

Regularized Nonlinear Acceleration.

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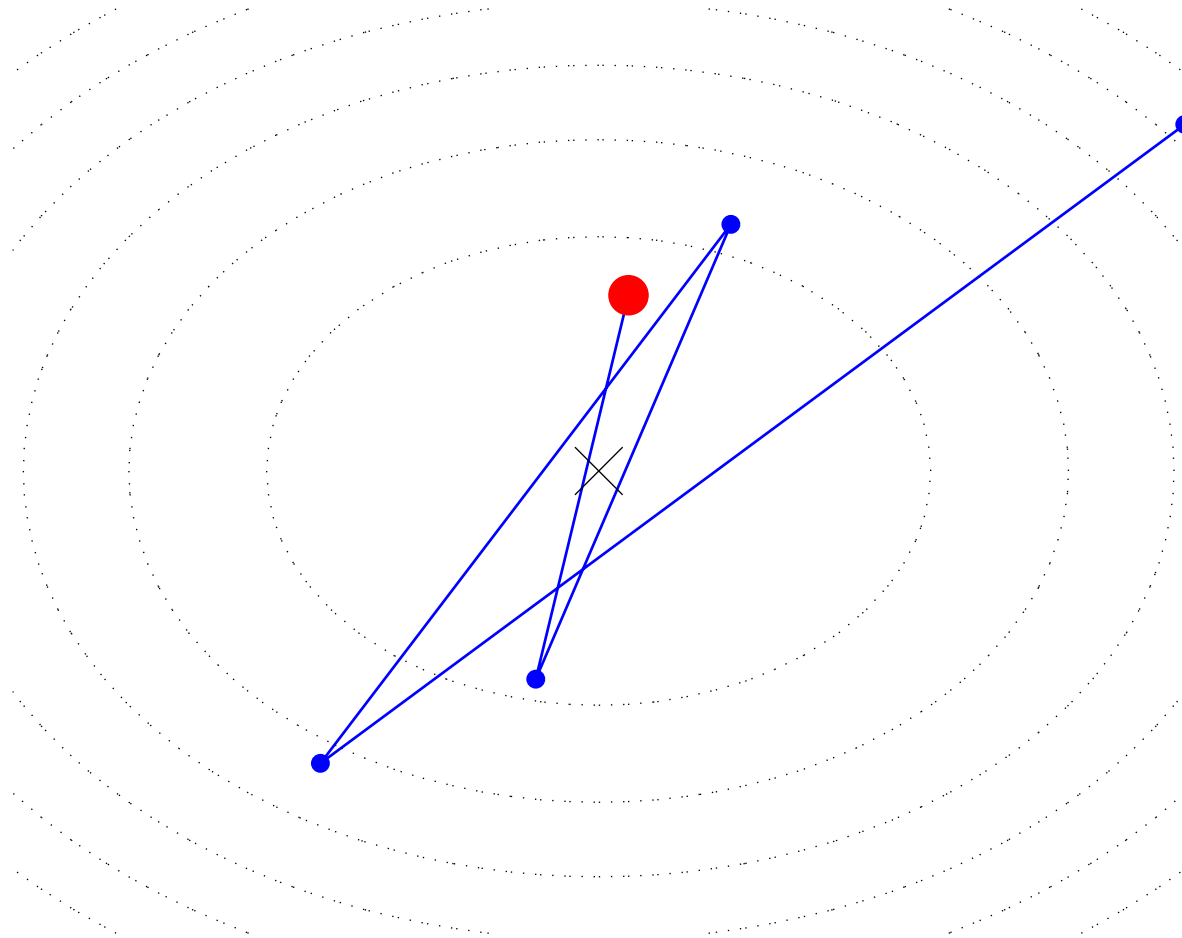
Introduction

Generic convex optimization problem

$$\min_{x \in \mathbb{R}^n} f(x)$$

Introduction

Algorithms produce a **sequence** of iterates.



We only keep the last (or best) one. . .

Introduction

Aitken's Δ^2 [Aitken, 1927]. Given a sequence $\{s_k\}_{k=1,\dots} \in \mathbb{R}^{\mathbb{N}}$ with limit s_* , and suppose

$$s_{k+1} - s_* = a(s_k - s_*), \quad \text{for } k = 1, \dots$$

We can compute a using

$$s_{k+1} - s_k = a(s_k - s_{k-1}) \quad \Rightarrow \quad a = \frac{s_{k+1} - s_k}{s_k - s_{k-1}}$$

and get the limit s^* by solving

$$s_{k+1} - s^* = \frac{s_{k+1} - s_k}{s_k - s_{k-1}}(s_k - s^*)$$

which yields

$$s^* = \frac{s_{k-1}s_{k+1} - s_k^2}{s_{k+1} - 2s_k + s_{k-1}}$$

This is **Aitken's Δ^2** and allows us to **compute s_* from $\{s_{k+1}, s_k, s_{k-1}\}$** .

Introduction

Convergence acceleration. Consider

$$s_k = \sum_{i=0}^k \frac{(-1)^i}{(2i+1)} \xrightarrow{k \rightarrow \infty} \frac{\pi}{4} = 0.785398 \dots$$

we have

k	$\frac{(-1)^k}{(2k+1)}$	$\sum_{i=0}^k \frac{(-1)^i}{(2i+1)}$	Δ^2
0	1	1.0000	–
1	-0.33333	0.66667	–
2	0.2	0.86667	0.79167
3	-0.14286	0.72381	0.78333
4	0.11111	0.83492	0.78631
5	-0.090909	0.74401	0.78492
6	0.076923	0.82093	0.78568
7	-0.066667	0.75427	0.78522
8	0.058824	0.81309	0.78552
9	-0.052632	0.76046	0.78531

Introduction

Convergence acceleration.

- Similar results apply to sequences satisfying

$$\sum_{i=0}^k a_i (s_{n+i} - s_*) = 0$$

using Aitken's ideas recursively.

- This produces **Wynn's ε -algorithm** [Wynn, 1956].
- See [Brezinski, 1977] for a survey on acceleration, extrapolation.
- Directly related to the Levinson-Durbin algo on AR processes.
- **Vector case:** focus on **Minimal Polynomial Extrapolation** [Sidi et al., 1986].

Overall: a simple **postprocessing** step.

Outline

- Introduction
- **Minimal Polynomial Extrapolation**
- Regularized MPE
- Numerical results

Minimal Polynomial Extrapolation

Quadratic example. Minimize

$$f(x) = \frac{1}{2} \|Bx - b\|_2^2$$

using the basic gradient algorithm, with

$$x_{k+1} := x_k - \frac{1}{L}(B^T Bx_k - b).$$

we get

$$x_{k+1} - x^* := \underbrace{\left(\mathbf{I} - \frac{1}{L} B^T B \right)}_A (x_k - x^*)$$

since $B^T Bx^* = b$.

This means $x_{k+1} - x^*$ follows a **vector autoregressive process**.

Minimal Polynomial Extrapolation

We have

$$\sum_{i=0}^k c_i (x_i - x^*) = \sum_{i=1}^k c_i A^i (x_0 - x^*)$$

and setting $\mathbf{1}^T c = 1$, yields

$$\left(\sum_{i=0}^k c_i x_i \right) - x^* = p(A)(x_0 - x^*), \quad \text{where } p(v) = \sum_{i=1}^k c_i v^i$$

- Setting c such that $p(A)(x_0 - x^*) = 0$, we would have

$$x^* = \sum_{i=0}^k c_i x_i$$

- Get the limit by **averaging iterates** (using weights depending on x_k).
- We typically do not observe A (or x^*).
- How do we extract c from the iterates x_k ?

Minimal Polynomial Extrapolation

We have

$$\begin{aligned}x_k - x_{k-1} &= (x_k - x^*) - (x_{k-1} - x^*) \\ &= (A - \mathbf{I})A^{k-1}(x_0 - x^*)\end{aligned}$$

hence if $p(A) = 0$, we must have

$$\sum_{i=1}^k c_i(x_i - x_{i-1}) = (A - \mathbf{I})p(A)(x_0 - x^*) = 0$$

so if $(A - \mathbf{I})$ is nonsingular, the coefficient vector c solves the **linear system**

$$\begin{cases} \sum_{i=1}^k c_i(x_i - x_{i-1}) = 0 \\ \sum_{i=1}^k c_i = 1 \end{cases}$$

and $p(\cdot)$ is the **minimal polynomial** of A w.r.t. $(x_0 - x^*)$.

Approximate Minimal Polynomial Extrapolation

Approximate MPE.

- For k smaller than the degree of the minimal polynomial, we find c that **minimizes the residual**

$$\|(A - \mathbf{I})p(A)(x_0 - x^*)\|_2 = \left\| \sum_{i=1}^k c_i (x_i - x_{i-1}) \right\|_2$$

- Setting $U \in \mathbb{R}^{n \times k+1}$, with $U_i = x_{i+1} - x_i$, this means solving

$$c^* \triangleq \underset{\mathbf{1}^T c = 1}{\operatorname{argmin}} \|Uc\|_2 \quad (\text{AMPE})$$

in the variable $c \in \mathbb{R}^{k+1}$.

- Also known as Eddy-Mešina method [Mešina, 1977, Eddy, 1979] or Reduced Rank Extrapolation with arbitrary k (see [Smith et al., 1987, §10]). Very similar to Anderson acceleration, GMRES, etc.

Uniform Bound

Chebyshev polynomials. Crude bound on $\|Uc^*\|_2$ using Chebyshev polynomials, to bound error as a function of k , with

$$\begin{aligned}\left\|\sum_{i=0}^k c_i^* x_i - x^*\right\|_2 &= \left\|(I - A)^{-1} \sum_{i=0}^k c_i^* U_i\right\|_2 \\ &\leq \|(I - A)^{-1}\|_2 \|p(A)(x_1 - x_0)\|_2\end{aligned}$$

We have

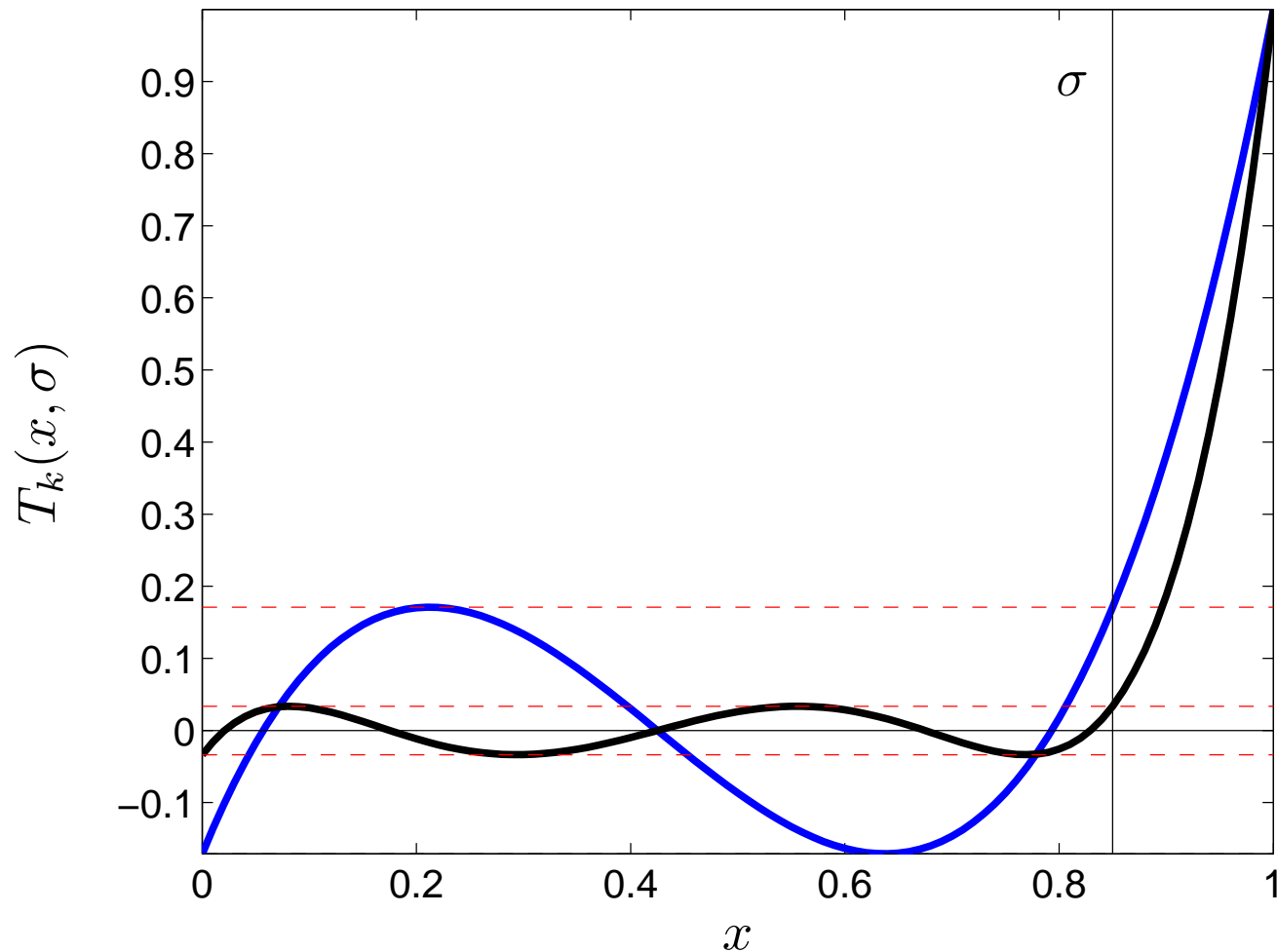
$$\begin{aligned}\|p(A)(x_1 - x_0)\|_2 &\leq \|p(A)\|_2 \|x_1 - x_0\|_2 \\ &= \max_{i=1, \dots, n} |p(\lambda_i)| \|x_1 - x_0\|_2\end{aligned}$$

where $0 \leq \lambda_i \leq \sigma$ are the eigenvalues of A . It suffices to find $p(\cdot) \in \mathbb{R}_k[x]$ solving

$$\inf_{\{p \in \mathbb{R}_k[x] : p(1)=1\}} \sup_{v \in [0, \sigma]} |p(v)|$$

Explicit solution using modified **Chebyshev polynomials**.

Uniform Bound using Chebyshev Polynomials



Chebyshev polynomials $T_3(x, \sigma)$ and $T_5(x, \sigma)$ for $x \in [0, 1]$ and $\sigma = 0.85$.
The maximum value of T_k on $[0, \sigma]$ decreases geometrically fast when k grows.

Approximate Minimal Polynomial Extrapolation

Proposition

AMPE convergence. Let A be symmetric, $0 \preceq A \preceq \sigma I$ with $\sigma < 1$ and c^* be the solution of (AMPE). Then

$$\left\| \sum_{i=0}^k c_i^* x_i - x^* \right\|_2 \leq \kappa(A - I) \frac{2\zeta^k}{1 + \zeta^{2k}} \|x_0 - x^*\|_2 \quad (1)$$

where $\kappa(A - I)$ is the condition number of the matrix $A - I$ and ζ is given by

$$\zeta = \frac{1 - \sqrt{1 - \sigma}}{1 + \sqrt{1 - \sigma}} < \sigma, \quad (2)$$

See also [Nemirovskiy and Polyak, 1984]. Gradient method, $\sigma = 1 - \mu/L$, so

$$\left\| \sum_{i=0}^k c_i^* x_i - x^* \right\|_2 \leq \kappa(A - I) \left(\frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}} \right)^k \|x_0 - x^*\|_2$$

Approximate Minimal Polynomial Extrapolation

AMPE versus Nesterov, conjugate gradient.

- Key difference with conjugate gradient: we do not observe A . . .
- Chebyshev polynomials satisfy a two-step recurrence. For quadratic minimization using the gradient method:

$$\begin{cases} z_{k-1} = y_{k-1} - \frac{1}{L}(By_{k-1} - b) \\ y_k = \frac{\alpha_{k-1}}{\alpha_k} \left(\frac{2z_{k-1}}{\sigma} - y_{k-1} \right) - \frac{\alpha_{k-2}}{\alpha_k} y_{k-2} \end{cases}$$

where $\alpha_k = \frac{2-\sigma}{\sigma}\alpha_{k-1} - \alpha_{k-2}$

- Nesterov's acceleration recursively computes a similar polynomial with

$$\begin{cases} z_{k-1} = y_{k-1} - \frac{1}{L}(By_{k-1} - b) \\ y_k = z_{k-1} + \beta_k(z_{k-1} - z_{k-2}), \end{cases}$$

see also [Hardt, 2013].

Approximate Minimal Polynomial Extrapolation

Accelerating optimization algorithms. For gradient descent, we have

$$\tilde{x}_{k+1} := \tilde{x}_k - \frac{1}{L} \nabla f(\tilde{x}_k)$$

- This means $\tilde{x}_{k+1} - x^* := A(\tilde{x}_k - x^*) + O(\|\tilde{x}_k - x^*\|_2^2)$ where

$$A = I - \frac{1}{L} \nabla^2 f(x^*),$$

meaning that $\|A\|_2 \leq 1 - \frac{\mu}{L}$, whenever $\mu I \preceq \nabla^2 f(x) \preceq LI$.

- Approximation error is a sum of three terms

$$\left\| \sum_{i=0}^k \tilde{c}_i \tilde{x}_i - x^* \right\|_2 \leq \underbrace{\left\| \sum_{i=0}^k c_i x_i - x^* \right\|_2}_{\text{AMPE}} + \underbrace{\left\| \sum_{i=0}^k (\tilde{c}_i - c_i) x_i \right\|_2}_{\text{Stability}} + \underbrace{\left\| \sum_{i=0}^k \tilde{c}_i (\tilde{x}_i - x_i) \right\|_2}_{\text{Nonlinearity}}$$

Stability is key here.

Approximate Minimal Polynomial Extrapolation

Stability.

- The iterations span a Krylov subspace

$$\mathcal{K}_k = \text{span} \{U_0, AU_0, \dots, A^{k-1}U_0\}$$

so the matrix U in AMPE is a **Krylov matrix**.

- Similar to **Hankel or Toeplitz** case. $U^T U$ has a condition number typically growing exponentially with dimension [Tyrtysnikov, 1994].
- In fact, the Hankel, Toeplitz and Krylov problems are directly connected, hence the link with Levinson-Durbin [Heinig and Rost, 2011].
- For generic optimization problems, eigenvalues are perturbed by deviations from the linear model, which can make the situation even worse.

Be wise, regularize

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Regularized Minimal Polynomial Extrapolation

Regularized AMPE. Add a regularization term to AMPE.

- Regularized formulation of problem (AMPE),

$$\begin{aligned} & \text{minimize} && c^T (U^T U + \lambda I) c \\ & \text{subject to} && \mathbf{1}^T c = 1 \end{aligned} \tag{RMPE}$$

- Solution given by a linear system of size $k + 1$.

$$c_{\lambda}^* = \frac{(U^T U + \lambda I)^{-1} \mathbf{1}}{\mathbf{1}^T (U^T U + \lambda I)^{-1} \mathbf{1}} \tag{3}$$

Regularized Minimal Polynomial Extrapolation

RMPE algorithm.

Input: Sequence $\{x_0, x_1, \dots, x_{k+1}\}$, parameter $\lambda > 0$

- 1: Form $U = [x_1 - x_0, \dots, x_{k+1} - x_k]$
- 2: Solve the linear system $(U^T U + \lambda I)z = \mathbf{1}$
- 3: Set $c = z / (z^T \mathbf{1})$

Output: Return $\sum_{i=0}^k c_i x_i$, approximating the optimum x^*

Regularized Minimal Polynomial Extrapolation

Regularized AMPE. Define

$$S(k, \alpha) \triangleq \min_{\{q \in \mathbb{R}_k[x] : q(1)=1\}} \left\{ \max_{x \in [0, \sigma]} ((1-x)q(x))^2 + \alpha \|q\|_2^2 \right\},$$

Proposition [Scieur, d'Aspremont, and Bach, 2016]

Error bounds Let matrices $X = [x_0, x_1, \dots, x_k]$, $\tilde{X} = [x_0, \tilde{x}_1, \dots, \tilde{x}_k]$ and scalar $\kappa = \|(A - I)^{-1}\|_2$. Suppose \tilde{c}_λ^* solves problem (RMPE) and assume $A = g'(x^*)$ symmetric with $0 \preceq A \preceq \sigma I$ where $\sigma < 1$. Let us write the perturbation matrices $P = \tilde{U}^T \tilde{U} - U^T U$ and $\mathcal{E} = (X - \tilde{X})$. Then

$$\|\tilde{X} \tilde{c}_\lambda^* - x^*\|_2 \leq C(\mathcal{E}, P, \lambda) S(k, \lambda / \|x_0 - x^*\|_2^2)^{\frac{1}{2}} \|x_0 - x^*\|_2$$

where

$$C(\mathcal{E}, P, \lambda) = \left(\kappa^2 + \frac{1}{\lambda} \left(1 + \frac{\|P\|_2}{\lambda} \right)^2 \left(\|\mathcal{E}\|_2 + \kappa \frac{\|P\|_2}{2\sqrt{\lambda}} \right)^2 \right)^{\frac{1}{2}}$$

Regularized Minimal Polynomial Extrapolation

Proposition [Scieur et al., 2016]

Asymptotic acceleration Using the gradient method with stepsize in $]0, \frac{2}{L}[$ on a L -smooth, μ -strongly convex function f with Lipschitz-continuous Hessian of constant M .

$$\|\tilde{X}\tilde{c}_\lambda^* - x^*\|_2 \leq \kappa \left(1 + \frac{(1 + \frac{1}{\beta})^2}{4\beta^2}\right)^{1/2} \frac{2\zeta^k}{1 + \zeta^{2k}} \|x_0 - x^*\|$$

with

$$\zeta = \frac{1 - \sqrt{\mu/L}}{1 + \sqrt{\mu/L}}$$

for $\|x_0 - x^*\|$ small enough, where $\lambda = \beta\|P\|_2$ and $\kappa = \frac{L}{\mu}$ is the condition number of the function $f(x)$.

We (asymptotically) recover the accelerated rate in [Nesterov, 1983].

Regularized Minimal Polynomial Extrapolation

Stochastic optimization. Noisy oracles on iterates (in practice, gradients)
 $\tilde{x}_{t+1} = g(\tilde{x}_t) + \eta_{t+1}$, where η_t is noise term (independent). Equivalent to

$$\tilde{x}_{t+1} = x^* + G(\tilde{x}_t - x^*) + \varepsilon_{t+1},$$

where $\|\mathbf{E}[\varepsilon_t]\| \leq \nu$ and ε_t has bounded variance $\Sigma_t \preceq (\sigma^2/d)I$ with

$$\tau \triangleq \frac{\nu + \sigma}{\|x_0 - x^*\|}.$$

Proposition [Scieur, d'Aspremont, and Bach, 2017]

Error bounds *The accuracy of AMPE applied to the sequence $\{\tilde{x}_0, \dots, \tilde{x}_k\}$ is bounded by*

$$\frac{\mathbf{E}\left[\left\|\sum_{i=0}^k \tilde{c}_i^\lambda \tilde{x}_i - x^*\right\|\right]}{\|x_0 - x^*\|} \leq \left(S_\kappa(k, \bar{\lambda}) \sqrt{\frac{1}{\kappa^2} + \frac{O(\tau^2(1+\tau)^2)}{\bar{\lambda}^3}} + O\left(\sqrt{\tau^2 + \frac{\tau^2(1+\tau^2)}{\bar{\lambda}}}\right) \right)$$

Regularized Minimal Polynomial Extrapolation

Stochastic optimization.

- When the noise scale $\tau \rightarrow 0$, if $\bar{\lambda} = \Theta(\tau^s)$ with $s \in]0, \frac{2}{3}[$, we recover the accelerated rate

$$\mathbf{E} \left[\left\| \sum_{i=0}^k \tilde{c}_i^\lambda \tilde{x}_i - x^* \right\| \right] \leq \frac{1}{\kappa} \left(\frac{1 - \sqrt{\kappa}}{1 + \sqrt{\kappa}} \right)^k \|x_0 - x^*\|.$$

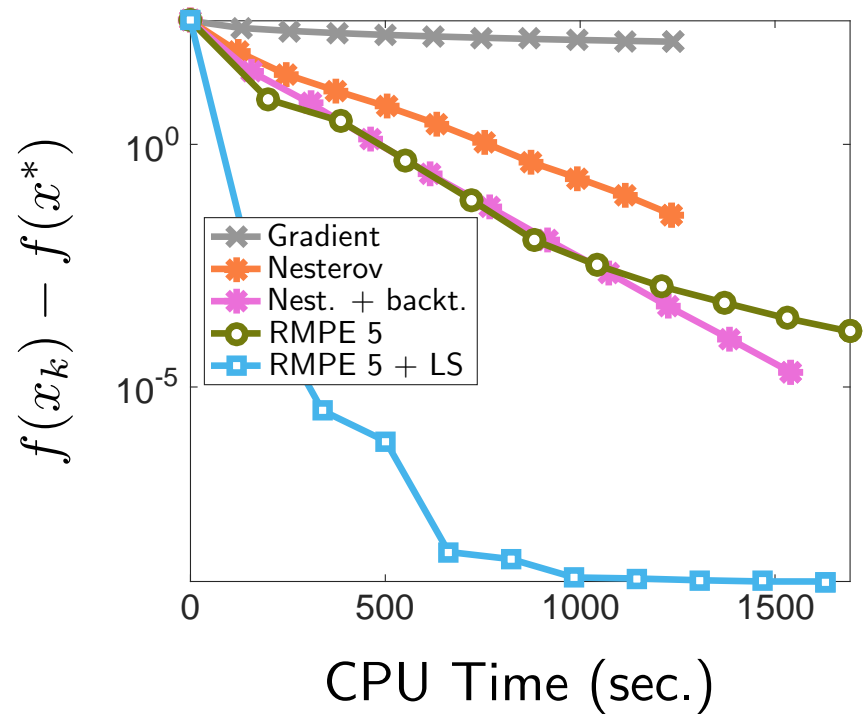
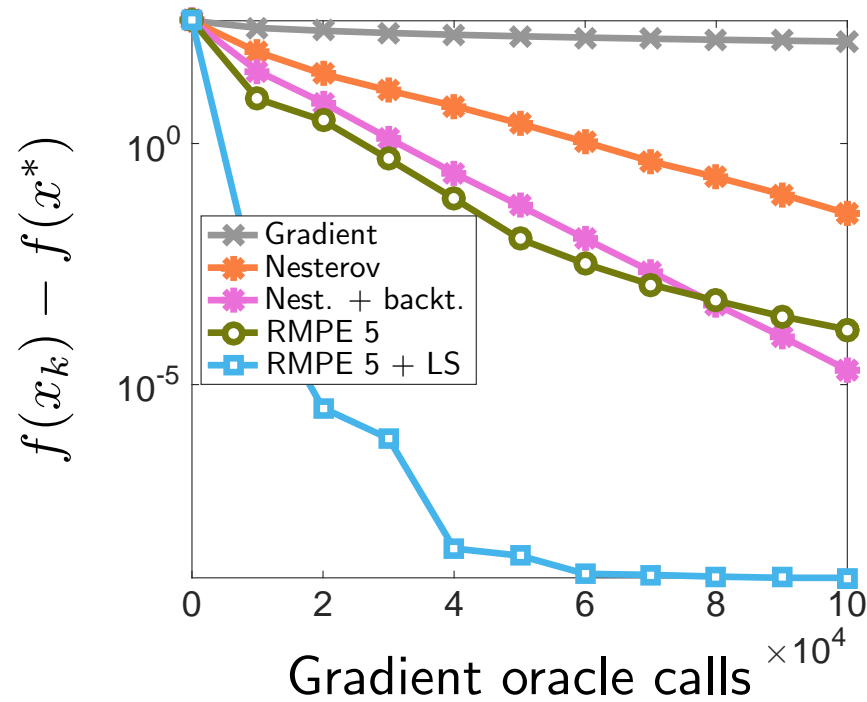
- If $\lambda \rightarrow \infty$, we recover the averaged gradient

$$\mathbf{E} \left[\left\| \sum_{i=0}^k \tilde{c}_i^\lambda \tilde{x}_i - x^* \right\| \right] \rightarrow \mathbf{E} \left[\left\| \frac{1}{k+1} \sum_{i=0}^k \tilde{x}_i - x^* \right\| \right]$$

Outline

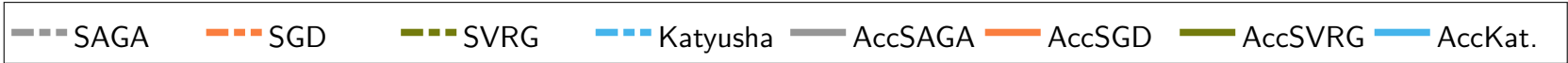
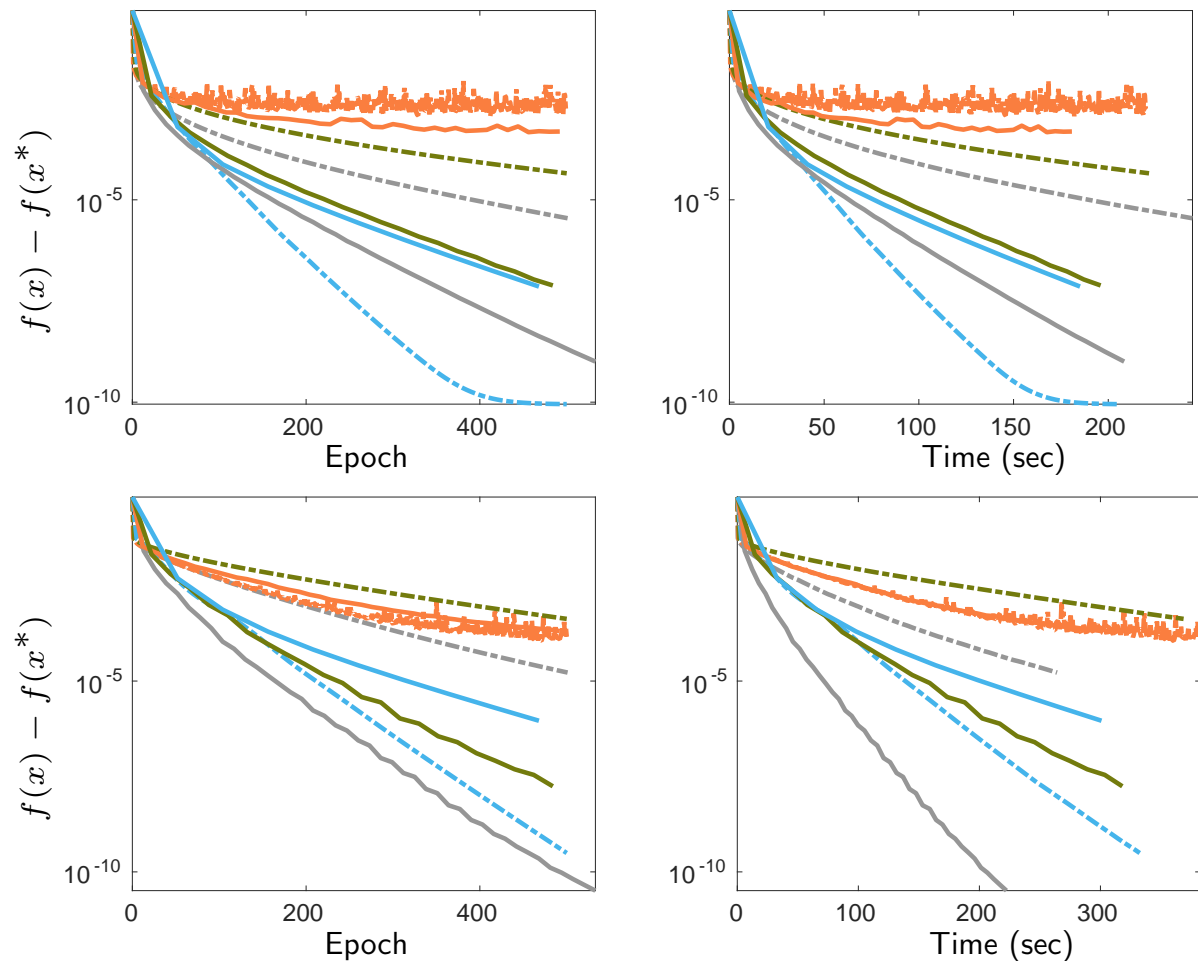
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Numerical Results



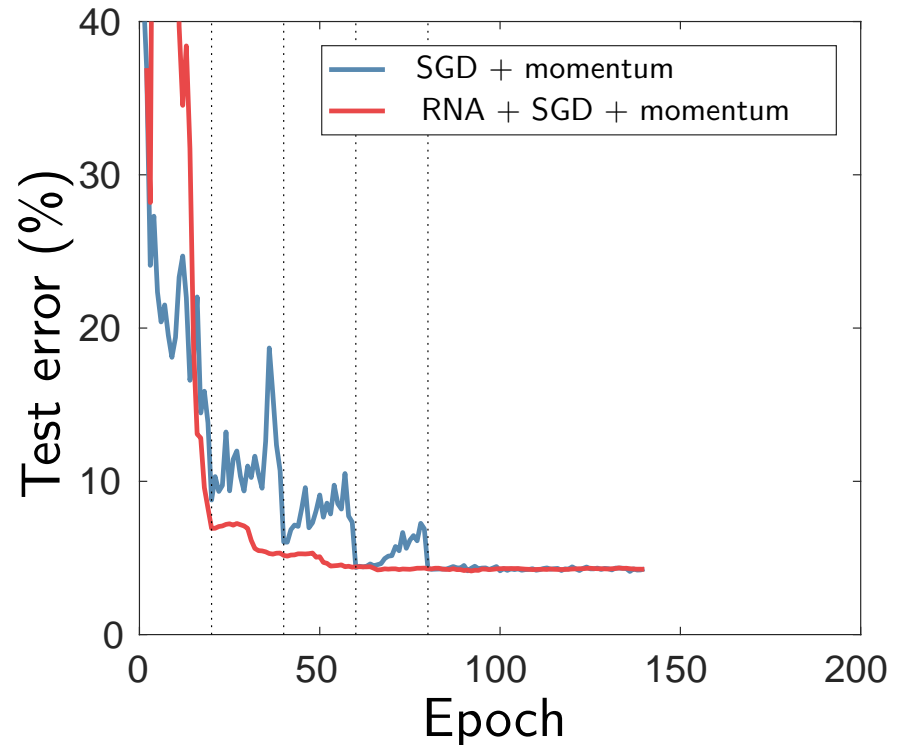
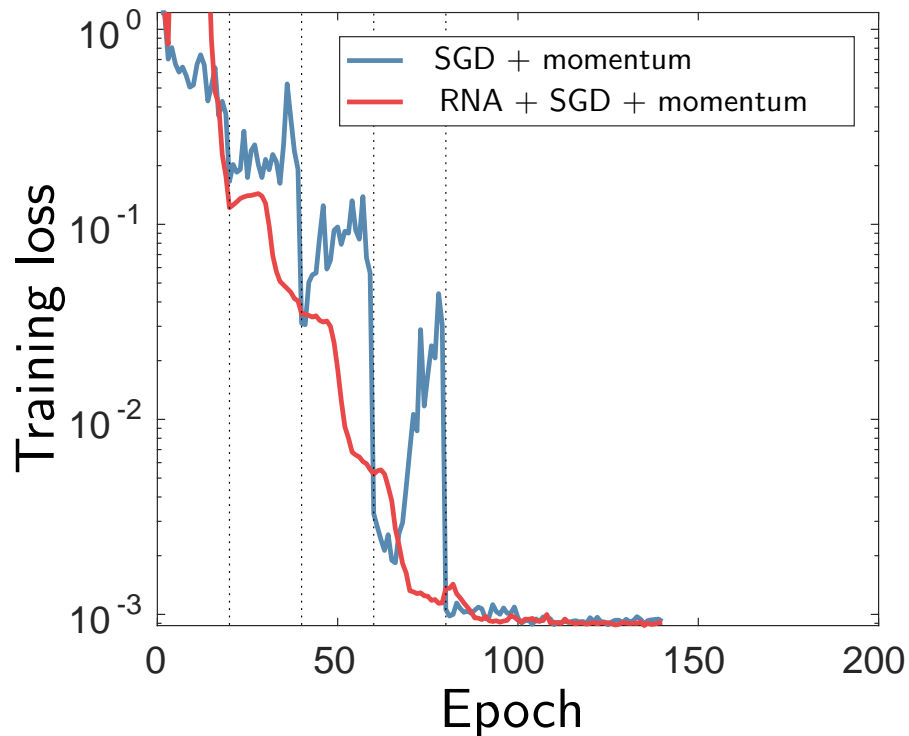
Logistic regression with ℓ_2 regularization, on *Madelon Dataset* (500 features, 2000 data points), solved using several algorithms. The penalty parameter has been set to 10^2 in order to have a condition number equal to 1.2×10^9 .

Numerical Results



Optimization of quadratic loss (*Top*) and logistic loss (*Bottom*) with several algorithms, using the Sid dataset with bad conditioning. The experiments are done in Matlab. *Left*: Error vs epoch number. *Right*: Error vs time.

Numerical Results



Convergence acceleration. Training Resnet-28-10 on CIFAR data set. Value reached by the current iterate versus extrapolated one (from the last 15 iterates). Training loss on the *left*, testing error on the *right*. Restarting the training periodically at the extrapolated point. Vertical lines mark learning rate decreases.

Conclusion

Postprocessing works. Regularized MPE yields asymptotically optimal rates.

- Simple **postprocessing** step.
- Marginal complexity, can be performed in parallel.
- Significant convergence speedup over optimal methods.
- Adaptive. Does not need knowledge of smoothness parameters.

Work in progress. . .

- Extrapolating accelerated methods.
- Constrained problems.
- Better handling of smooth functions.
- . . .

Open problems

- **Regularization.** How do we account for the fact that we are estimating the limit of a VAR sequence with a fixed point?
- The VAR matrix A is formed implicitly, but we have some information on its spectrum through smoothness.
- Explicit bounds on the **regularized Chebyshev problem**,

$$S(k, \alpha) \triangleq \min_{\{q \in \mathbb{R}_k[x] : q(1)=1\}} \left\{ \max_{x \in [0, \sigma]} ((1-x)q(x))^2 + \alpha \|q\|_2^2 \right\}.$$

Preprints on ArXiv, NIPS 2016, 2017.



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