

Smooth over-parameterized solvers for non-smooth structured optimisation

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Joint work with Gabriel Peyré (ENS Paris)

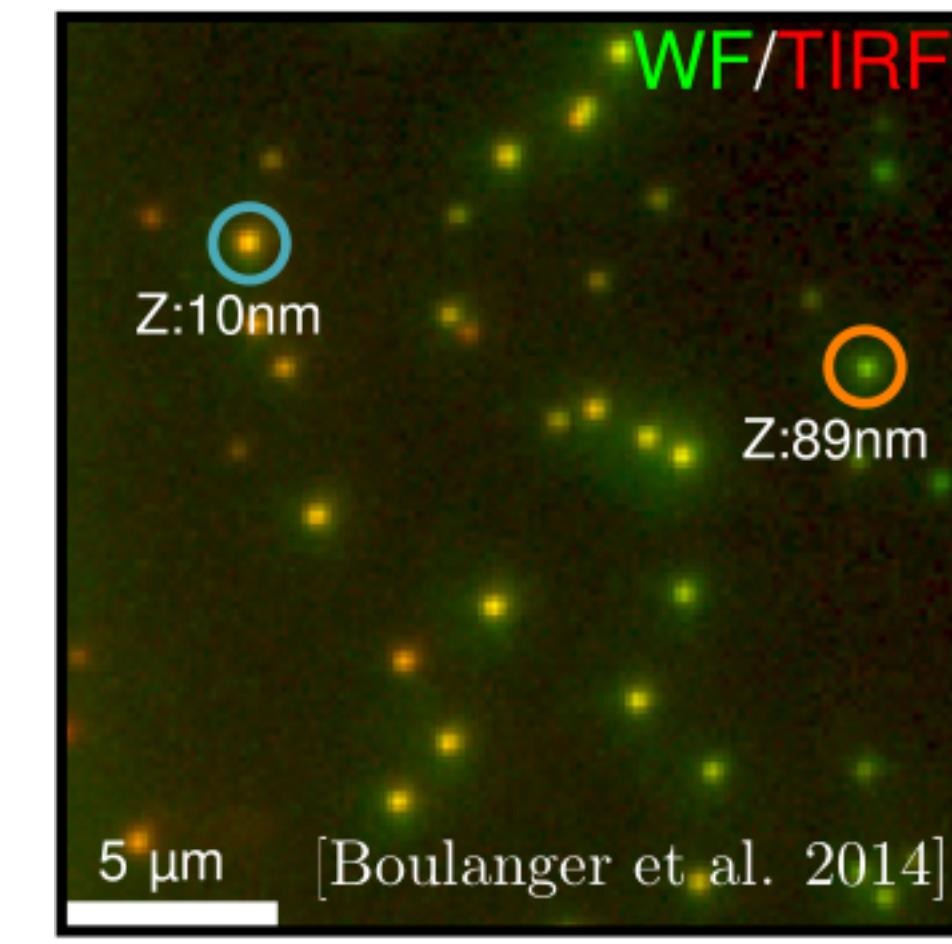
References:

1. [Smooth Bilevel Programming for Sparse Regularization](#), Neurips 2021.
2. [Smooth over-parameterized solvers for non-smooth structured optimization](#). (preprint)

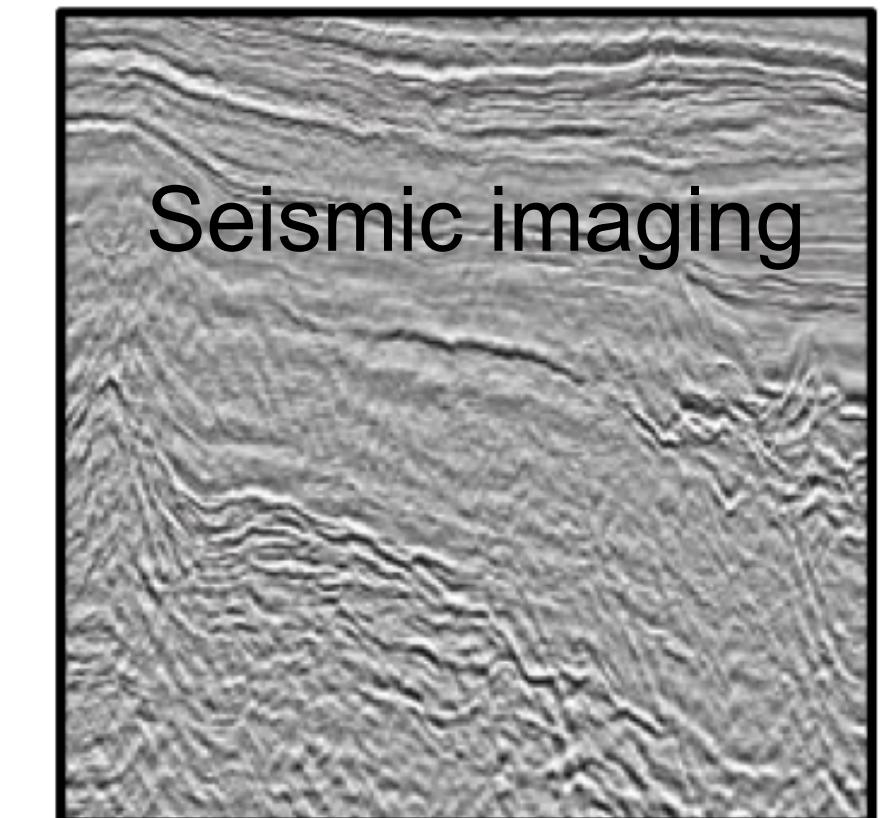
Structure promoting regularisation

Given $A \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$, solve $Ax = y$.

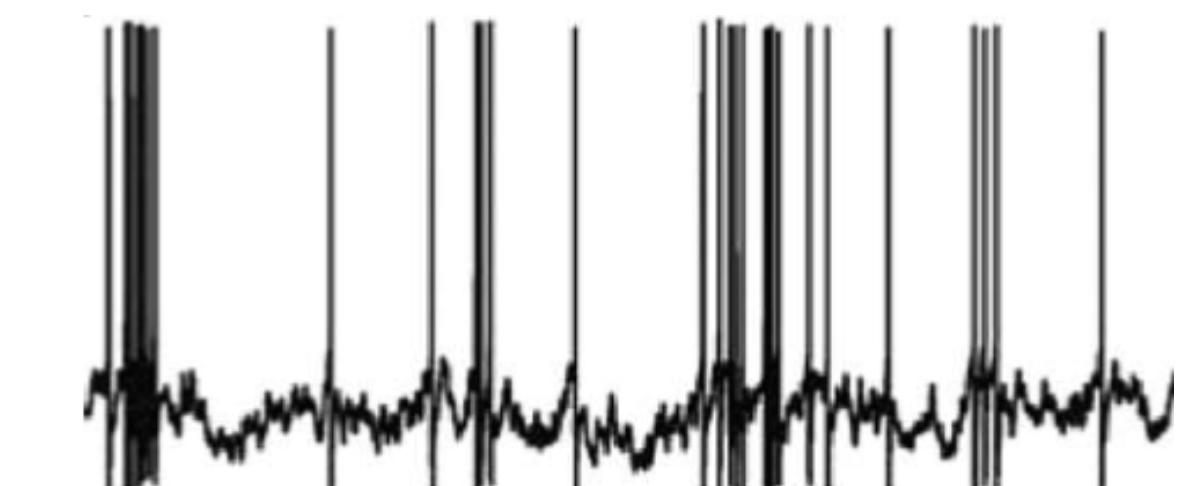
- $m \ll n$ is ill conditioned setting.
- $n \ll m$ with noise is typical ML setting



Fluorescence microscopy



Seismic imaging

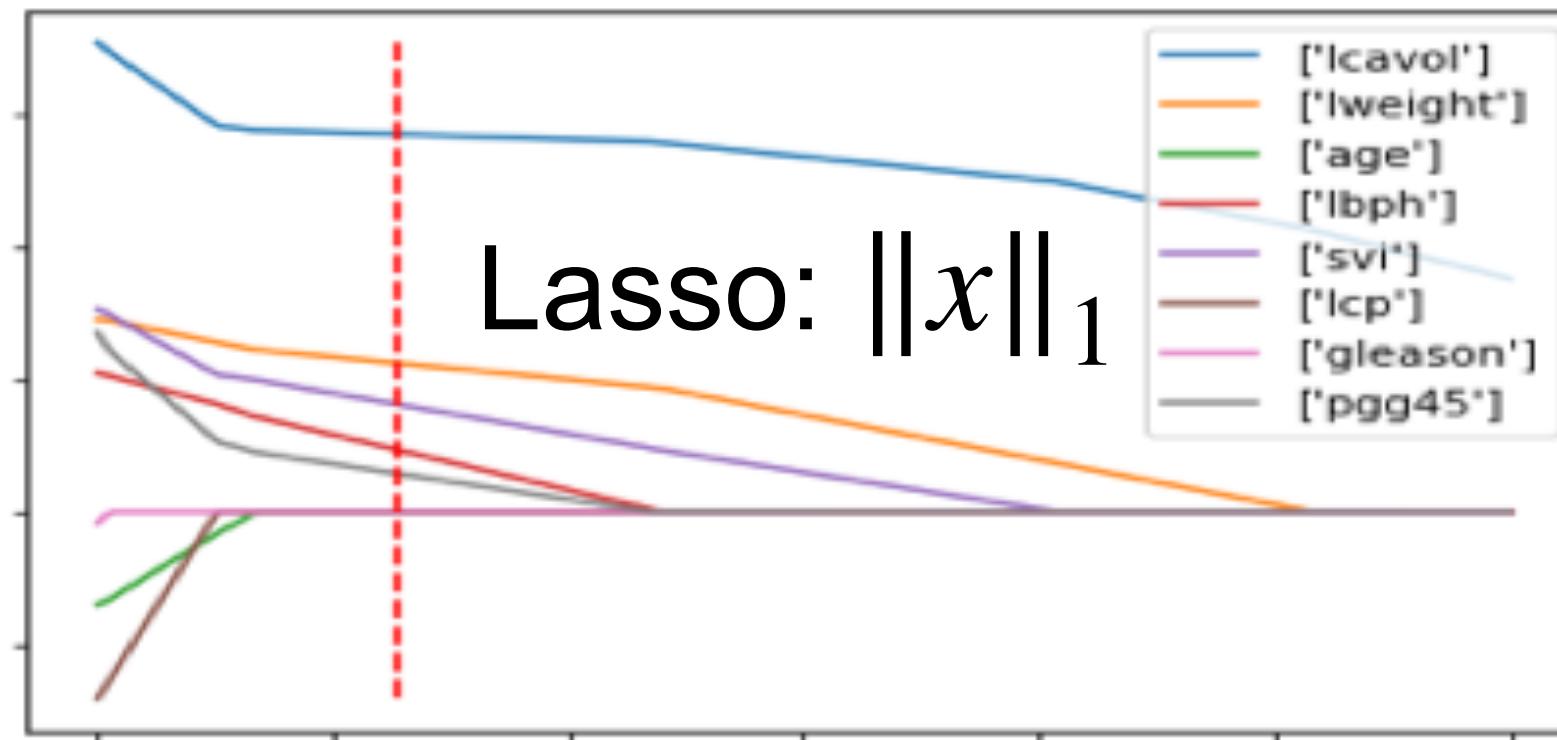
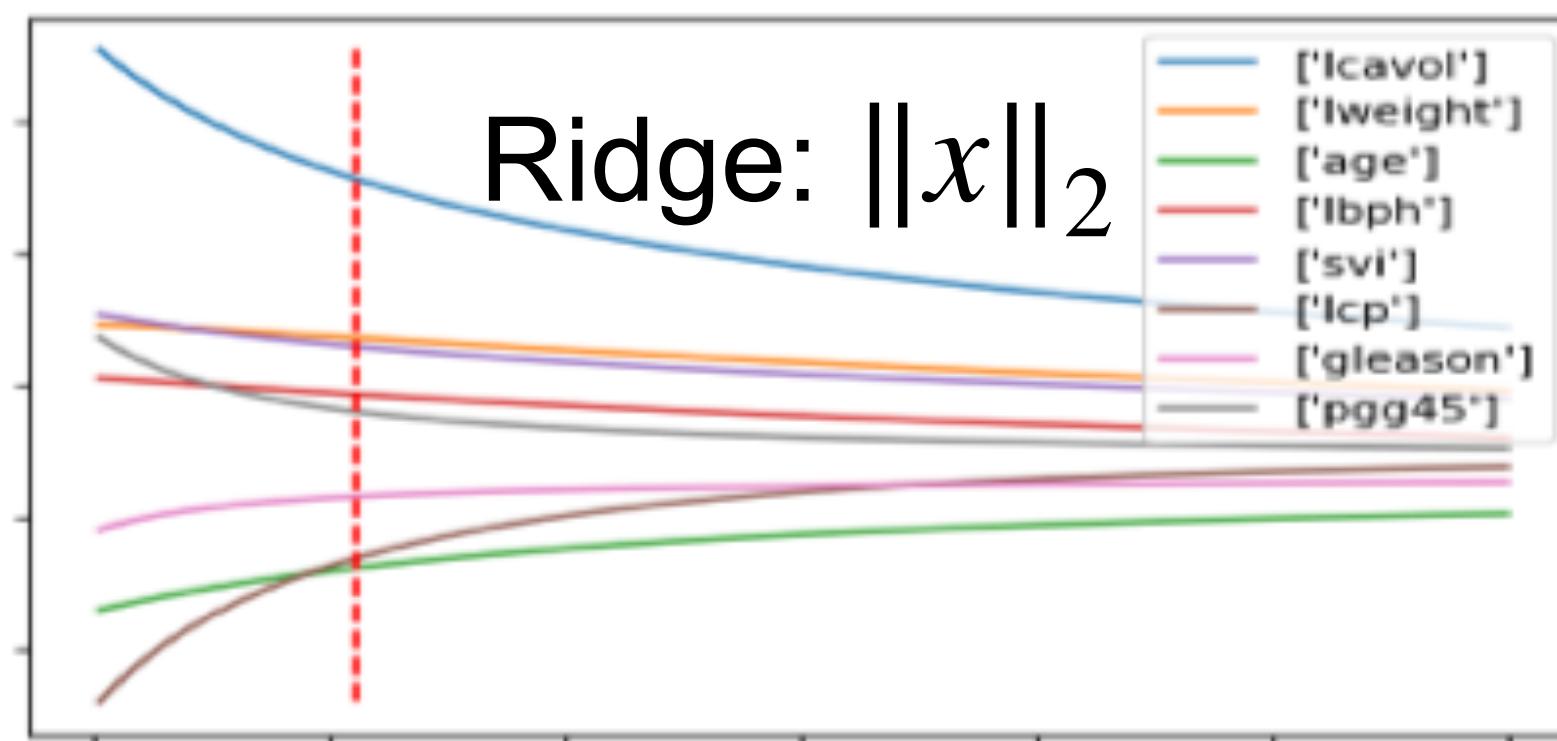


Neural spikes(1D)

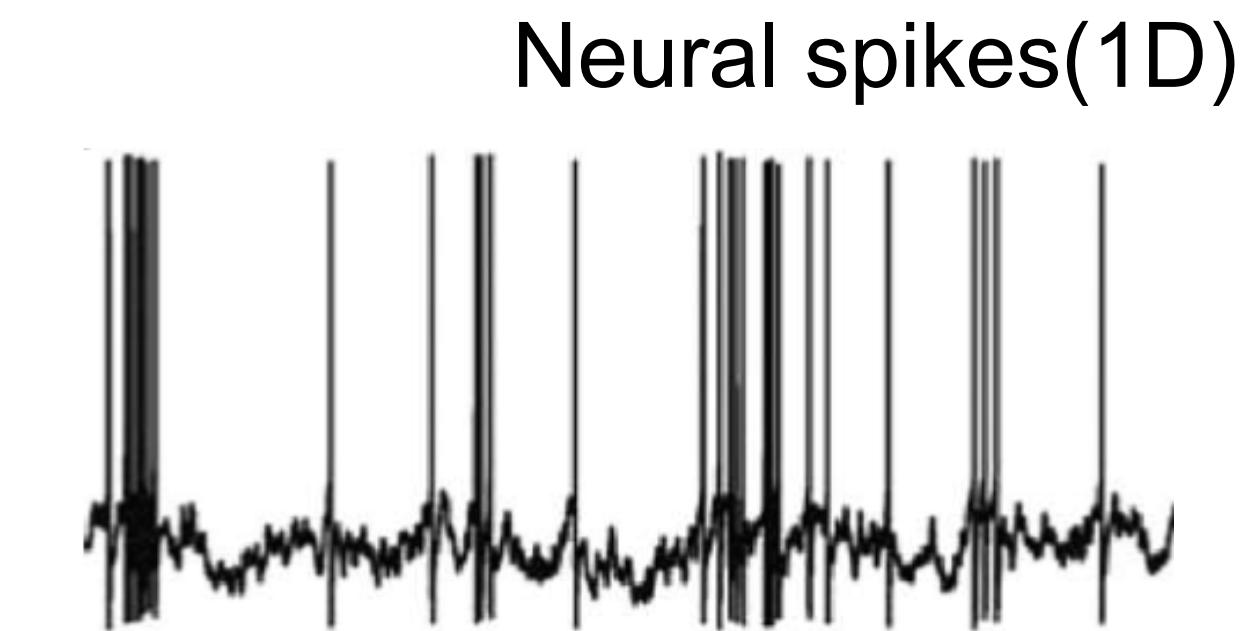
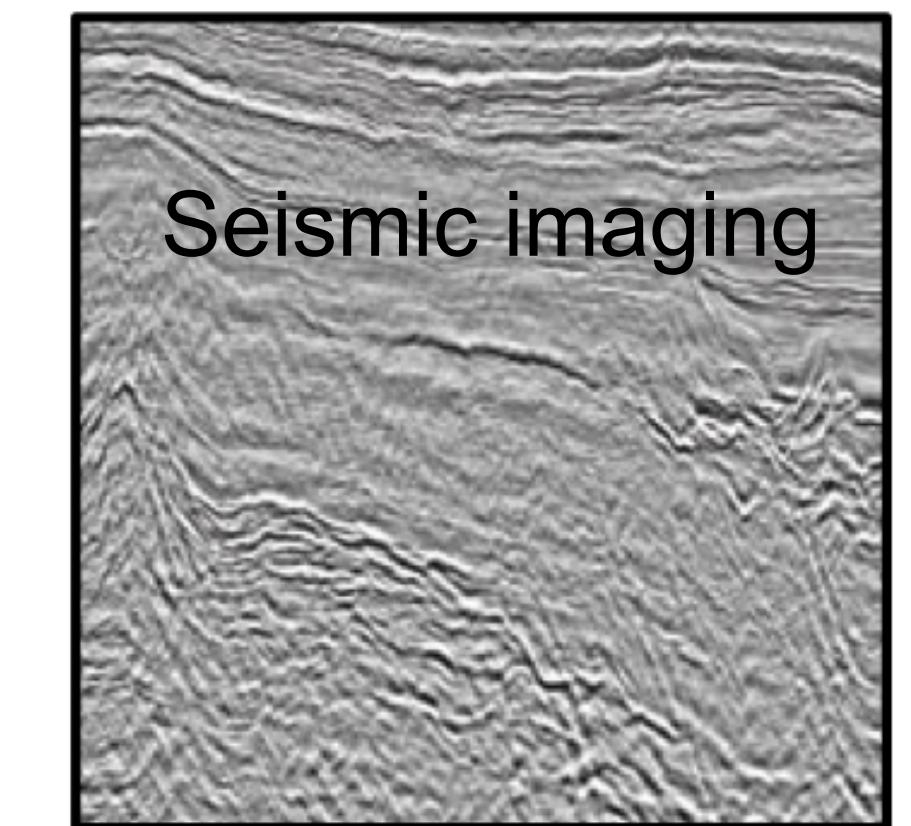
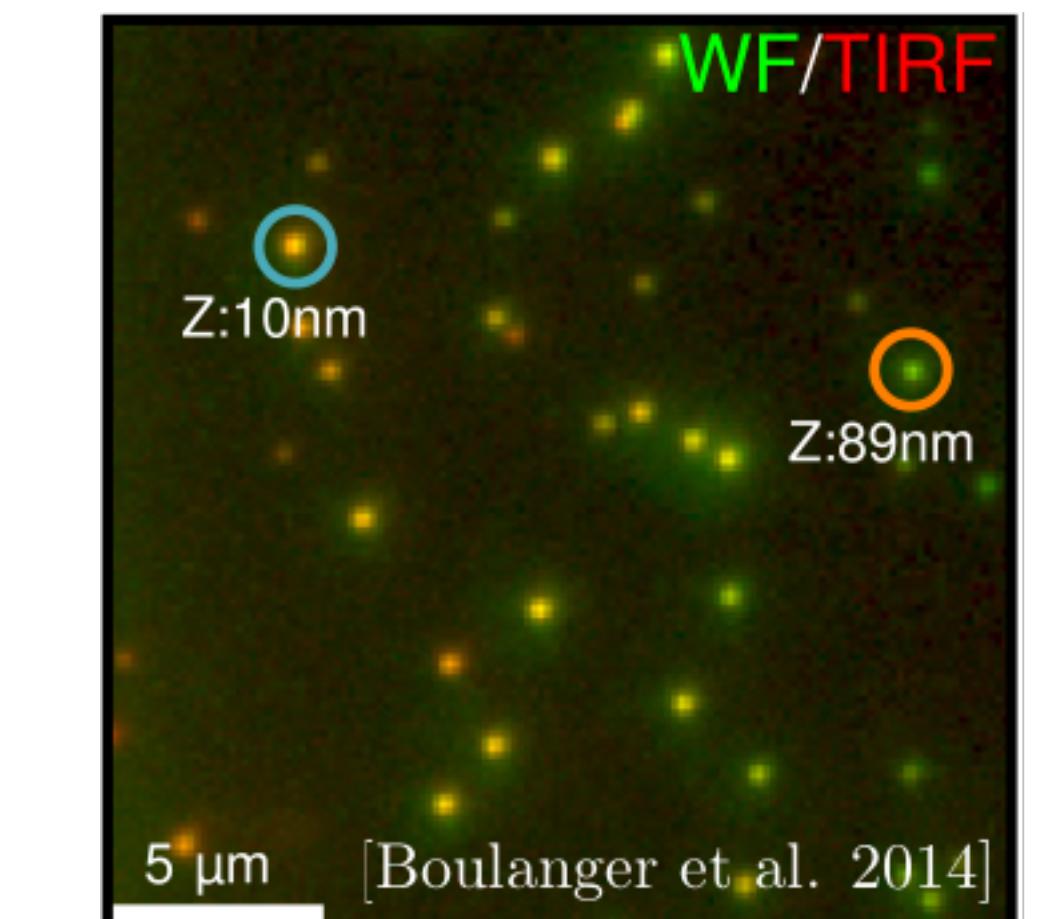
Structure promoting regularisation

Given $A \in \mathbb{R}^{m \times n}$ and $y \in \mathbb{R}^m$, solve $Ax = y$.

$$\min_{x \in \mathbb{R}^n} \Phi(x) := R(x) + F(Ax, y)$$



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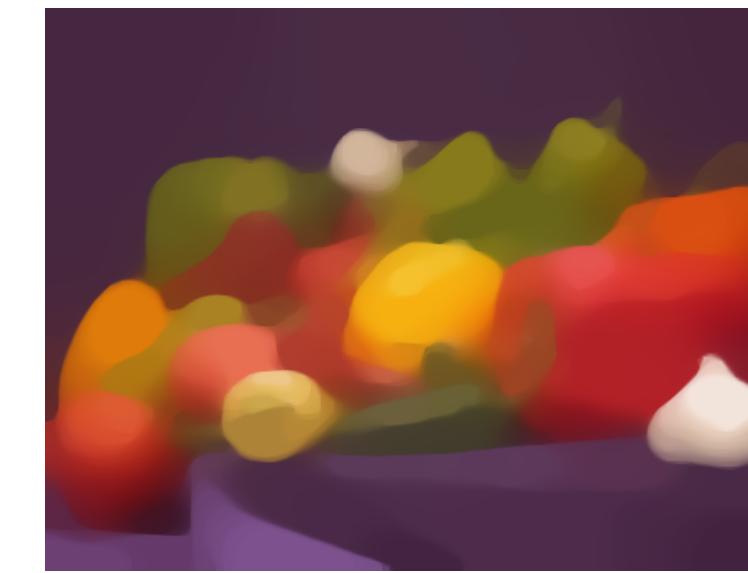
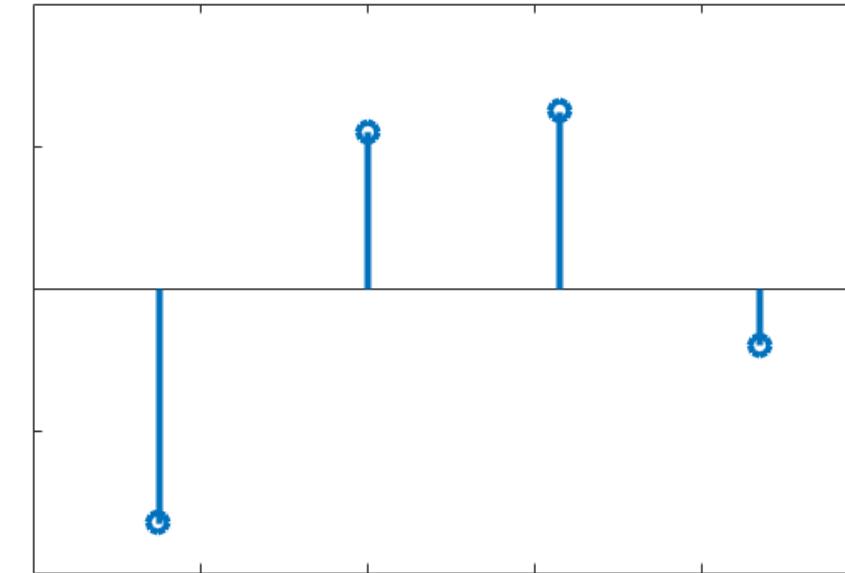


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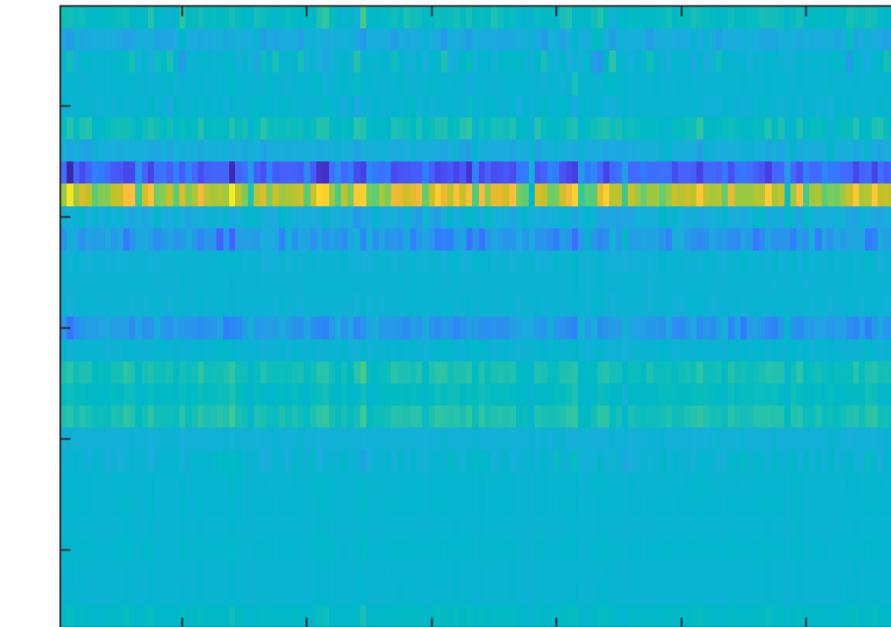
$$\min_{x \in \mathbb{R}^n} R(x) + F(Ax, y)$$

Nonsmooth R promotes structure:

- $R(x) = \|Dx\|_1$



- $R(x) = \|x\|_* = \sum_{i=1}^n \sigma_i(x)$



F is loss function:

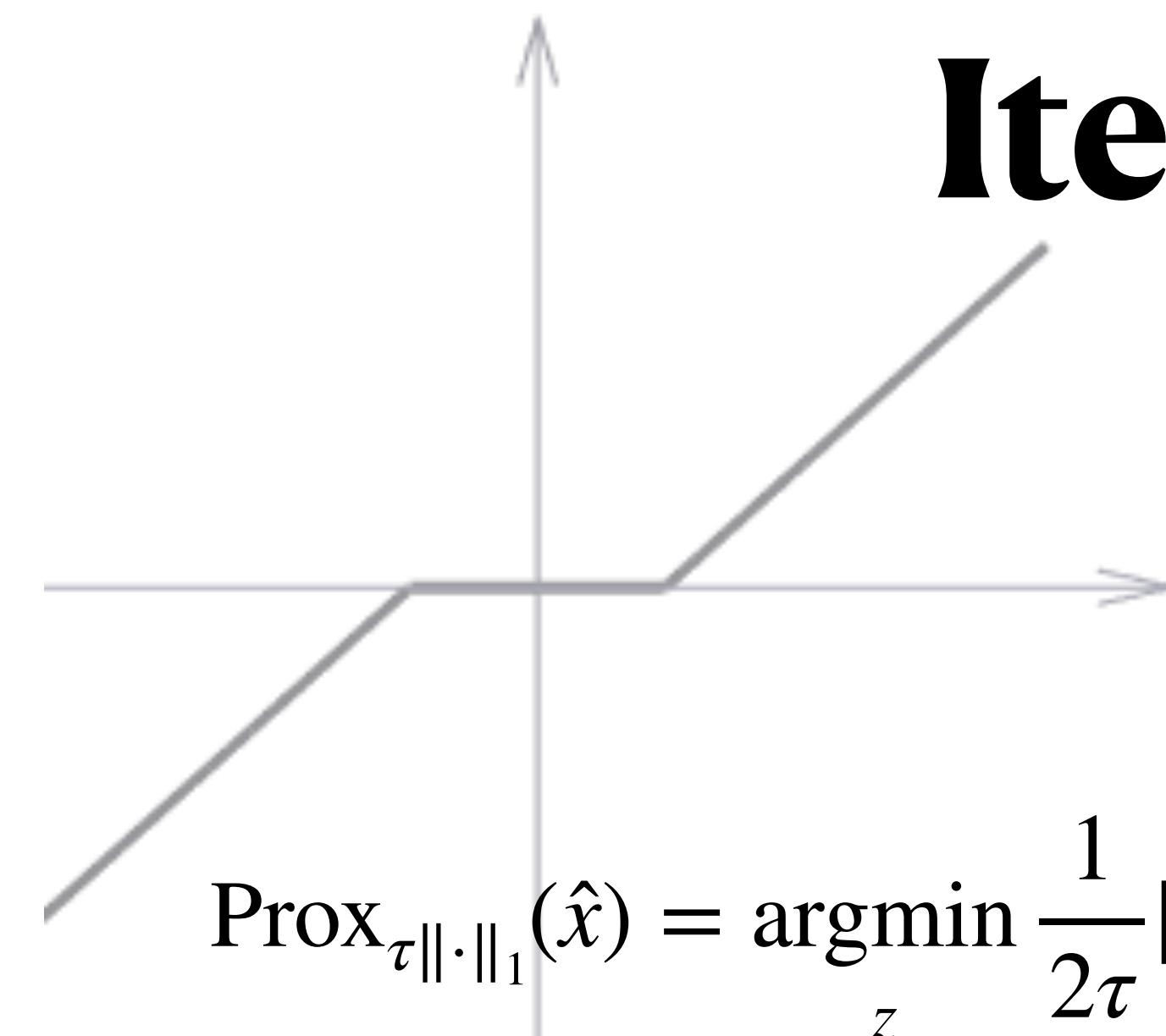
- $F(x, y) = \frac{1}{2} \|x - y\|^2$

- $F(x, y) = \iota_{x=y}$

- $F(x, y) = \|x - y\|_1$

Typical optimisation approach: Proximal-based methods such as Primal-Dual, ADMM, ISTA, ...

Iterative Soft Thresholding

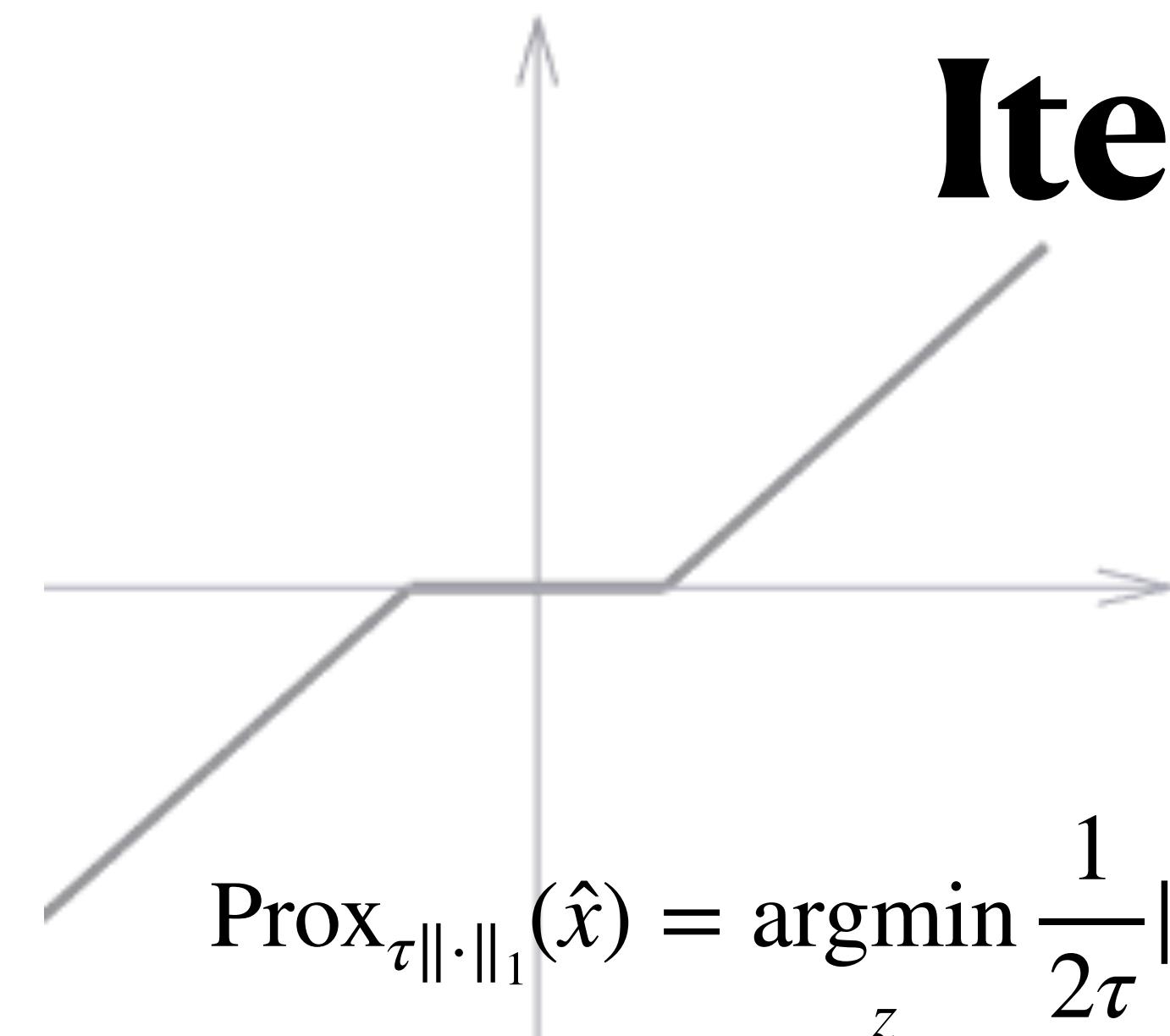


$$\begin{aligned}\text{Prox}_{\tau \|\cdot\|_1}(\hat{x}) &= \underset{z}{\operatorname{argmin}} \frac{1}{2\tau} \|z - \hat{x}\|^2 + \|z\|_1 \\ &= \text{sign}(\hat{x})(|\hat{x}| - \tau)_+\end{aligned}$$

$$\min_{x \in \mathbb{R}^n} \Phi(x) = \frac{1}{2\lambda} \|Ax - y\|^2 + \|x\|_1$$

$$\begin{cases} \hat{x}_{k+1} &= x_k - \tau A^\top (Ax_k - y) \\ x_{k+1} &= \text{Prox}_{\tau \|\cdot\|_1}(\hat{x}_{k+1}) \end{cases}$$

Iterative Soft Thresholding



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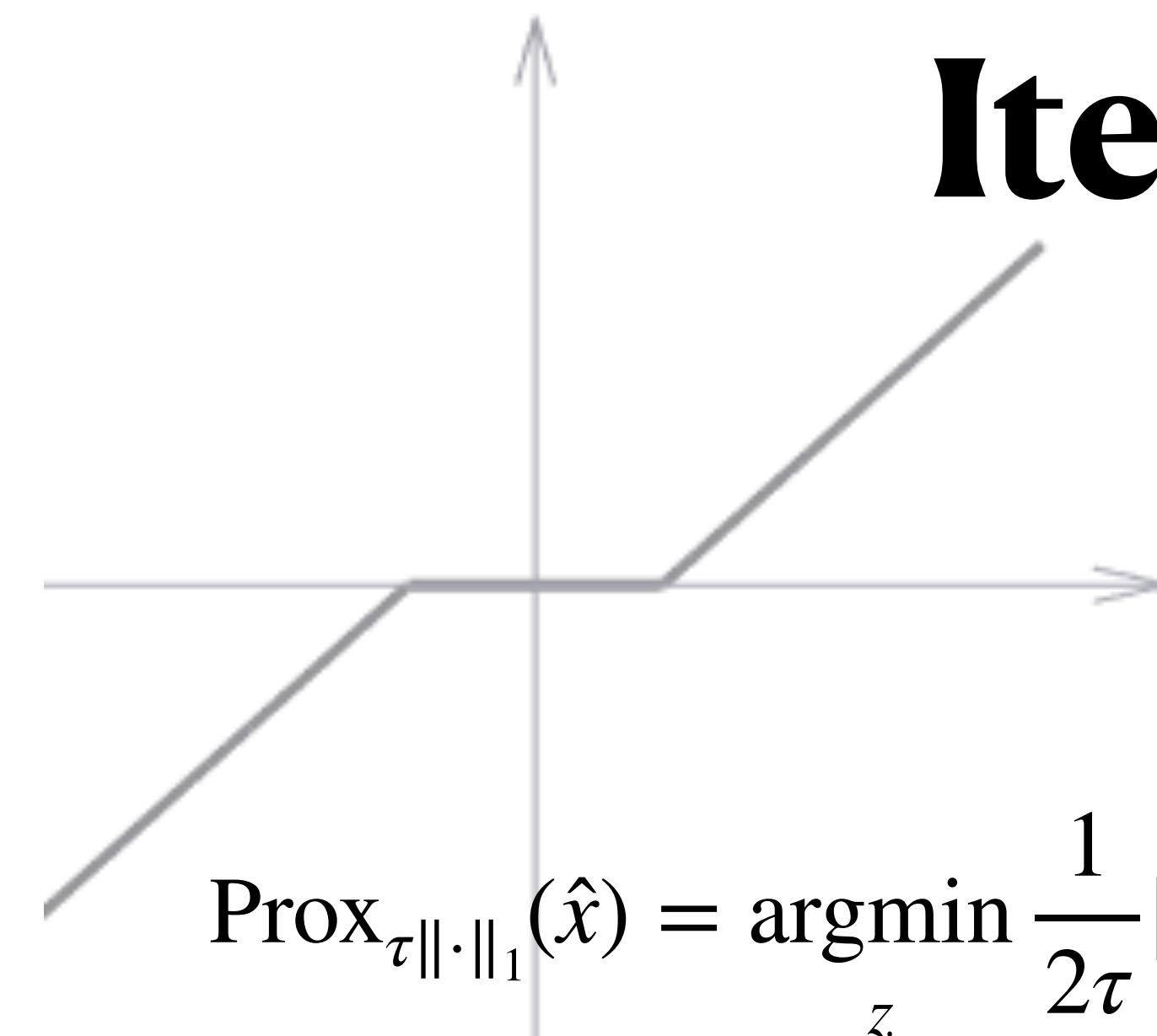
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Convergence rates (Beck & Teboulle 2009):

$$\Phi(x_k) - \min_x \Phi(x) \leq \frac{C_n}{k}$$

Iterative Soft Thresholding



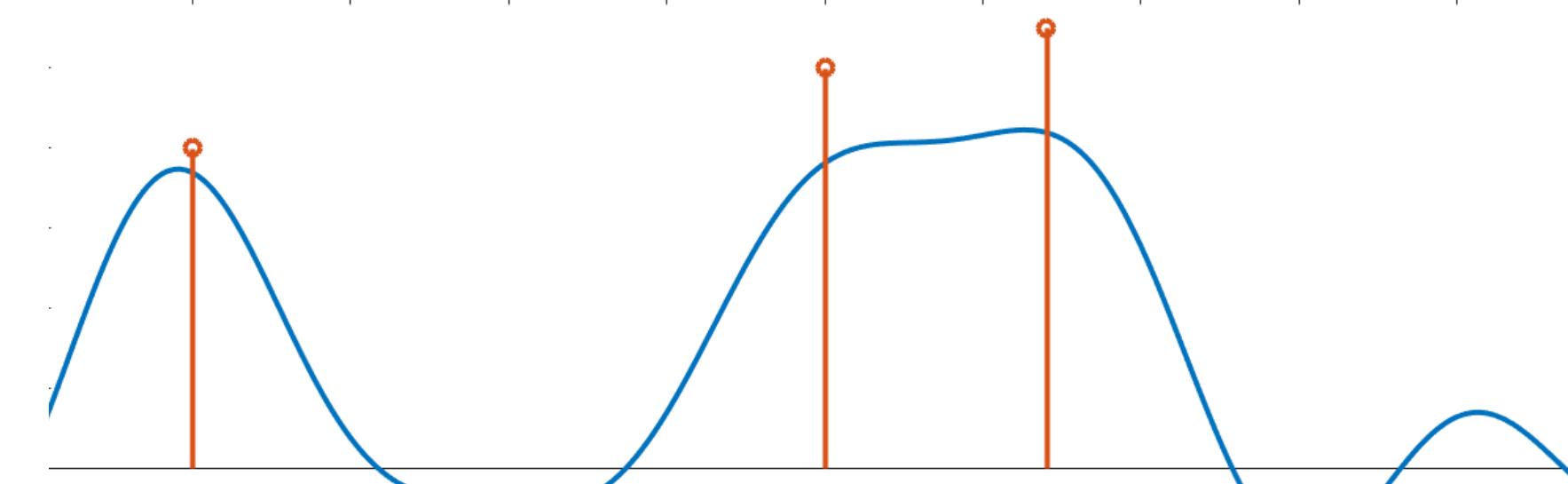
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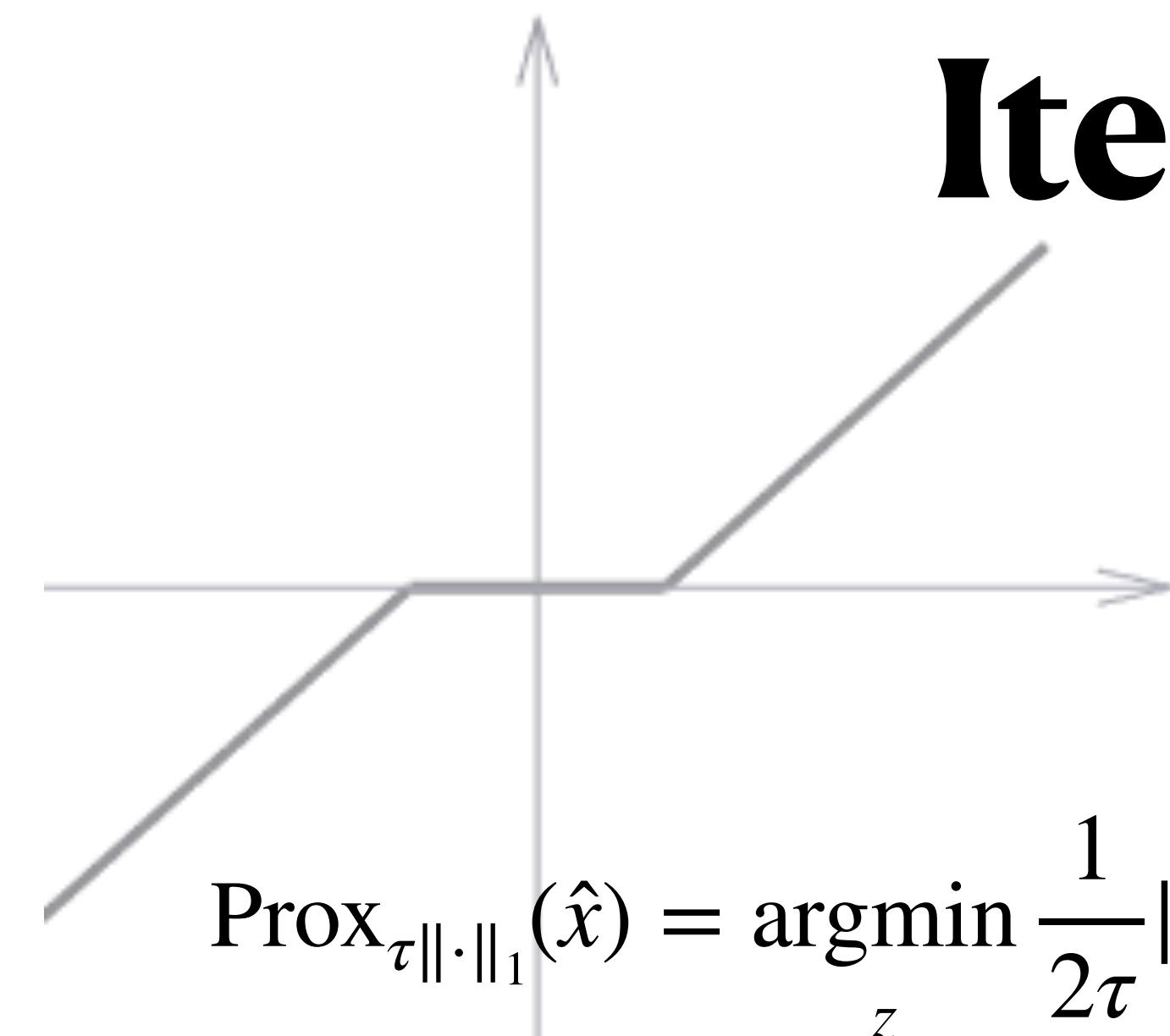
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$$\text{Column } i : A_i = \left(\exp(2\pi\sqrt{-1}x_i^\top \omega_k) \right)_k$$

$C_n = \mathcal{O}(p^{-d})$ if $[x_i] \subseteq [0,1]^d$ spaced p apart

Iterative Soft Thresholding



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Grid-free convergence rates (Chizat 2021):

$$\Phi(x_k) - \min_x \Phi(x) \leq k^{-2/(d+1)}$$

NB: Result is independent of n

Proximal Mirror descent

Entropy function:

η strongly convex and smooth.

Bregman distance:

$$D_\eta(a, b) = \eta(a) - \eta(b) - \langle \nabla \eta(b), a - b \rangle$$

$$x_{k+1} \in \operatorname{argmin} F(x_k) + \langle \nabla F(x_k), x - x_k \rangle + \lambda \|x\|_1 + \frac{1}{\tau} D_\eta(x, x_k)$$

[Chizat 2021]:

- $\eta(x) = \frac{1}{2} \|x\|^2$ corresponds to ISTA with convergence rate $\mathcal{O}(k^{-2/(d+2)})$
- $\eta(x) = \gamma \text{arsinh}(x/\gamma) - \sqrt{x^2 + \gamma^2} + \gamma$ with $\gamma > 0$ with convergence rate $\mathcal{O}(k^{-1} \log(k))$

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One can improve to $\mathcal{O}(1/k^2)$ rates, however, standard acceleration techniques such as BB step, Quasi-Newton, etc are non-trivial to apply.

Use of other proximal based methods (e.g. Primal Dual, ADMM) require tuning of several parameters.

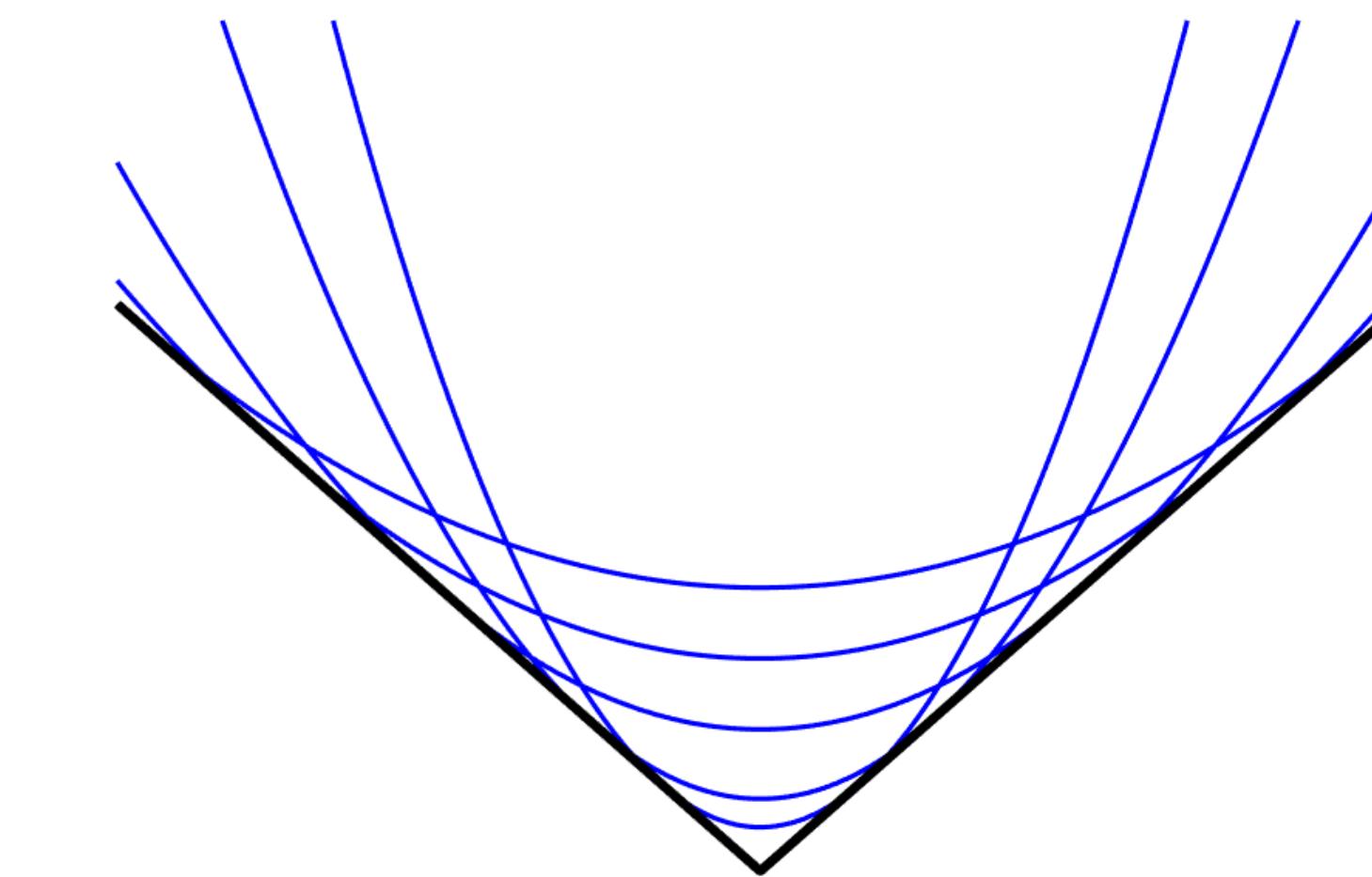
This Talk:

New class of algo for nonsmooth structured optimisation

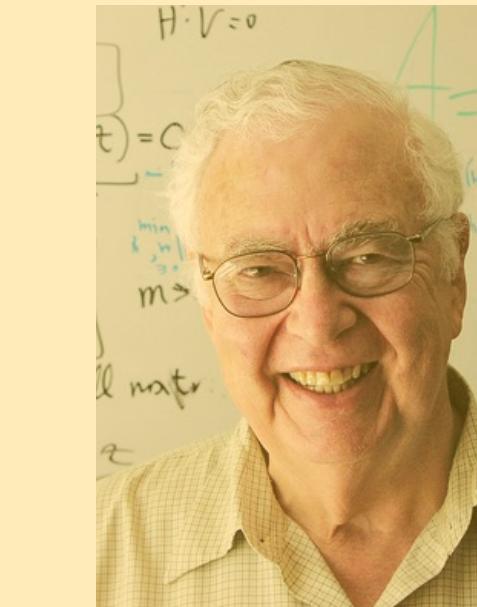
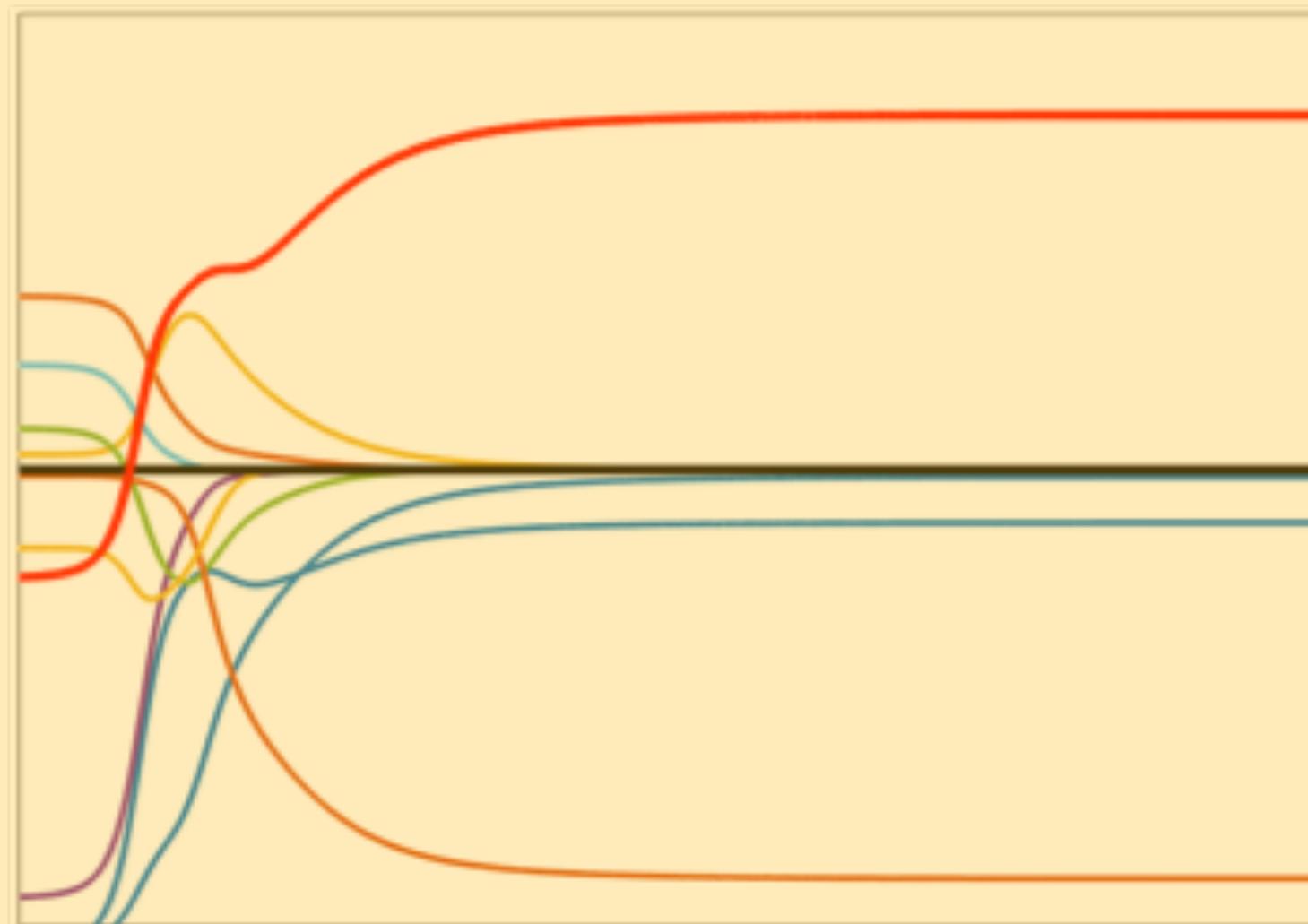
- (1) Overparametrize to obtain a **smooth and nonconvex** problem.
- (2) **VarPro**: Place into a bilevel form for better problem conditioning.
- (3) Over-parameterization lets us stay in Euclidean geometry with **dimension and grid independent** convergence analysis.
- (4) Use BFGS to obtain fast convergence behaviour.

I will focus on the Lasso but our method can be applied in many settings, including total variation/group ℓ_1 /nuclear norm regularisation and nonsmooth loss functions.

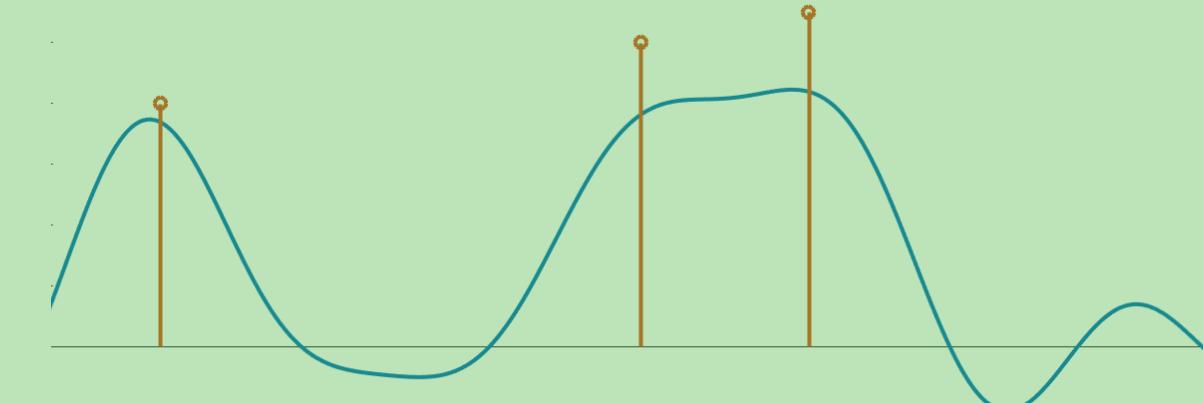
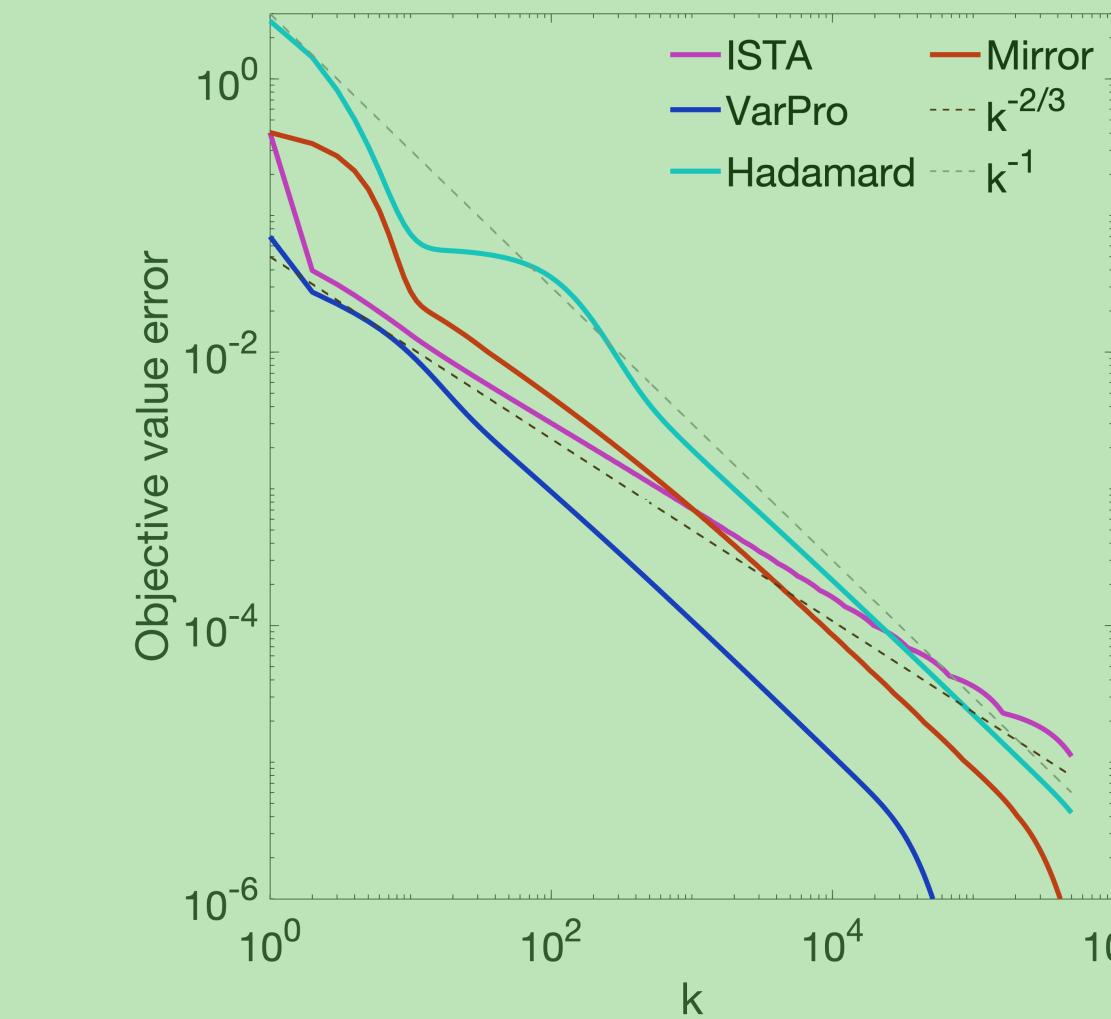
Overparameterization



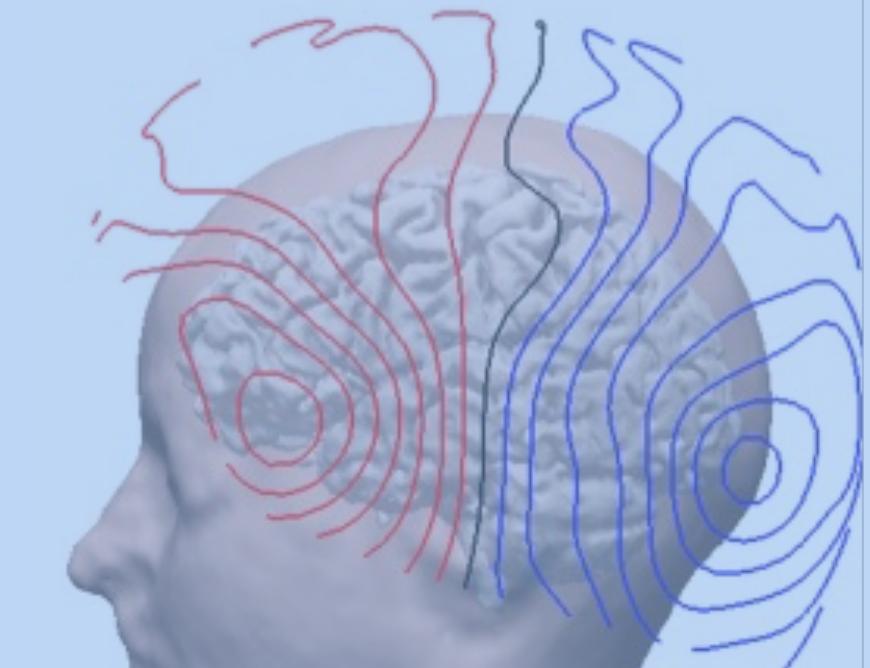
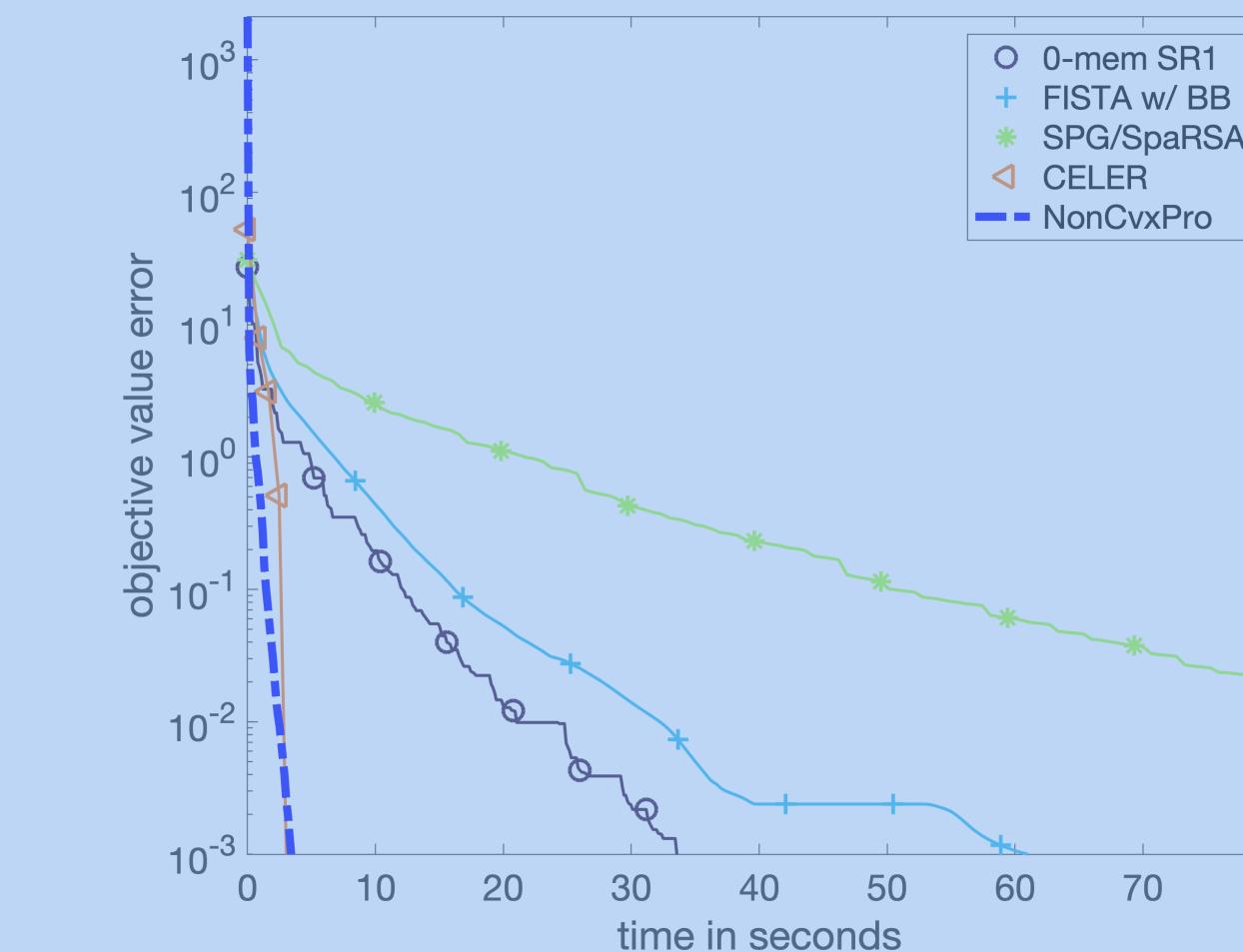
VarPro



Convergence



Numerical Results



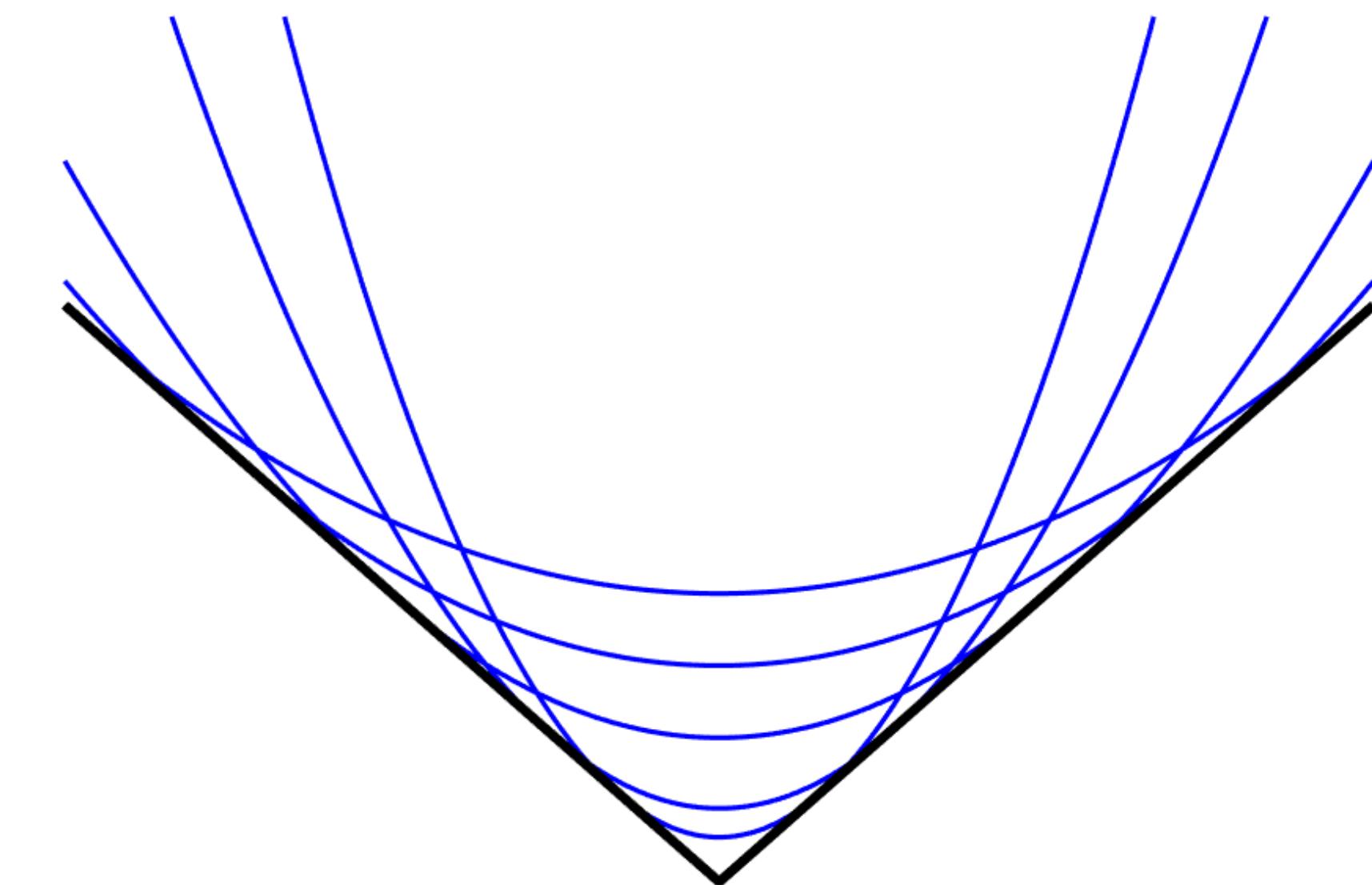
Iterative Reweighted Least Squares

The η -trick :

$$|x| = \inf_{\eta > 0} \frac{1}{2} \frac{x^2}{\eta} + \frac{1}{2} \eta$$

Jointly convex in x and η

$$\min_{x \in \mathbb{R}^n} \Phi(x) = \frac{1}{2\lambda} \|Ax - y\|^2 + \|x\|_1$$



Iterative Reweighted Least Squares

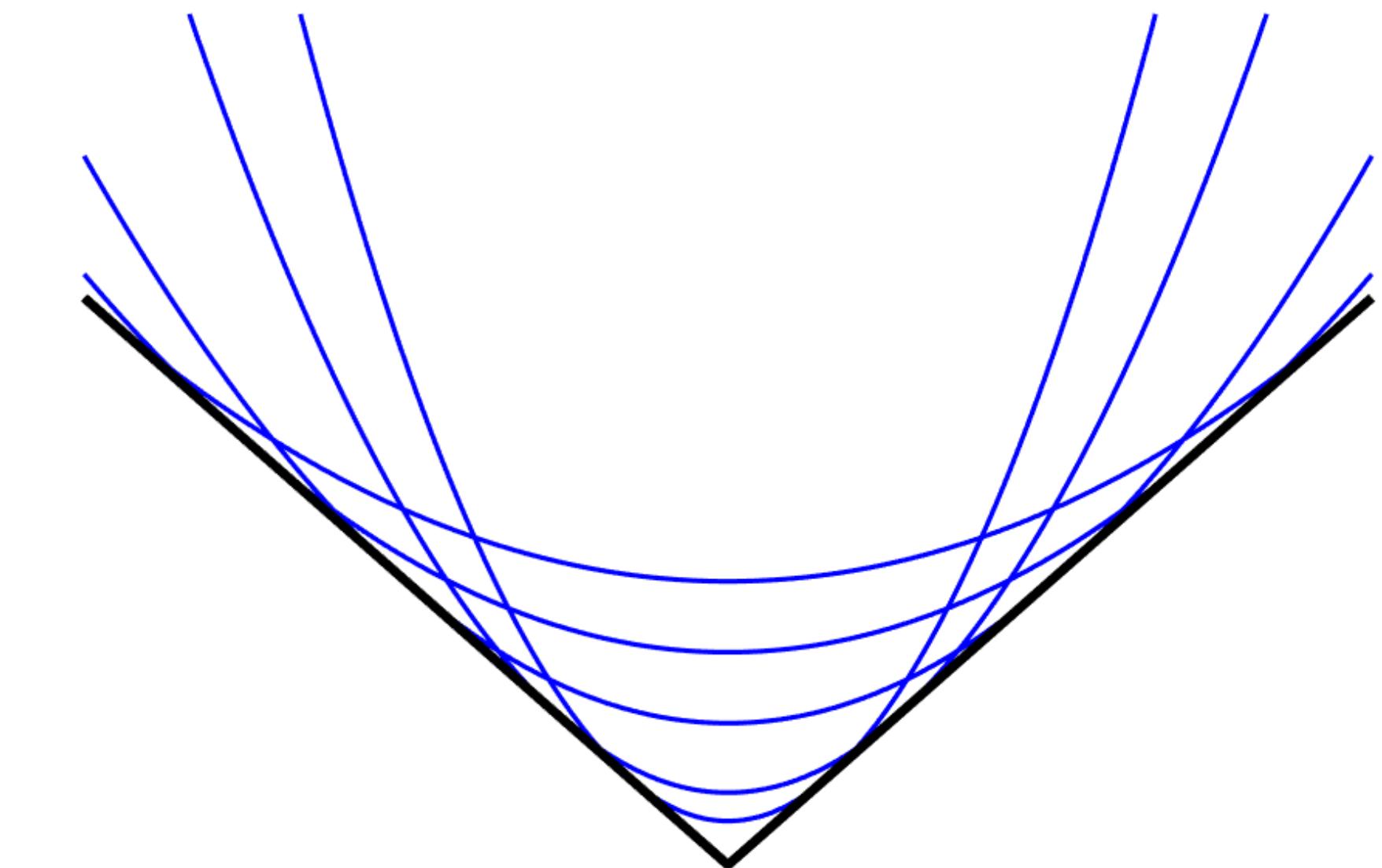
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Jointly convex in x and η

$$\min_{x \in \mathbb{R}^n} \frac{1}{2} \sum_i \left(\frac{x_i^2}{\eta_i} + \eta_i \right) + \frac{1}{2\lambda} \|Ax - y\|^2 + \frac{\epsilon}{2} \sum_i \frac{1}{\eta_i}$$

$$\min_{x \in \mathbb{R}^n} \Phi(x) = \frac{1}{2\lambda} \|Ax - y\|^2 + \|x\|_1$$



Alternating minimisation

$$\begin{cases} x_{k+1} = (A^\top A + \lambda \text{diag}(1/\eta_k))^{-1} A^\top y \\ \eta_{k+1} = \sqrt{\epsilon + x_k^2} \end{cases}$$

The Hadamard parametrization

$$|x| = \inf_{\eta > 0} \frac{1}{2} \frac{x^2}{\eta} + \frac{1}{2}\eta$$

$$\begin{array}{c} u = x/\sqrt{\eta} \\ \longrightarrow \\ v = \sqrt{\eta} \end{array}$$

$$|x| = \inf_{x=u \odot v} u^2/2 + v^2/2$$

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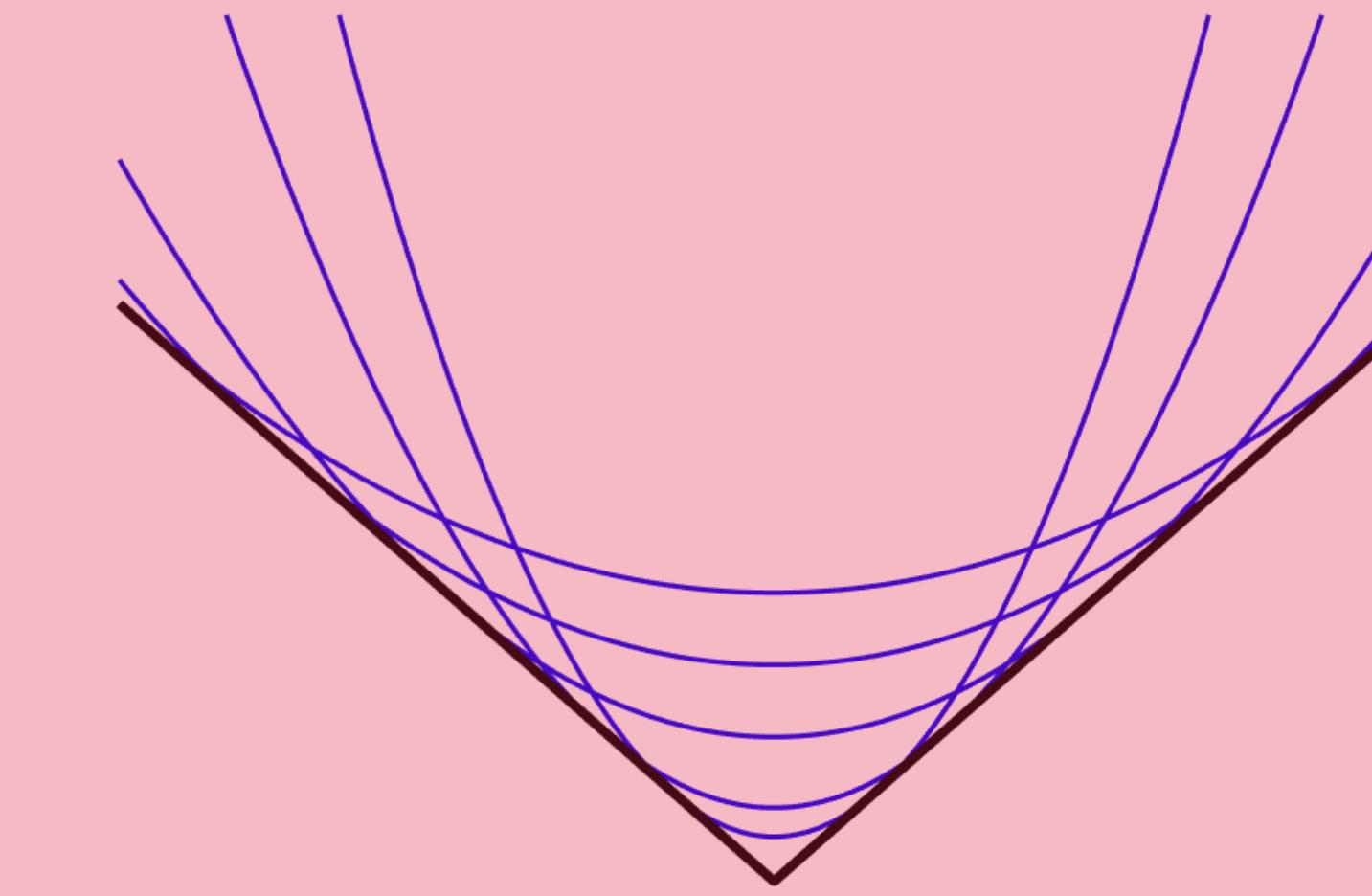
$$\min_{u, v \in \mathbb{R}^n} \frac{1}{2\lambda} \|Au \odot v - y\|^2 + \frac{1}{2} \|u\|^2 + \frac{1}{2} \|v\|^2$$

Convex and nonsmooth

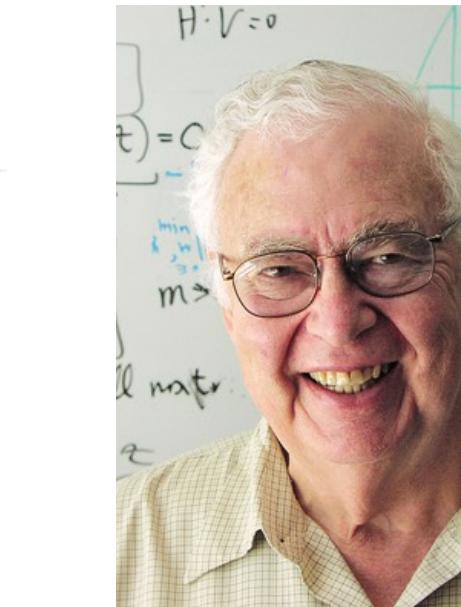
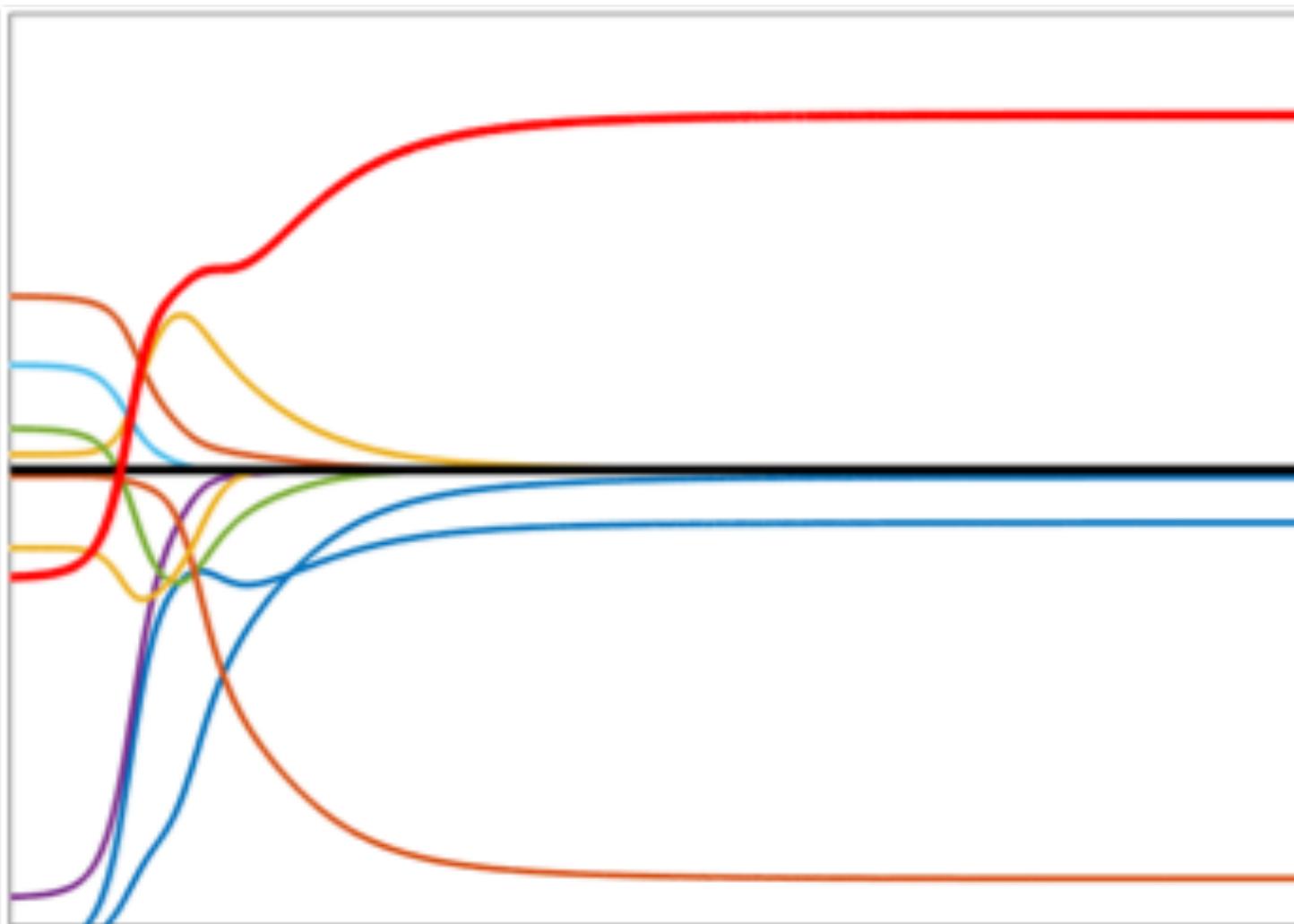
Non-Convex and smooth

One can either do alternating minimisation or gradient descent on u, v

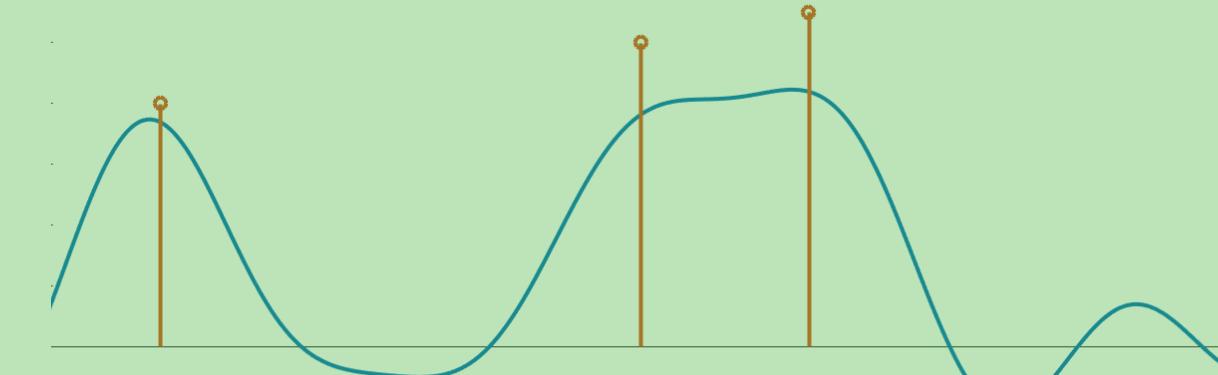
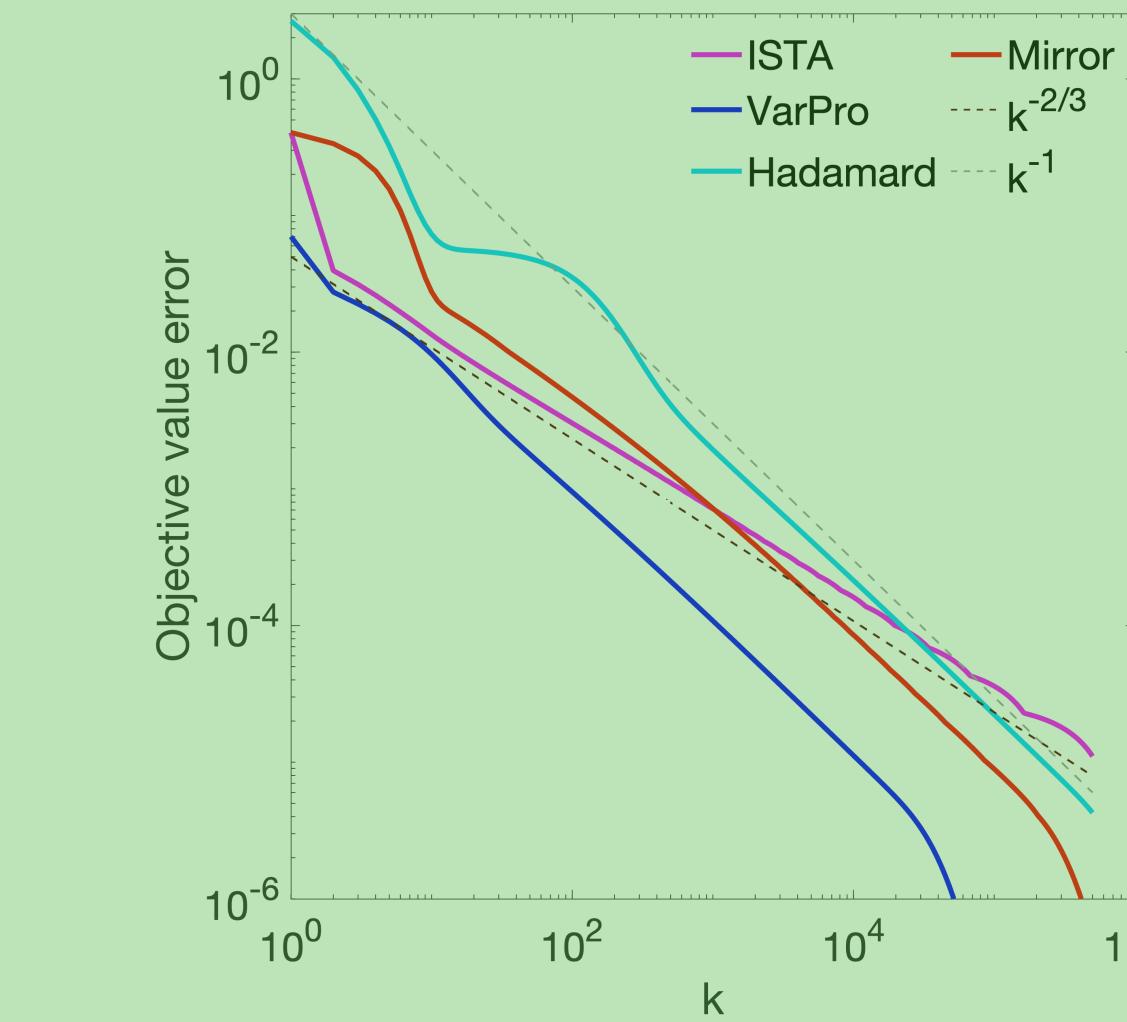
Overparameterization



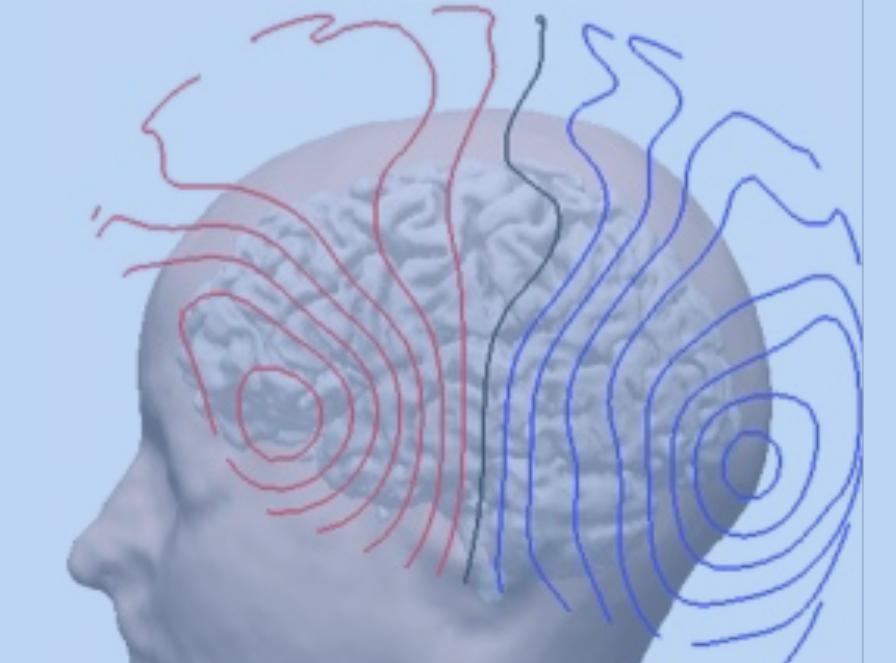
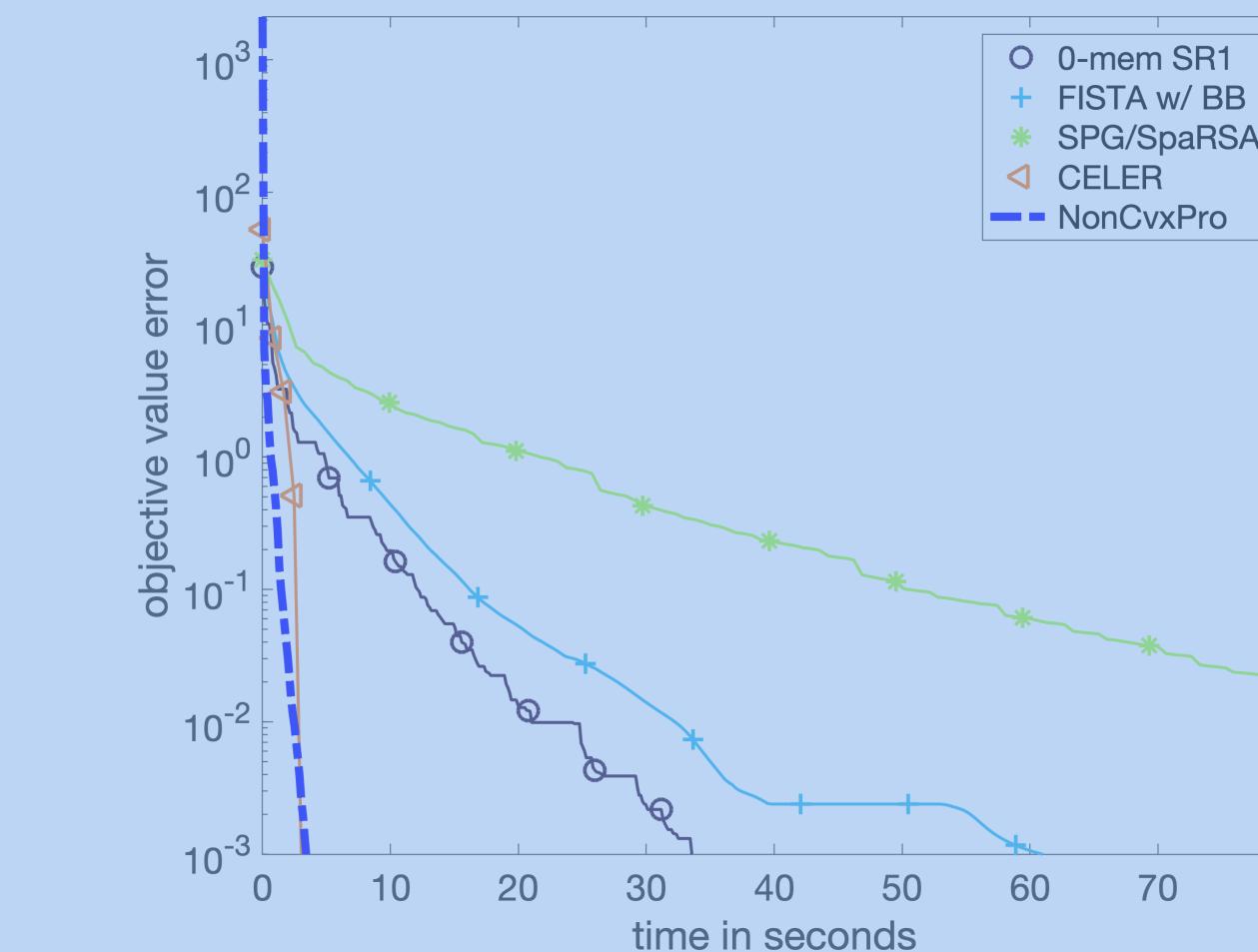
VarPro



Convergence



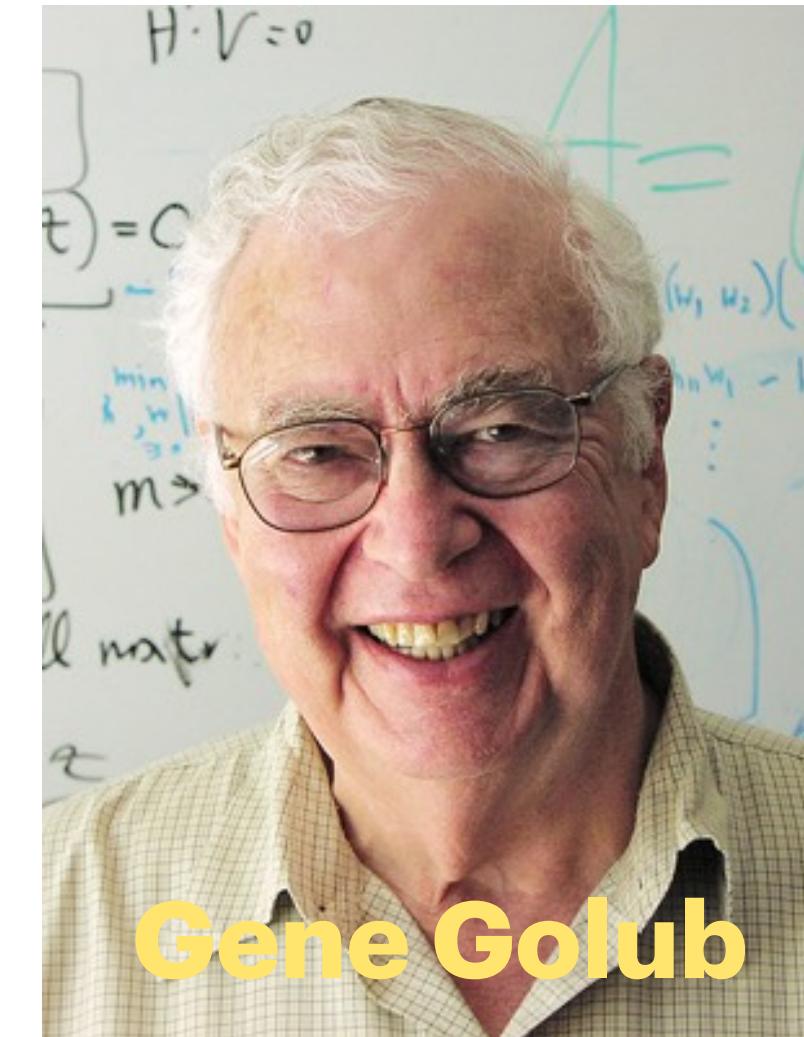
Numerical Results



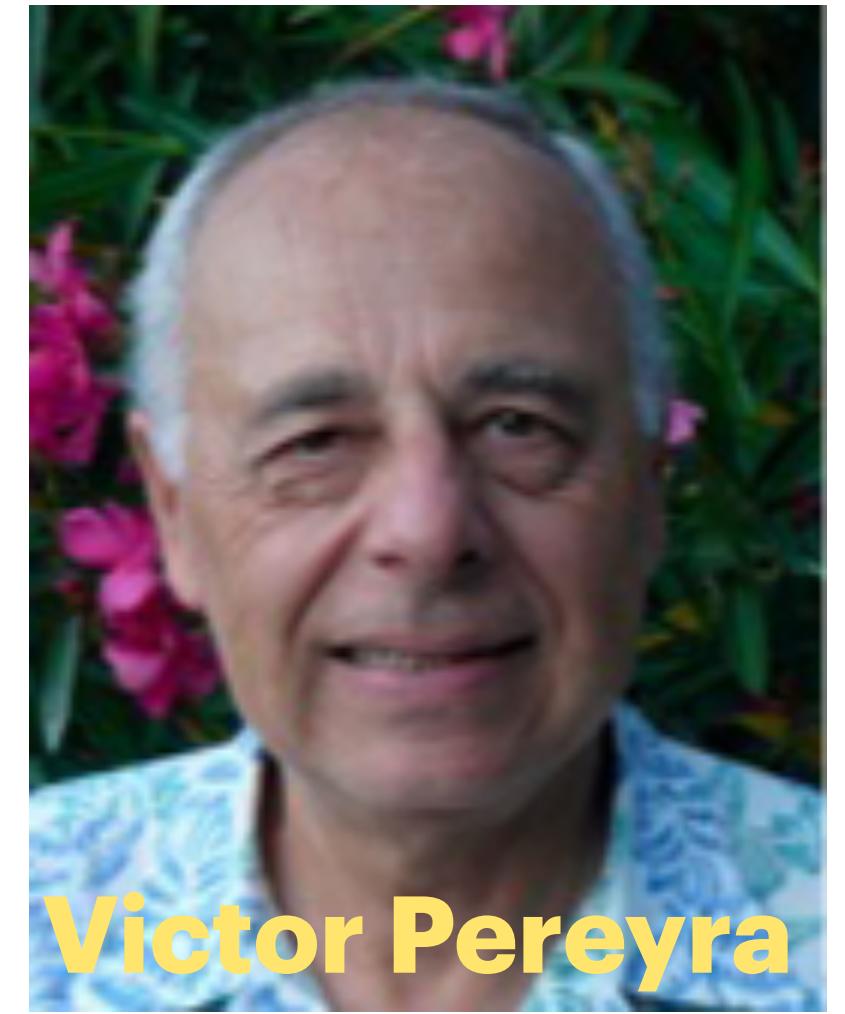
VarPro

VarPro: Instead of $\min_{u,v} F(u, v)$

Solve $\min_v f(v) = F(u(v), v)$ with
 $u(v) \in \operatorname{argmin}_u F(u, v)$



Gene Golub



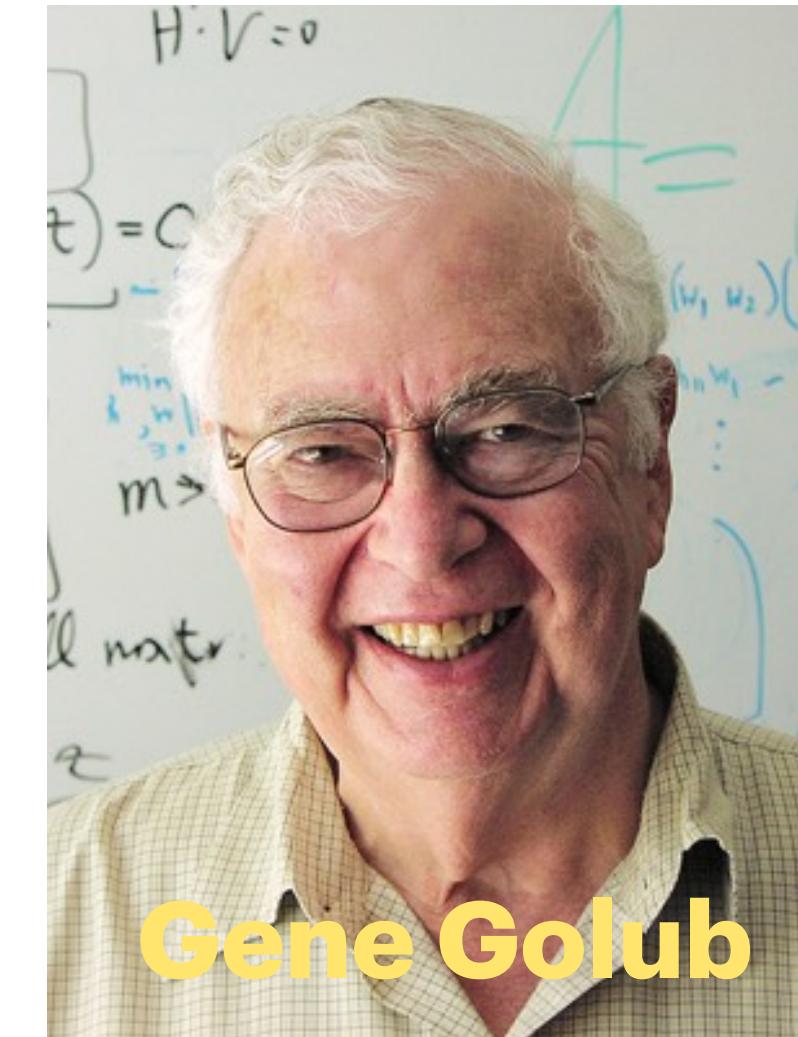
Victor Pereyra

VarPro

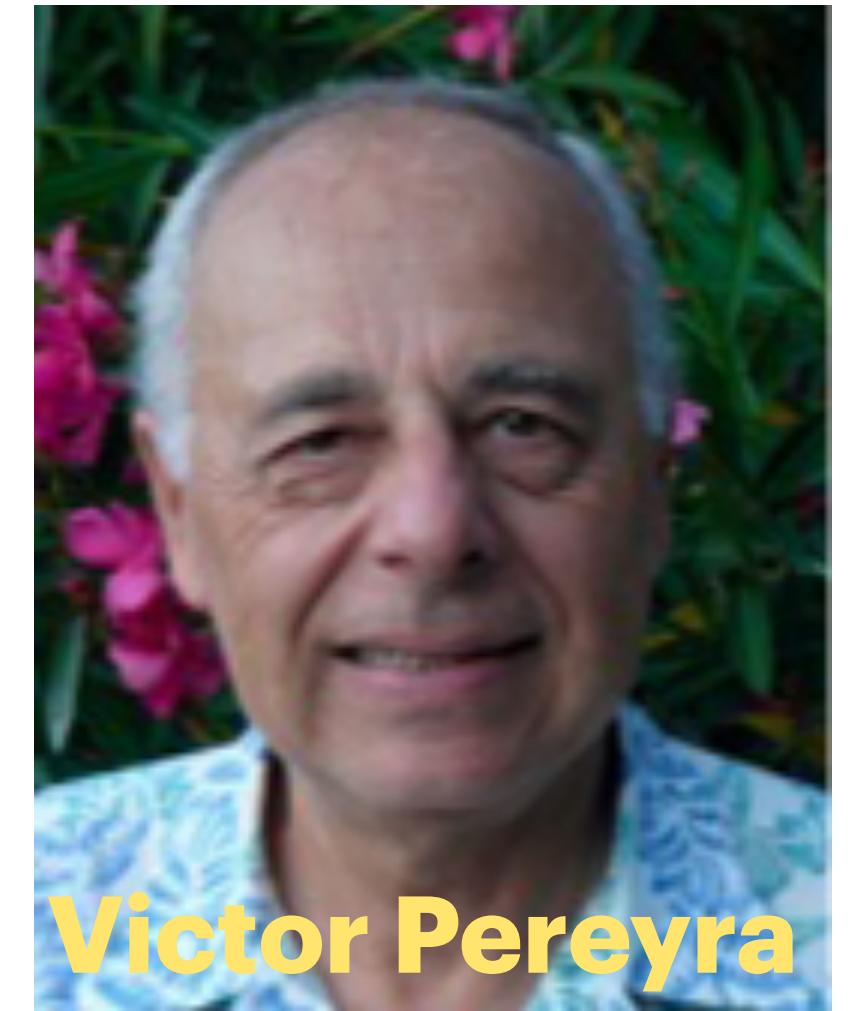
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Easy to compute derivative:

Envelope theorem: $\nabla f(v) = \partial_v F(u(v), v)$

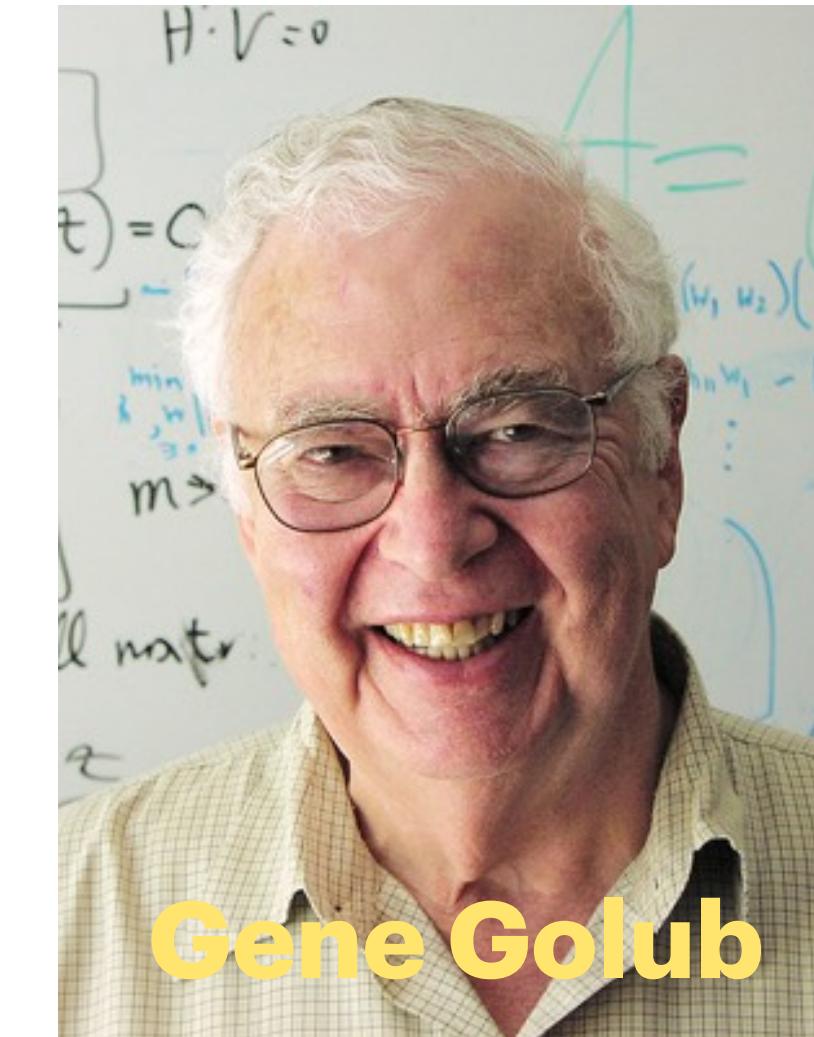
Chain rule: $\nabla f(v) = \partial_v F(u(v), v) + \partial_u F(u(v), v) \nabla u(v)$

VarPro

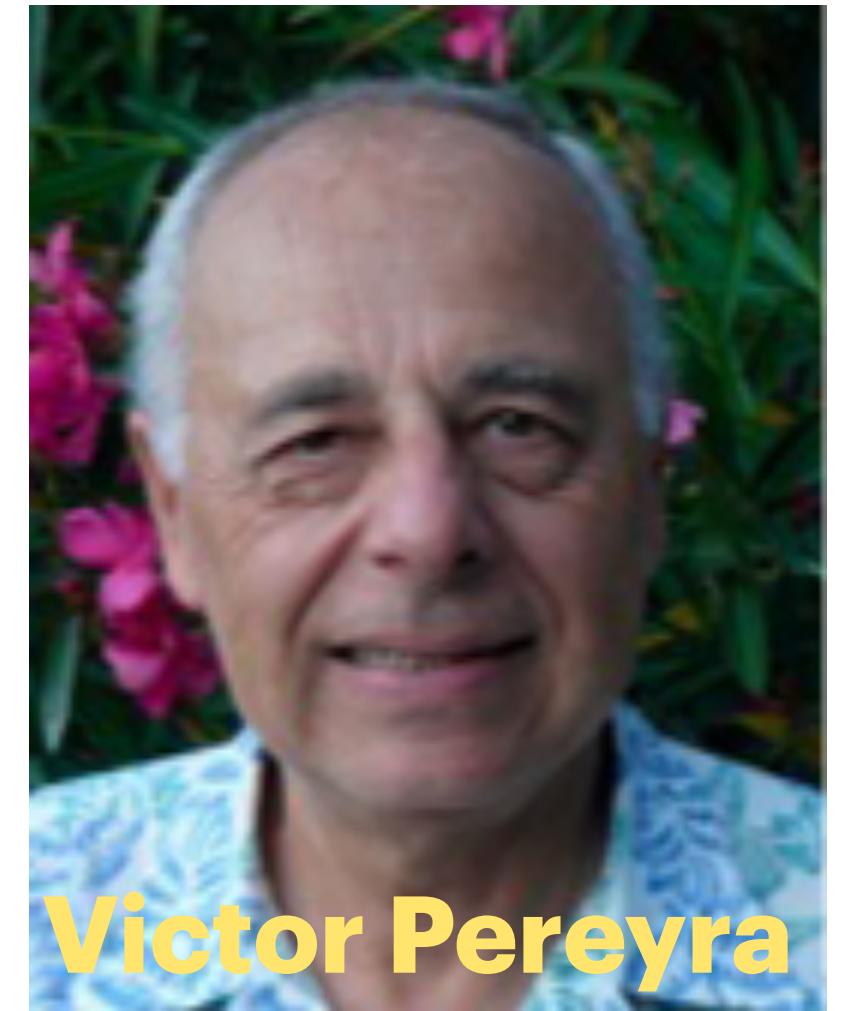
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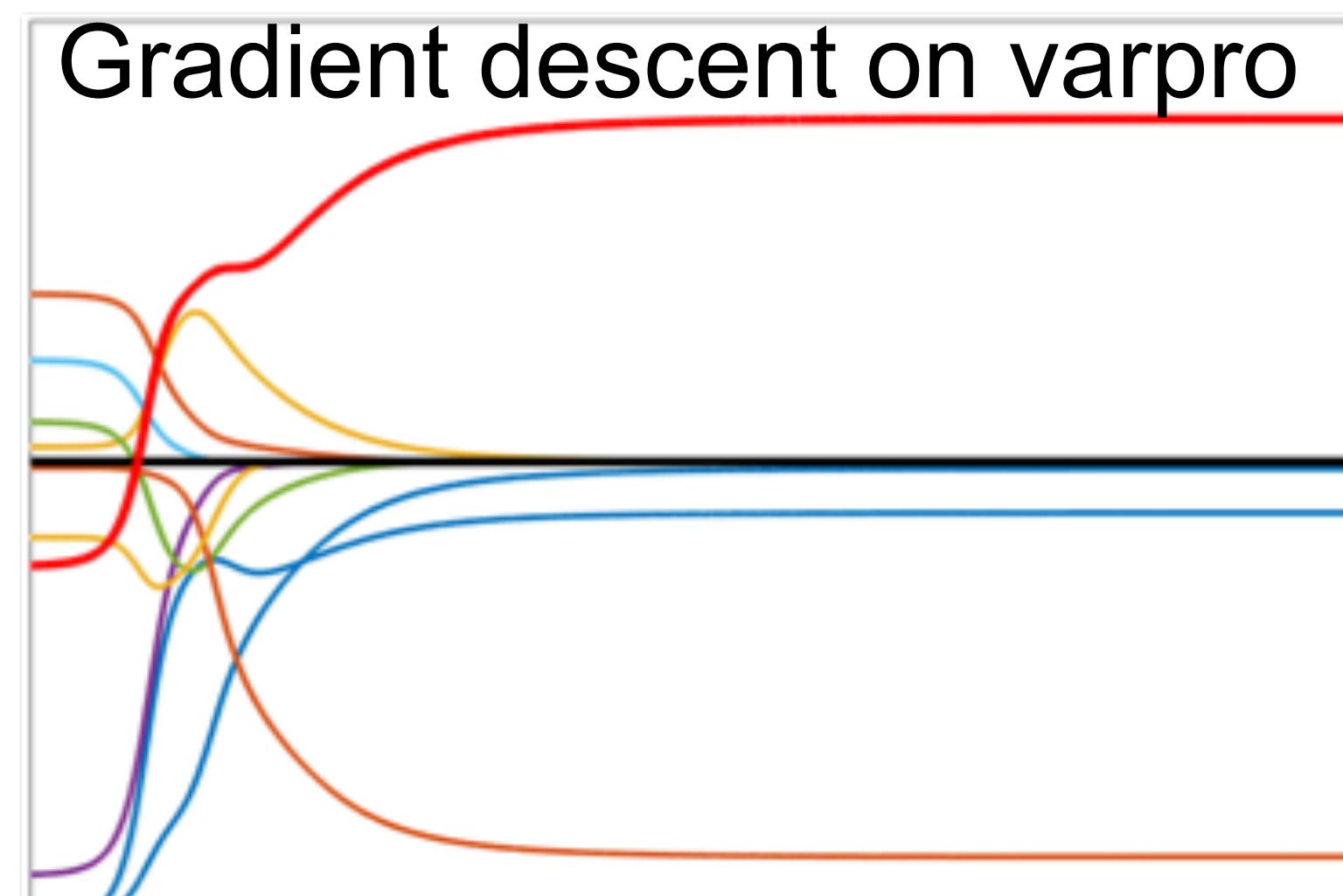
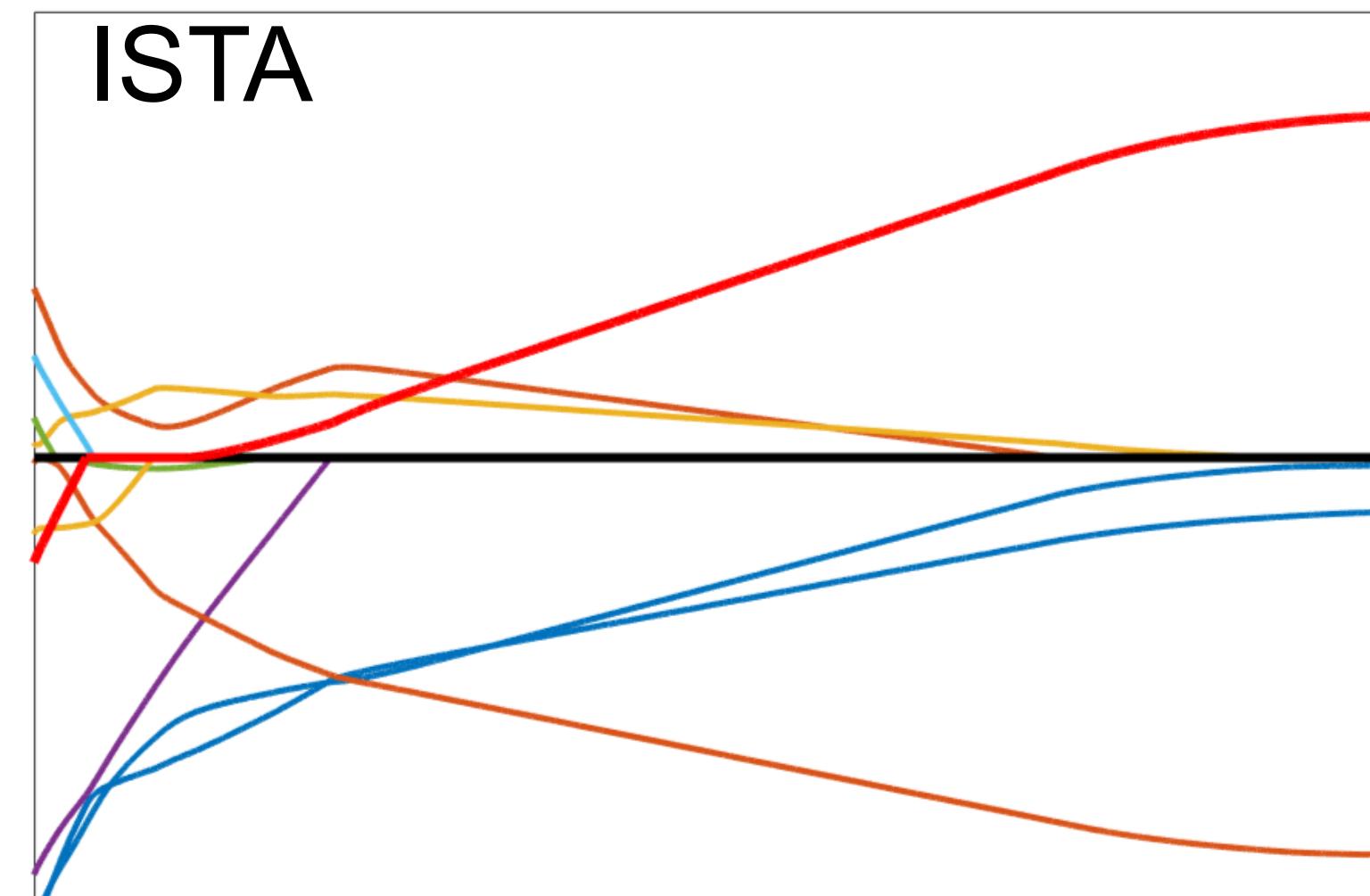
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$\nabla^2 f$ is the **Schur complement** of $\nabla^2 F(u, v)$ and is typically better conditioned

Bilevel formulation

$$\min_v f(v)$$

$$f(v) := \min_u \frac{1}{2} \|u\|^2 + \frac{1}{2} \|v\|^2 + \frac{1}{2\lambda} \|Au \odot v - y\|^2$$



Bilevel formulation

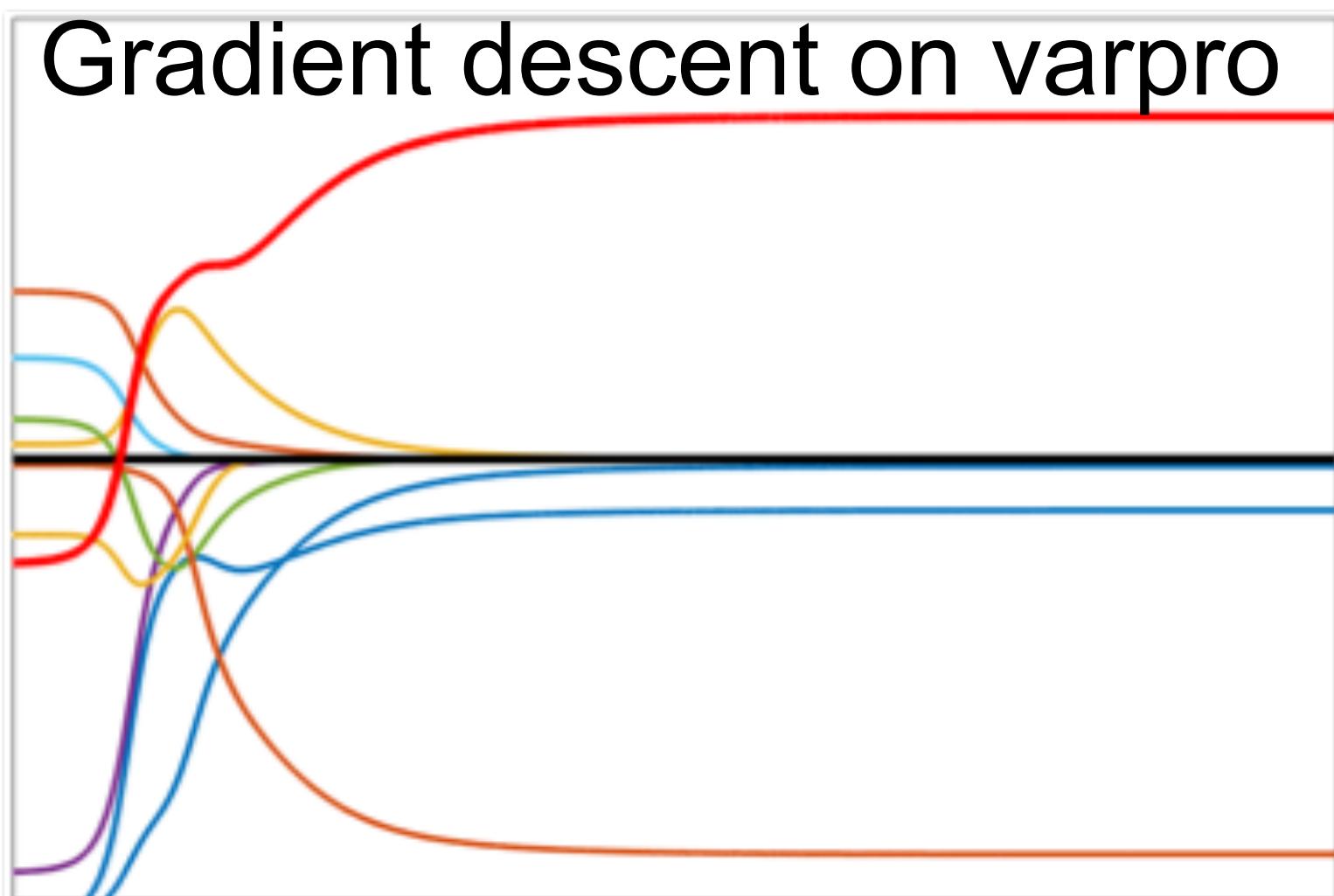
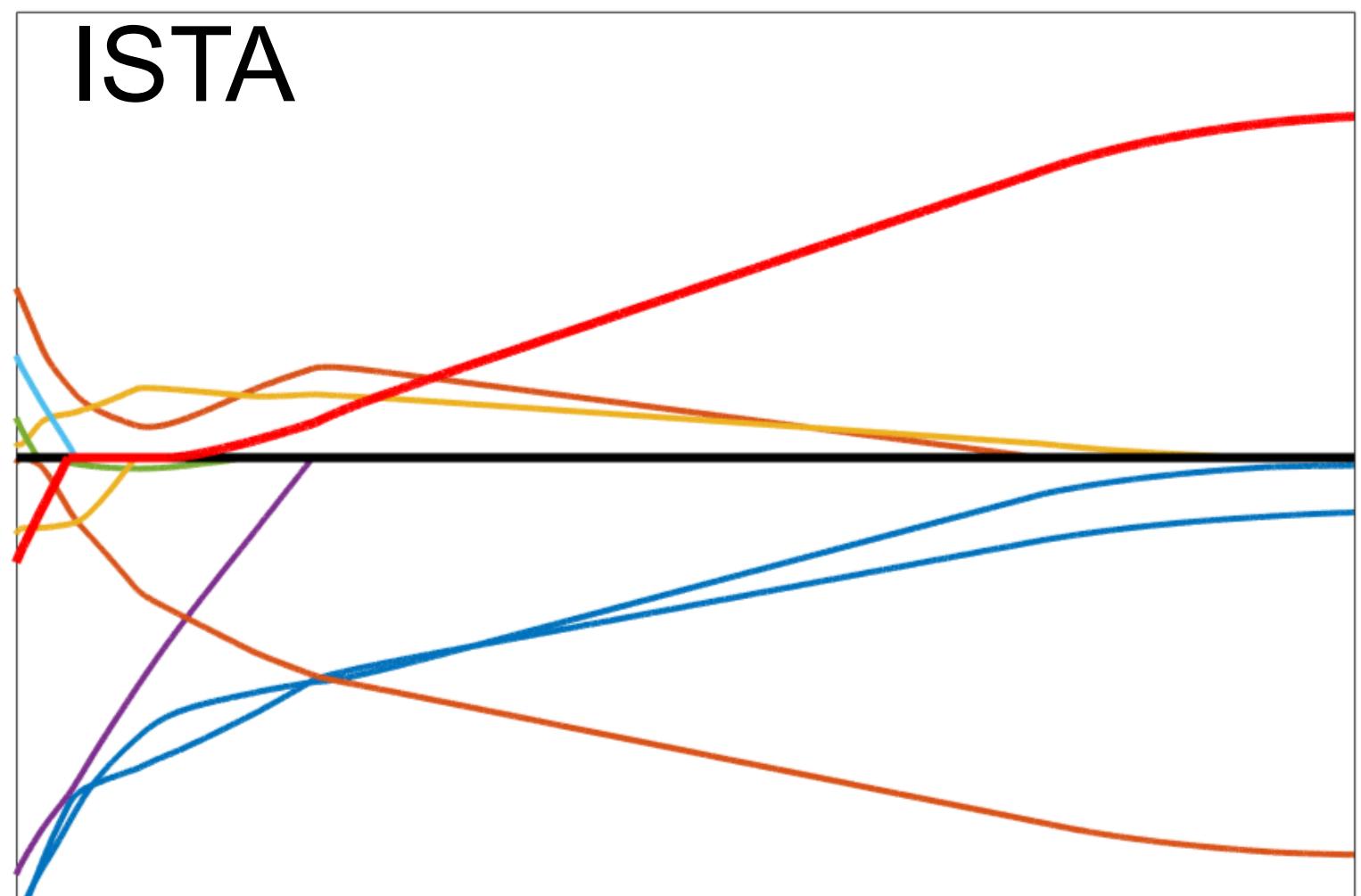
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Computing the gradient:

$$\nabla f(v) = v + \frac{1}{\lambda} u \odot A^\top (Au \odot v - y)$$

$$u = (\lambda I + \text{diag}(v)A^\top A \text{diag}(v))^{-1}(v \odot A^\top y)$$



Bilevel formulation

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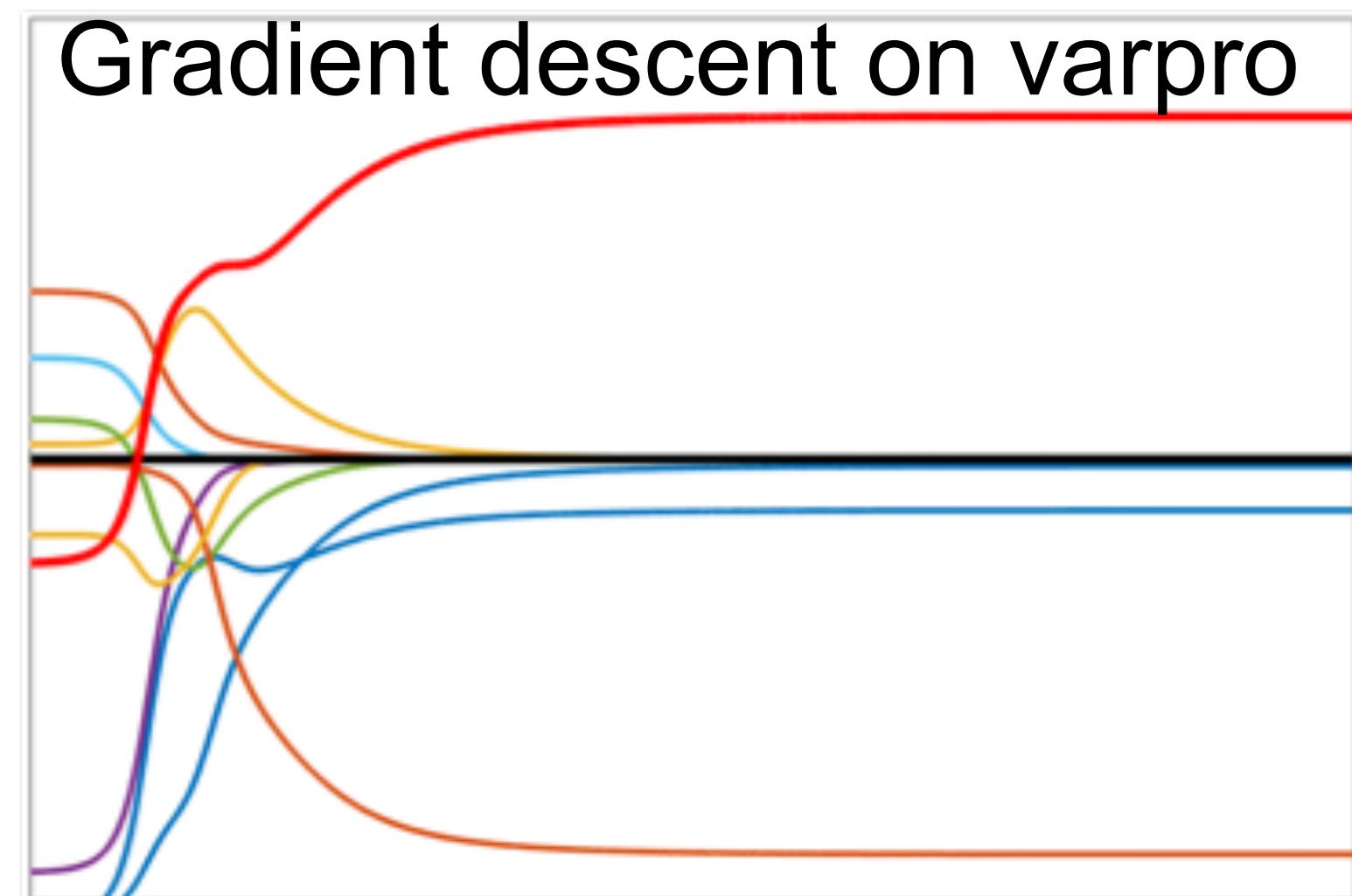
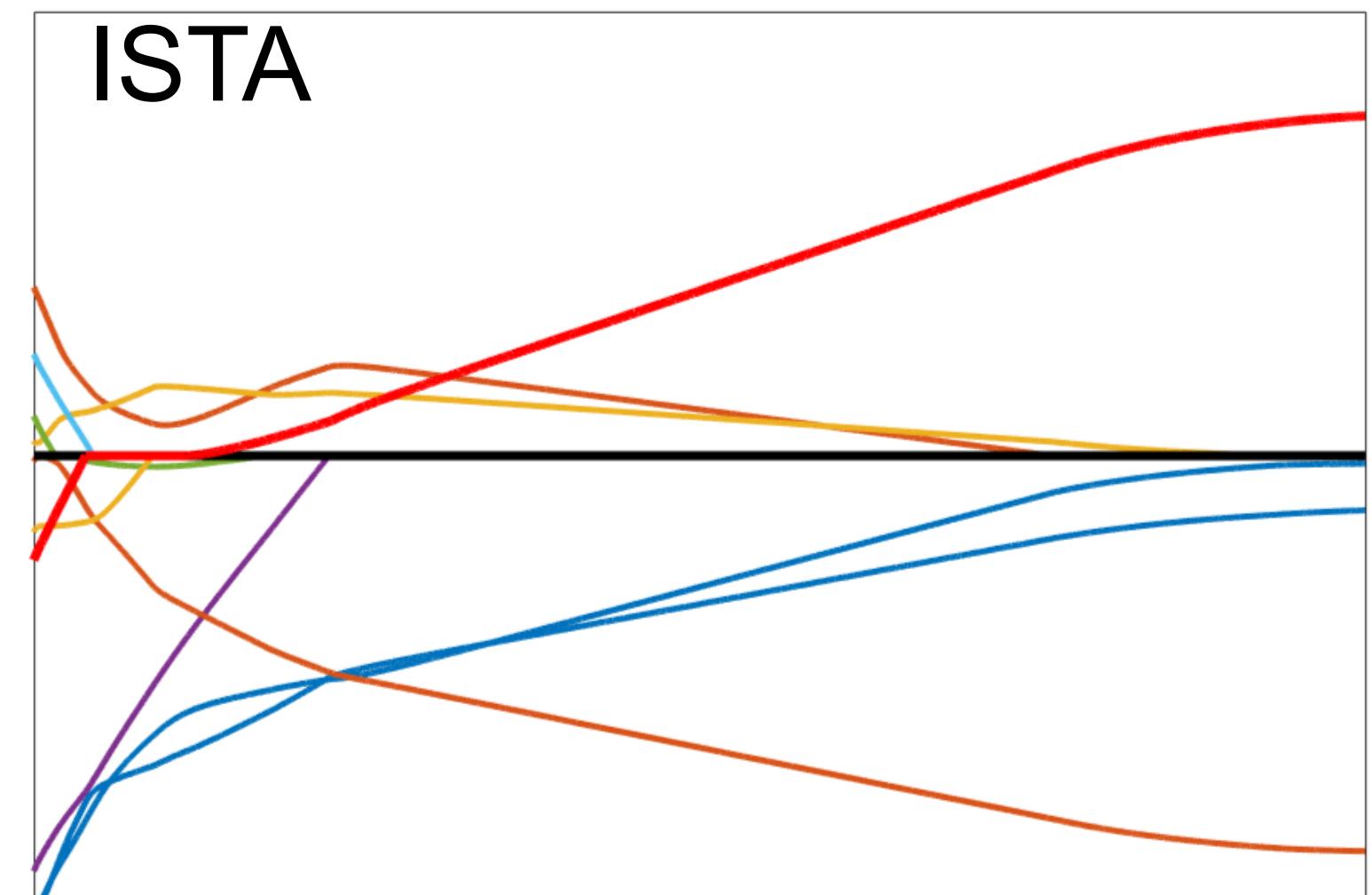
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Woodbury identity: $\nabla f(v) = v - v \odot (X^\top a)^2$

(allows $\lambda = 0$)

$$a = (\text{Adiag}(v^2)A^\top + \lambda I)^{-1}y$$



Bilevel formulation

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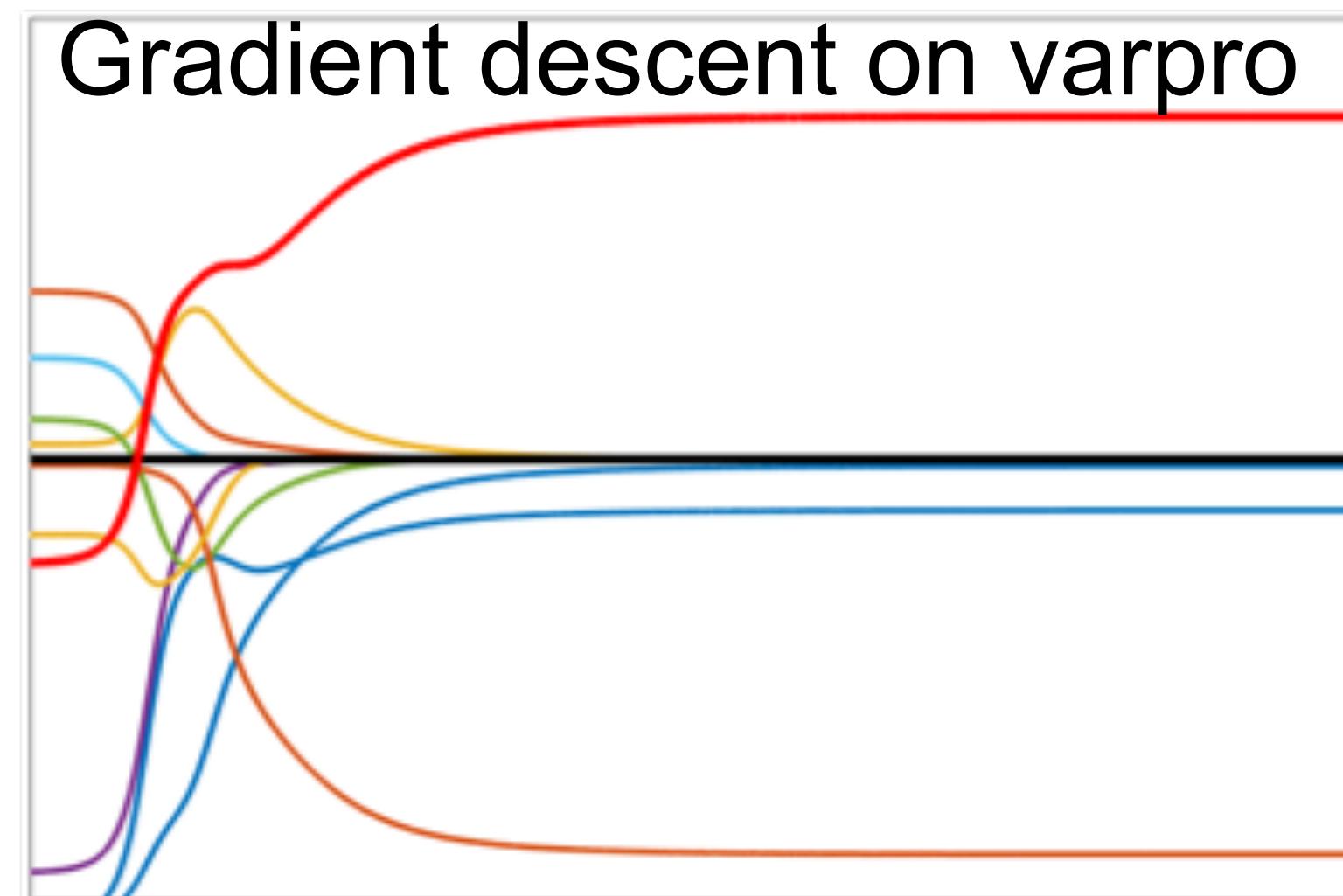
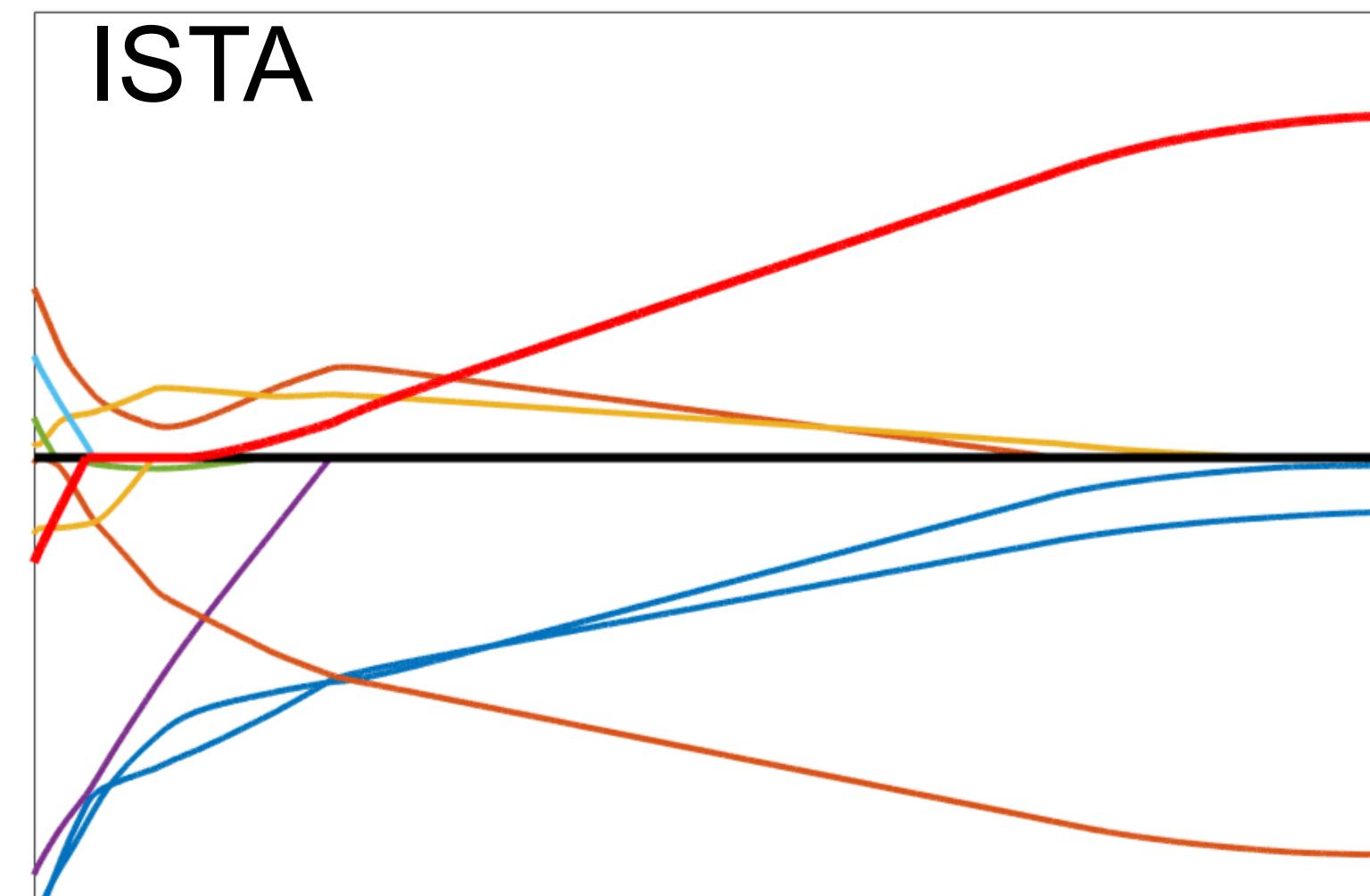
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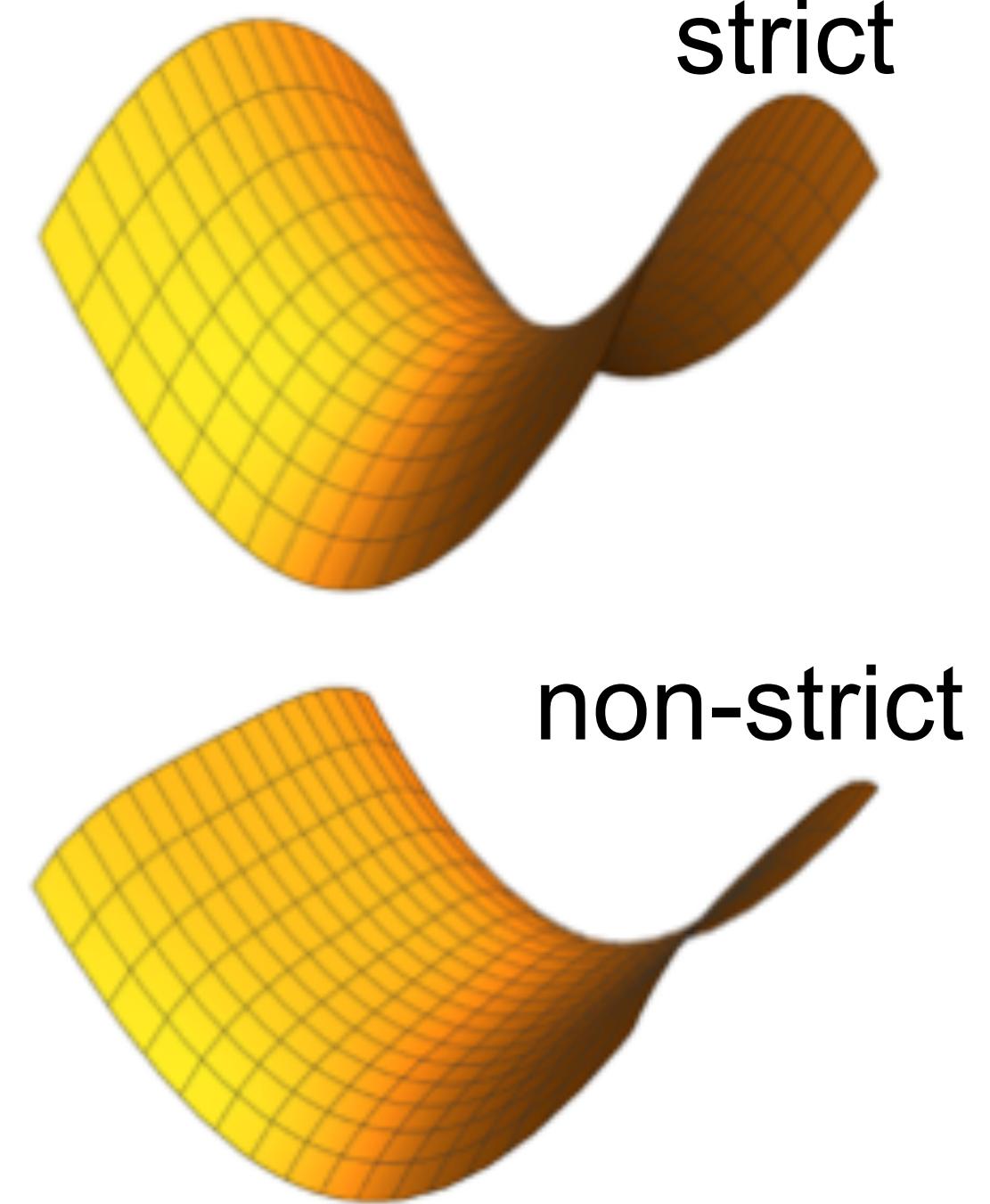
Need to handle $m \times m$ or $n \times n$ symmetric positive-definite linear system.

Mildly non-convex

Definition: v is a strict saddle point if

$\nabla f(v) = 0$ but $\nabla^2 f(v) \succeq 0$ does not hold

Lee et al (2017): Gradient descent almost always avoid strict saddles.



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$$\text{Primal: } x = u(v) \odot v$$

x global minimum

$$\text{Dual: } \xi = \frac{1}{\lambda} A^\top (Ax - y)$$

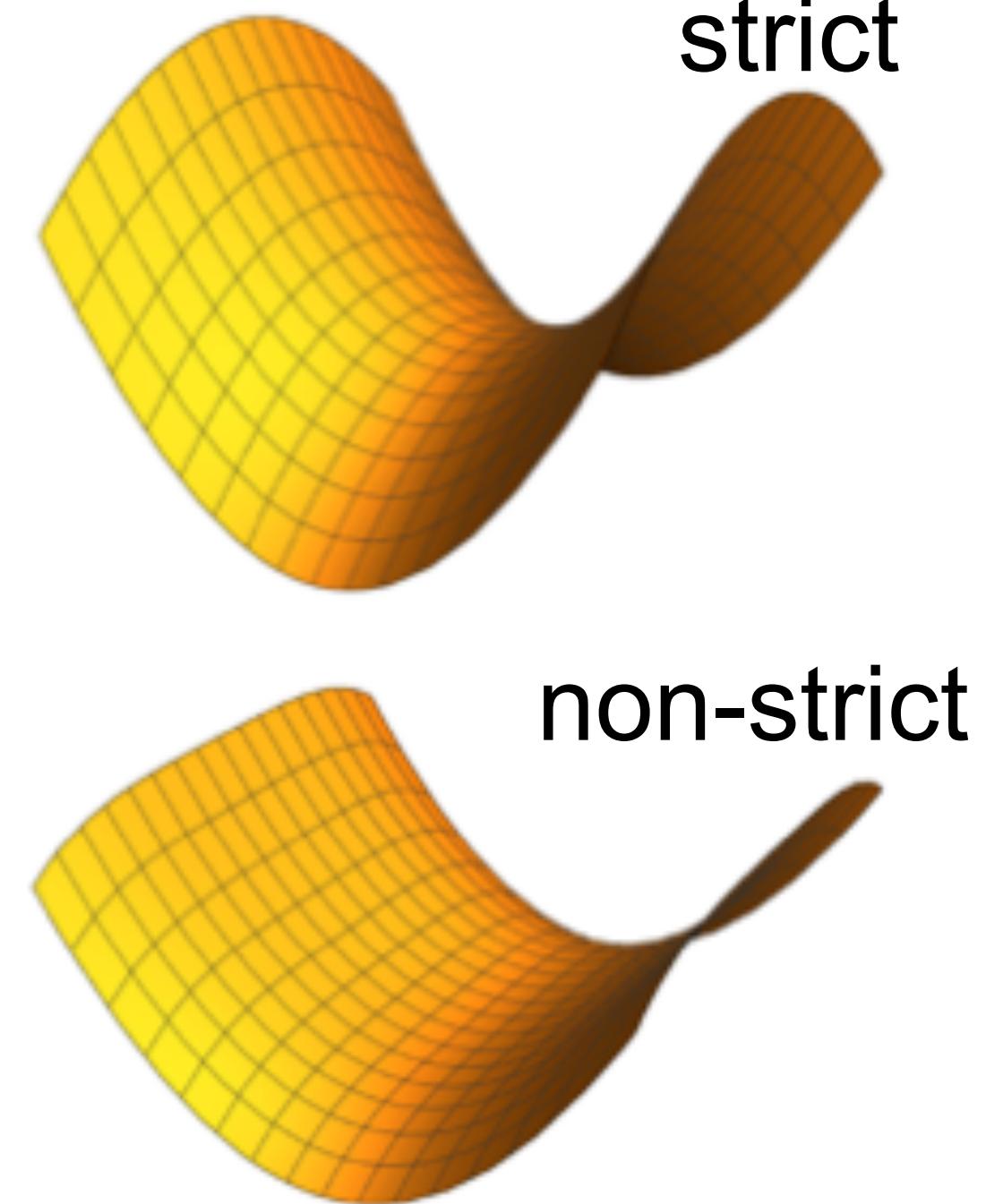
$$\xi_I = \text{sign}(x_I) \text{ and } \|\xi\|_\infty \leq 1, I = \text{Supp}(x)$$

Theorem: All stationary points of f are either global minima or strict saddles.

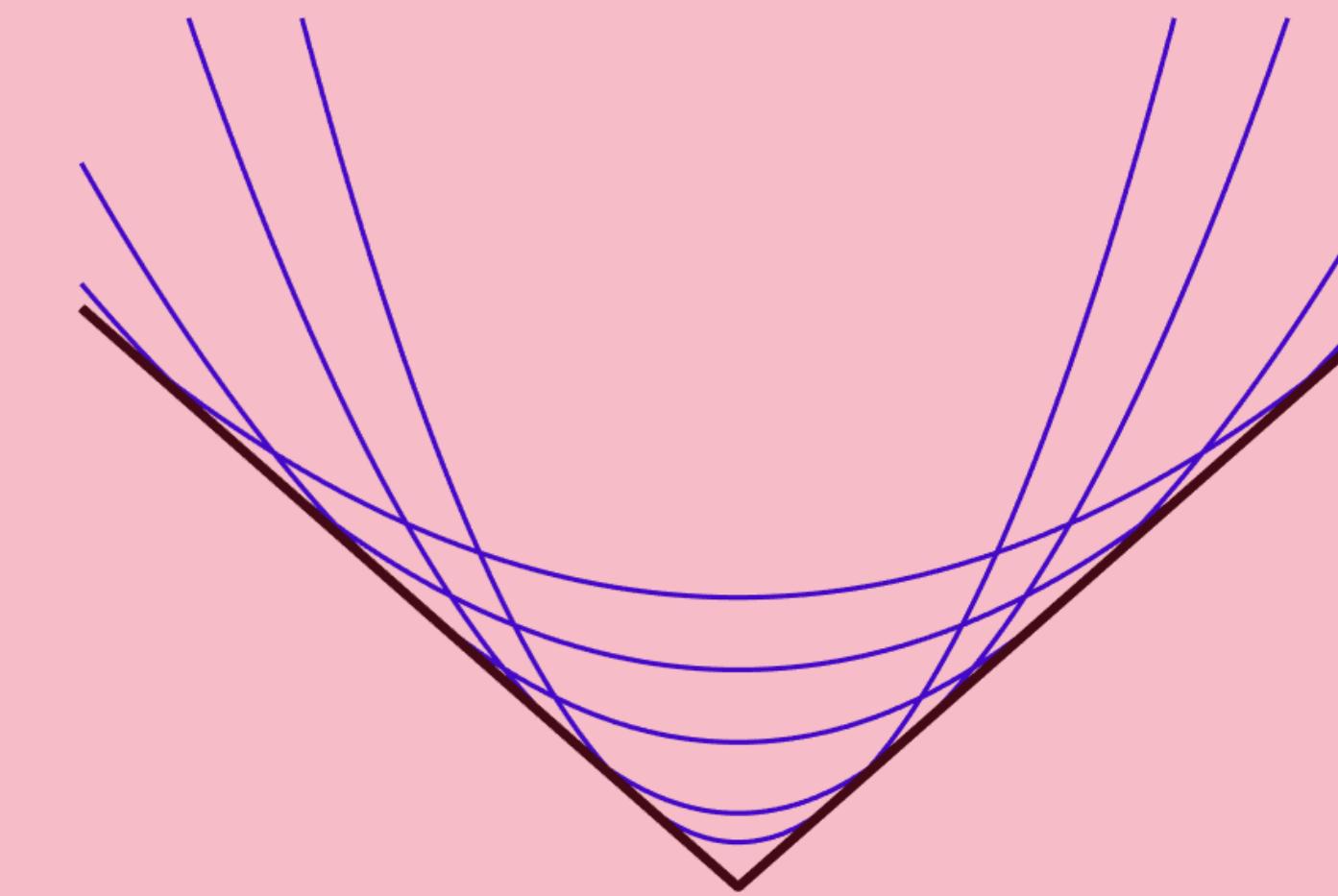
$$\nabla f(v) = 0 \text{ implies}$$

$$\text{Eig}(\nabla^2 f(v)) \subseteq [1 - \|\xi_{I_c}\|_\infty, 4]$$

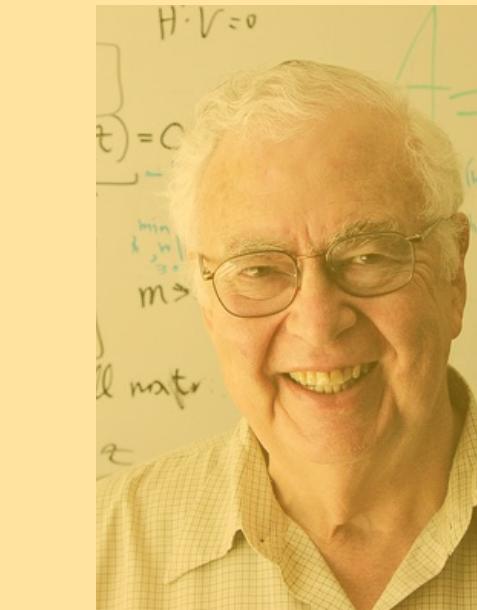
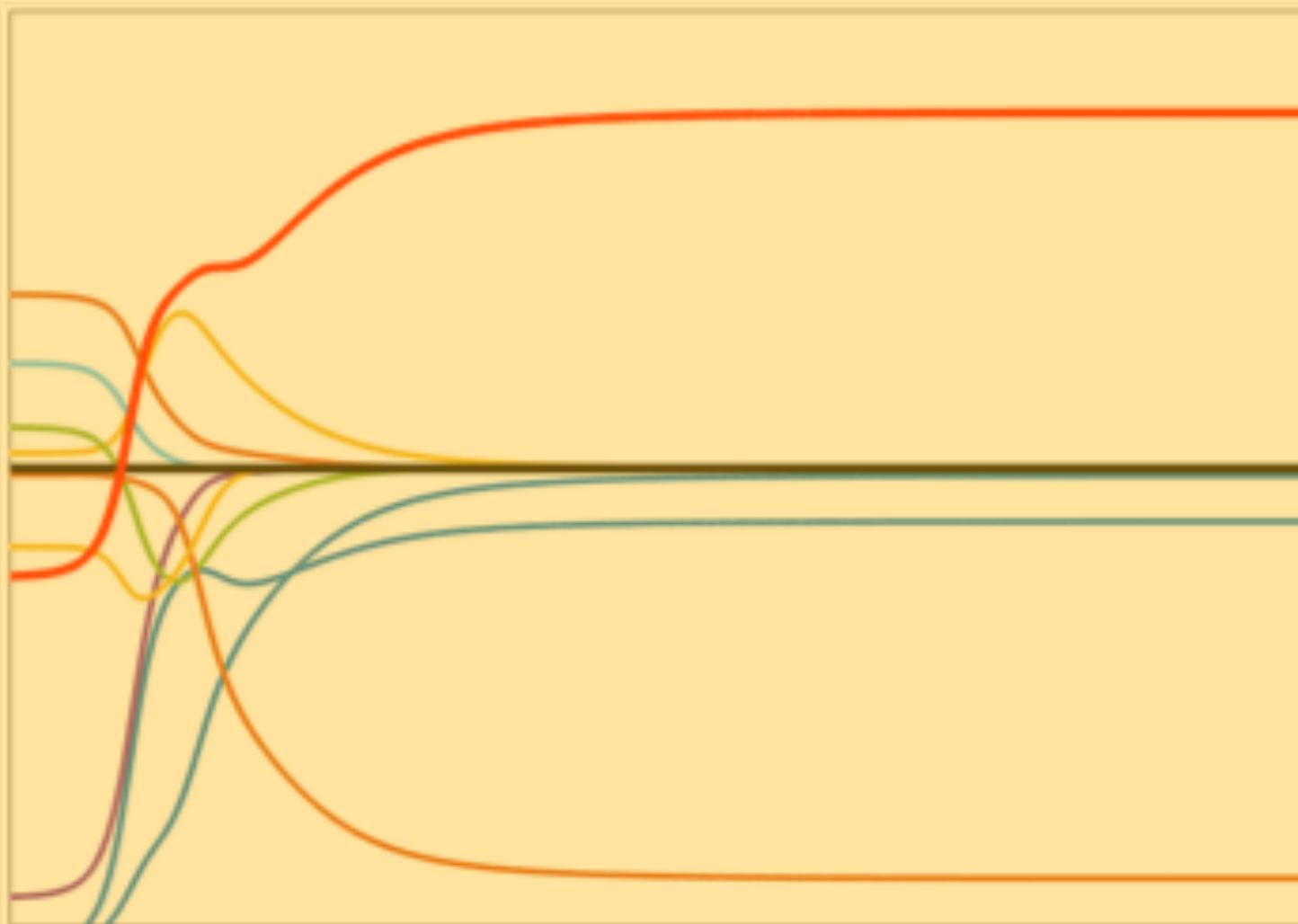
If the solution is nondegenerate $\|\xi_{I_c}\|_\infty < 1$, then quasi-Newton methods achieve local super-linear convergence.



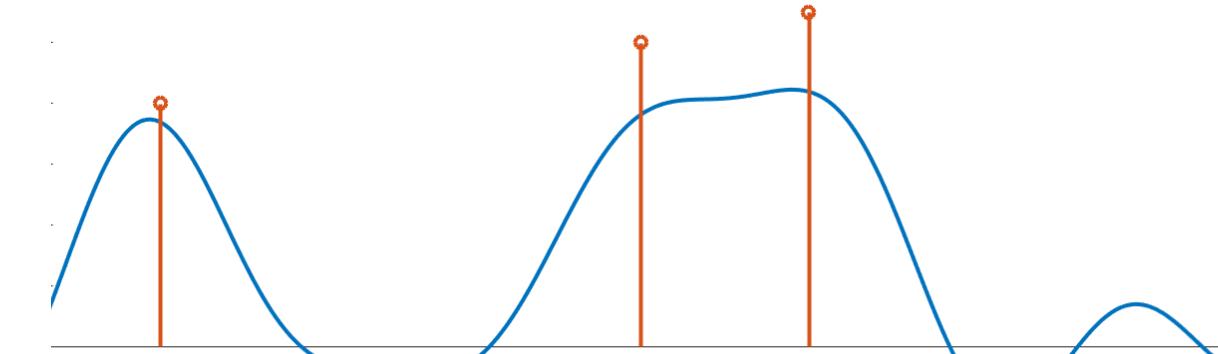
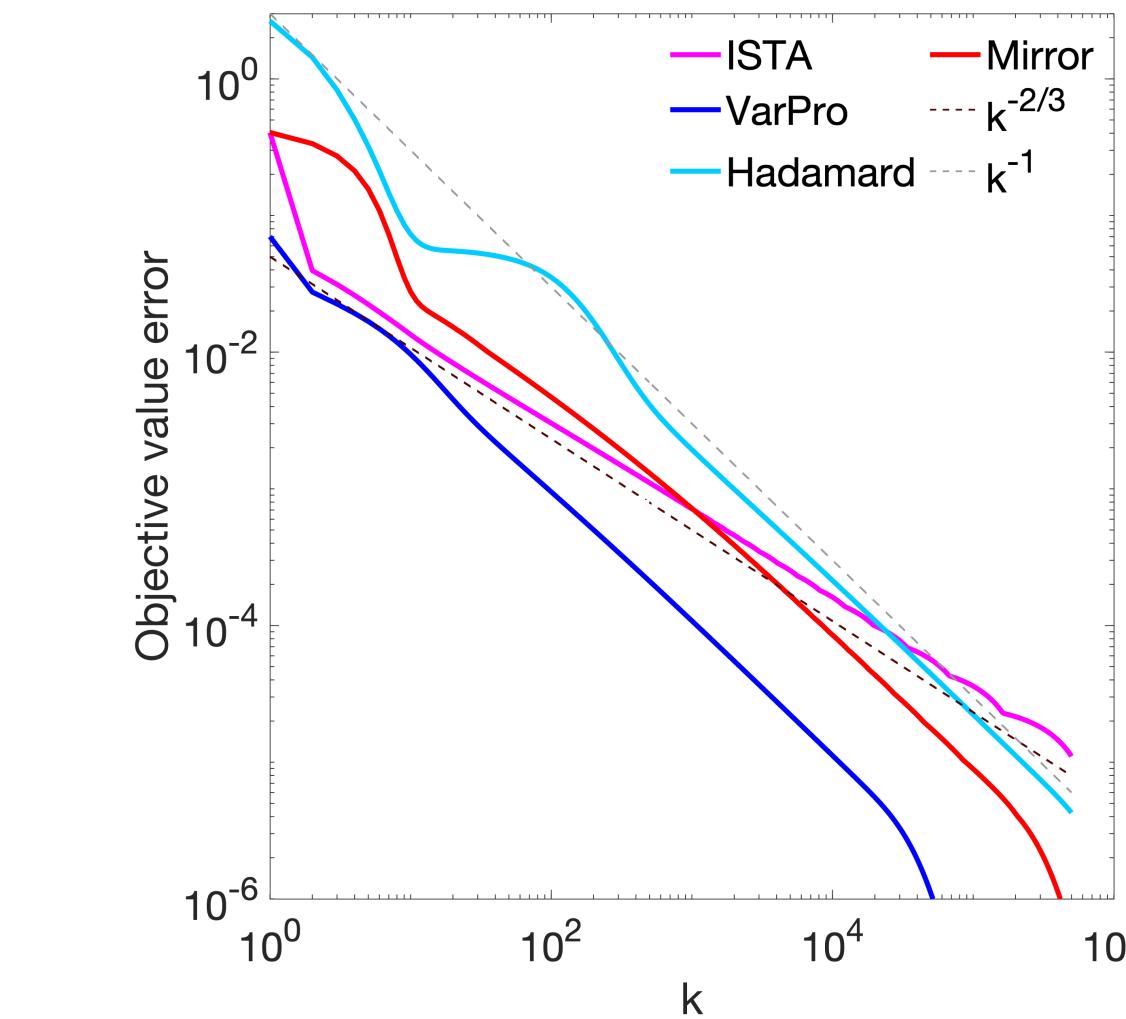
Quadratic Variational Forms



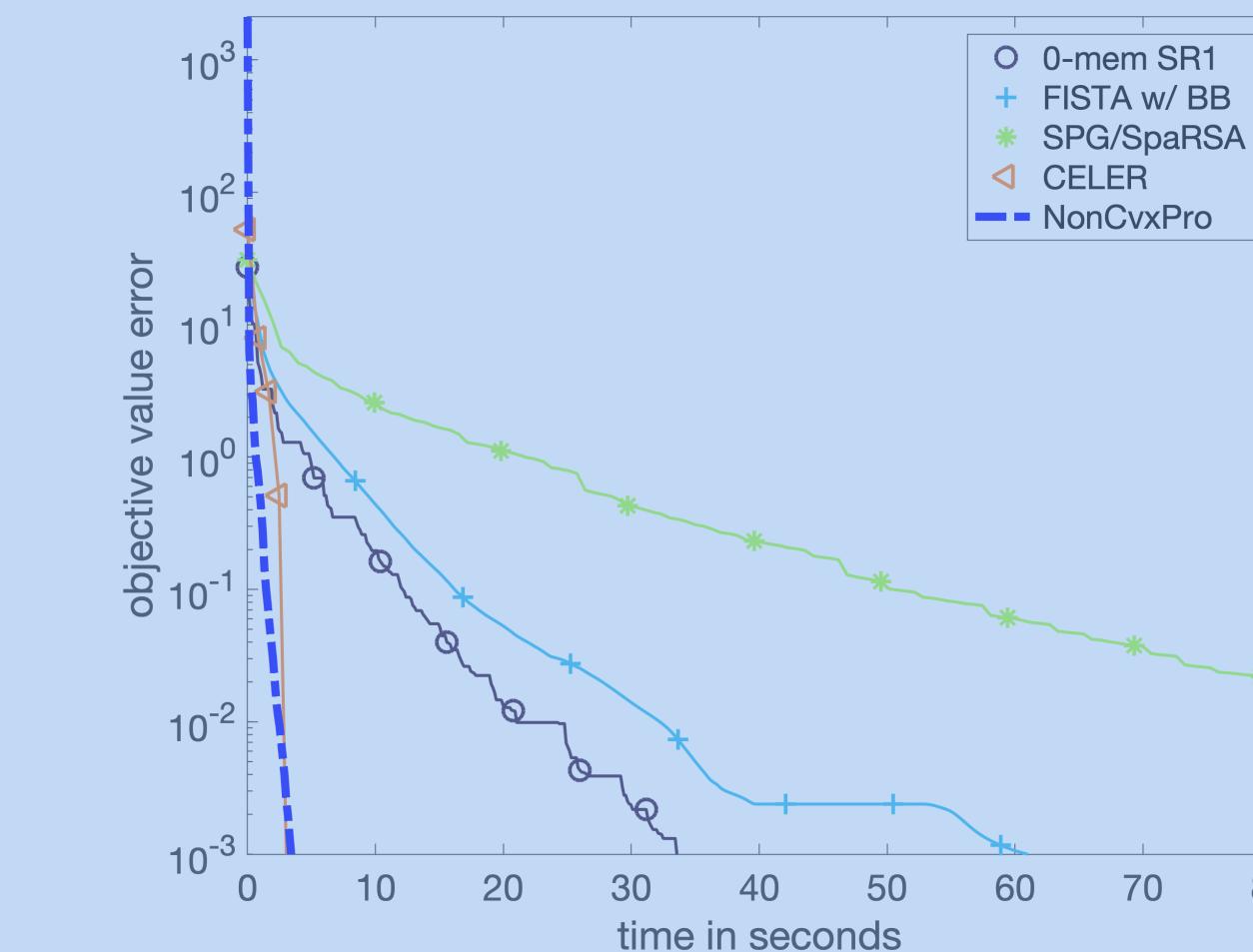
VarPro



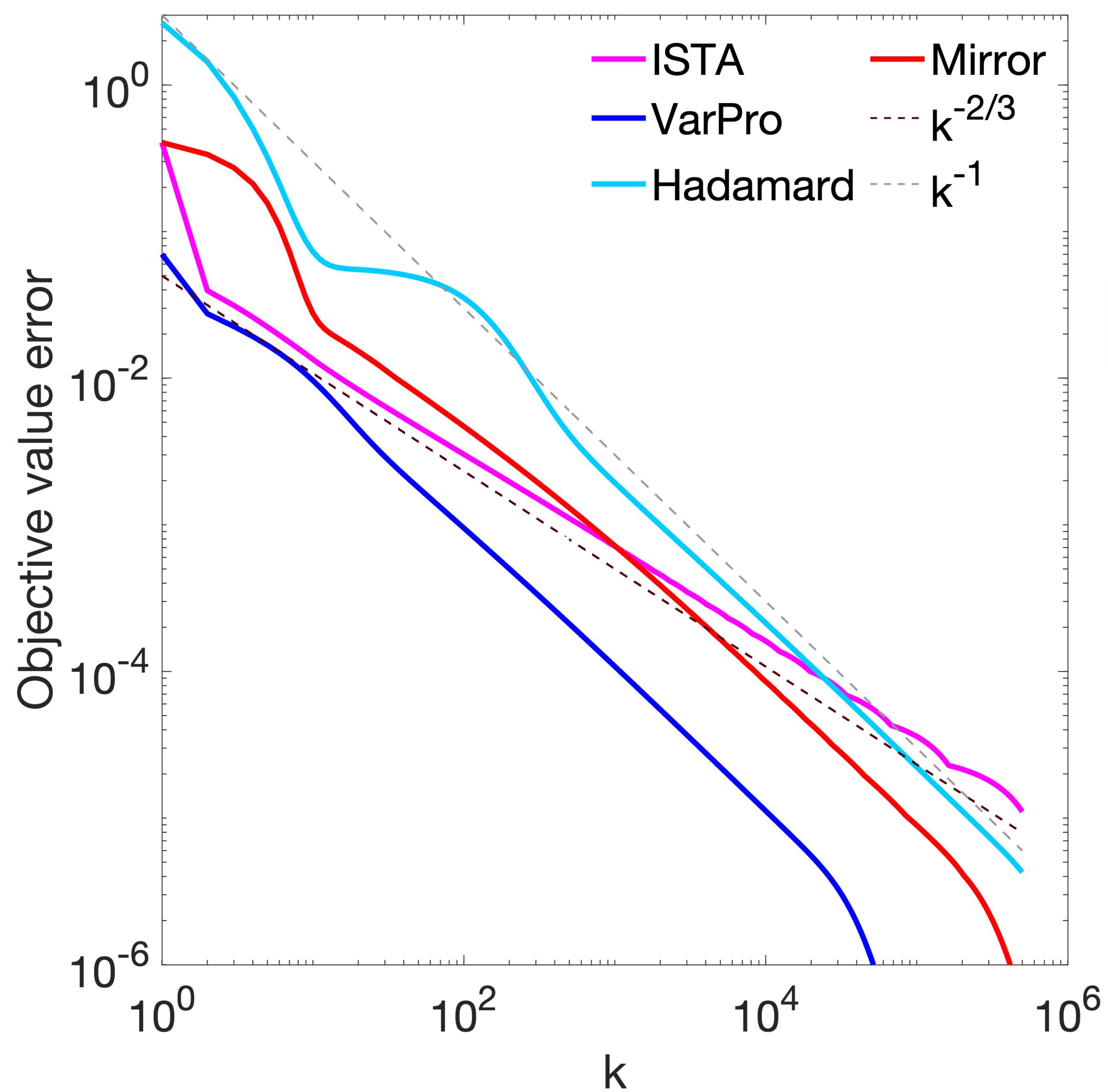
Convergence



Numerical Results

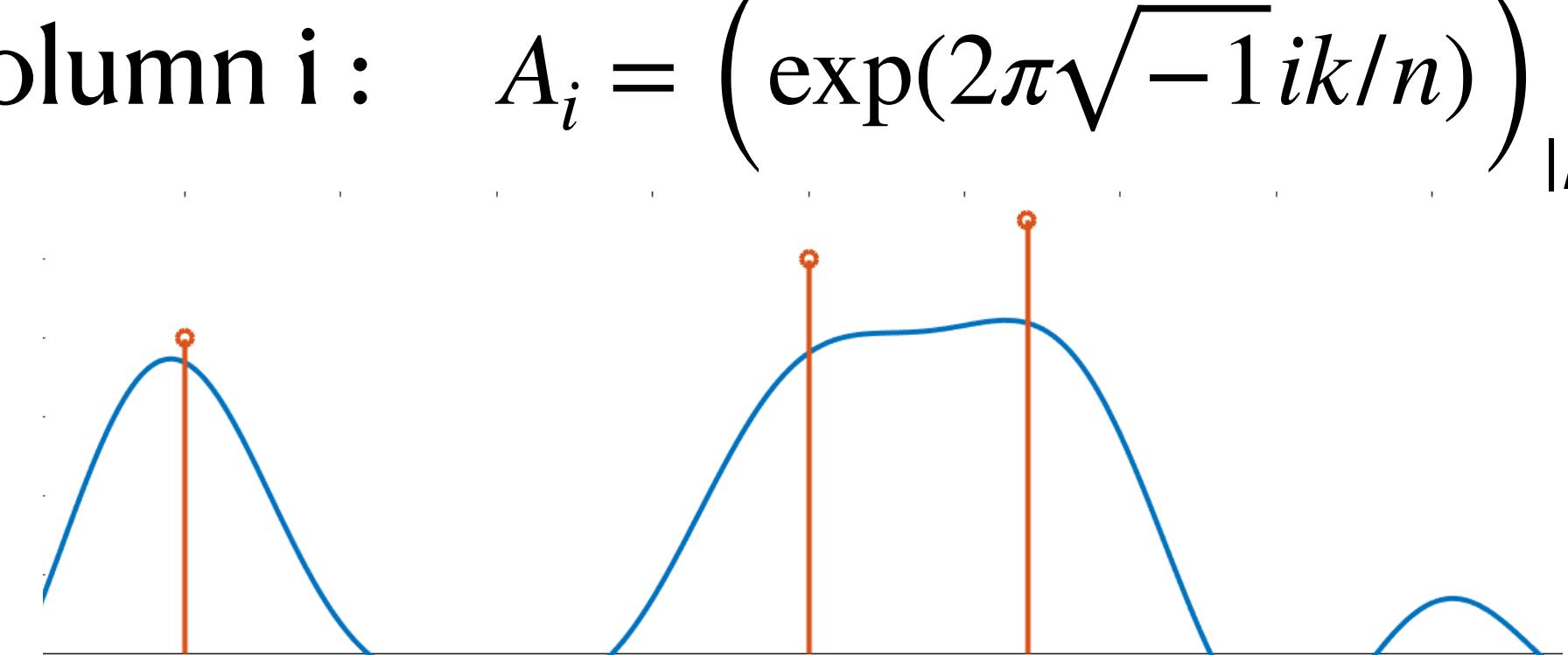


Observation

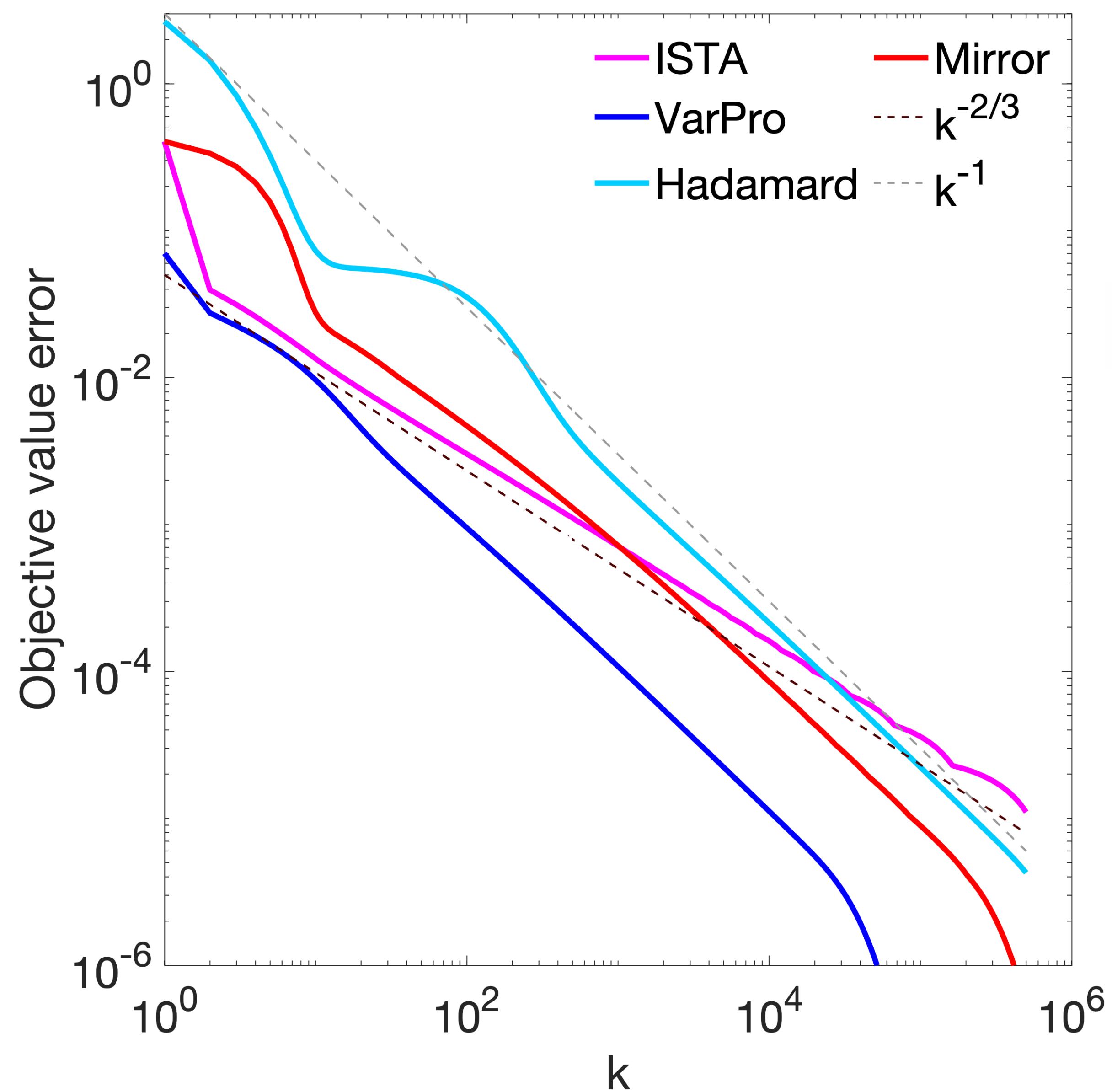


Solving the Lasso with a discretised Fourier operator ($n = 500$):

Column i : $A_i = \left(\exp(2\pi\sqrt{-1}ik/n) \right)_{|k| \leq m}$

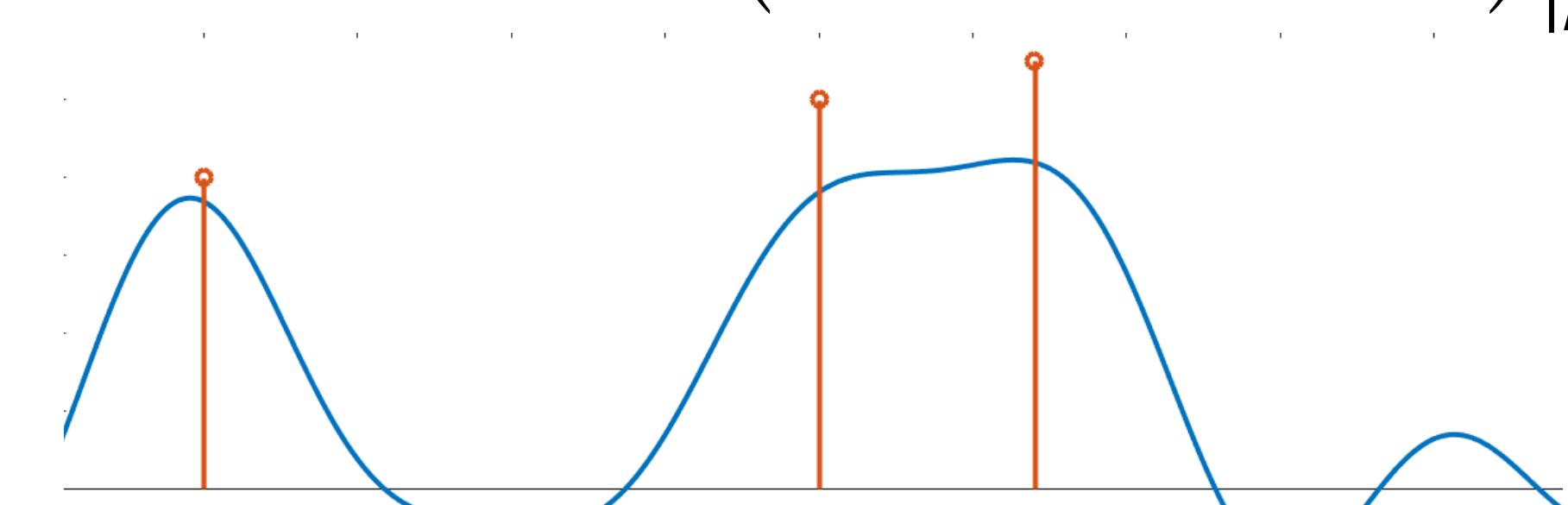


Observation



Solving the Lasso with a discretised Fourier operator ($n = 500$):

Column i : $A_i = \left(\exp(2\pi\sqrt{-1}ik/n) \right)_{|k| \leq m}$



Observations:

- ISTA converges at $\mathcal{O}(k^{-2/3})$ while proximal mirror descent converges at $\mathcal{O}(k^{-1})$ as shown by Chizat (2021).
- The Hadamard parameterisations also converge at $\mathcal{O}(k^{-1})$

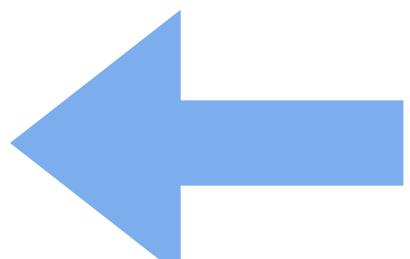
Gradient Descent Convergence

$$G(u, v) = \frac{1}{2} \|u\|^2 + \frac{1}{2} \|v\|^2 + F(u \odot v)$$

$$\begin{cases} u_{k+1} = u_k - \tau(u_k + v_k \nabla F(u_k \odot v_k)) \\ v_{k+1} = v_k - \tau(v_k + u_k \nabla F(u_k \odot v_k)) \end{cases}$$

Assume:

- $\|\nabla F(x) - \nabla F(x')\|_\infty \leq L_1 \|x - x'\|_1$
- $\sup_{\|x\|_1 \leq B} \|\nabla F(x)\|_\infty \leq K$ where $B := G(u_0, v_0)$



If $F(x) = \|Ax - y\|^2$ and A has normalised columns, then
 $L_1, K = \mathcal{O}(1)$

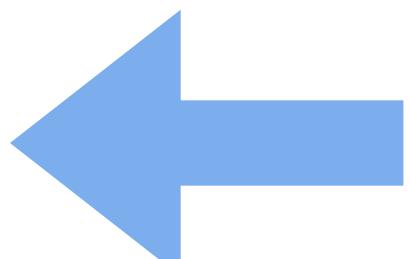
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If $F(x) = \|Ax - y\|^2$ and A has normalised columns, then $L_1, K = \mathcal{O}(1)$

Proposition: $\nabla G(u, v)$ is Lipschitz with constant $L \sim K + L_1 B^2$,

$$\min_{j \leq k} \|\nabla G(u_j, v_j)\|^2 \leq \frac{2L}{k} (G(u_0, v_0) - \min_{u, v} G(u, v))$$

Corollary: If $u_k v_k \rightarrow x_*$ and $\|\nabla G(u_k, v_k)\| = \mathcal{O}(1/k)$, then $\Phi(u_k v_k) - \Phi(x_*) = \mathcal{O}(1/k)$

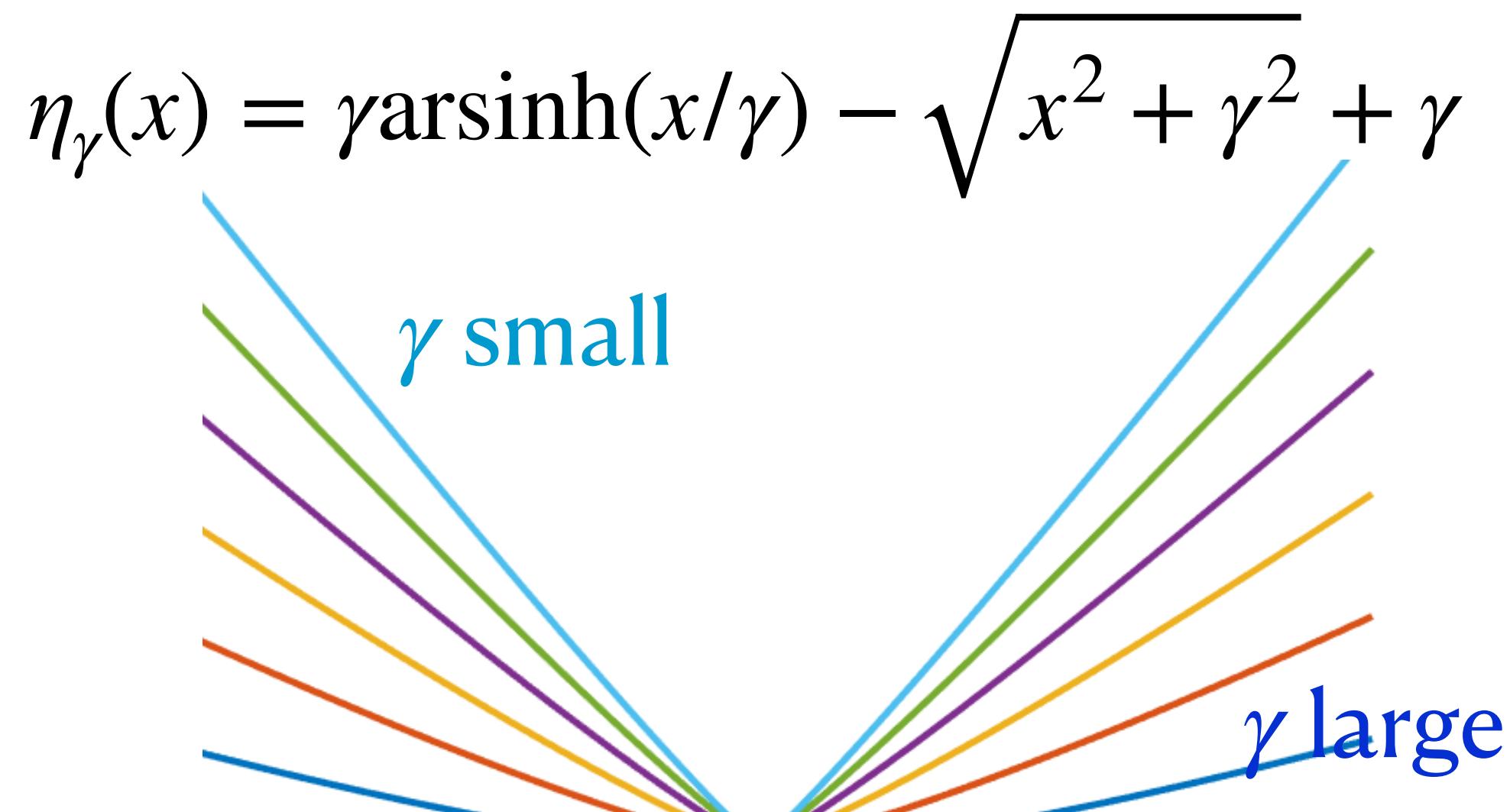
Mirror flow interpretation

Hadamard parametrised gradient flow as $\tau \rightarrow 0$

Let $x(t) := u(t) \odot v(t)$ and η_γ be the hyperbolic entropy with parameter $\gamma > 0$.

$$\frac{d}{dt} \nabla \eta_{\gamma(t)}(x(t)) = -2 \nabla F(x(t))$$

$$\gamma(t) = \frac{1}{2} e^{-2\lambda t} |u(0) - v(0)|$$



Recall Mirror Descent:

$$x_{k+1} \in \operatorname{argmin} F(x_k) + \frac{1}{n} \langle \nabla F(x_k), x - x_k \rangle + \frac{1}{\tau} D_\eta(x, x_k)$$



$$\nabla \eta(x_{k+1}) = \nabla \eta(x_k) - \tau \nabla F(x_k)$$

$$\frac{d}{dt} \nabla \eta(x(t)) = -\nabla F(x(t))$$



If $\lambda = 0$, then $\gamma(t) = \gamma(0)$ and links to works on implicit regularisation [e.g. Vaškevičius et al 2019]

From Gradient Descent to Quasi-Newton

Observations:

- $x_k = u_k \odot v_k$ is implicitly optimised in Hyperbolic geometry
- The parameters u_k, v_k operate in Euclidean geometry.

**Robust acceleration tools are available
(BB step, Quasi-Newton, BFGS, etc)!**

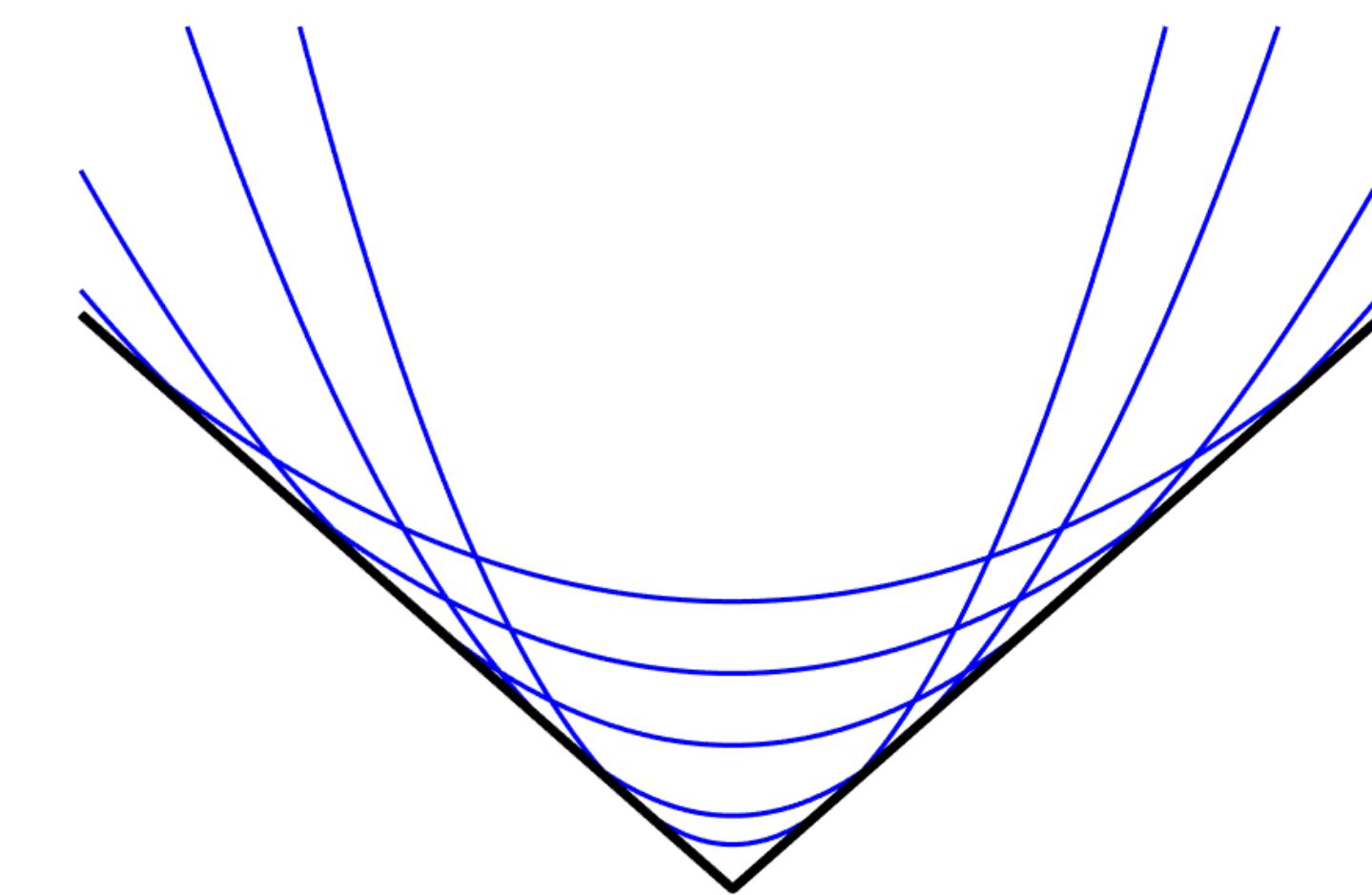
$$\begin{cases} v_{k+1} &= v_k - \tau_k B_k \nabla f(v_k) \\ B_k &\approx [\nabla^2 f(v_k)]^{-1} \end{cases}$$

Secant condition:

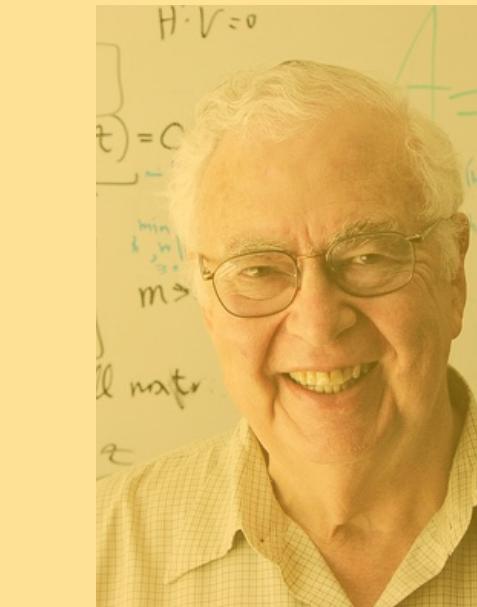
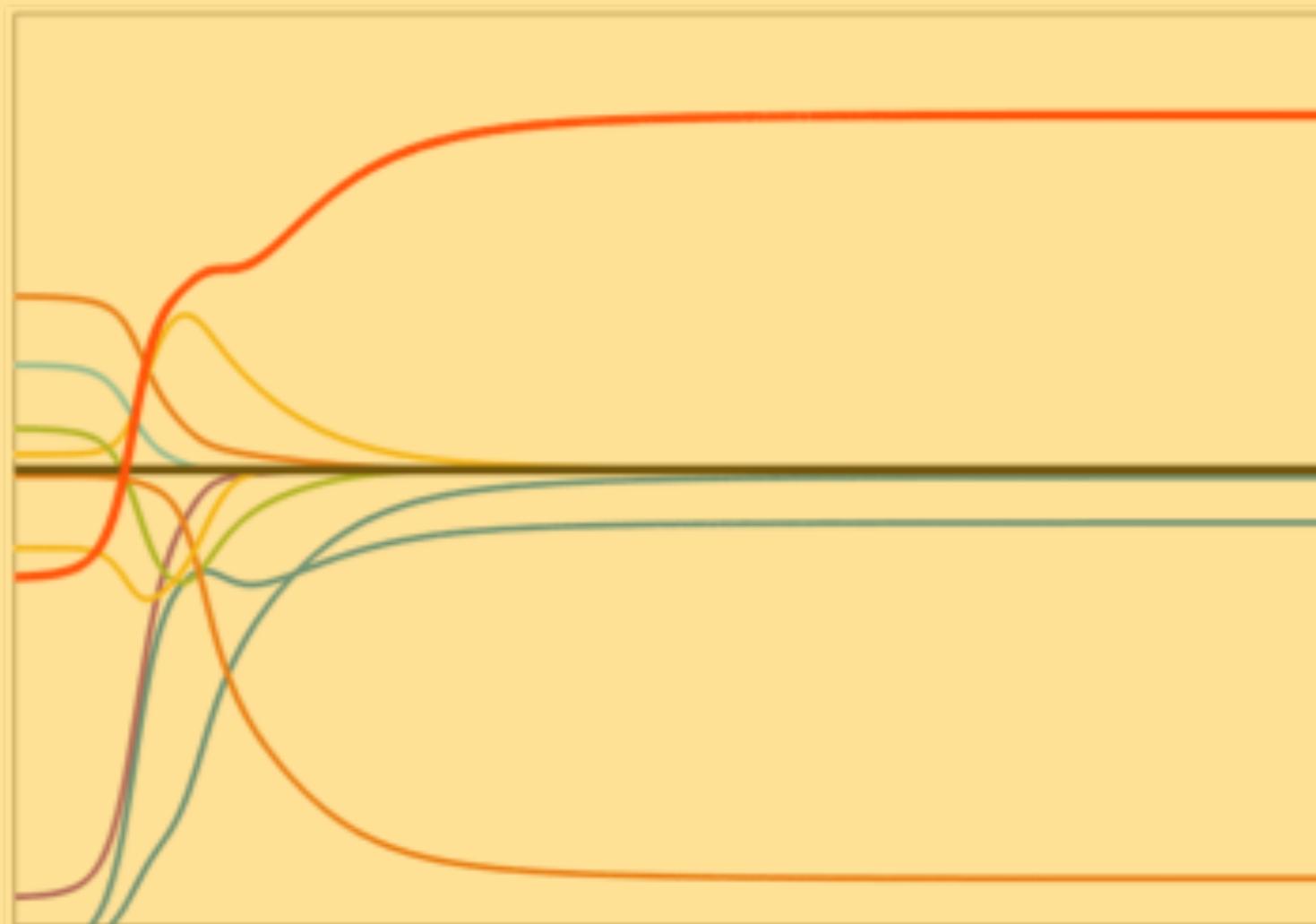
$$\overrightarrow{\quad} \quad \nabla f(v_{k+1}) - \nabla f(v_k) = \nabla^2 f(v_k)(v_{k+1} - v_k) + o(\|v_{k+1} - v_k\|)$$
$$\overrightarrow{\quad} \quad B_{k+1}(\nabla f(v_{k+1}) - \nabla f(v_k)) = v_{k+1} - v_k$$

In practice, **L-BFGS + Varpro** leads to substantial performance gains over SOTA methods.

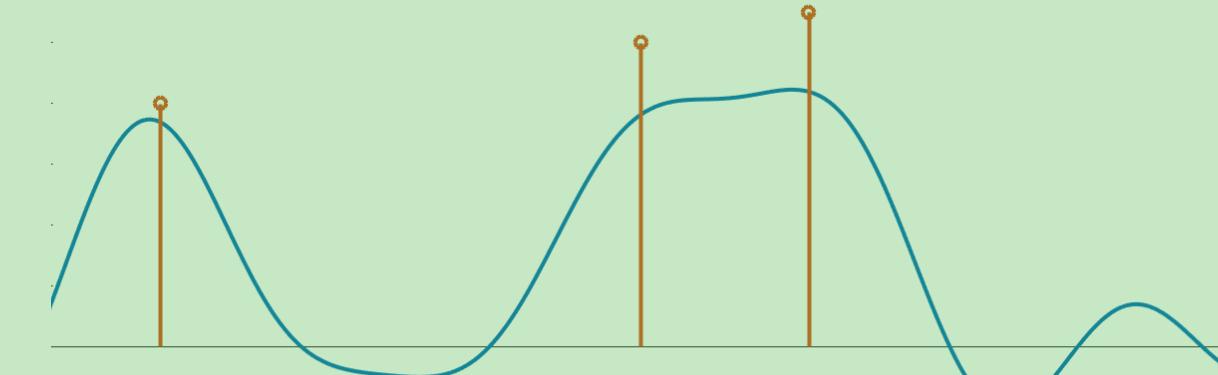
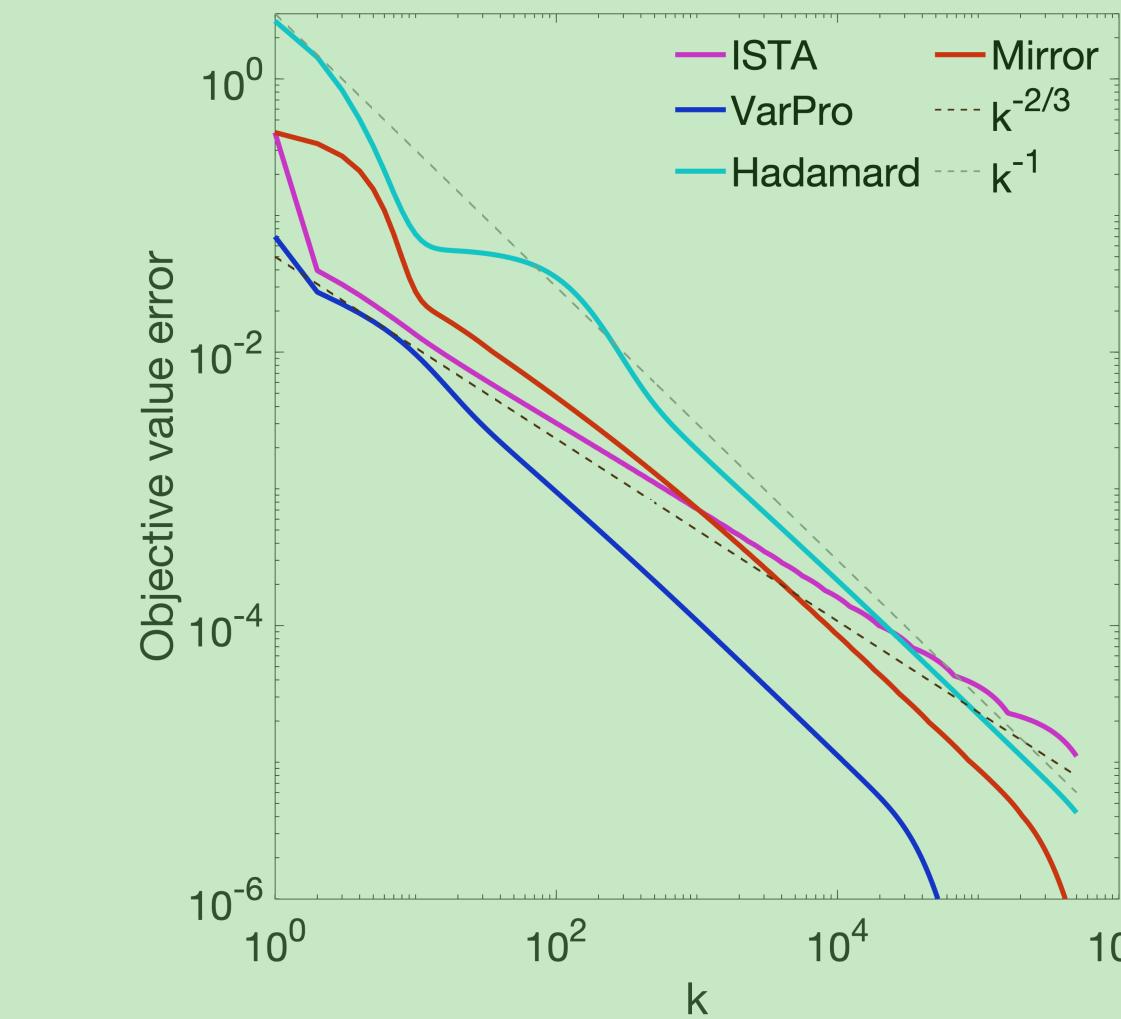
Quadratic Variational Forms



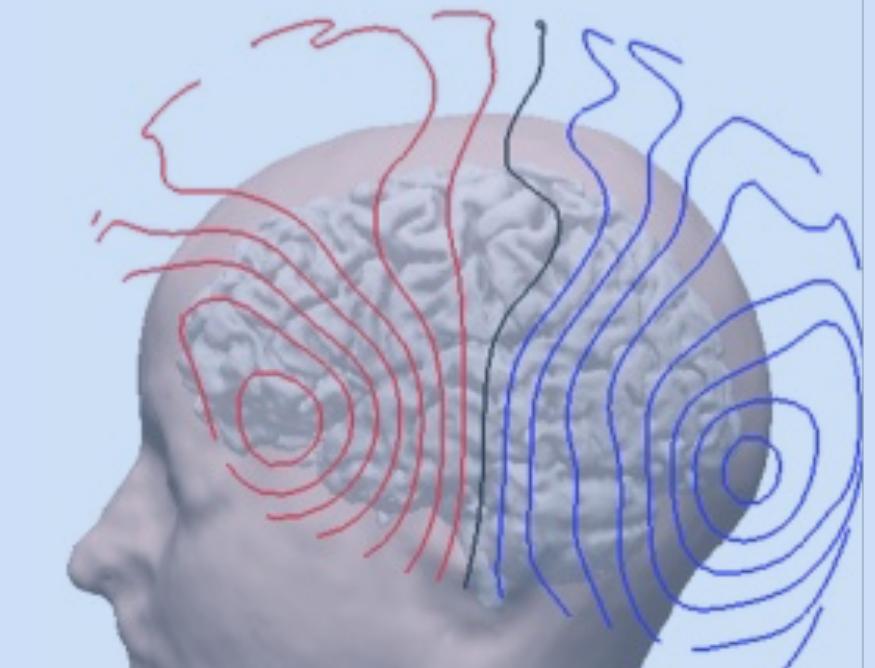
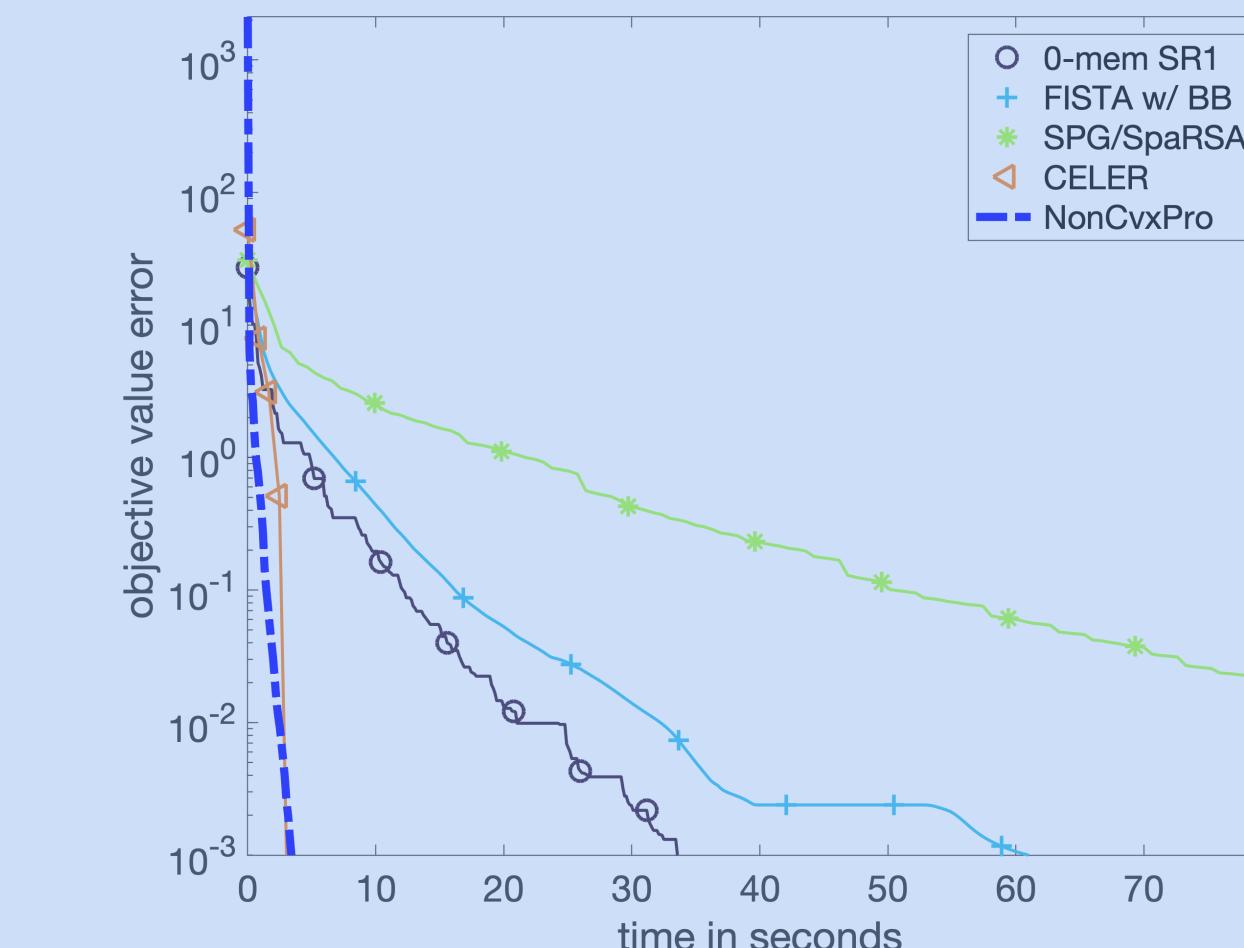
VarPro



Convergence



Numerical Results



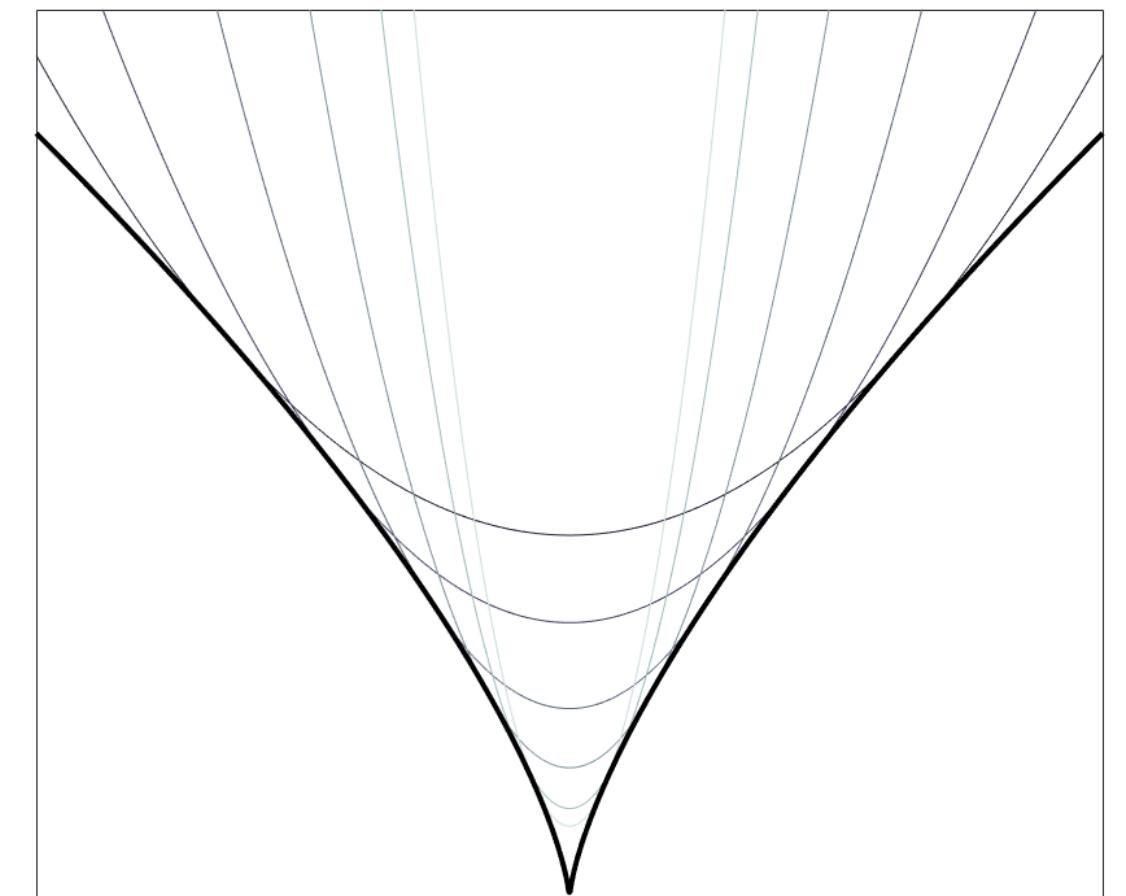
When do quadratic variational forms exist?

Group ℓ_1 : Given disjoint $\cup_g g = \{1, \dots, n\}$

$$\|x\|_{1,2} = \sum_g \|x_g\| = \min_{x_g = u_g v_g} \sum_g \frac{\|u_g\|^2}{2} + \frac{v_g^2}{2}$$

$$|x|^q \propto \min_{x=uv} u^2 + v^p, \quad q = \frac{2p}{p+2}$$

$$\|X\|_* = \min_{X=UV} \frac{\|U\|_F^2 + \|V\|_F^2}{2}$$



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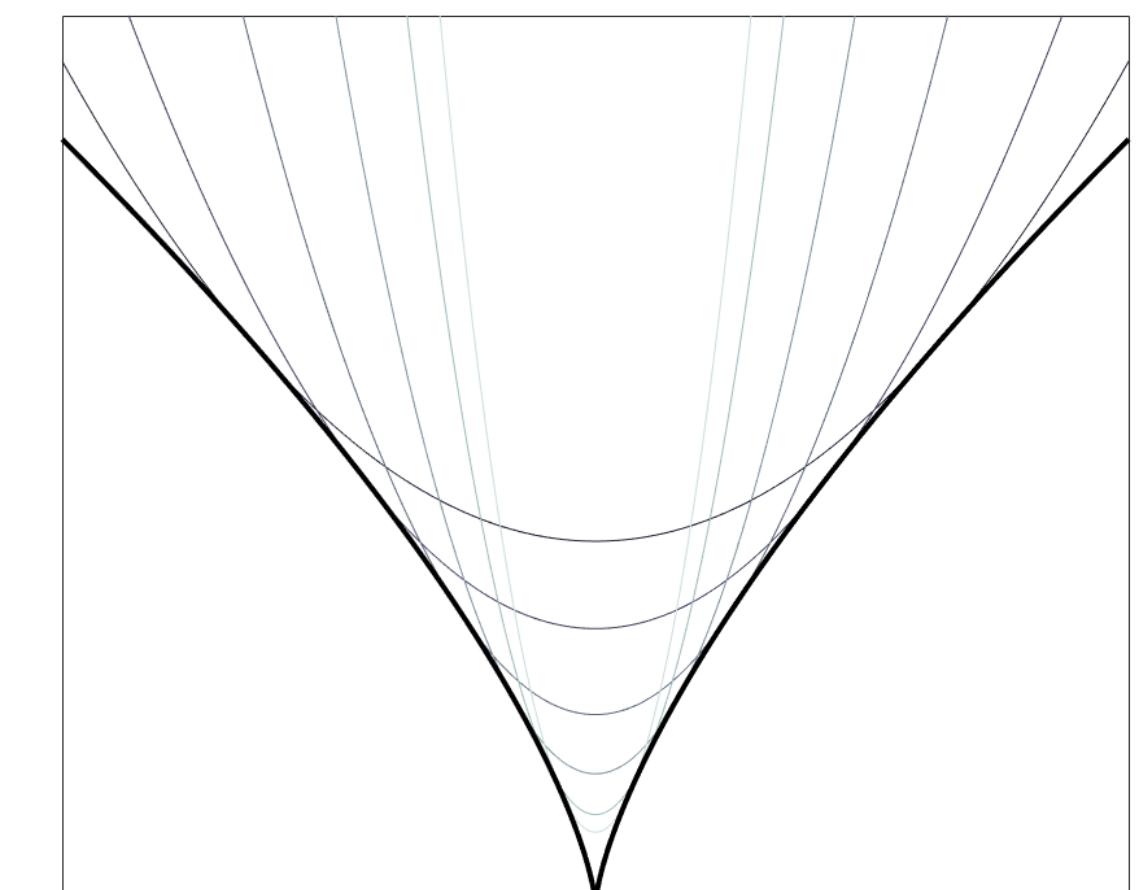
$$\|X\|_* = \min_{X=UV} \frac{\|U\|_F^2 + \|V\|_F^2}{2}$$

[Black & Rangarajan 1992]

[Geman & Reynolds 1992]

Let $R : \mathbb{R}^n \rightarrow [0, \infty]$. The following are equivalent:

- $R(x) = \phi(x^2)$ where ϕ is concave.
- $R(x) = \inf_{\eta \in \mathbb{R}_+^n} \frac{1}{2} \sum_i \frac{x_i^2}{\eta_i} + h(\eta)$ where $h(\eta) = (-\phi)^*(-1/2\eta)$



General formulation

$$\min_{x \in \mathbb{R}^n} R(Lx) + F(Ax)$$

Assume:

$$L \in \mathbb{R}^{p \times n}, A \in \mathbb{R}^{m \times n}$$

$$R(x) = \inf_{\eta \in \mathbb{R}_+^n} \frac{1}{2} \sum_i \frac{|x_i|^2}{\eta_i} + h(\eta)$$

Over-parametrized form: $\min_{u,v} G(u, v)$

$$G(u, v) = h(v) + \min \left\{ \frac{1}{2} \|u\|^2 + F(Ax); \ Lx = u \odot v \right\}$$

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Bilevel function.
 $f(v) := \min_u G(u, v).$

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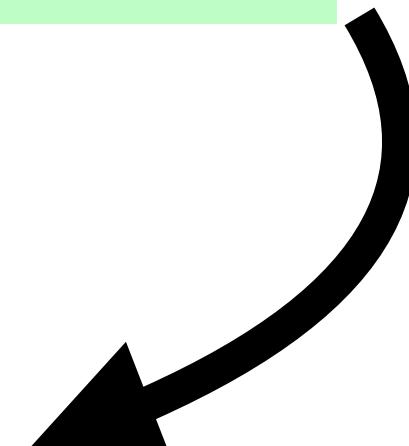
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Bilevel function.
 $f(v) := \min_u G(u, v).$

Dual of inner function:

$$f(v) = h(v) + \max_{\xi \in \mathbb{R}^m, \alpha \in \mathbb{R}^p} -\frac{1}{2} \|v\alpha\|^2 - F^*(\xi) - \iota_{\{L^\top \alpha + A^\top \xi = 0\}}(\alpha, \xi)$$



General formulation

$$\min_{x \in \mathbb{R}^n} R(Lx) + F(Ax)$$

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Gradient formula:

$$\nabla f(v) = \nabla h(v) - v\alpha_v^2$$

- If $F \in C^{1,1}$, then f is differentiable.
- If $F = \iota_{\{y\}}$, f is differentiable at v if $Ax = y$ for some x and $\text{Supp}(v) \supseteq \text{Supp}(Lx)$

Nonsmooth Loss functions

$$\min_x R_1(Dx) + R_2(Ax - y)$$

$$R_i(z) = \min_{\eta \in \mathbb{R}_+^n} \frac{1}{2} \sum_i \frac{x_i^2}{\eta_i} + h_i(\eta) \text{ with } h_i \text{ smooth}$$

$$\min_x \lambda \|x\|_1 + \|Ax - y\|$$

Square root Lasso

$$\min_x \lambda \|Dx\|_1 + \|Ax - y\|_1$$

TV-L1

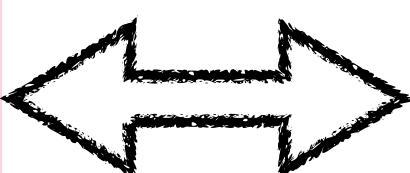
$$\min_X \lambda \|X\|_{1,2} + \|AX - Y\|_*$$

Multitask learning

Nonsmooth Loss functions

$$\min_x R_1(Dx) + R_2(Ax - y)$$

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$$\min_{v,w} f(v,w) := h_1(v) + h_2(w) + \phi(v,w)$$

$$\phi(v,w) = \max_{D^\top \alpha + A^\top \xi = 0} -\frac{1}{2} \|v\alpha\|^2 - \frac{1}{2} \|w\xi\|^2 + \langle \xi, y \rangle$$

Gradient formulas:

$$\partial_v f = \nabla h_1(v) - v\alpha^2$$

$$\partial_w f = \nabla h_2(w) + w\xi^2$$

NB: inner problem is a quadratic problem

$$\min_x \lambda \|x\|_1 + \|Ax - y\|$$

Square root Lasso

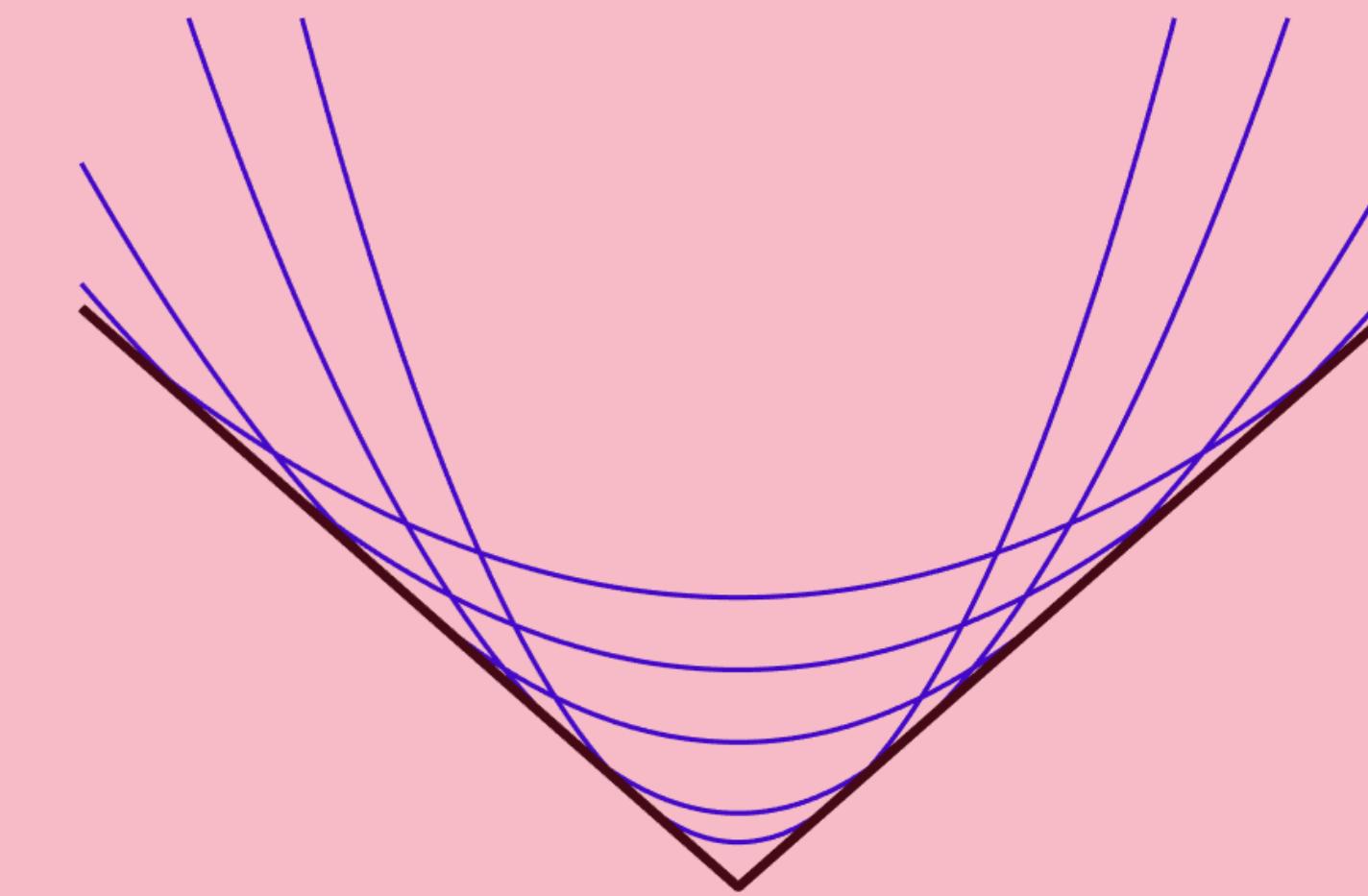
$$\min_x \lambda \|Dx\|_1 + \|Ax - y\|_1$$

TV-L1

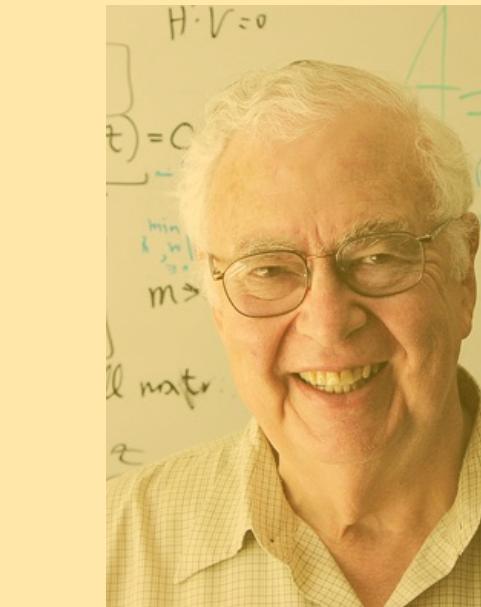
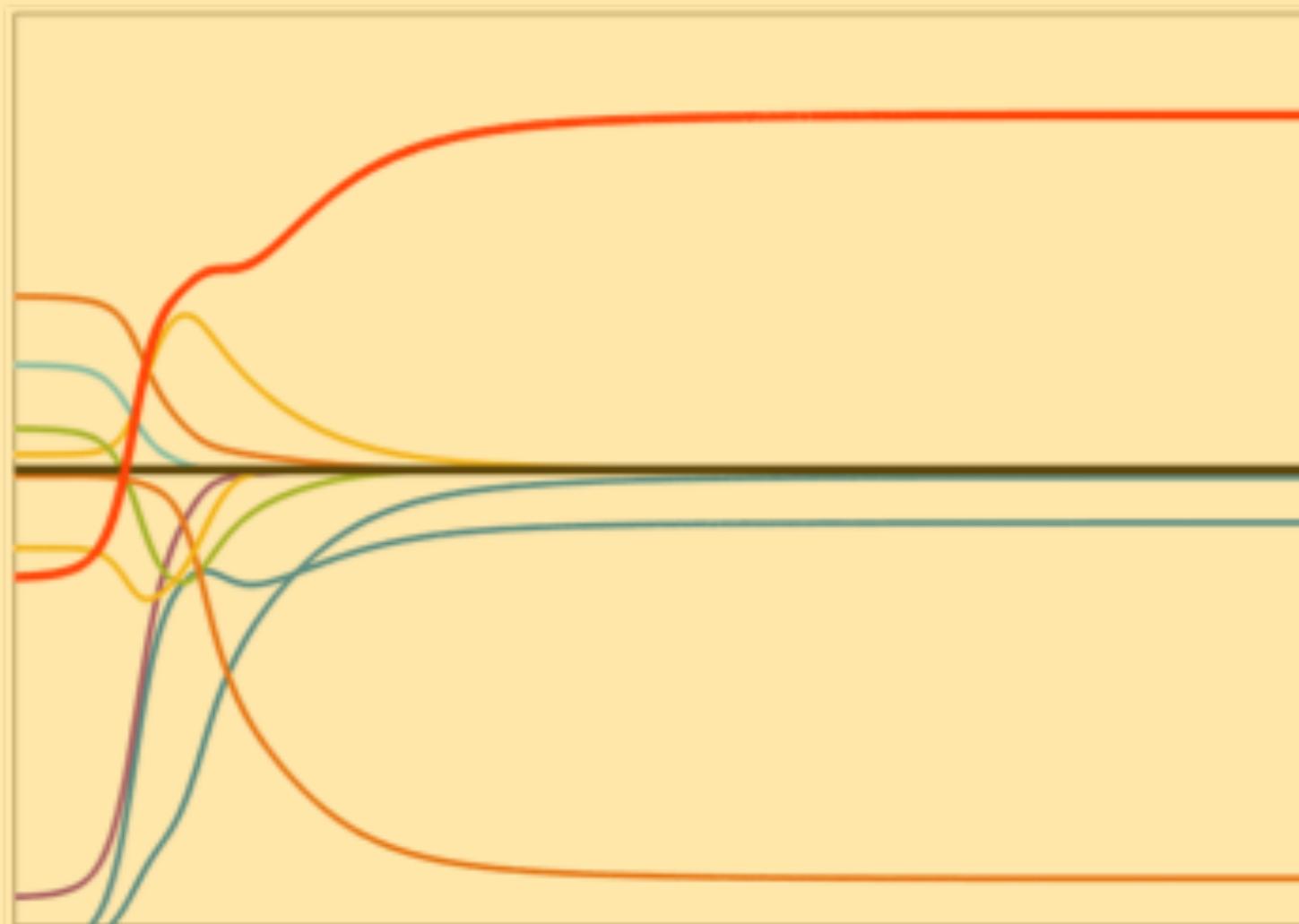
$$\min_X \lambda \|X\|_{1,2} + \|AX - Y\|_*$$

Multitask learning

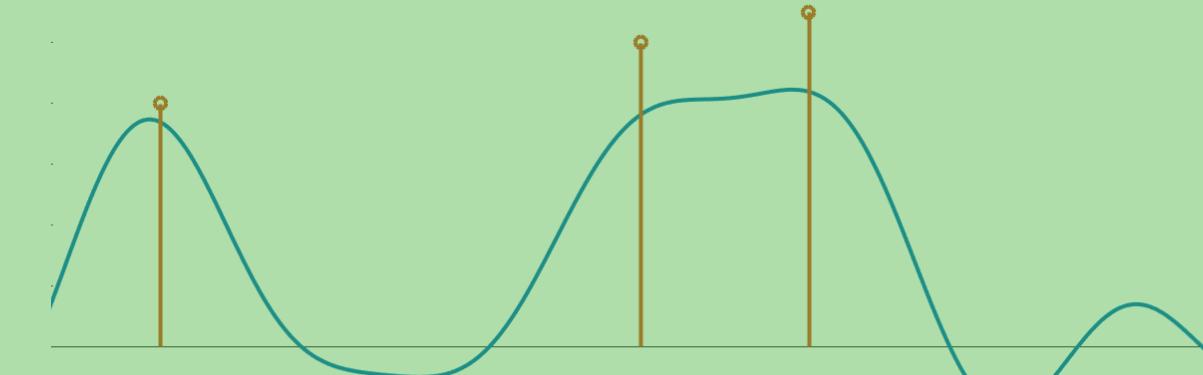
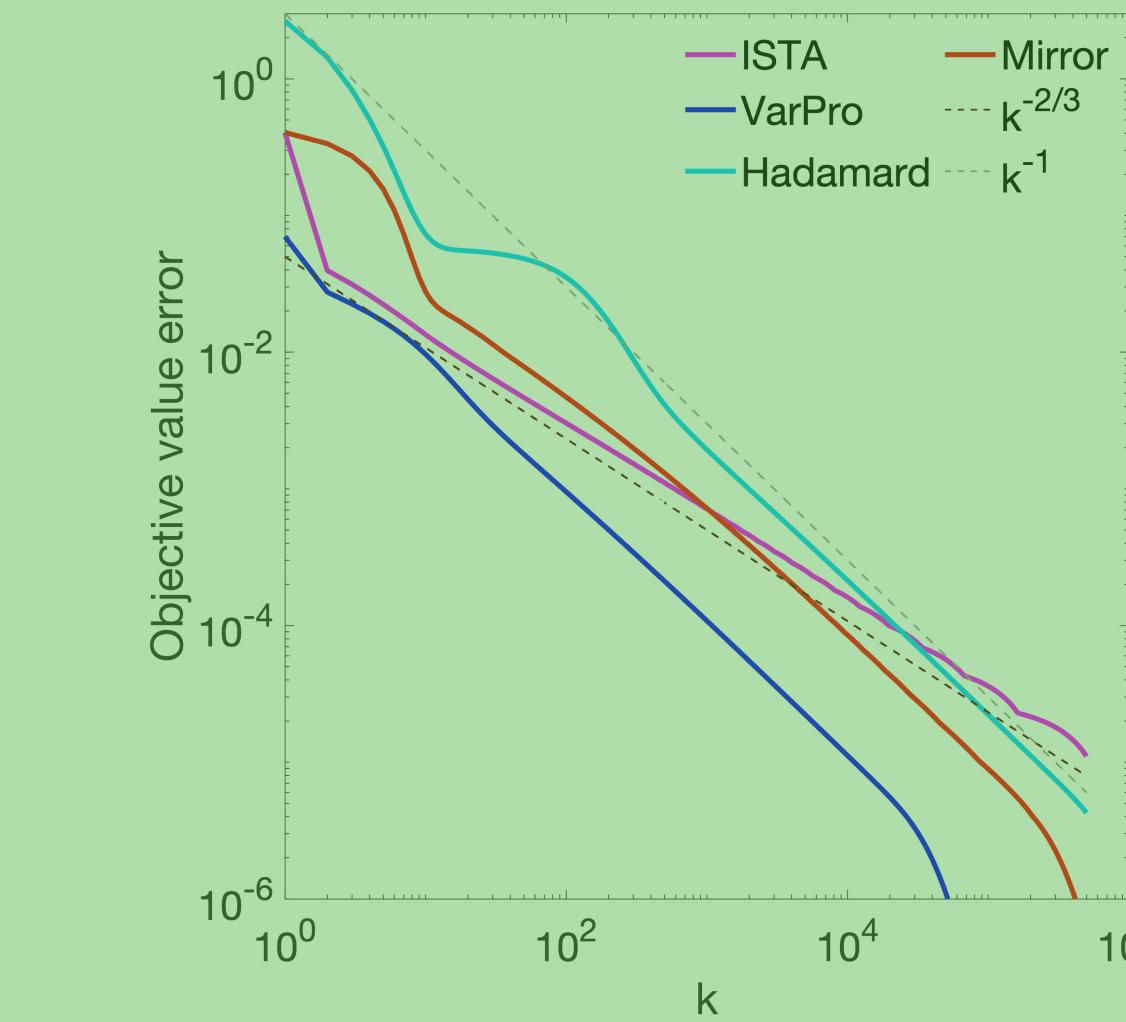
Quadratic Variational Forms



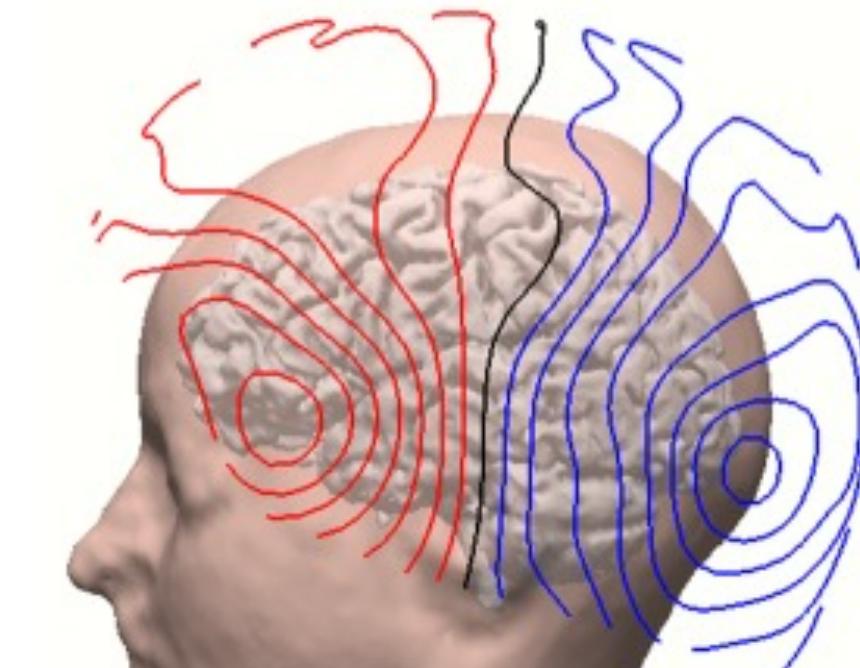
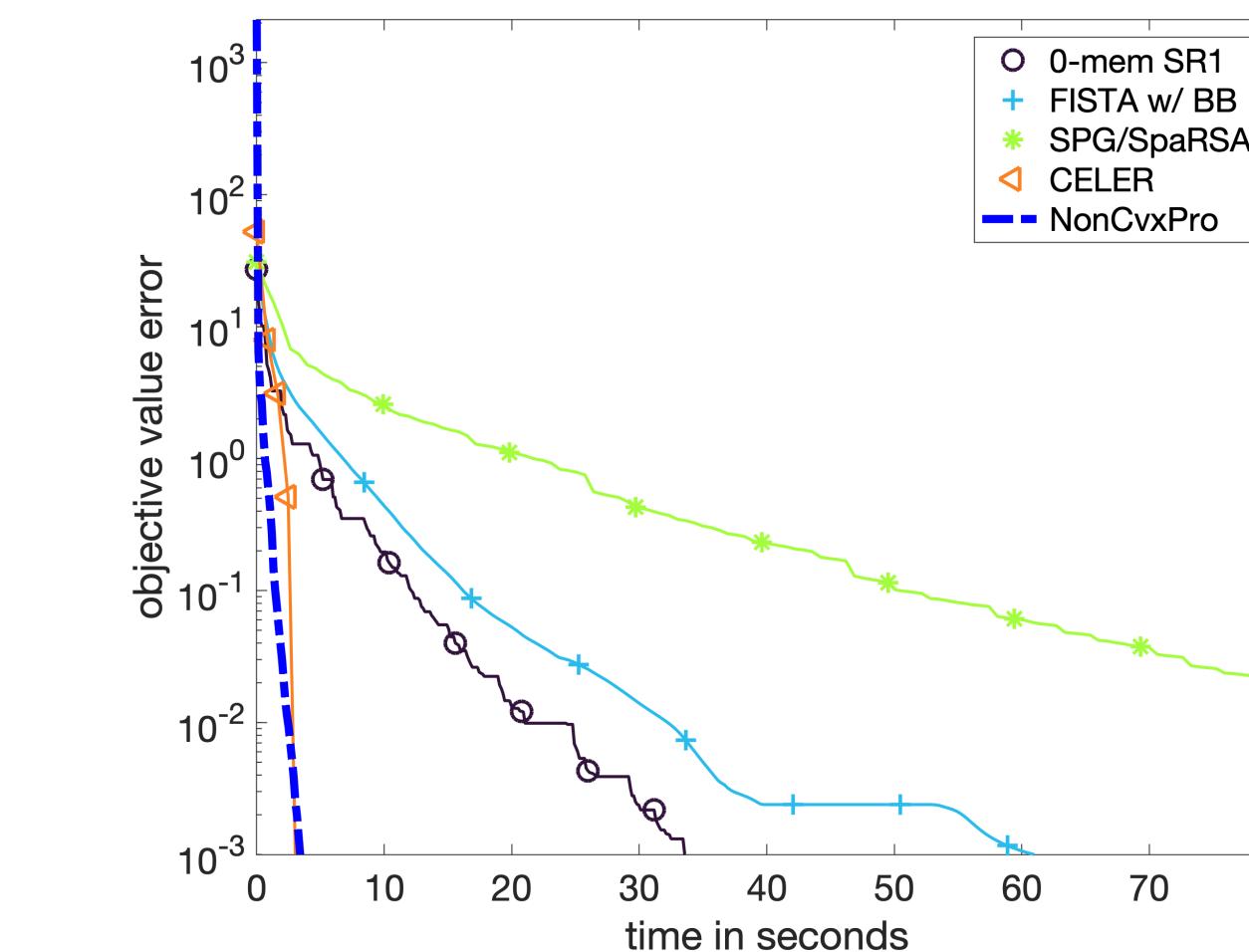
VarPro



Convergence



Numerical Results

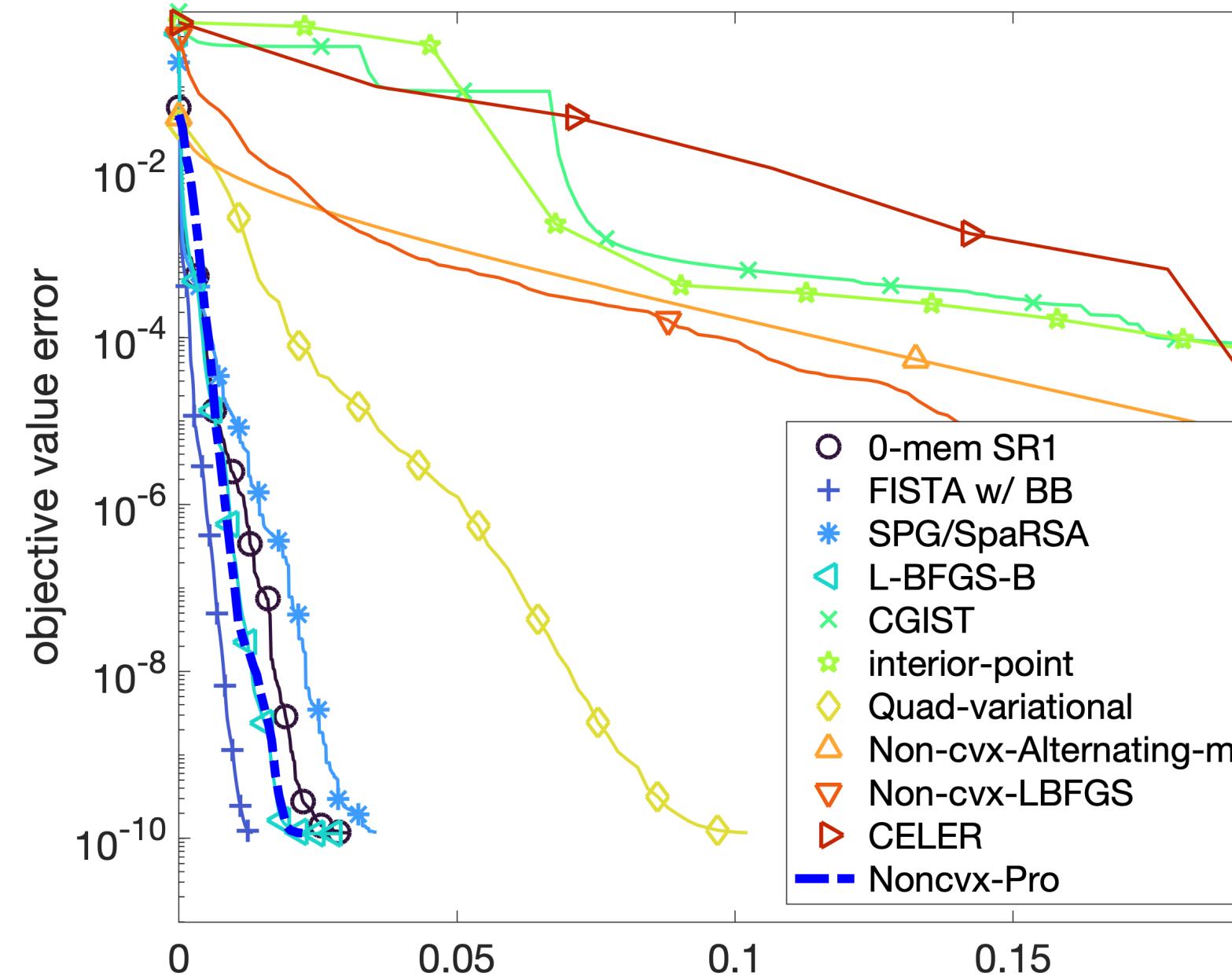


UCI/Adult income prediction

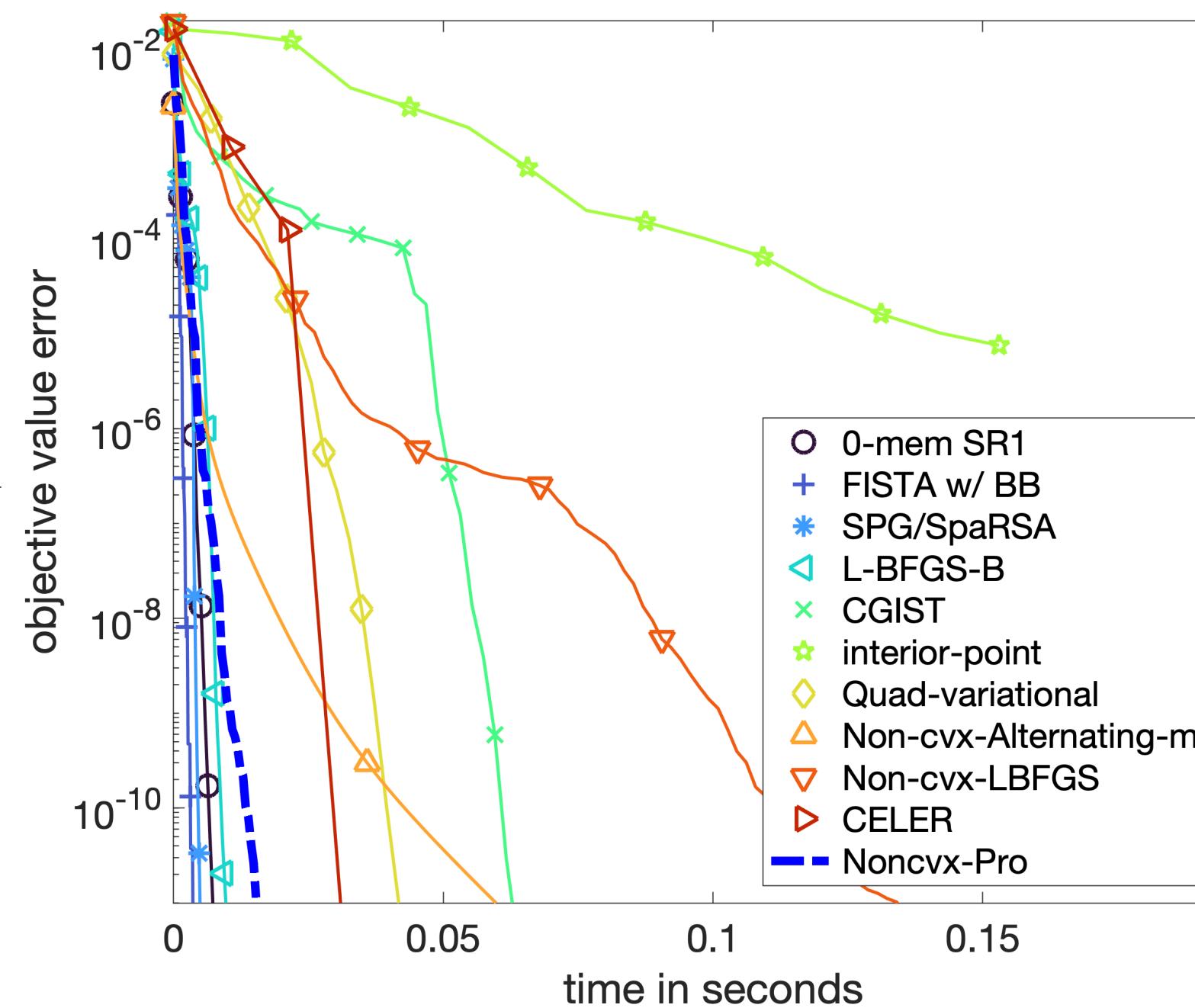
Lasso

a8a (m, n) = (22696, 122)

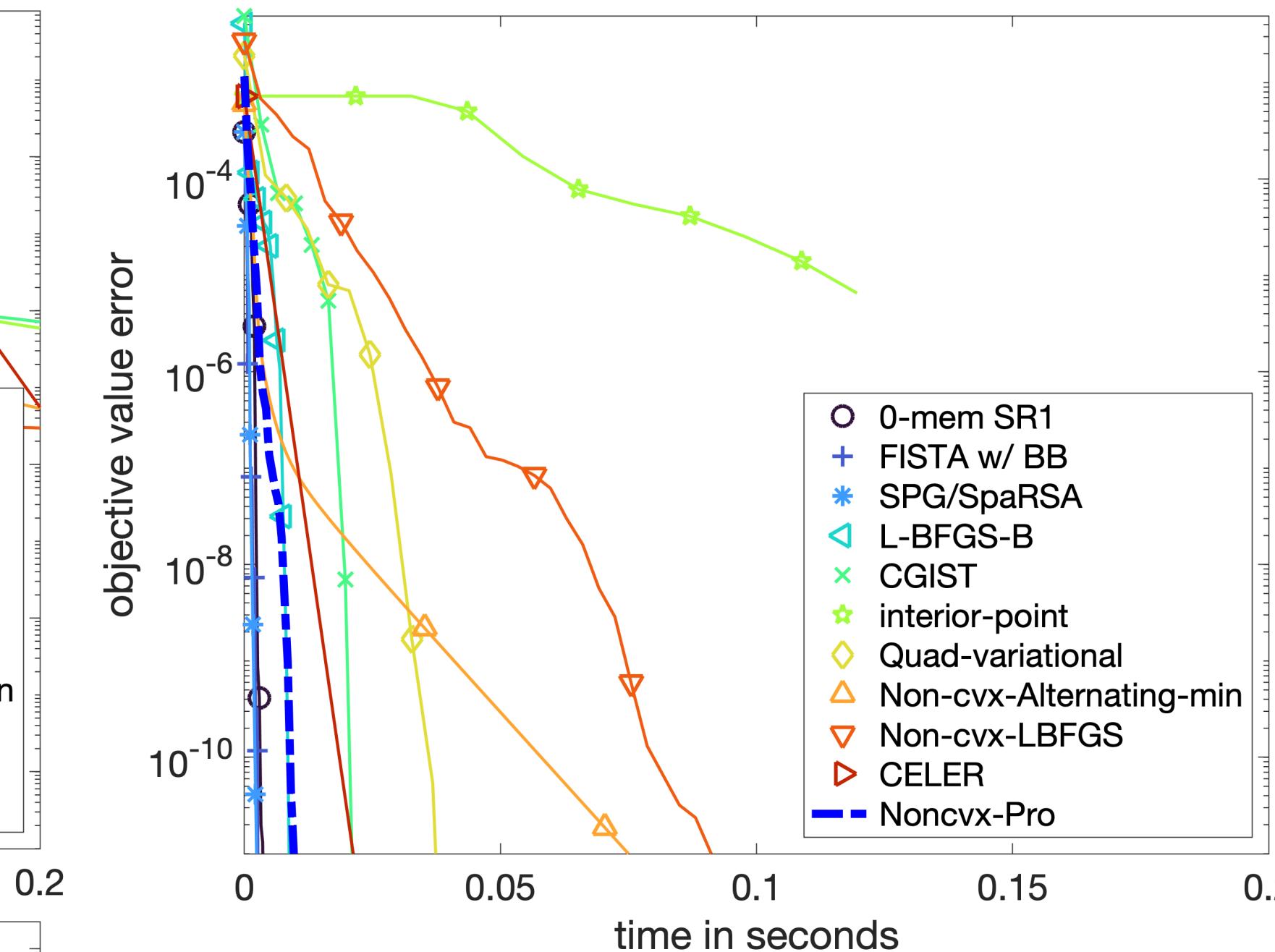
λ_*



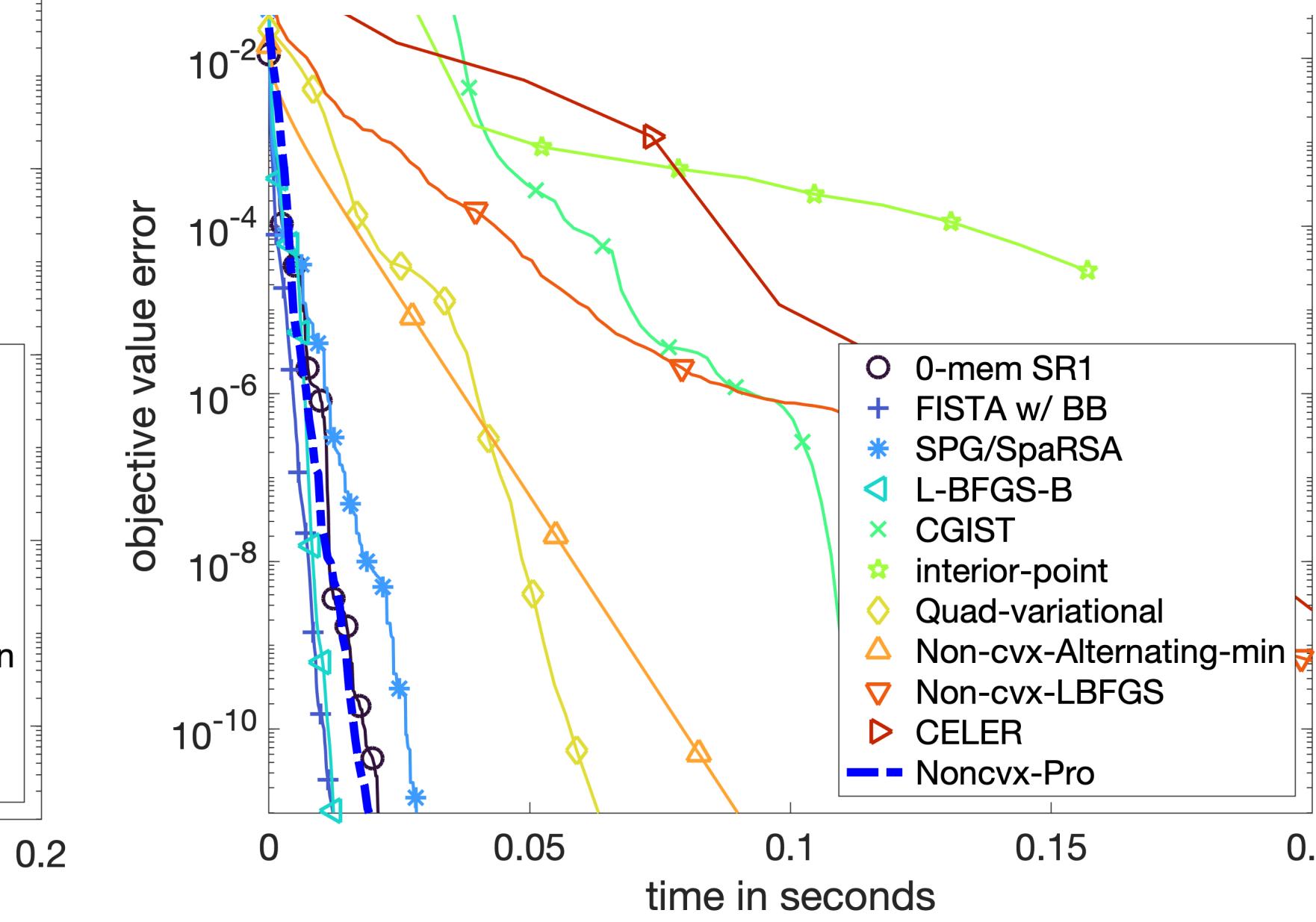
$\frac{1}{10} \lambda_{\max}$



$\frac{1}{2} \lambda_{\max}$



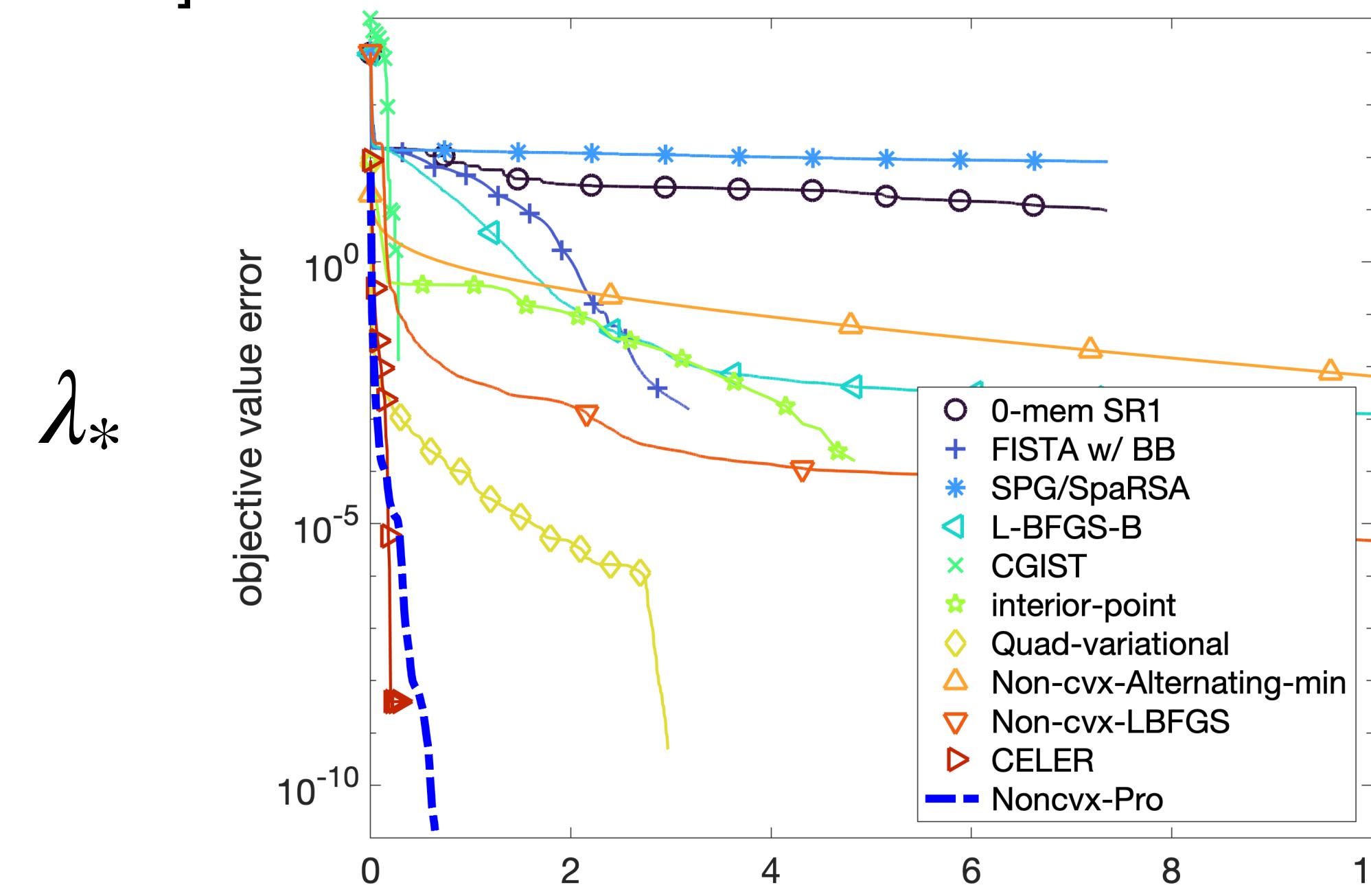
$\frac{1}{50} \lambda_{\max}$



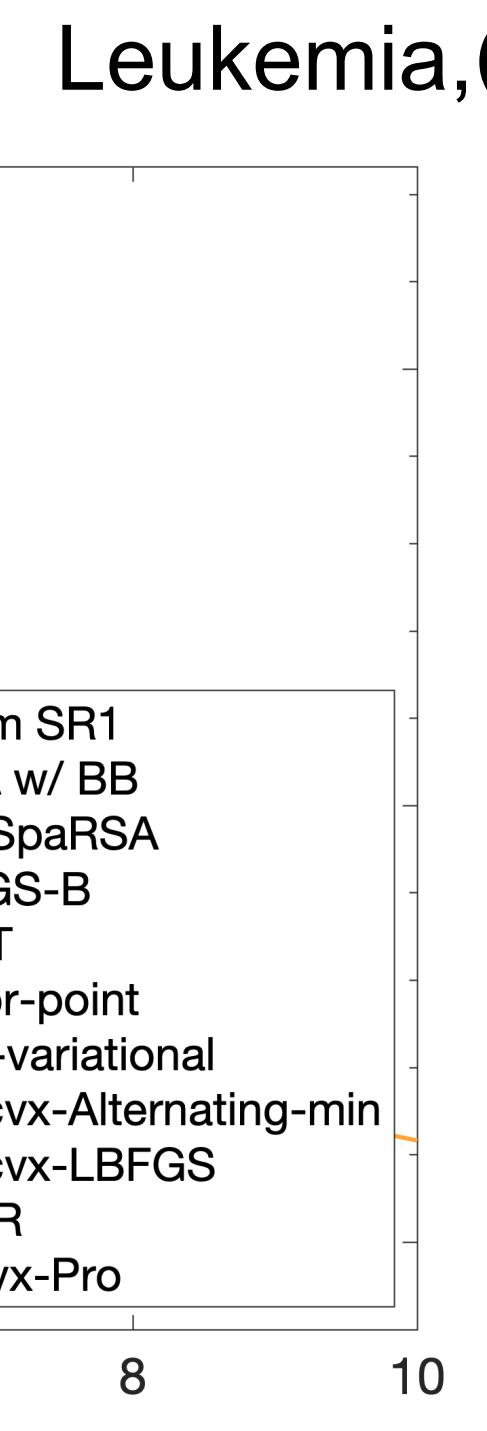
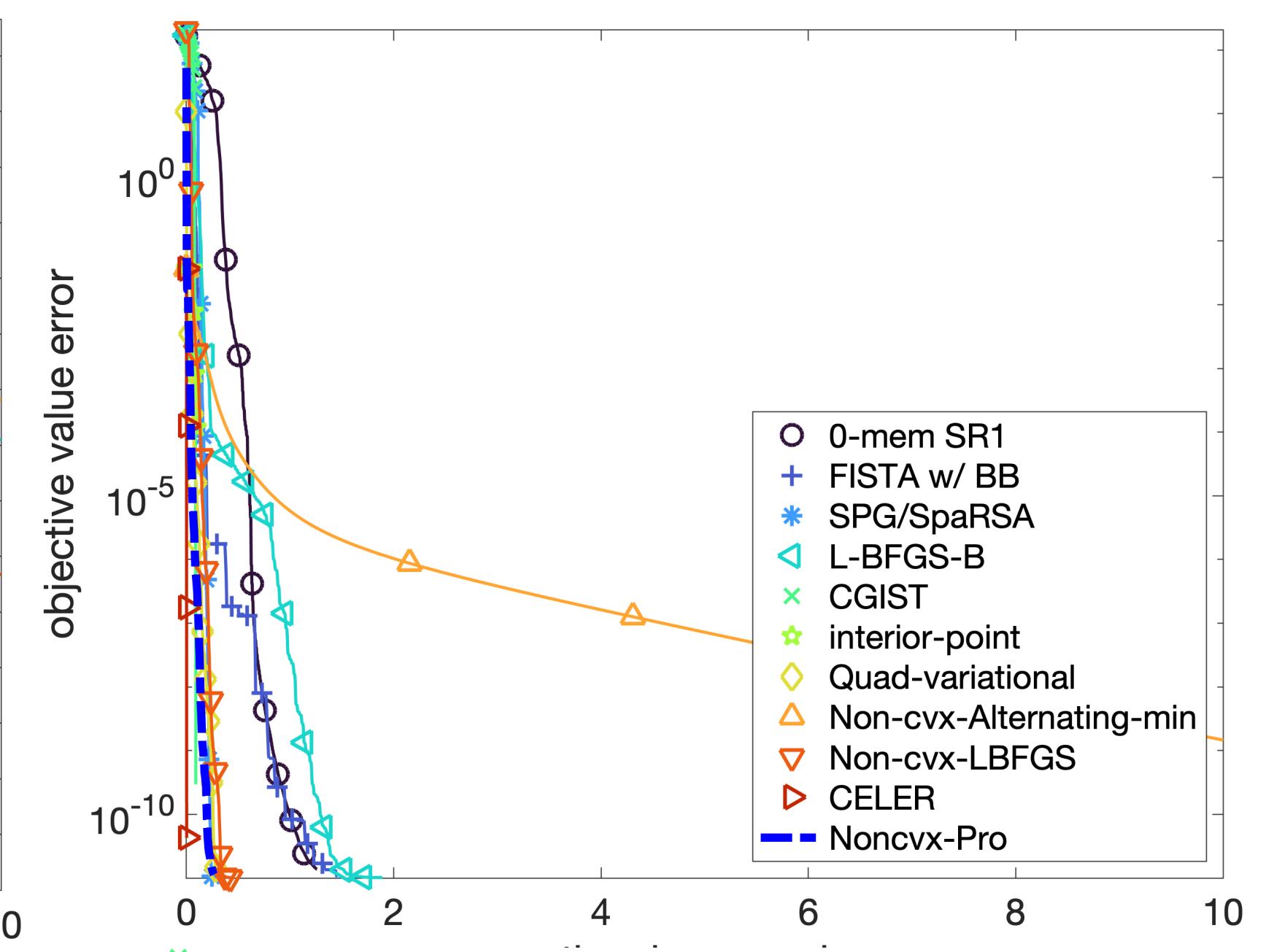
[Golub et al 1999] Molecular classification of cancer

Lasso

Leukemia, $(m, n) = (38,7129)$

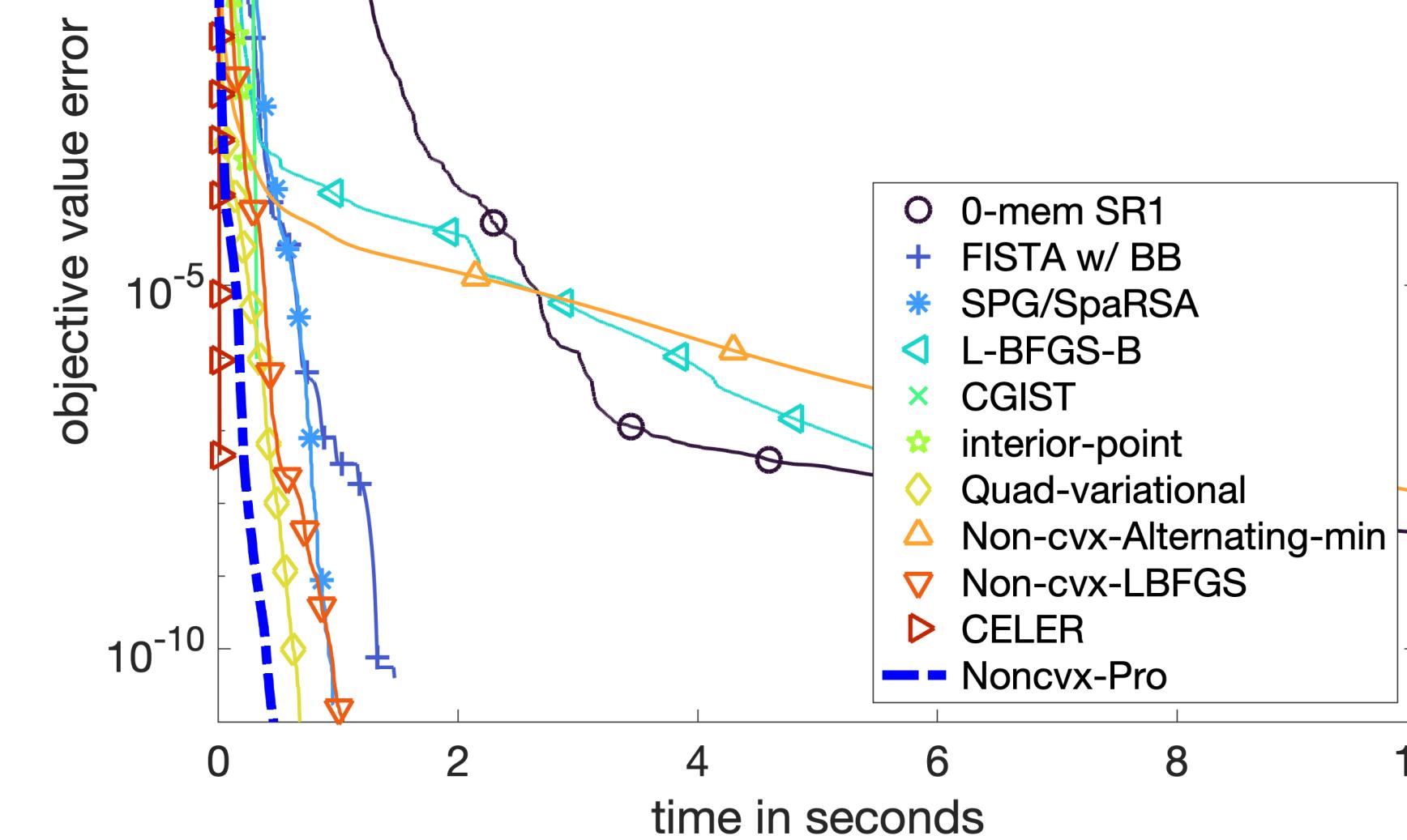


$$\lambda_*$$



$$\frac{1}{2}\lambda_{\max}$$

$$\frac{1}{10}\lambda_{\max}$$

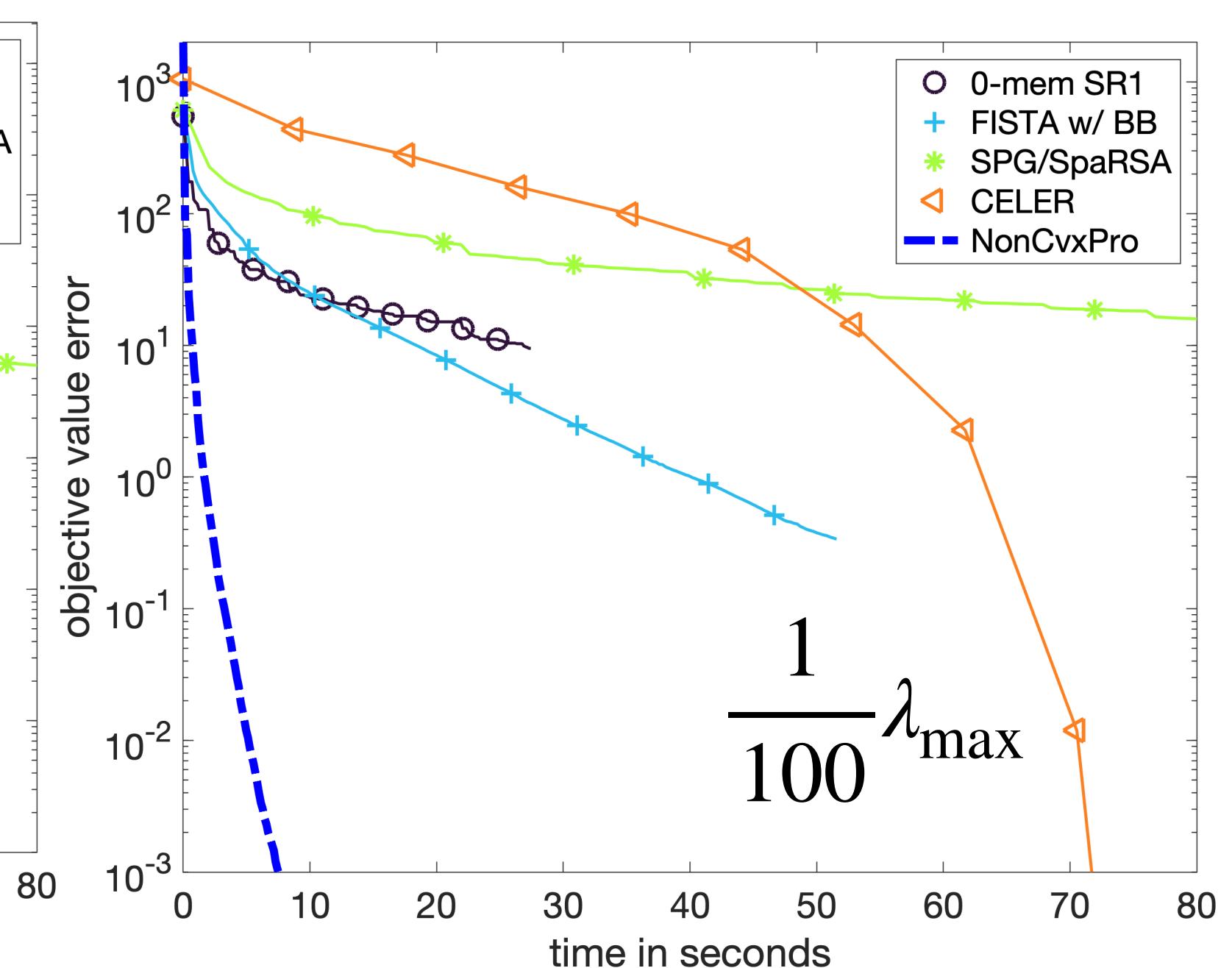
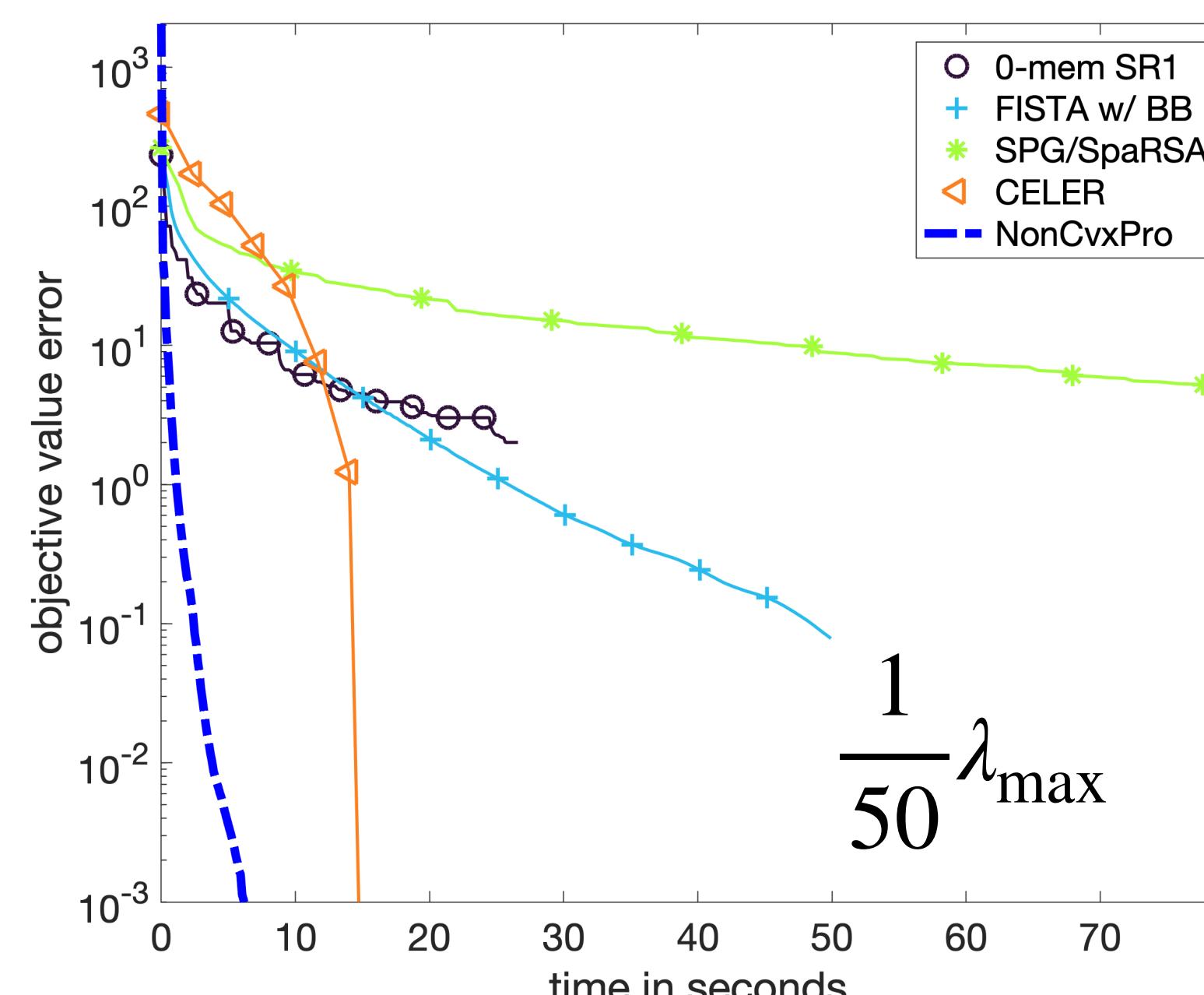
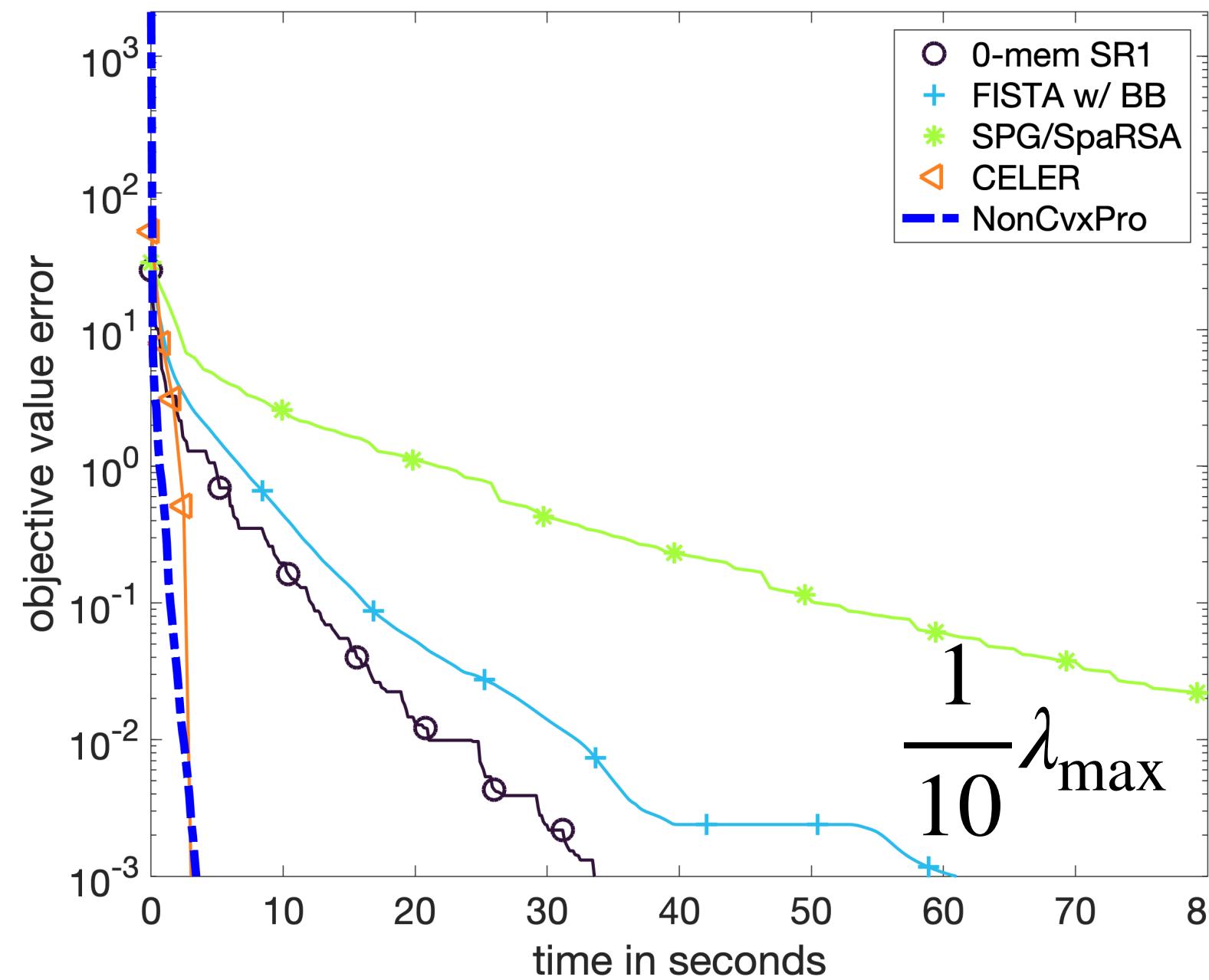
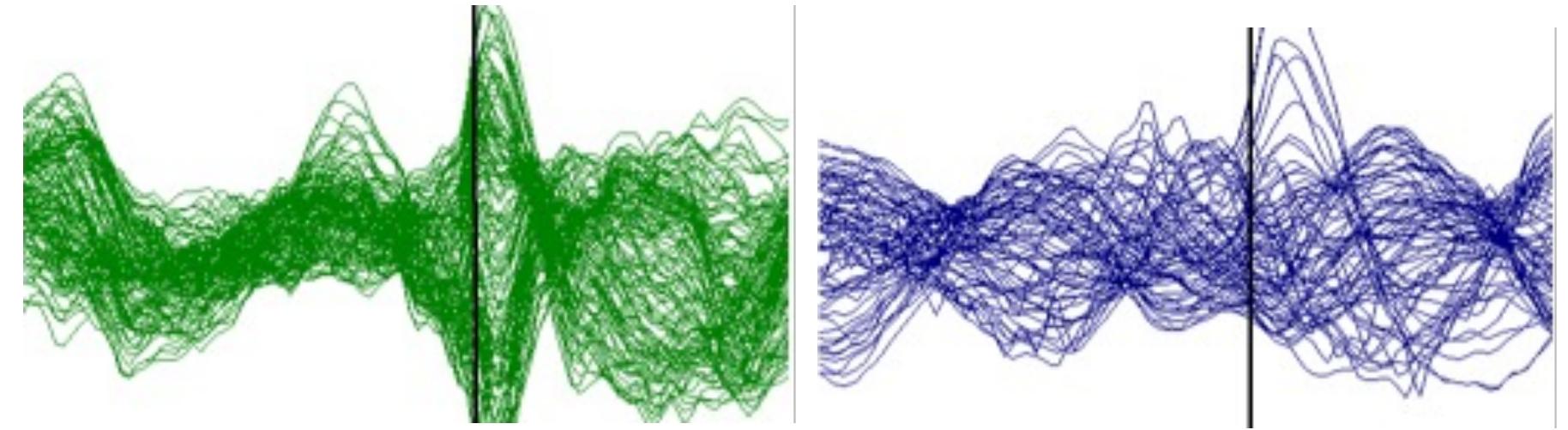
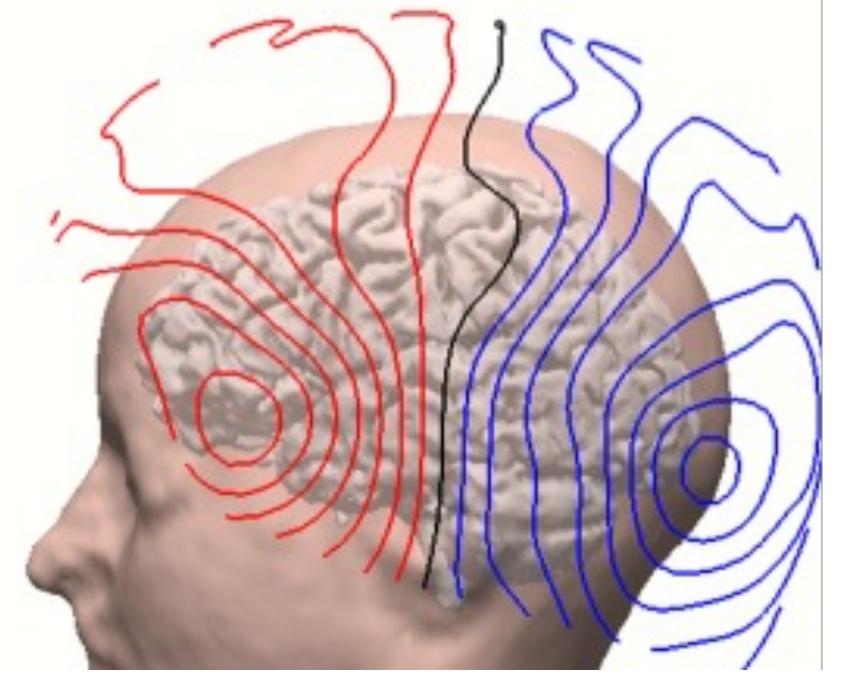


[Ndiaye et al, 2015]

Group Lasso - MEG/EEG

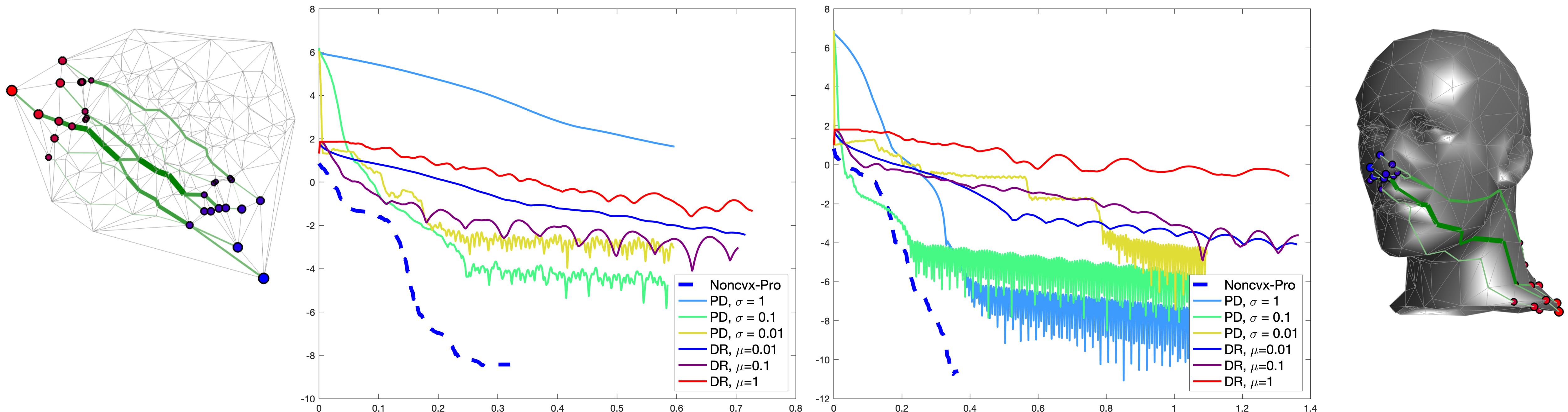
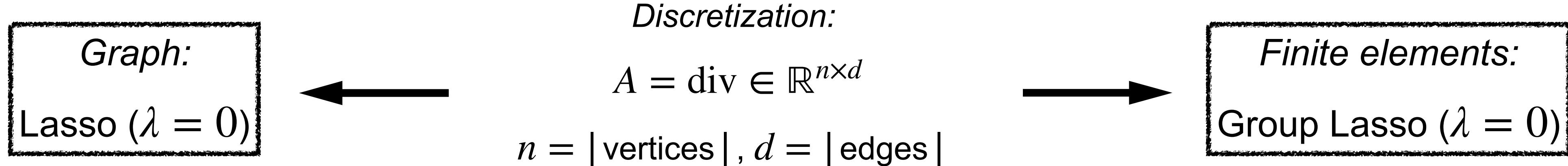
$$\left. \begin{array}{l} 2294 \text{ source locations} \\ \text{Group in time, } |g| = 181 \end{array} \right\} \longrightarrow n = 2294 \times 181$$

$$301 \text{ MEG} + 59 \text{ EEG Sensors} \longrightarrow m = 360 \times 181$$



Optimal Transport

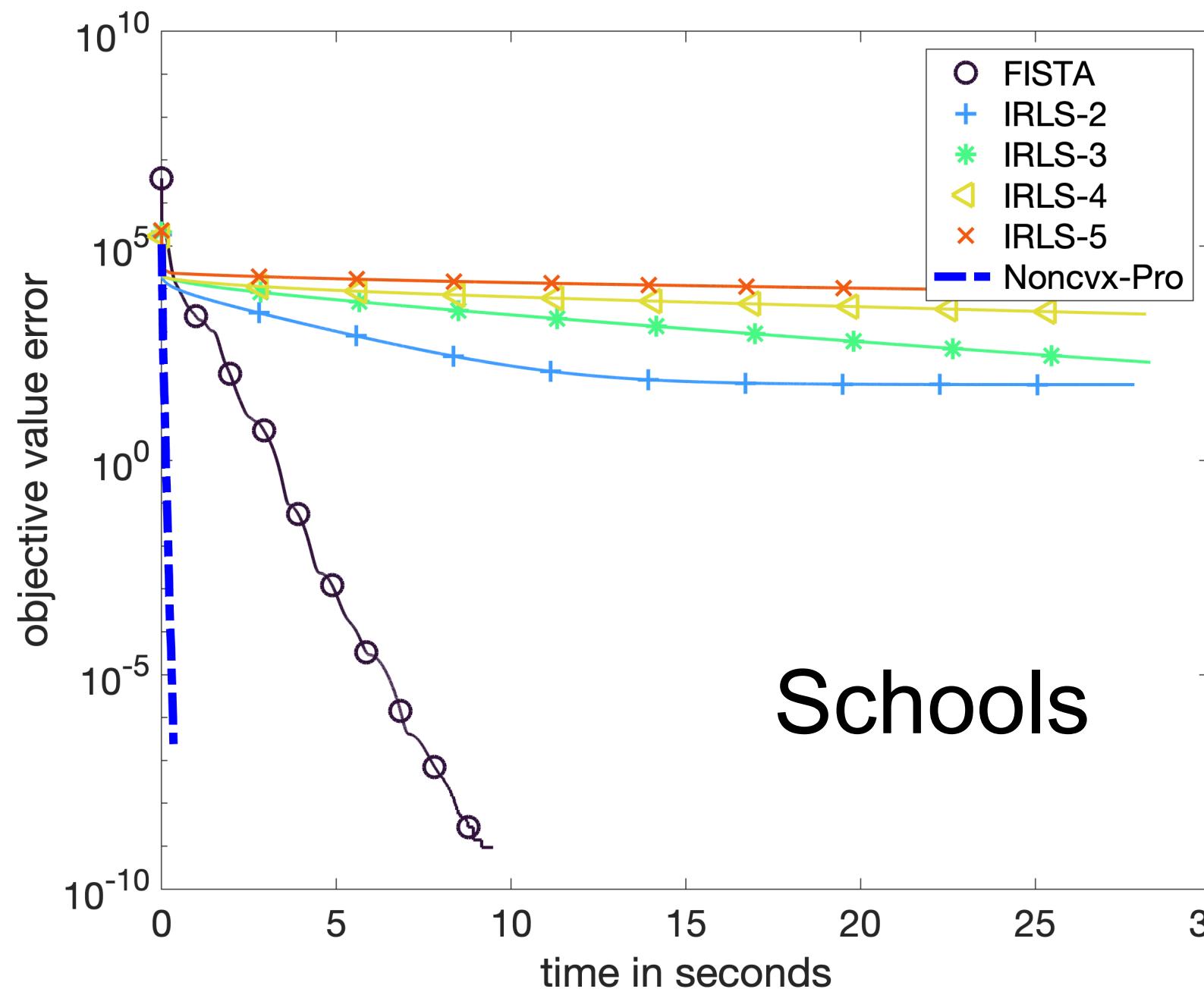
$$W_1(\alpha, \beta) = \min_{\vec{w}} \left\{ \int \|\vec{w}(x)\|; \operatorname{div}(\vec{w}) = \alpha - \beta \right\}$$



Multitask learning

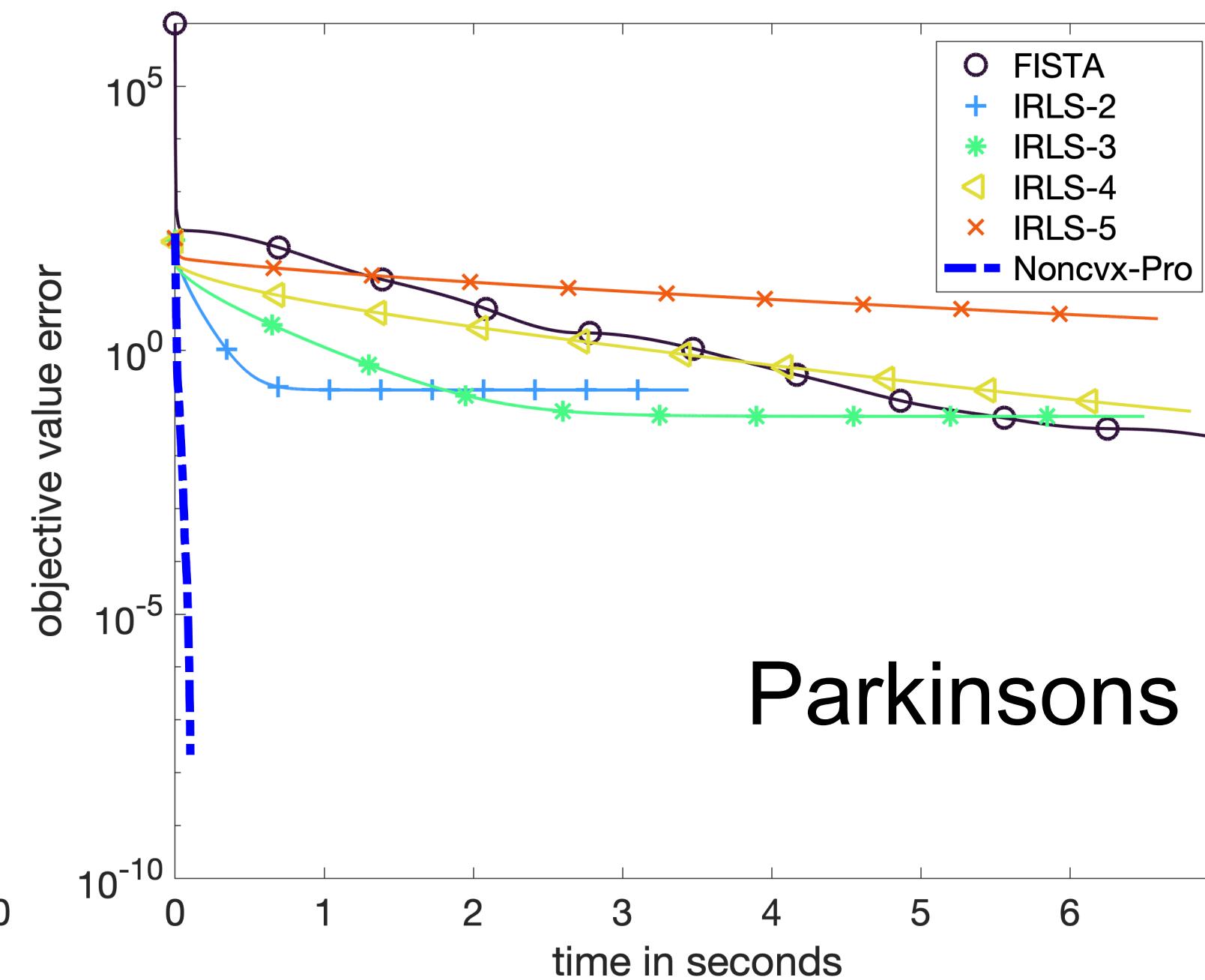
$$\min_{X=(x_t)_{t=1}^T} \frac{1}{2\lambda} \sum_{t=1}^T \|A_t x_t - y_t\|^2 + \|X\|_*$$

$y = \text{exam scores}$
 T schools
 n students



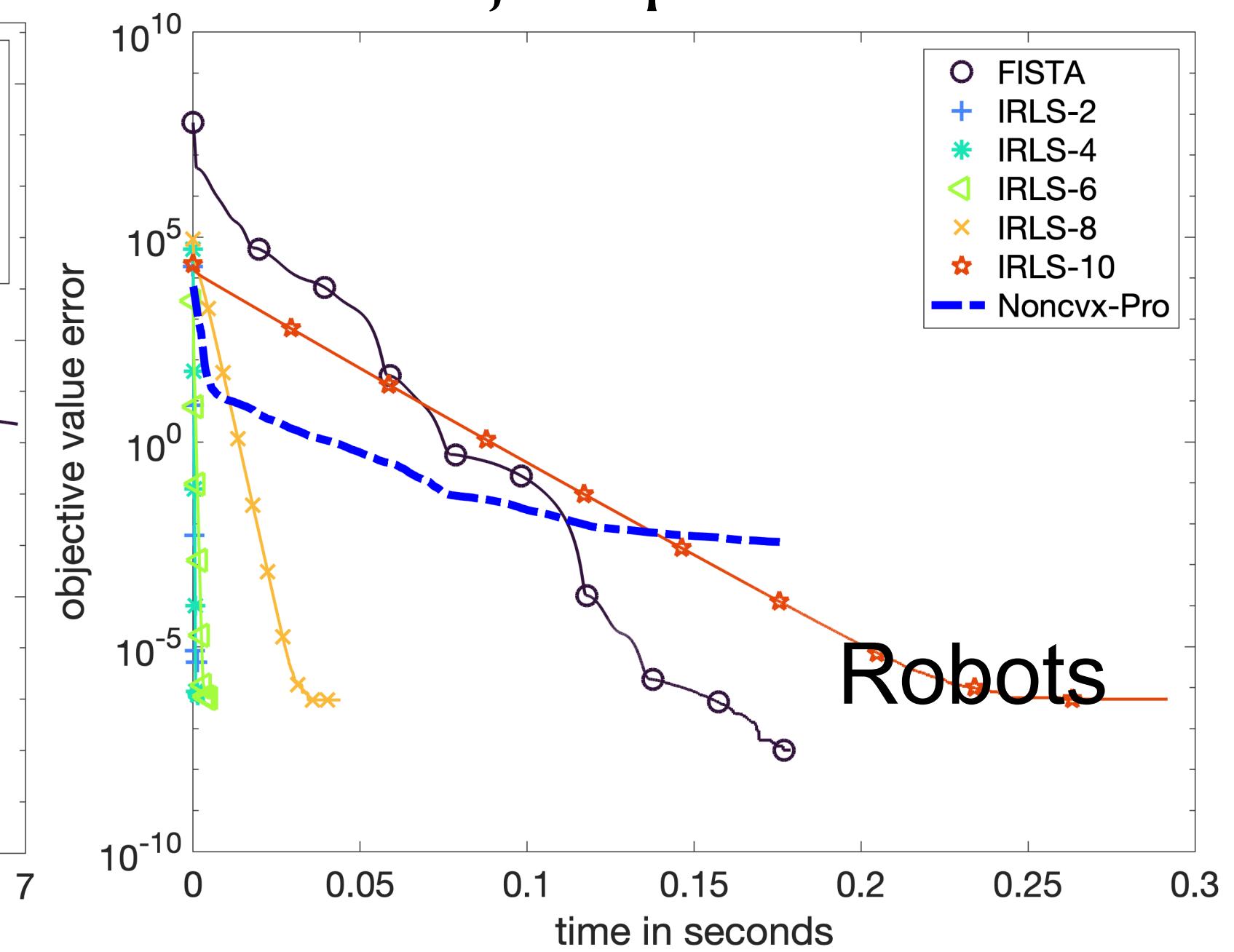
$$(T, n, d) = (139, 15362, 27)$$

$y = \text{symptoms}$
 T patients
 d bio-medical features



$$(T, n, d) = (42, 5875, 19)$$

$y = \text{motor}$
 T robot arms
 d joint positions



$$(T, n, d) = (7, 48933, 21)$$

IRLS-d implies regularisation 10^{-d}

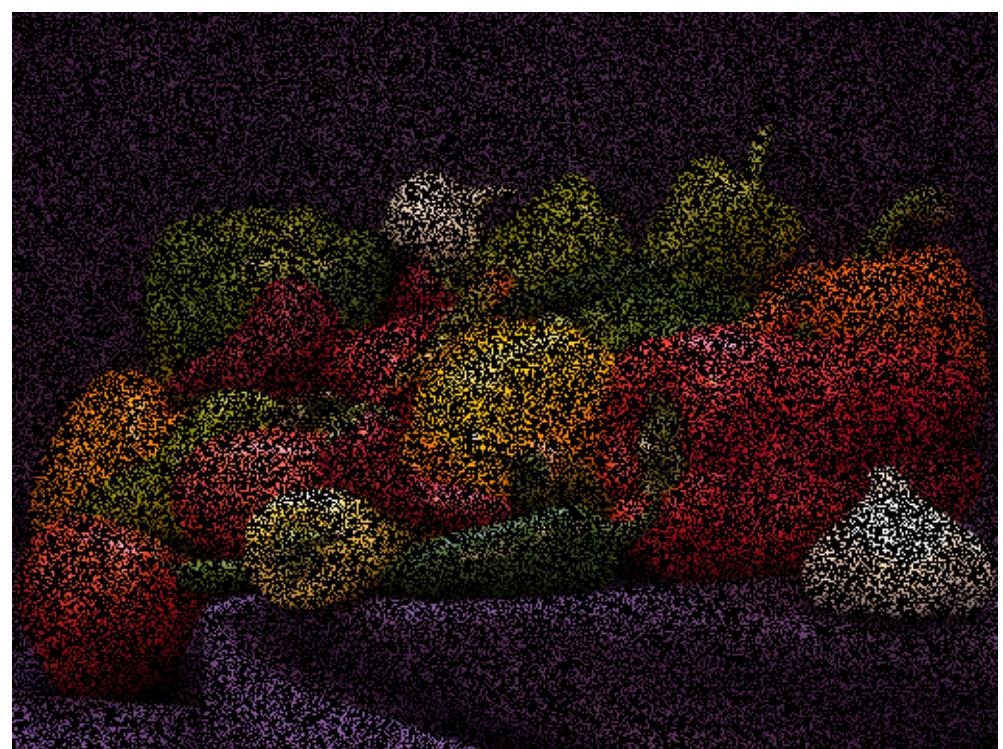
A = masking operator

$$\text{Loss: } \frac{1}{2\lambda} \|Ax - y\|^2$$

Image inpainting

$$D : \mathbb{R}^{d \times d \times T} \rightarrow \mathbb{R}^{d \times d \times 2T}$$

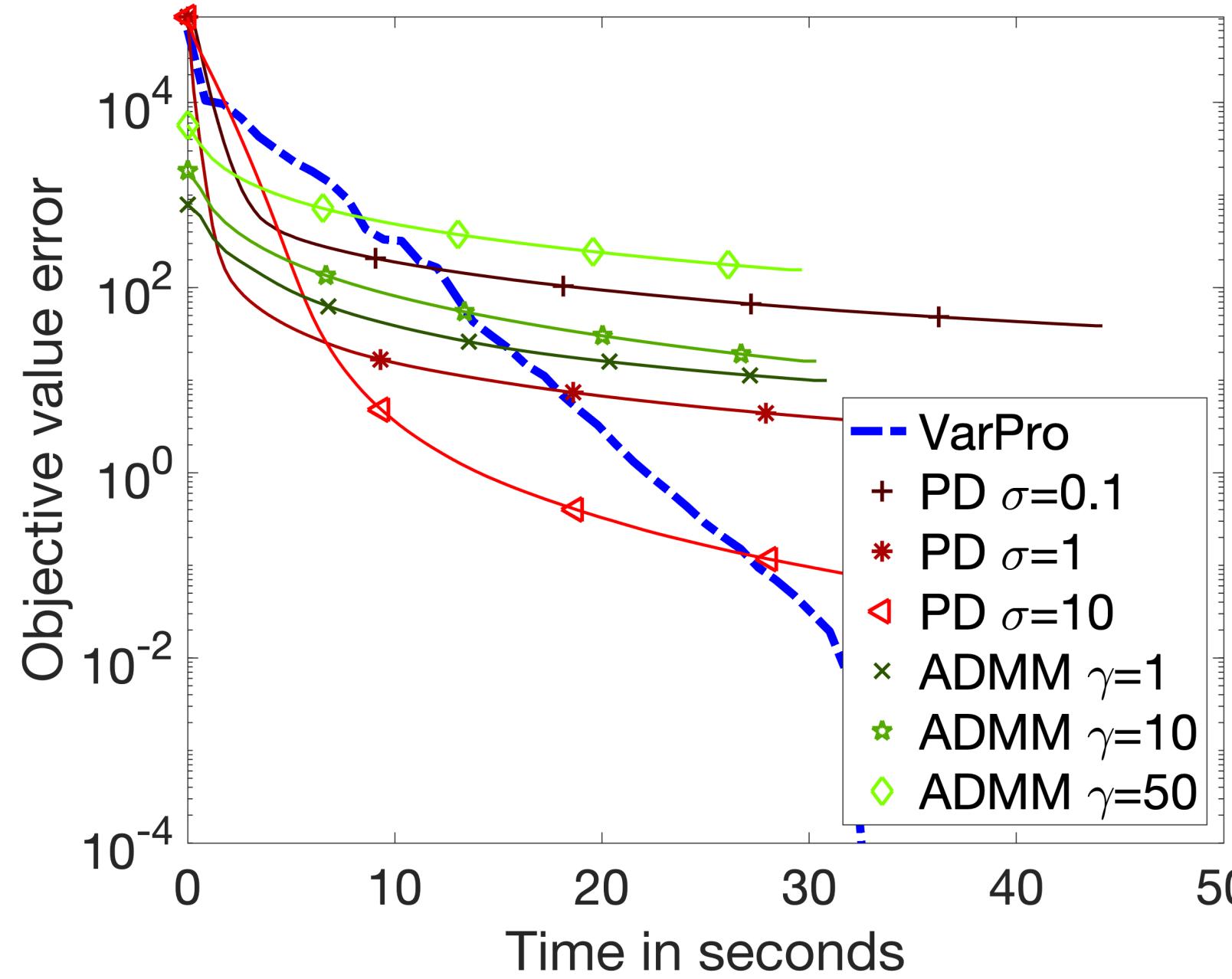
$$Dx = ((D^h x^t, D^v x^t))_{t=1}^T$$



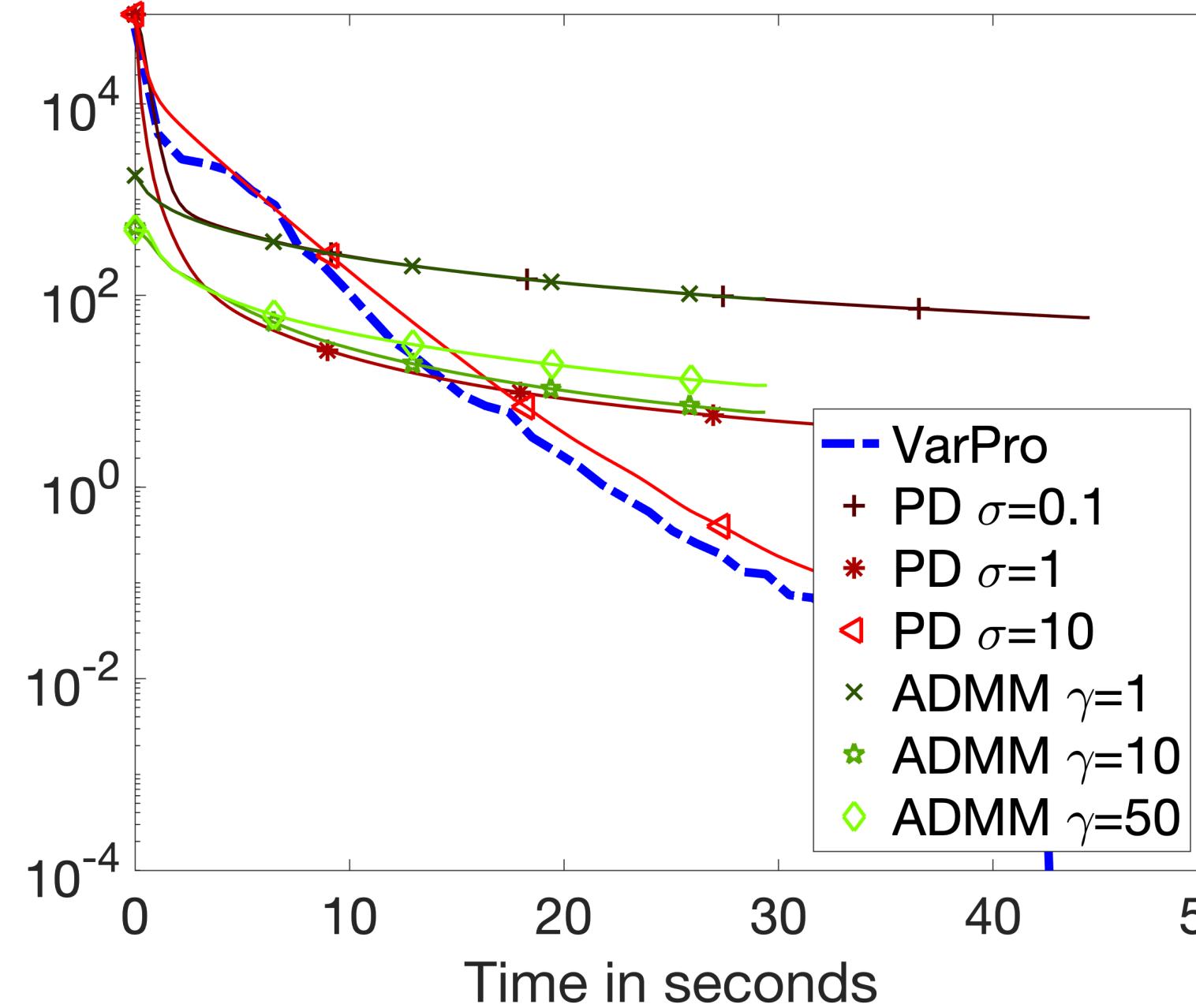
384 × 512

Group TV:

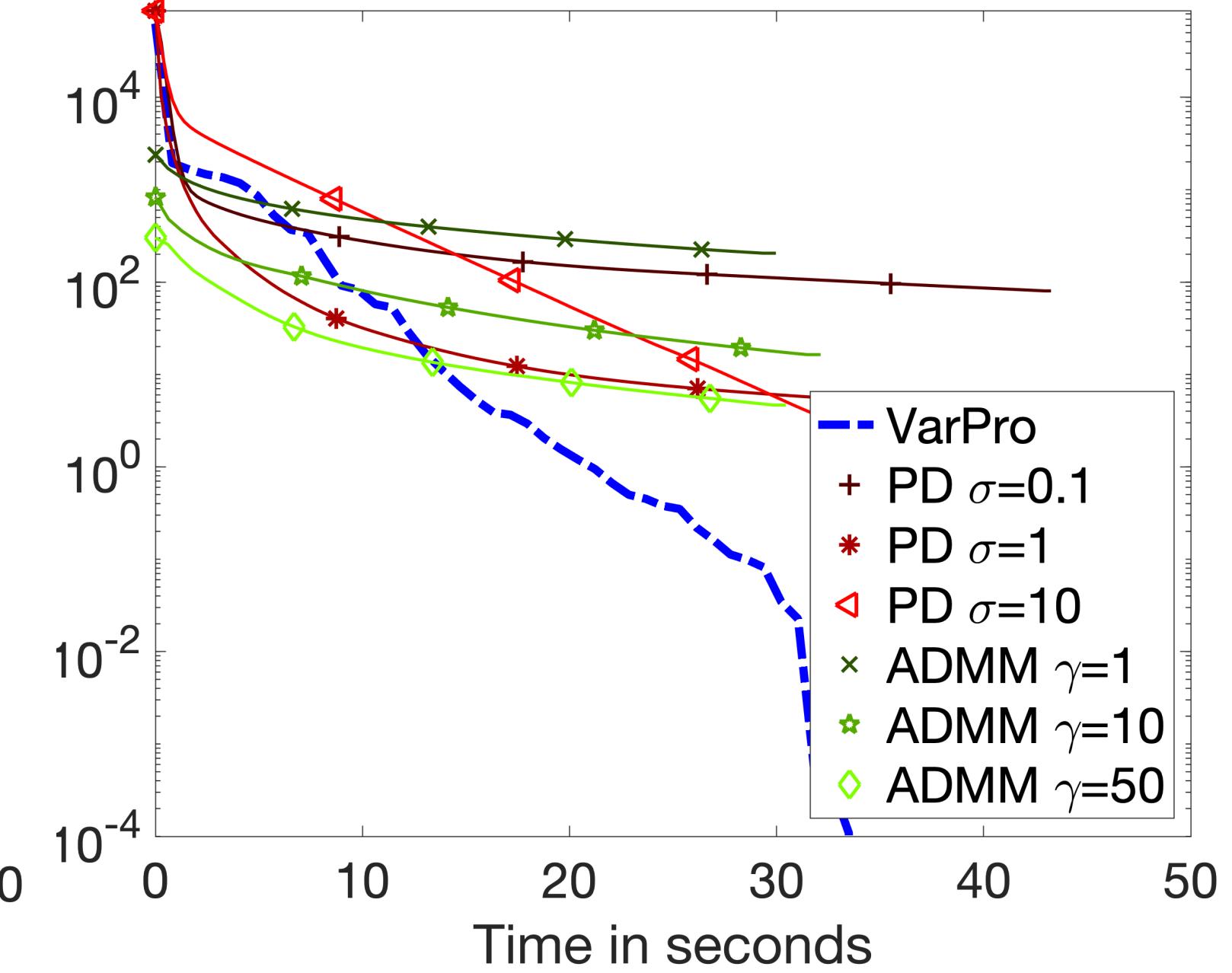
$$R(x) = \|Dx\|_{2,1} = \sum_{i,j=1}^d \sqrt{\sum_{t=1}^T (D^h x^t)_{i,j}^2 + (D^v x^t)_{i,j}^2}$$



$$\lambda = 0.1$$



$$\lambda = 0.5$$



$$\lambda = 1$$

Hyperspectral imaging

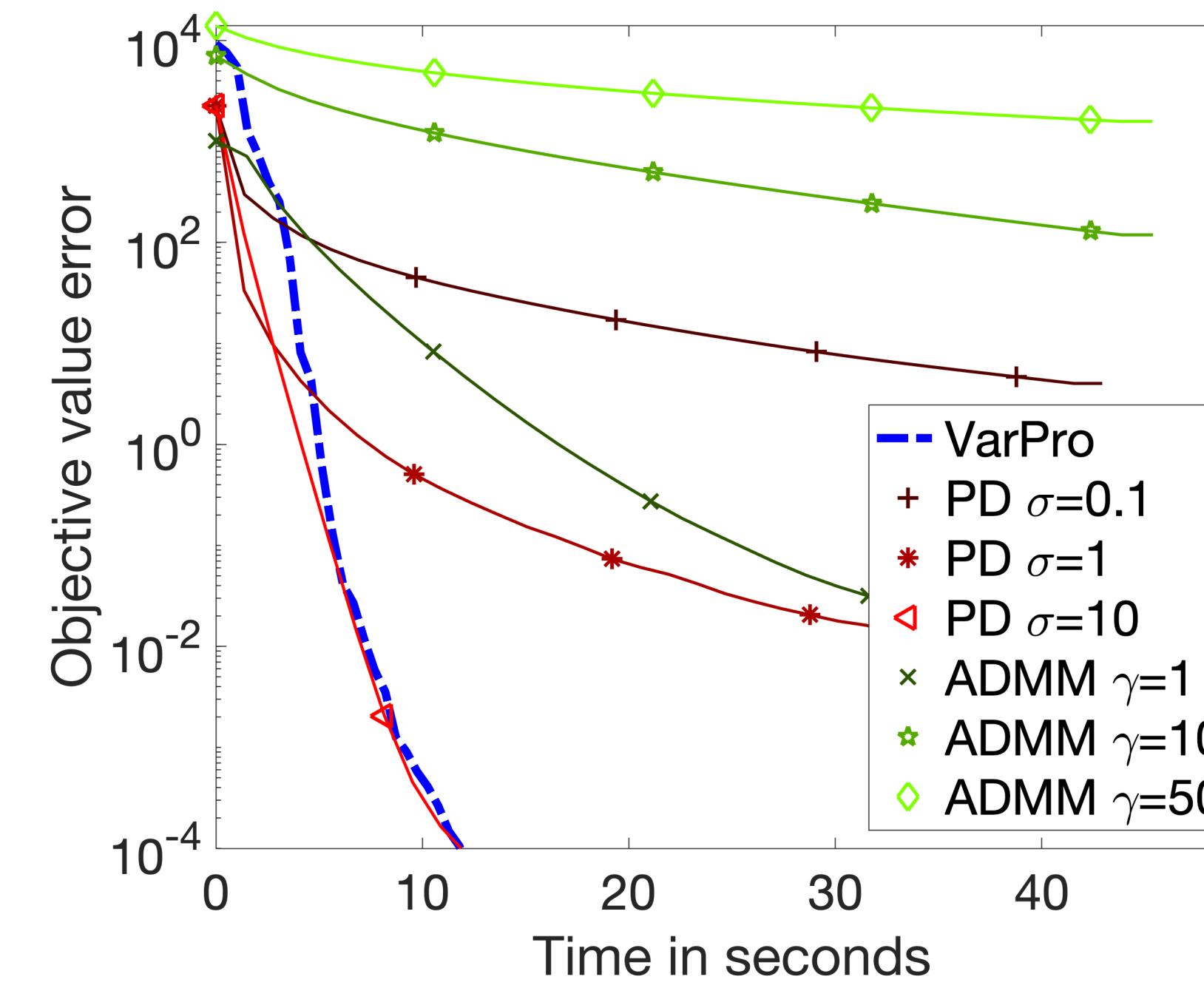
Group TV image denoising: $A = I$



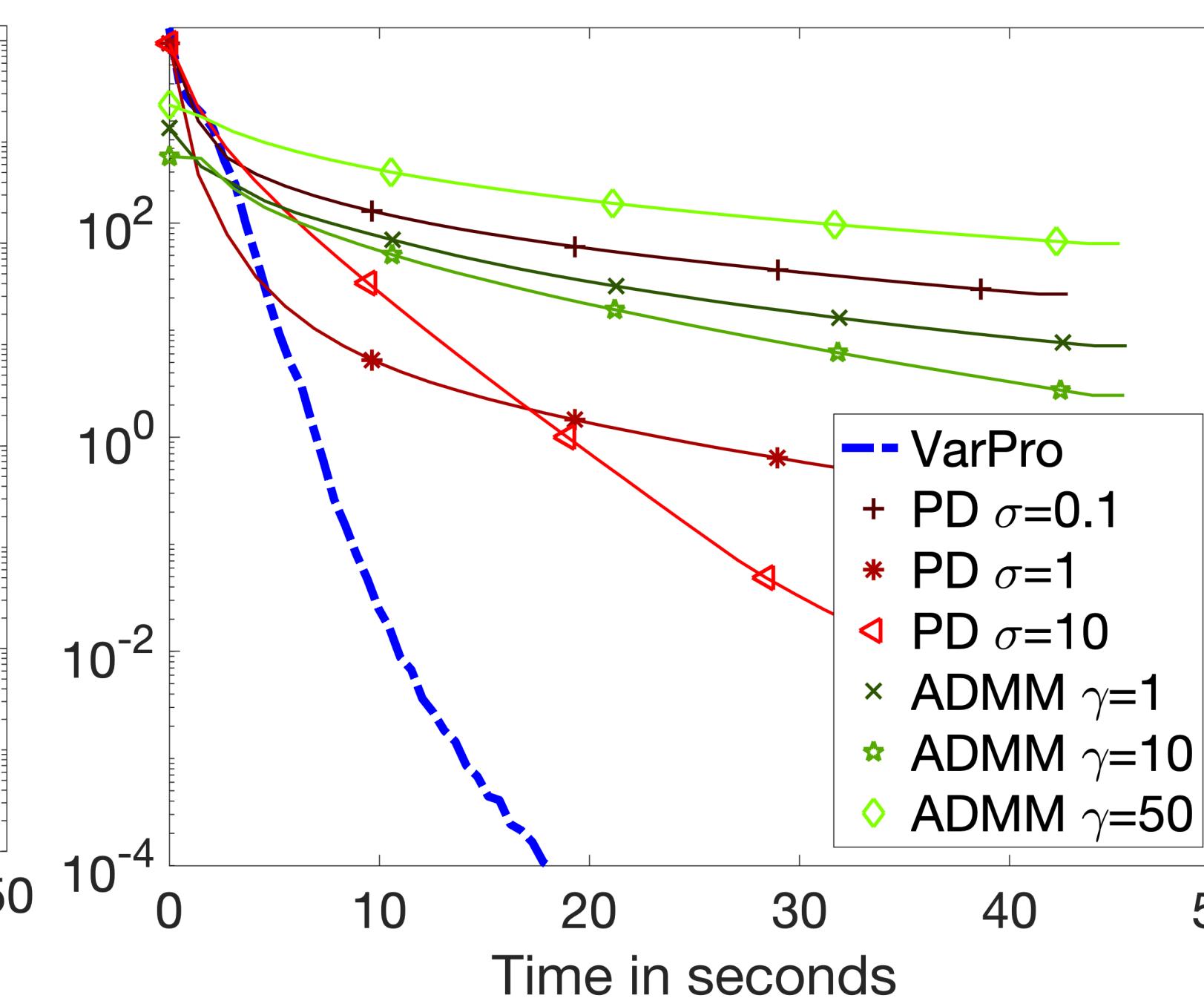
Indian Pines dataset

Input: noisy images of dimension $d = 145$ with $T = 224$ spectral bands

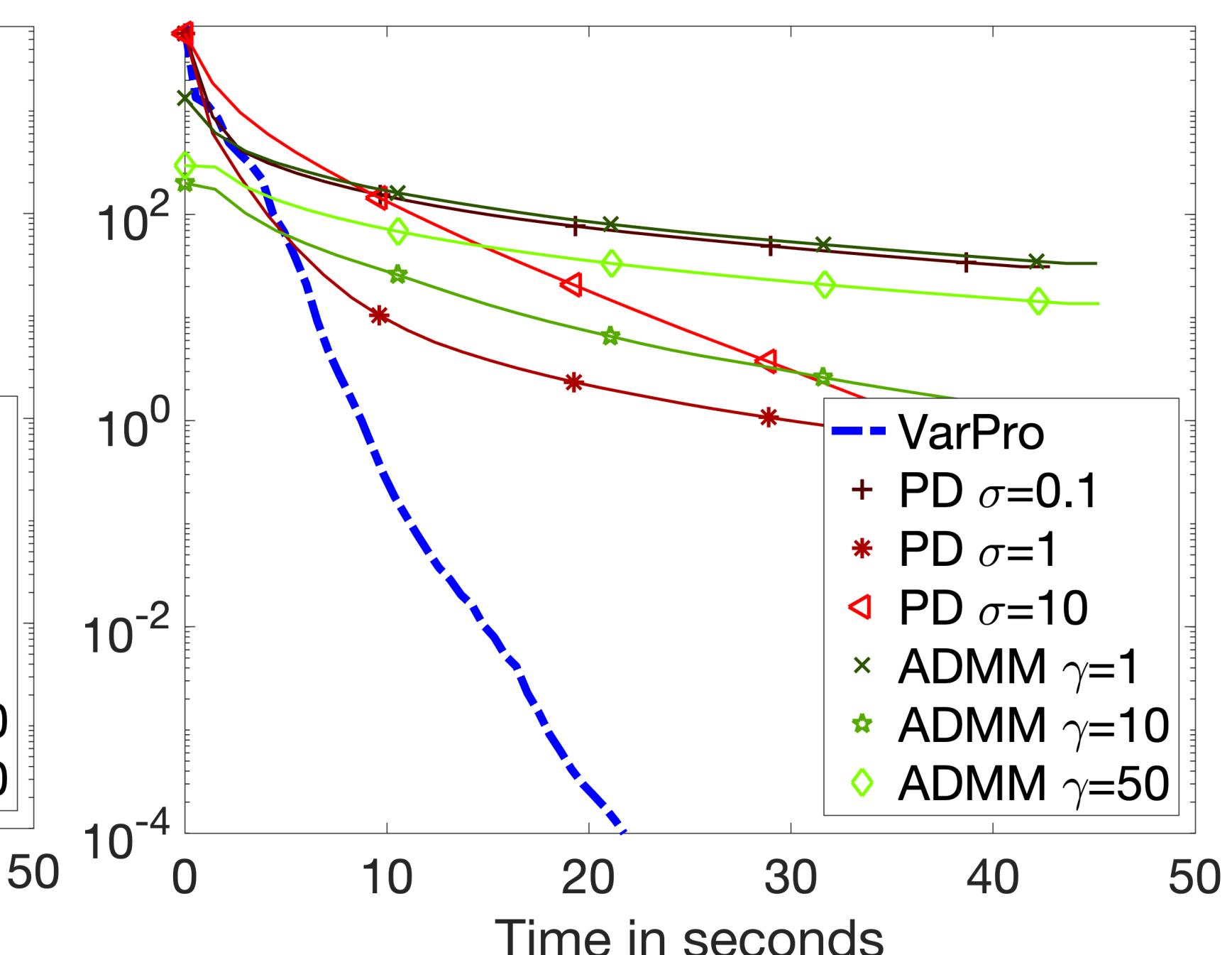
145×145



$$\lambda = 0.1$$



$$\lambda = 0.5$$



$$\lambda = 1$$

Conclusion

