    - $S_k = [s^{k-m_k} \ldots s^{k-1}]$ with $s^i = v^{i+1} - v^i$ for each i.
  - $H_k = \text{argmin}_{HY_k = S_k} \|H - I\|_F$: **approximate inverse Jacobian** of G.
  - multi-secant type-II Broyden's (quasi-Newton) method.

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- $v^{k+1} = v^k - B_k^{-1} g^k$, with $B_k^{-1} = I + (S_k - Y_k)(S_k^T Y_k)^{-1} S_k^T$.

Type-I Anderson acceleration

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Algorithm 2 Type-I Anderson Acceleration (AA-I)

1: **for** $k = 0, 1, \ldots$ **do**
2: Choose $m_k \leq m$ (*e.g.*, $m_k = \min\{m, k\}$ for some integer $m \geq 0$).
3: Compute $\tilde{\gamma}^k = (S_k^T Y_k)^{-1}(S_k^T g^k)$.
4: $\alpha_0^k = \tilde{\gamma}_0^k$, $\alpha_i^k = \tilde{\gamma}_i^k - \tilde{\gamma}_{i-1}^k$ $(1 \leq i \leq m_k - 1)$ and $\alpha_{m_k}^k = 1 - \tilde{\gamma}_{m_k-1}^k$.
5: $v^{k+1} = \sum_{j=0}^{m_k} \alpha_j^k F(v^{k-m_k+j})$.

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Good news:

- Compared to **LBFGS** and **restarted Broyden**:
  - AA is *memory efficient* (AA-I with $m = 5 - 10$ beats LBFGS/restarted Broyden with $m = 200 - 500$)

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  - AA is *line-search free*: just accept or reject is the best practice
  - AA is suitable to be used in a completely *black-box* way
    - PGD: don't separate the gradient step and projection
    - ADMM: don't separate the primal and dual steps

Good news:

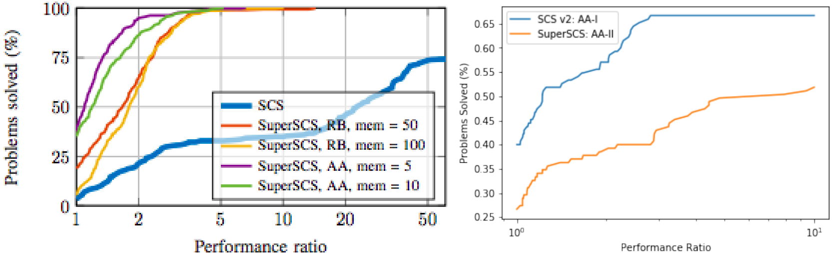

Figure: Sparse PCA: DM profiles of run time. Left: AA-II v.s. restarted Broyden, both in SuperSCS. Right: AA-I (SCS 2.x) v.s. AA-II (SuperSCS).

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Bad news:

- **Numerical challenge**: both AA-I and AA-II are subject to potential *numerical instability*, and AA-I is more severe.
  - AA-II: $Y_k^T Y_k$ (close to) singular (degenerate least-squares system).
  - AA-I: B_k can be (close to) singular.

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- **Theoretical challenge**: local convergence theory exists with further smoothness assumptions, but *no global convergence*.

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Bad news: **Numerical challenge**

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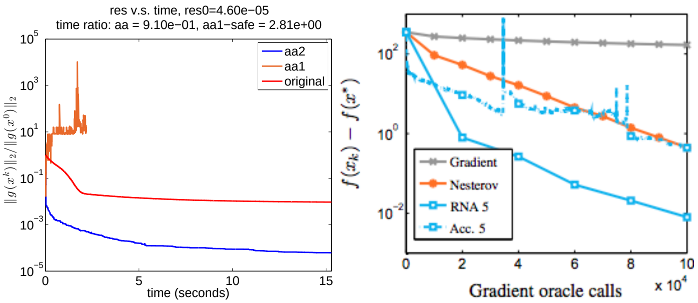

Figure: Divergence of AA + gradient descent on ℓ_2 regularized logistic regression **without** stabilization. Left: Failure of AA-I. Right: Failure of AA-II (*Regularized Nonlinear Acceleration*, Scieur et al., 2016).

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  - (Scieur et al., 2016) showed that adding **constant quadratic regularization** to the objective leads to local convergence improvement.
  - **Insufficient** for global convergence both in theory and practice.
- In general, most of the literature has been focused on AA-II:
  - AA-I is generally *missing both in theory and practice*.

Goal and contribution

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Goal and contribution

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  - The FP mapping of SCS is non-smooth and singular.
  - **Surprise:** stabilization also improves convergence consistently over both the original AA-I and AA-II.
- Develop a "plug-and-play" acceleration scheme based on the stabilized AA
  - View an arbitrary unaccelerated algorithm as a **black-box** fixed-point iteration problem.
  - For example, concatenate successive iterates in momentum algorithms.

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- Iterates for $k = 1, 2, \ldots$, $(D,\ \epsilon > 0,\ M$ positive integer)

1. Compute $v_{\text{FP}}^{k+1} = F_\alpha(v^k), \quad g^k = v^k - v_{\text{FP}}^{k+1}$.
2. Update Y_k and S_k to include the new information
   & Compute a **modified** α^k (H_k/B_k)
3. Compute $v_{\text{AA}}^{k+1} = \sum_{j=0}^{M} \alpha_j^k v_{\text{FP}}^{k-M+j+1}$.
4. If the residual $\|G(v^k)\|_2 \le D\|g^0\|_2/n_{\text{AA}}^{1+\epsilon}$: (**safeguard**)
   Adopt $v^{k+i} = v_{\text{AA}}^{k+i}$ for $i = 1, \ldots, M$.
   (n_{AA}: # of adopted AA candidates)
5. Otherwise, take $v^{k+1} = v_{\text{FP}}^{k+1}$.

Motivations of the stabilization tricks

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  - Can be seen as a much cheaper alternative to the expensive line-search.

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Stabilization of AA-I: rank-one update

AA-I $\Longleftrightarrow$ Type-I Broyden's rank-one update with **orthogonalization**:

Proposition

Suppose that S_k is full rank, then B_k can be computed inductively from $B_k^0 = I$ as follows:

$$B_k^{i+1} = B_k^i + \frac{(y^{k-m_k+i} - B_k^i s^{k-m_k+i})(\hat{s}^{k-m_k+i})^T}{(\hat{s}^{k-m_k+i})^T s^{k-m_k+i}}, \quad i = 0, \ldots, m_k - 1$$

with $B_k = B_k^{m_k}$. Here $\{\hat{s}^i\}_{i=k-m_k}^{k-1}$ is the Gram-Schmidt orthogonalization of $\{s^i\}_{i=k-m_k}^{k-1}$, i.e., $\hat{s}^i = s^i - \sum_{j=k-m_k}^{i-1} \frac{(\hat{s}^j)^T s^i}{(\hat{s}^j)^T \hat{s}^j} \hat{s}^j, \quad i = k - m_k, \ldots, k-1.$

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- AA-II: add ridge penalty (regularized nonlinear acceleration, 2016)

$$\text{minimize}_{\sum_{j=0}^{m_k} \alpha_j = 1} \quad \| \sum_{j=0}^{m_k} \alpha_j G(v^{k-m_k+j}) \|_2^2 + \lambda \|\alpha\|_2^2$$

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- AA-I: Powell-type trick (turns out very helpful also **in practice**!)
  - Replace y^{k-m_k+i} with $\tilde{y}^{k-m_k+i} = \theta_k^i y^{k-m_k+i} + (1-\theta_k^i) B_k^i s^{k-m_k+i}$, where $\theta_k^i = \phi_{\bar{\theta}}(\eta_k^i)$, with $\eta_k^i = \frac{\hat{s}^{k-m_k+i\,T} (B_k^i)^{-1} y^{k-m_k+i}}{\|\hat{s}^{k-m_k+i}\|_2^2}$,

$$\phi_{\bar{\theta}}(\eta) = \begin{cases} 1 & \text{if } |\eta| \geq \bar{\theta} \\ \frac{1 - \mathbf{sign}(\eta)\bar{\theta}}{1-\eta} & \text{if } |\eta| < \bar{\theta}. \end{cases}$$

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  Help in extreme cases, but impede the convergence in general.

- AA-I: Powell-type trick (turns out very helpful also **in practice**!)
  - Replace y^{k-m_k+i} with $\tilde{y}^{k-m_k+i}=\theta_k^i y^{k-m_k+i}+(1-\theta_k^i)B_k^i s^{k-m_k+i}$, where $\theta_k^i=\phi_{\bar{\theta}}(\eta_k^i)$, with $\eta_k^i=\frac{\hat{s}^{k-m_k+i\,T}(B_k^i)^{-1}y^{k-m_k+i}}{\|\hat{s}^{k-m_k+i}\|_2^2}$,

$$\phi_{\bar{\theta}}(\eta)=\begin{cases}1 & \text{if } |\eta|\geq\bar{\theta}\\ \frac{1-\textbf{sign}(\eta)\bar{\theta}}{1-\eta} & \text{if } |\eta|<\bar{\theta}.\end{cases}$$

  - $|\det(B_k)|\geq\bar{\theta}^{m_k}>0$, and in particular, B_k is **invertible**!

Stabilization of AA-I: 2. Re-start checking

Goal of re-start: avoid blow-up ("upper bound" on B_k).

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- Solution: update $m_k = m_{k-1} + 1$. If $m_k = m + 1$ or $\|\hat{s}^{k-1}\|_2 < \tau\|s^{k-1}\|_2$, then reset $m_k = 1$.
- Then $\|B_k\|_2 \leq 3(1 + \bar{\theta} + \tau)^m/\tau^m - 2$!
- (Re)define $H_k := B_k^{-1}$: $\|H_k\|_2 \leq \left(3\left(\frac{1+\bar{\theta}+\tau}{\tau}\right)^m - 2\right)^{n-1} / \bar{\theta}^m$.

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Stabilization of AA-II: Adaptive Regularization

Our approach:

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- Adaptive quadratic regularization: (adaptive LS)

$$\text{minimize} \quad \|g^k - Y_k\gamma^k\|_2^2 + \eta\left(\|S_k\|_F^2 + \|Y_k\|_F^2\right)\|\gamma^k\|_2^2,$$

where $\eta \geq 0$ is a regularization parameter and

$$g^k = G(v^k), \quad y^k = g^{k+1} - g^k, \quad Y_k = [y^{k-M} \ \ldots \ y^{k-1}]$$
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Lemma (Bounded approximate inverse Jacobian)

We have $v_{AA}^{k+1} = v^k - H_k g^k$, where $g^k = G(v^k)$ is the FP residual at v^k, and $\|H_k\|_2 \le 1 + 2/\eta$, where $\eta > 0$ is the regularization parameter in the adaptive LS subproblem.

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Global convergence

Theorem

Suppose that f **has a fixed-point**. *Also suppose that f is non-expansive in l_2-norm or contractive in an arbitrary norm. Assume that $\{x^k\}_{k=0}^{\infty}$ is generated by the generic stabilization scheme wth α^k (H_k/B_k) chosen by either the stabilized AA-I or AA-II . Then we have*

$$\lim_{k\to\infty} x^k = x^\star,$$

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What if f does not have a fixed-point? Pathological settings to be discussed later.

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Effect of stabilization: AA-II + constant regularization

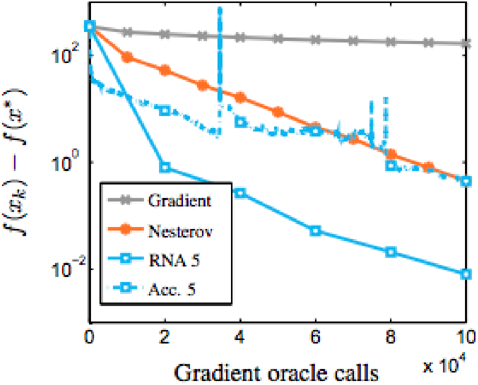

Figure: Effect of constant regularization (RNA, Scieur et al., 2016): ℓ_2 regularized logistic regression.

Effect of stabilization: AA-II + adaptive regularization

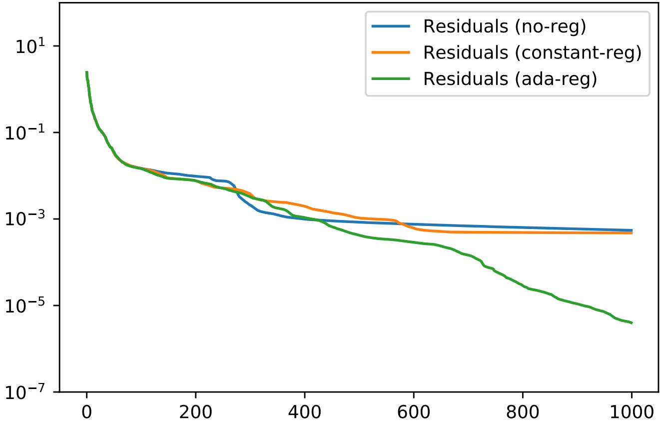

Figure: Further improvement of adaptive regularization (A2DR, FZB 2019): Nonnegative least squares.

Gradient Descent: stabilization from **divergence** to **convergence**

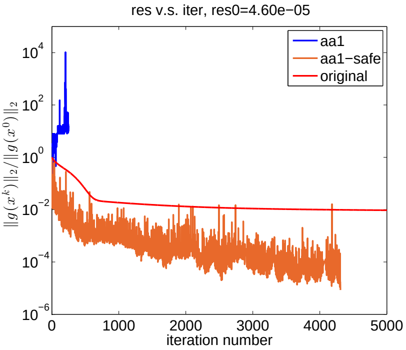

Figure: Gradient descent: regularized logistic regression. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

ISTA: elastic net regression – nonsmoothness coming from shrinkage

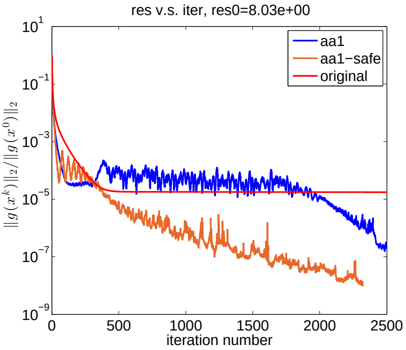

Figure: Iterative Shrinkage-Thresholding Algorithm: elastic-net linear regression. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

Effect of stabilization: AA-I

MDP (value iteration) (discount factor $\gamma = 0.99$):

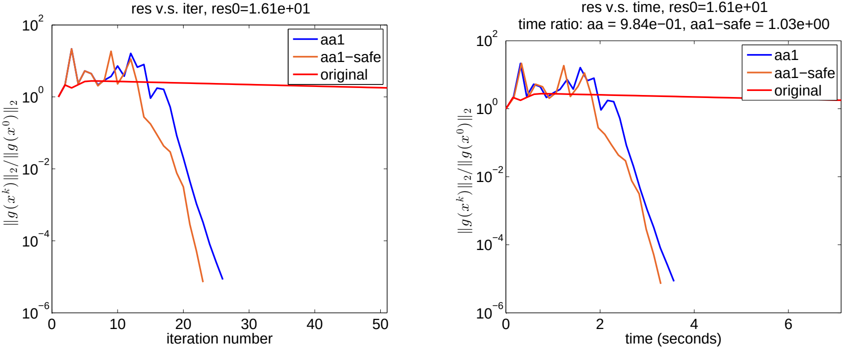

Figure: Value iteration: MDP. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

Effect of **different memories** *m*:

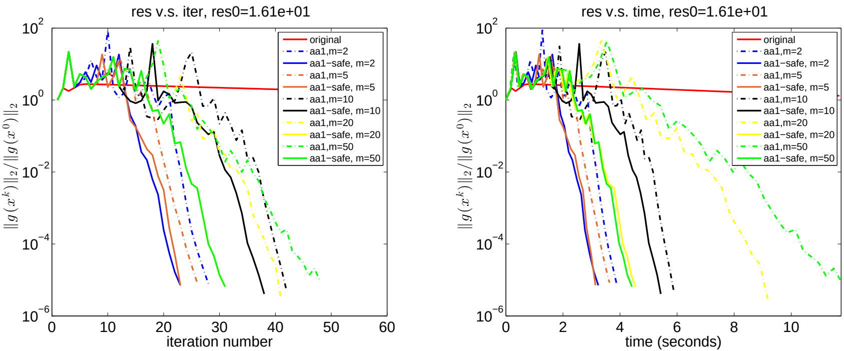

Figure: Value iteration: memory effect. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

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SCS as FP

- Problem: minimize$_x$ $c^T x$, subject to $Ax + s = b,\ s \in \mathcal{K}$.

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- Algorithm – SCS ($\mathcal{C} = \mathbb{R}^n \times \mathcal{K}^* \times \mathbb{R}_+$):

$$\begin{aligned}
\tilde{u}^{k+1} &= (I + Q)^{-1}(u^k + v^k) \\
u^{k+1} &= \Pi_{\mathcal{C}}(\tilde{u}^{k+1} - v^k) \\
v^{k+1} &= v^k - \tilde{u}^{k+1} + u^{k+1}.
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- FP (don't apply AA to u and v separately):

$$F(u,v) = \begin{bmatrix} \Pi_{\mathcal{C}}((I+Q)^{-1}(u+v) - v) \\ v - (I+Q)^{-1}(u+v) + u \end{bmatrix}.$$

- F is non-expansive (in ℓ_2), and 0 is always a fixed-point, and so the global convergence theorem goes through.

- We apply the stabilized AA-I to SCS.
- **Hyper-parameters choice**: $\bar{\theta} = 0.01$, $\tau = 0.001$, $D = 10^6$, $\epsilon = 10^{-6}$, memory $m = 5$, averaging weight $\alpha = 0.1$.
- **Matrix-free updates**: instead of computing and storing H_k, we store $H_{k-j}\tilde{y}_{k-j}$ and $\frac{H_{k-j}^T \hat{s}_{k-j}}{\hat{s}_{k-j}^T (H_{k-j}\tilde{y}_{k-j})}$ for $j = 1, \ldots, m_k$, compute

$$d_k = g_k + \sum_{j=1}^{m_k} (s_{k-j} - (H_{k-j}\tilde{y}_{k-j})) \left(\frac{H_{k-j}^T \hat{s}_{k-j}}{\hat{s}_{k-j}^T (H_{k-j}\tilde{y}_{k-j})} \right)^T g_k,$$

  and then update $\tilde{x}^{k+1} = x^k - d_k$.
- **Problem scaling** is helpful when matrices are involved.

- Compared to **restarted Broyden**:

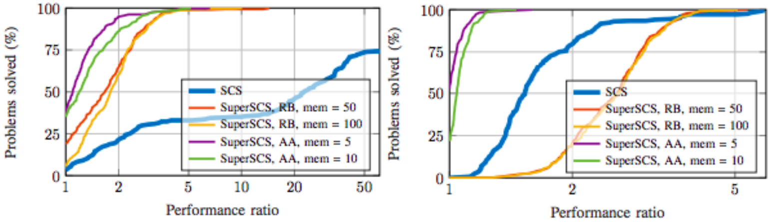

Figure: DM profile. left: sparse PCA; right: sparse logistic regression. *SuperSCS: fast and accurate large-scale conic optimization.* Sopasakis, et al., 2019.

Further success of AA-I: SCS 2.x

- Compared to **AA-II**:

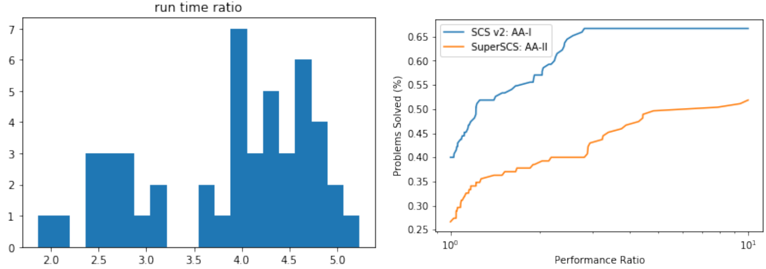

Figure: Sparse PCA. Left: histogram of run time ratio between SuperSCS (AA-II) and SCS 2.x (AA-I). Right: DM profile of run time.

- Still fail for 35% of the test cases.

Even further success with stabilized AA-I

SCS: LP – nonsmoothness coming from projections

- Implementation in progress in the next version of SCS.

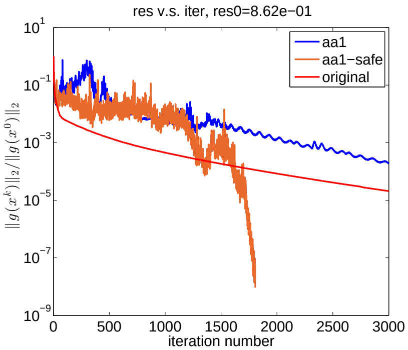

Figure: SCS: linear program. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

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SCS: SOCP – nonsmoothness coming from projections

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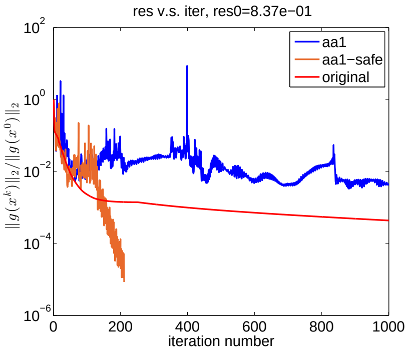

Figure: SCS: second-order cone program. Left: residual norm versus iteration. Right: residual norm versus time (seconds).

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- Open-sourced Python Solver for Prox-Affine Distributed Convex Optimization
- Combining AA-II with DRS (Douglas-Rachford Splitting).
- Available at `https://github.com/cvxgrp/a2dr`

Prox-affine form of generic convex optimization

We consider the following **prox-affine** representation/formulation of a **generic** convex optimization problem:

$$
\begin{array}{ll}
\text{minimize} & \sum_{i=1}^N f_i(x_i) \\
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\end{array}
$$

with variable $x = (x_1, \ldots, x_N) \in \mathbf{R}^{n_1 + \cdots + n_N}$, $A_i \in \mathbf{R}^{m \times n_i}$, $b \in \mathbf{R}^m$.

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- $f_i : \mathbf{R}^{n_i} \to \mathbf{R} \cup \{+\infty\}$ is closed, convex and proper (CCP).
- Each f_i can **only** be accessed through its proximal operator:

$$\mathbf{prox}_{tf_i}(v_i) = \mathrm{argmin}_{x_i} \ \left(f_i(x_i) + \frac{1}{2t}\|x_i - v_i\|_2^2\right).$$

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Why **prox-affine** form?

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x_vals, primal, dual, num_iters, solve_time = a2dr(p_list, A_list, b)
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Try it out! Simply provide a list of proximal functions $\mathbf{prox}_{tf_i}(v_i)$ (p_list), list of A_i's (A_list), and b (b), and you are done!

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Finally: CVXPY + a2dr – Expression tree complier exists: Epsilon (Wytock et al., 2015).

Previous Work

Most common approaches for prox-affine formulation (sometimes goes by the name "distributed optimization"):

- Alternating direction method of multipliers (ADMM).
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These are typically slow to converge – acceleration techniques:

- Adaptive penalty parameters.
- Momentum methods.
- Quasi-Newton or Newton-type method with line search.

Our Method

A2DR: Stabilized AA-II applied to DRS

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- Why **AA-II**?
  - Work better with DRS + prox-affine than type-I AA
  - Better stability for **general purpose** solvers and distributed settings.
    - **prox** operators have much larger diversity than solvable cones in SCS.
- Why **DRS**?
  - Allows for a natural NEFP representation (ADMM not), and amenable to proximal evaluation (ALM not).

Challenges and contribution

Major Challenge:

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Theory: First globally convergent type-II AA variant in non-smooth and potentially **pathological** settings.

Practice: An open-source Python solver `a2dr` based on **A2DR**:

`https://github.com/cvxgrp/a2dr`.

DRS Algorithm

- Rewrite problem as ($\mathcal{I}_S$ is the indicator of set S)

$$\text{minimize} \quad \overbrace{\sum_{i=1}^{N} f_i(x_i)}^{f(x)} + \overbrace{\mathcal{I}_{Ax=b}(x)}^{g(x)}.$$

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- DRS iterates for $k = 1, 2, \ldots,$

$$\begin{aligned} x_i^{k+1/2} &= \mathbf{prox}_{tf_i}(v^k), \quad i = 1, \ldots, N \\ v^{k+1/2} &= 2x^{k+1/2} - v^k \\ x^{k+1} &= \Pi_{Av=b}(v^{k+1/2}) \\ v^{k+1} &= v^k + x^{k+1} - x^{k+1/2} \end{aligned}$$

$\Pi_S(v)$ is Euclidean projection of v onto S.

Convergence of DRS

- DRS iterations can be conceived as a fixed point (FP) mapping

$$v^{k+1} = F(v^k)$$

- F is **firmly non-expansive**.
- v^k converges to a fixed point of F (if it exists).
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So we add AA-II.

Performance/Stopping Criterion of A2DR

- Stop and output $x^{k+1/2}$ when $\|r^k\|_2 \le \epsilon_{\text{tol}} = \epsilon_{\rm abs} + \epsilon_{\rm rel}\|r^0\|_2$:

$$\begin{aligned} r^k_{\text{prim}} &= Ax^{k+1/2} - b, \\ r^k_{\text{dual}} &= \frac{1}{t}(v^k - x^{k+1/2}) + A^T\lambda^k, \\ r^k &= (r^k_{\rm prim}, r^k_{\rm dual}). \end{aligned}$$

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\end{aligned}
$$

- Remark:
  - Just KKT conditions. Notice that $(v^k - x^{k+1/2})/t \in \partial f(x^{k+1/2})$.
  - $\mathbf{prox}_f$ is enough, and no need for access to f or its sub-gradient.
- Dual variable is solution to least-squares problem

$$
\lambda^k = \mathrm{argmin}_\lambda \; \|r_{\mathsf{dual}}^k\|_2
$$

Key lemma to the proof

Lemma (Connecting FP residuals with OPT residuals)

Suppose that $\liminf_{j\to\infty} \|G(v^j)\|_2 \leq \epsilon$ *for some* $\epsilon > 0$*, then*

$$\liminf_{j\to\infty} \|r^j_{\mathrm{prim}}\|_2 \leq \|A\|_2\epsilon, \quad \liminf_{j\to\infty} \|r^j_{\mathrm{dual}}\|_2 \leq \frac{1}{t}\epsilon.$$

Convergence of A2DR

Theorem (Solvable Case)

If the problem is solvable (e.g., feasible and bounded), then

$$\liminf_{k\to\infty} \|r^k\|_2 = 0$$

and the AA candidates are adopted infinitely often. Furthermore, if F has a fixed point, then

$$\lim_{k\to\infty} v^k = v^\star \text{ and } \lim_{k\to\infty} x^{k+1/2} = x^\star,$$

where $v^\star$ is a fixed-point of F and $x^\star$ is a solution to our problem.

Remark. when the proximal operators and projections are evaluated with *errors* bounded by ϵ, then $\liminf_{k\to\infty} \|r^k\|_2 = O(\sqrt{\epsilon})$.

Convergence of A2DR

Theorem (Pathological Case)

If the problem is pathological (strongly primal infeasible or strongly dual infeasible), then

$$\lim_{k\to\infty}\left(v^k - v^{k+1}\right) = \delta v \neq 0.$$

Furthermore, if $\lim_{k\to\infty} Ax^{k+1/2} = b$*, then the problem is unbounded and* $\|\delta v\|_2 = t\,\mathbf{dist}(\mathbf{dom}\, f^*, \mathbf{range}(A^T))$*.*
Otherwise, it is infeasible and $\|\delta v\|_2 \geq \mathbf{dist}(\mathbf{dom}\, f, \{x : Ax = b\})$ *with equality when the dual problem is feasible.*

Implementation

Pre-conditioning (convergence greatly improved by rescaling problem):

- Replace original A, b, f_i with

$$\hat{A} = DAE, \quad \hat{b} = Db, \quad \hat{f}_i(\hat{x}_i) = f_i(e_i \hat{x}_i)$$

- D and E are diagonal positive, $e_i > 0$ corresponds to ith block diagonal entry of E, and chosen by equilibrating A
- Proximal operator of $\hat{f}_i$ can be evaluated using proximal operator of f_i

$$\mathbf{prox}_{t\hat{f}_i}(\hat{v}_i) = \frac{1}{e_i}\mathbf{prox}_{(e_i^2 t)f_i}(e_i \hat{v}_i)$$

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Parallelization: `multiprocessing` package in Python.

Nonnegative Least Squares (NNLS)

$$
\begin{array}{ll}
\text{minimize} & \|Fz - g\|_2^2 \\
\text{subject to} & z \geq 0
\end{array}
$$

with respect to $z \in \mathbf{R}^q$

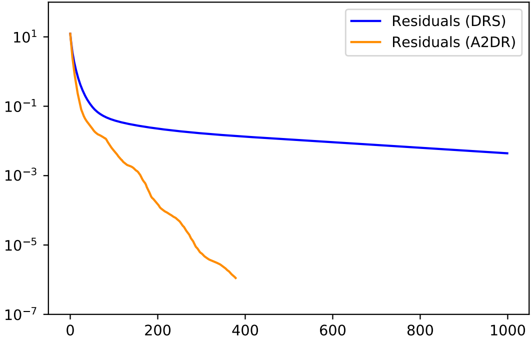
- Problem data: $F \in \mathbf{R}^{p \times q}$ and $g \in \mathbf{R}^p$
- Can be written in standard form with

$$
f_1(x_1) = \|Fx_1 - g\|_2^2, \quad f_2(x_2) = \mathcal{I}_{\mathbf{R}_+^n}(x_2)
$$
$$
A_1 = I, \quad A_2 = -I, \quad b = 0
$$

- We evaluate proximal operator of f_1 using LSQR

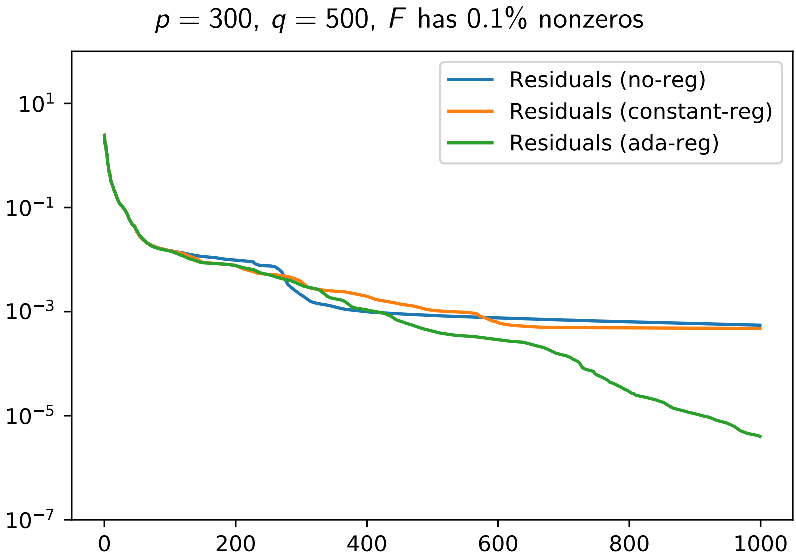
NNLS: Convergence of $\|r^k\|_2$

$p = 10^4$, $q = 8000$, F has 0.1% nonzeros



OSQP and SCS took respectively 349 and 327 seconds, while A2DR only took 55 seconds.

NNLS: Effect of regularization



Sparse Inverse Covariance Estimation

- Samples $z_1, \ldots, z_p$ IID from $\mathcal{N}(0, \Sigma)$
- Know covariance $\Sigma \in \mathbf{S}^q_+$ has **sparse** inverse $S = \Sigma^{-1}$
- One way to estimate S is by solving the penalized log-likelihood problem

$$\text{minimize} \quad -\log\det(S) + \mathrm{tr}(SQ) + \alpha\|S\|_1,$$

  where Q is the sample covariance, $\alpha \geq 0$ is a parameter
- Note $\log\det(S) = -\infty$ when $S \not\succ 0$

Sparse Inverse Covariance Estimation

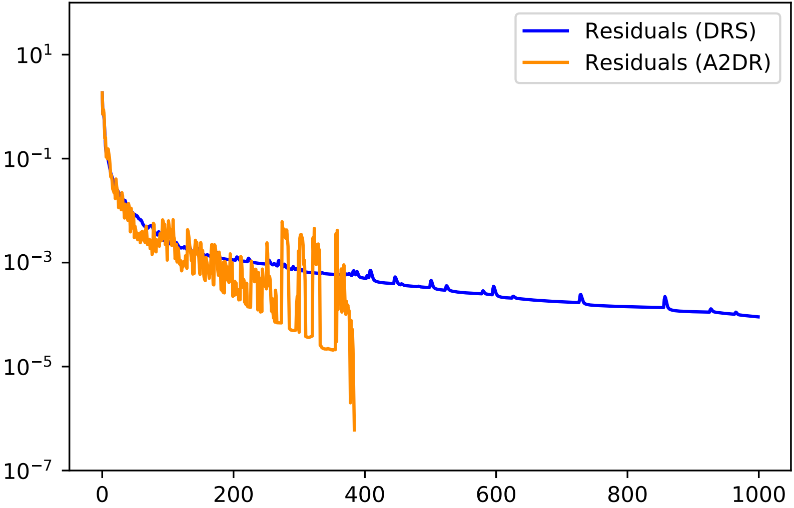
- Problem can be written in standard form with

$$f_1(S_1) = -\log\det(S_1) + \mathrm{tr}(S_1 Q), \quad f_2(S_2) = \alpha\|S_2\|_1,$$
$$A_1 = I, \quad A_2 = -I, \quad b = 0.$$

- Both proximal operators have closed-form solutions.

Covariance Estimation: Convergence of $\|r^k\|_2$

$p = 1000$, $q = 100$, S has 10% nonzeros



Covariance Estimation: larger examples

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- In the latter case, A2DR converged in 2.6 hours to a tolerance of 10^{-3}, while SCS failed immediately with an out-of-memory error.

Multi-Task Logistic Regression

$$\text{minimize} \quad \phi(W\theta, Y) + \alpha \textstyle\sum_{l=1}^{L} \|\theta_l\|_2 + \beta\|\theta\|_*$$

with respect to $\theta = [\theta_1 \cdots \theta_L] \in \mathbf{R}^{s \times L}$

- Problem data: $W \in \mathbf{R}^{p \times s}$ and $Y = [y_1 \cdots y_L] \in \mathbf{R}^{p \times L}$
- Regularization parameters: $\alpha \geq 0, \beta \geq 0$
- Logistic loss function

$$\phi(Z, Y) = \sum_{l=1}^{L} \sum_{i=1}^{p} \log\left(1 + \exp(-Y_{il} Z_{il})\right)$$

Multi-Task Logistic Regression

- Rewrite problem in standard form with:

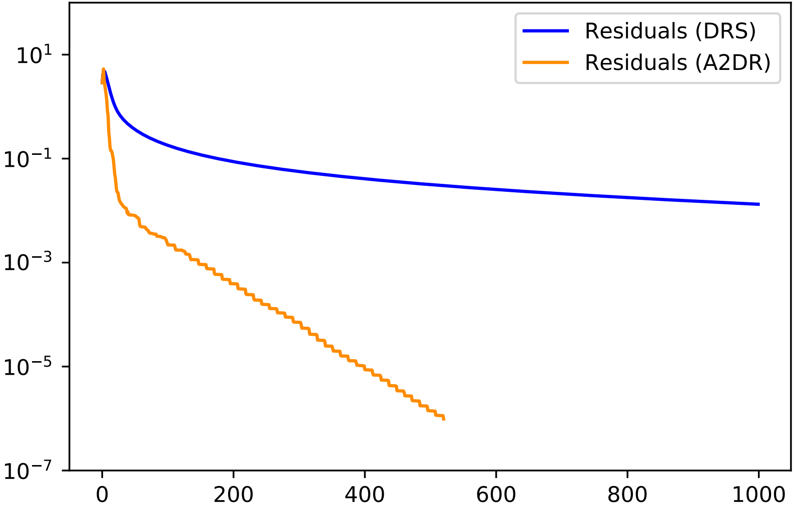
$$f_1(Z) = \phi(Z, Y), \quad f_2(\theta) = \alpha \sum_{l=1}^{L} \|\theta_l\|_2, \quad f_3(\tilde{\theta}) = \beta \|\tilde{\theta}\|_*,$$

$$A = \begin{bmatrix} I & -W & 0 \\ 0 & I & -I \end{bmatrix}, \quad x = \begin{bmatrix} Z \\ \theta \\ \tilde{\theta} \end{bmatrix}, \quad b = 0$$

- We evaluate proximal operator of f_1 using Newton-CG method, and the rest with closed-form formulae.

Multi-Task Logistic: Convergence of $\|r^k\|_2$

$p = 300,\ s = 500,\ L = 10,\ \alpha = \beta = 0.1$



Other examples

A (very) brief summary of other examples (see the paper for more details):

- l_1 trend filtering.
- Stratified models.
- Single commodity flow optimization (match the performance of OSQP, and largely outperform SCS).
- Optimal control (largely outperform both SCS and OSQP).
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Remark. The advantage compared to OSQP probably comes from the inclusion of AA, while the advantage compared to SCS (which includes type-I AA) is probably due to the more compact standard form representation.

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- Python library:

`https://github.com/cvxgrp/a2dr`

Future Work on A2DR

- More work on feasibility detection.
- Expand library of proximal operators (non-convex proximal).
- User-friendly interface with CVXPY (with the help of `Epsilon`).
- GPU parallelization and cloud computing,

1 Motivation and Problem Statement

2 Acceleration: connecting quasi-Newton with extrapolation
- Good news and bad news

3 A generic stabilization scheme
- Stabilization of AA-I
- Stabilization of AA-II
- Global convergence: solvable settings
- A browse through effect of stabilization

4 Applications
- Conic optimization + SCS 2.x
- Prox-affine optimization + A2DR

5 Beyond convexity

Beyond non-expansiveness (convexity)

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  - **Safe-guard** becomes central here (unlike non-expansive cases), and need to be exclusive designed for each algorithm.
  - Example: We proposed **Anderson accelerated iPALM** [GHXZ2018] with an exclusive safe-guard for iPALM for computing the MLEs multivariate Hawkes processes.

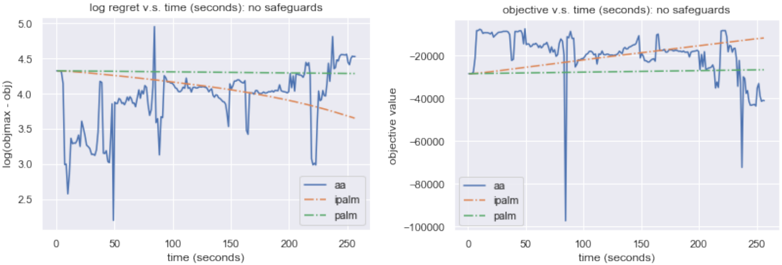

Figure: MLE of MHPs: exponential hawkes. No safe-guards. Left: log-regret v.s. time (seconds). Right: objective v.s. time (seconds).

Safe-guards in non-convex optimization

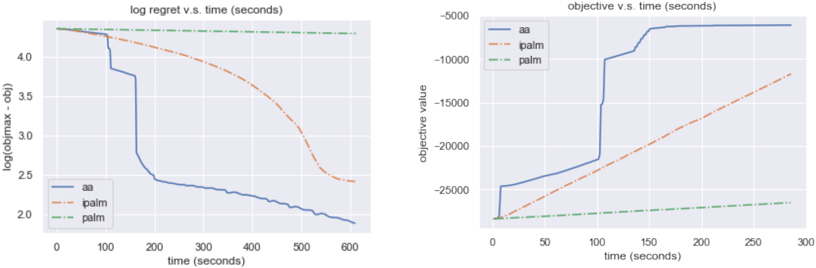

Figure: MLE of MHPs: synthetic exponential hawkes. With safe-guards. Left: log-regret v.s. time (seconds). Right: objective v.s. time (seconds).

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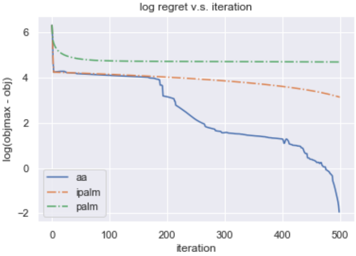

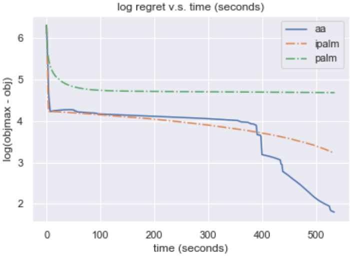

Figure: MLE of MHPs: synthetic power law hawkes. With safe-guards. Left: log-regret v.s. iterations Right: log-regret v.s. time (seconds).

Safe-guards in non-convex optimization

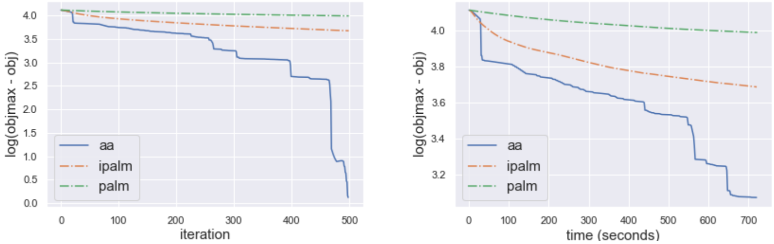

Figure: MLE of MHPs: memetracker dataset + exponential hawkes. With safe-guards. Left: log-regret v.s. iterations Right: log-regret v.s. time (seconds).

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- Adaptive choices/line-search of the hyper-parameters in our stabilized AA-I.

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    - Zhang, J., O'Donoghue, B. and Boyd, S. P. (2018).
- Thanks to Anqi Fu for the input to the A2DR part of the slides.

Thanks for listening!

Any questions?