

Optimized first-order minimization methods

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Low-dose X-ray CT image reconstruction



Thin-slice FBP

Seconds



ASIR

A bit longer



Statistical

Much longer

Image reconstruction as an optimization problem:

$$\hat{\mathbf{x}} = \arg \min_{\mathbf{x} \succeq 0} \frac{1}{2} \|\mathbf{y} - \mathbf{A}\mathbf{x}\|_W^2 + R(\mathbf{x})$$

(Same sinogram, so all at same **dose**)

Outline

- Motivation (done)
- Problem definition
- Existing algorithms
 - Gradient descent
 - Nesterov's "optimal" first-order methods
 - General first-order methods
- Optimizing first-order minimization methods
- Drori & Teboulle's numerical bounds
- Donghwan Kim's analytically optimized ("more optimal") first-order methods
- Example (logistic regression for machine learning)
- Summary / Future work

Problem setting

Optimization problem setting

$$\hat{\mathbf{x}} = \underset{\mathbf{x}}{\operatorname{arg\,min}} f(\mathbf{x})$$

- Unconstrained
- Large-scale (Hessian too big to store)
 - image reconstruction
 - big-data / machine learning
 - ...
- Cost function assumptions (throughout)
 - $f : \mathbb{R}^M \mapsto \mathbb{R}$
 - convex (need not be strictly convex)
 - non-empty set of global minimizers:

$$\hat{\mathbf{x}} \in \mathcal{X}^* = \{\mathbf{x}_* \in \mathbb{R}^M : f(\mathbf{x}_*) \leq f(\mathbf{x}), \forall \mathbf{x} \in \mathbb{R}^M\}$$

- smooth (differentiable with L -Lipshitz gradient)

$$\|\nabla f(\mathbf{x}) - \nabla f(\mathbf{z})\|_2 \leq L \|\mathbf{x} - \mathbf{z}\|_2, \quad \forall \mathbf{x}, \mathbf{z} \in \mathbb{R}^M$$

Example: Machine learning

To learn weights \mathbf{x} of binary classifier given feature vectors $\{\mathbf{v}_i\}$ and labels $\{y_i\}$:

$$f(\mathbf{x}) = \sum_i \psi(y_i \langle \mathbf{x}, \mathbf{v}_i \rangle),$$

where $y_i = \pm 1$.

loss functions $\psi(t)$

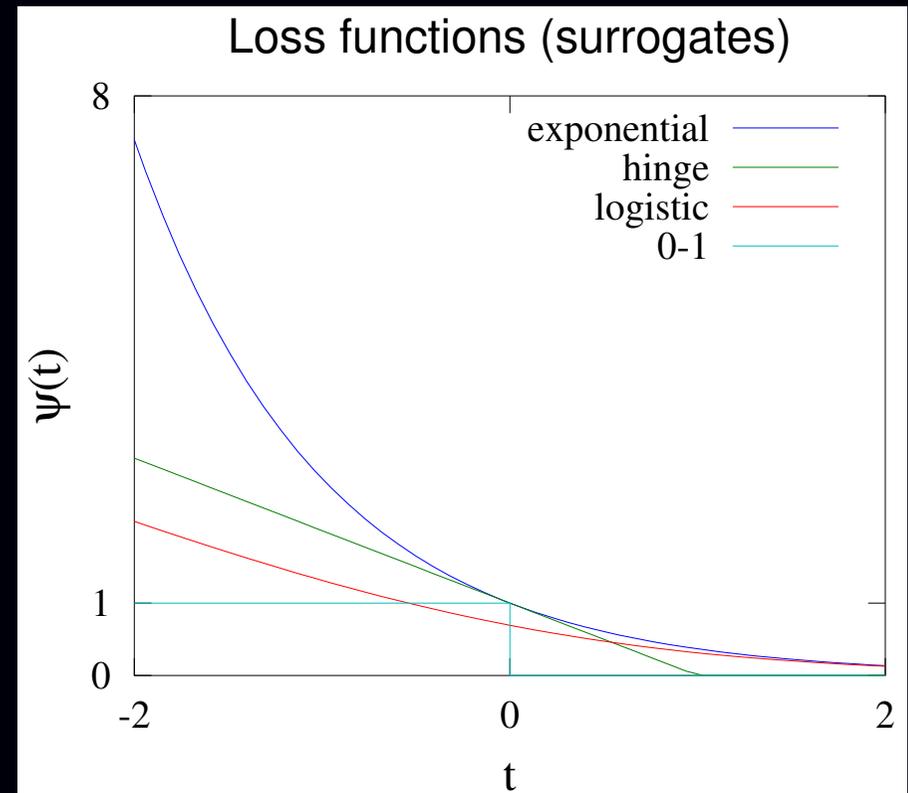
0-1: $1_{\{t \leq 0\}}$

exponential: $\exp(-t)$

logistic: $\log(1 + \exp(-t))$

hinge: $\max\{0, 1 - t\}$

Which of these fit our conditions?



Algorithms

Gradient descent

iteration with step size $1/L$ ensures monotonic descent of f :

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \nabla f(\mathbf{x}_n)$$

stacking:

$$\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_{N-1} \\ \mathbf{x}_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N-2} \\ \mathbf{x}_{N-1} \end{bmatrix} - \frac{1}{L} \begin{bmatrix} \nabla f(\mathbf{x}_0) \\ \nabla f(\mathbf{x}_1) \\ \vdots \\ \nabla f(\mathbf{x}_{N-2}) \\ \nabla f(\mathbf{x}_{N-1}) \end{bmatrix}$$

i.e.:

$$\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_{N-1} \\ \mathbf{x}_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N-2} \\ \mathbf{x}_{N-1} \end{bmatrix} - \frac{1}{L} \left(\underbrace{\begin{bmatrix} 1 & 0 & 0 & \dots & 0 \\ 0 & 1 & 0 & \dots & 0 \\ \vdots & & \ddots & & \\ 0 & \dots & 0 & 1 & 0 \\ 0 & \dots & 0 & 0 & 1 \end{bmatrix}}_{H_{\text{GD}}} \otimes \mathbf{I} \right) \begin{bmatrix} \nabla f(\mathbf{x}_0) \\ \nabla f(\mathbf{x}_1) \\ \vdots \\ \nabla f(\mathbf{x}_{N-2}) \\ \nabla f(\mathbf{x}_{N-1}) \end{bmatrix}$$

Note: $N \times N$ coefficient matrix H_{GD} is diagonal (a special case of lower triangular).

Gradient descent convergence rate

Classic $O(1/n)$ convergence rate of cost function descent:

$$\underbrace{f(\mathbf{x}_n) - f(\mathbf{x}_*)}_{\text{inaccuracy}} \leq \frac{L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{2n}.$$

Drori & Teboulle (2013) derive tightest inaccuracy bound:

$$f(\mathbf{x}_n) - f(\mathbf{x}_*) \leq \frac{L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{4n + 2}.$$

They construct a Huber-like function f for which GD achieves that bound.
Case closed for GD.

$O(1/n)$ rate is undesirably slow.

Heavy ball method

iteration (Polyak, 1987):

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{\alpha}{L} \nabla f(\mathbf{x}_n) + \underbrace{\beta (\mathbf{x}_n - \mathbf{x}_{n-1})}_{\text{momentum!}} \quad (\text{for implementation})$$

$$= \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n \underbrace{\alpha \beta^{n-k}}_{\text{coefficients}} \nabla f(\mathbf{x}_k) \quad (\text{for analysis})$$

stacking:

$$\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_{N-1} \\ \mathbf{x}_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N-2} \\ \mathbf{x}_{N-1} \end{bmatrix} - \frac{1}{L} \left(\underbrace{\begin{bmatrix} \alpha & 0 & 0 & \dots & 0 \\ \alpha\beta & \alpha & 0 & \dots & 0 \\ & & \ddots & & \\ \alpha\beta^{N-2} & \dots & \alpha\beta & \alpha & 0 \\ \alpha\beta^{N-1} & \dots & \alpha\beta^2 & \alpha\beta & \alpha \end{bmatrix}}_{H_{\text{HB}}} \otimes \mathbf{I} \right) \begin{bmatrix} \nabla f(\mathbf{x}_0) \\ \nabla f(\mathbf{x}_1) \\ \vdots \\ \nabla f(\mathbf{x}_{N-2}) \\ \nabla f(\mathbf{x}_{N-1}) \end{bmatrix}$$

Here, $N \times N$ coefficient matrix H_{HB} is lower triangular.

- How to choose α and β ?
- How to optimize $N \times N$ coefficient matrix H more generally?

General first-order method class

General “first-order” (FO) iteration:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n h_{n+1,k} \nabla f(\mathbf{x}_k)$$

stacking:

$$\begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \vdots \\ \mathbf{x}_{N-1} \\ \mathbf{x}_N \end{bmatrix} = \begin{bmatrix} \mathbf{x}_0 \\ \mathbf{x}_1 \\ \vdots \\ \mathbf{x}_{N-2} \\ \mathbf{x}_{N-1} \end{bmatrix} - \frac{1}{L} \left(\underbrace{\begin{bmatrix} h_{1,0} & 0 & 0 & \dots & 0 \\ h_{2,0} & h_{2,1} & 0 & \dots & 0 \\ & & \ddots & & \\ h_{N,0} & h_{N,1} & \dots & h_{N,N-2} & h_{N,N-1} \end{bmatrix}}_{H_{\text{FO}}} \otimes \mathbf{I} \right) \begin{bmatrix} \nabla f(\mathbf{x}_0) \\ \nabla f(\mathbf{x}_1) \\ \vdots \\ \nabla f(\mathbf{x}_{N-2}) \\ \nabla f(\mathbf{x}_{N-1}) \end{bmatrix}$$

Primary goals:

- Analyze convergence rate of FO for any given H
- Optimize $N \times N$ lower-triangular (“causal”) step-size coefficient matrix H .
 - fast convergence
 - efficient recursive implementation
 - universal (design *prior* to iterating)

Not: Barzilai-Borwein gradient method

Barzilai & Borwein, 1988

$$\mathbf{g}^{(n)} \triangleq \nabla f(\mathbf{x}_n)$$
$$\alpha_n = \frac{\|\mathbf{x}_n - \mathbf{x}_{n-1}\|^2}{\langle \mathbf{x}_n - \mathbf{x}_{n-1}, \mathbf{g}^{(n)} - \mathbf{g}^{(n-1)} \rangle}$$
$$\mathbf{x}_{n+1} = \mathbf{x}_n - \alpha_n \nabla f(\mathbf{x}_n).$$

Not in “first-order” class FO.

Neither are methods like

- steepest descent (with line search),
- conjugate gradient,
- quasi-Newton ...

Nesterov's fast gradient method (FGM1)

Nesterov (1983) iteration: Initialize: $t_0 = 1, \mathbf{z}_0 = \mathbf{x}_0$

$$\begin{aligned} \mathbf{z}_{n+1} &= \mathbf{x}_n - \frac{1}{L} \nabla f(\mathbf{x}_n) && \text{(usual GD update)} \\ t_{n+1} &= \frac{1}{2} \left(1 + \sqrt{1 + 4t_n^2} \right) && \text{(magic momentum factors)} \\ \mathbf{x}_{n+1} &= \mathbf{z}_{n+1} + \frac{t_n - 1}{t_{n+1}} (\mathbf{z}_{n+1} - \mathbf{z}_n) && \text{(update with momentum)}. \end{aligned}$$

Reverts to GD if $t_n = 1, \forall n$.

FGM1 is in class FO:
$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n h_{n+1,k} \nabla f(\mathbf{x}_k)$$

$$h_{n+1,k} = \begin{cases} \frac{t_n - 1}{t_{n+1}} h_{n,k}, & k = 0, \dots, n-2 \\ \frac{t_n - 1}{t_{n+1}} (h_{n,n-1} - 1), & k = n-1 \\ 1 + \frac{t_n - 1}{t_{n+1}}, & k = n. \end{cases} \quad \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1.25 & 0 & 0 & 0 & 0 \\ 0 & 0.10 & 1.40 & 0 & 0 & 0 \\ 0 & 0.05 & 0.20 & 1.50 & 0 & 0 \\ 0 & 0.03 & 0.11 & 0.29 & 1.57 & 0 \\ 0 & 0.02 & 0.07 & 0.18 & 0.36 & 1.62 \end{bmatrix}$$

Nesterov FGM1 optimal convergence rate

Shown by Nesterov to be $O(1/n^2)$ for “auxiliary” sequence:

$$f(\mathbf{z}_n) - f(\mathbf{x}_*) \leq \frac{2L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{(n+1)^2}.$$

Nesterov constructed a function f such that FGM1 achieves

$$\frac{\frac{3}{32}L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{(n+1)^2} \leq f(\mathbf{x}_n) - f(\mathbf{x}_*).$$

Thus $O(1/n^2)$ rate of FGM1 is optimal.

New results (Donghwan Kim, 2014):

- Bound on convergence rate of primary sequence $\{\mathbf{x}_n\}$:

$$f(\mathbf{x}_n) - f(\mathbf{x}_*) \leq \frac{2L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{(n+2)^2}.$$

- Verifies (numerically inspired) conjecture of Drori & Teboulle (2013).

Overview

General first-order (FO) iteration:

$$\mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n h_{n+1,k} \nabla f(\mathbf{x}_k)$$

- Analyze (*i.e.*, bound) convergence rate as a function of
 - number of iterations N
 - Lipschitz constant L
 - step-size coefficients $H = \{h_{n+1,k}\}$
 - Distance to a solution: $R = \|\mathbf{x}_0 - \mathbf{x}_\star\|$
- Optimize H by minimizing the bound

Ideal “universal” bound for first-order methods

For given

- number of iterations N
- Lipschitz constant L
- step-size coefficients $H = \{h_{n+1,k}\}$
- distance to a solution: $R = \|\mathbf{x}_0 - \mathbf{x}_*\|$

bound the worst-case convergence rate of FO algorithm:

$$B_1(H, R, L, N) \triangleq \max_{f \in \mathcal{F}_L} \max_{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^M} \max_{\substack{\mathbf{x}_* \in \mathcal{X}^*(f) \\ \|\mathbf{x}_0 - \mathbf{x}_*\| \leq R}} f(\mathbf{x}_N) - f(\mathbf{x}_*)$$

$$\text{such that } \mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n h_{n+1,k} \nabla f(\mathbf{x}_k), \quad n = 0, \dots, N-1.$$

Clearly for any FO method:

$$f(\mathbf{x}_N) - f(\mathbf{x}_*) \leq B_1(H, R, L, N)$$

Towards practical bounds for first-order methods

For convex functions with L -Lipschitz gradients

$$\frac{1}{2L} \|\nabla f(\mathbf{x}) - \nabla f(\mathbf{z})\|^2 \leq f(\mathbf{x}) - f(\mathbf{z}) - \langle \nabla f(\mathbf{z}), \mathbf{x} - \mathbf{z} \rangle, \quad \forall \mathbf{x}, \mathbf{z} \in \mathbb{R}^M.$$

Drori & Teboulle (2013) use this inequality to propose a “more tractable” bound:

$$B_2(H, R, L, N) \triangleq \max_{\mathbf{g}_0, \dots, \mathbf{g}_N \in \mathbb{R}^M} \max_{\delta_0, \dots, \delta_N \in \mathbb{R}} \max_{\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_N \in \mathbb{R}^M} \max_{\mathbf{x}_*: \|\mathbf{x}_0 - \mathbf{x}_*\| \leq R} LR\delta_N^2$$

$$\text{such that } \mathbf{x}_{n+1} = \mathbf{x}_n - \frac{1}{L} \sum_{k=0}^n h_{n+1,k} R \mathbf{g}_k, \quad n = 0, \dots, N-1,$$

$$\frac{1}{2} \|\mathbf{g}_i - \mathbf{g}_j\|^2 \leq \delta_i - \delta_j - \frac{1}{R} \langle \mathbf{g}_j, \mathbf{x}_i - \mathbf{x}_j \rangle, \quad i, j = 0, \dots, N, *$$

where $\mathbf{g}_n = \frac{1}{LR} \nabla f(\mathbf{x}_n)$ and $\delta_n = \frac{1}{LR} (f(\mathbf{x}_n) - f(\mathbf{x}_*))$.

For any FO method:

$$f(\mathbf{x}_N) - f(\mathbf{x}_*) \leq B_1(H, R, L, N) \leq B_2(H, R, L, N)$$

However, even B_2 is as of yet unsolved.

Numerical bounds for first-order methods

Drori & Teboulle (2013) further relax the bound leading eventually to a still simpler optimization problem (with no known closed-form solution):

$$f(\mathbf{x}_N) - f(\mathbf{x}_*) \leq B_1(H, R, L, N) \leq B_2(H, R, L, N) \leq B_3(H, R, L, N).$$

For given step-size coefficients H , and given number of iterations N , they use a semi-definite program (SDP) to compute B_3 numerically.

The find numerically that for the FGM1 choice of H , the convergence bound B_3 is slightly tighter than $\frac{2L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{(N+1)^2}$.

Optimizing step-size coefficients numerically

Drori & Teboulle (2013) also compute numerically the minimizer over H of their relaxed bound for given N using a semi-definite program (SDP):

$$H^* = \arg \min_H B_3(H, R, L, N).$$

Numerical solution for H^* for $N = 5$ iterations: [Fig. from Drori & Teboulle (2013)]

$$\begin{aligned} 0. & \text{ Input: } f \in C_L^{1,1}(\mathbb{R}^d), x_0 \in \mathbb{R}^d, \\ 1. & x_1 = x_0 - \frac{1.6180}{L} f'(x_0), \\ 2. & x_2 = x_1 - \frac{0.1741}{L} f'(x_0) - \frac{2.0194}{L} f'(x_1), \\ 3. & x_3 = x_2 - \frac{0.0756}{L} f'(x_0) - \frac{0.4425}{L} f'(x_1) - \frac{2.2317}{L} f'(x_2), \\ 4. & x_4 = x_3 - \frac{0.0401}{L} f'(x_0) - \frac{0.2350}{L} f'(x_1) - \frac{0.6541}{L} f'(x_2) - \frac{2.3656}{L} f'(x_3), \\ 5. & x_5 = x_4 - \frac{0.0178}{L} f'(x_0) - \frac{0.1040}{L} f'(x_1) - \frac{0.2894}{L} f'(x_2) - \frac{0.6043}{L} f'(x_3) - \\ & \frac{2.0778}{L} f'(x_4). \end{aligned}$$

Drawbacks

- Must choose N in advance
- Requires $O(N)$ memory for all gradient vectors $\{\nabla f(\mathbf{x}_n)\}_{n=1}^N$
- $O(N^2)$ computation for N iterations

Benefit: convergence bound (for specific N) $\approx 2 \times$ lower than for Nesterov's FGM1.

New analytical solution

- Analytical solution for optimized step-size coefficients (Donghwan Kim, 2014):

$$H^* : h_{n+1,k} = \begin{cases} \frac{\theta_{n-1}}{\theta_{n+1}} h_{n,k}, & k = 0, \dots, n-2 \\ \frac{\theta_{n-1}}{\theta_{n+1}} (h_{n,n-1} - 1), & k = n-1 \\ 1 + \frac{2\theta_{n-1}}{\theta_{n+1}}, & k = n. \end{cases}$$

$$\theta_n = \begin{cases} 1, & n = 0 \\ \frac{1}{2} \left(1 + \sqrt{1 + 4\theta_{n-1}^2} \right), & n = 1, \dots, N-1 \\ \frac{1}{2} \left(1 + \sqrt{1 + 8\theta_{n-1}^2} \right), & n = N. \end{cases}$$

- Analytical convergence bound for these optimized step-size coefficients:

$$f(\mathbf{x}_N) - f(\mathbf{x}_*) \leq B_3(H^*, R, L, N) = \frac{1L \|\mathbf{x}_0 - \mathbf{x}_*\|_2^2}{(N+1)(N+1+\sqrt{2})}.$$

Of course bound is $O(1/N^2)$, but constant is twice better than that of Nesterov.
No numerical SDP needed \implies feasible for large N .

Optimized gradient method (OGM1)

Donghwan Kim (2014) found efficient recursive iteration:

Initialize: $\theta_0 = 1, \mathbf{z}_0 = \mathbf{x}_0$

$$\mathbf{z}_{n+1} = \mathbf{x}_n - \frac{1}{L} \nabla f(\mathbf{x}_n) \quad (\text{usual GD update})$$

$$\theta_n = \begin{cases} \frac{1}{2} \left(1 + \sqrt{1 + 4\theta_{n-1}^2} \right), & n = 1, \dots, N-1 \\ \frac{1}{2} \left(1 + \sqrt{1 + 8\theta_{n-1}^2} \right), & n = N \end{cases} \quad (\text{momentum factors})$$

$$\mathbf{x}_{n+1} = \mathbf{z}_{n+1} + \frac{\theta_n - 1}{\theta_{n+1}} (\mathbf{z}_{n+1} - \mathbf{z}_n) + \underbrace{\frac{\theta_n}{\theta_{n+1}} (\mathbf{z}_{n+1} - \mathbf{x}_n)}_{\text{new momentum}}.$$

Reverts to Nesterov's FGM1 if the **new terms** are removed.

- Very simple modification of existing Nesterov code
- No need to choose N in advance (or solve SDP);
use favorite stopping rule then run one last “decreased momentum” step.
- Factor of 2 better upper bound than Nesterov's “optimal” FGM1.

(Proofs omitted.)

Numerical Example(s)

Machine learning (logistic regression)

To learn weights \mathbf{x} of binary classifier given feature vectors $\{\mathbf{v}_i\}$ and labels $\{y_i\}$:

$$\hat{\mathbf{x}} = \arg \min_{\mathbf{x}} f(\mathbf{x}), \quad f(\mathbf{x}) = \sum_i \psi(y_i \langle \mathbf{x}, \mathbf{v}_i \rangle) + \beta \frac{1}{2} \|\mathbf{x}\|_2^2,$$

where $y_i = \pm 1$.

$$\text{logistic: } \psi(t) = \log(1 + e^{-t}), \quad \dot{\psi}(t) = \frac{-1}{e^t + 1}, \quad \ddot{\psi}(t) = \frac{e^t}{(e^t + 1)^2} \in \left(0, \frac{1}{4}\right]$$

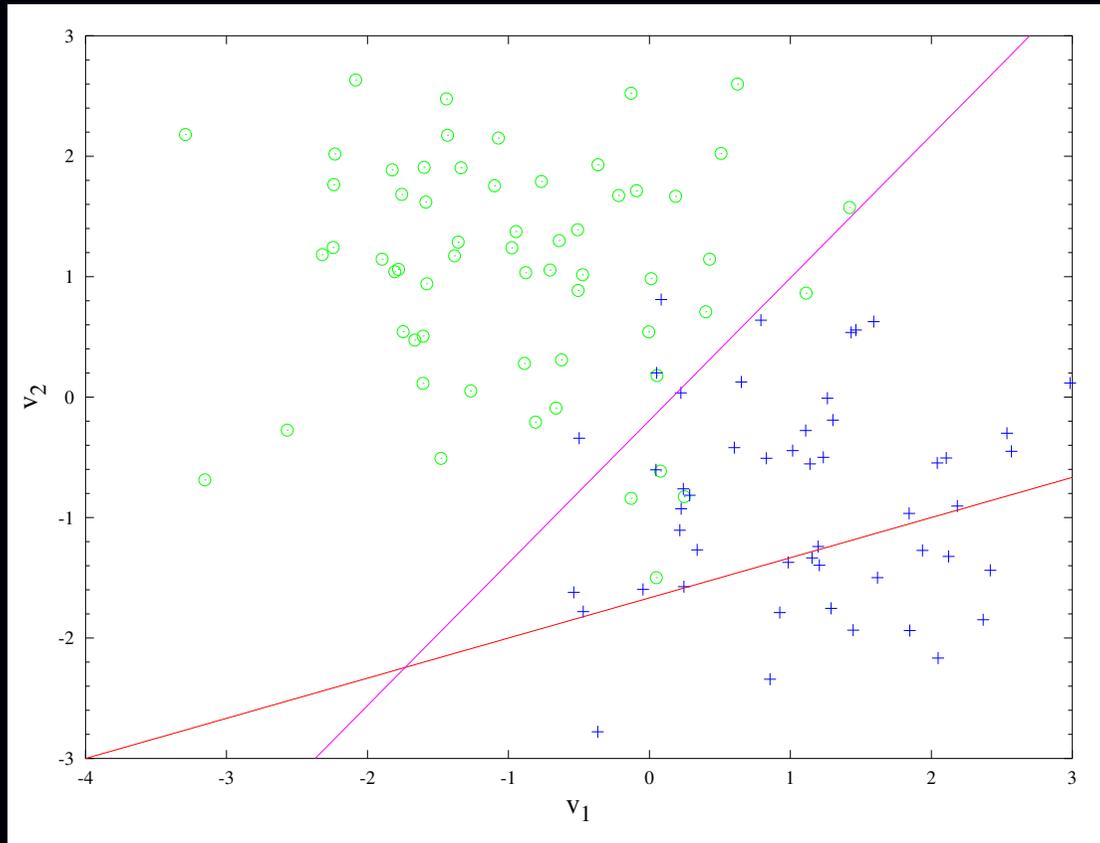
$$\text{Gradient } \nabla f(\mathbf{x}) = \sum_i y_i \mathbf{v}_i \dot{\psi}(y_i \langle \mathbf{x}, \mathbf{v}_i \rangle) + \beta \mathbf{x}$$

Hessian is positive definite so strictly convex:

$$\nabla^2 f(\mathbf{x}) = \sum_i \mathbf{v}_i \ddot{\psi}(y_i \langle \mathbf{x}, \mathbf{v}_i \rangle) \mathbf{v}_i' + \beta \mathbf{I} \preceq \frac{1}{4} \sum_i \mathbf{v}_i \mathbf{v}_i' + \beta \mathbf{I}$$

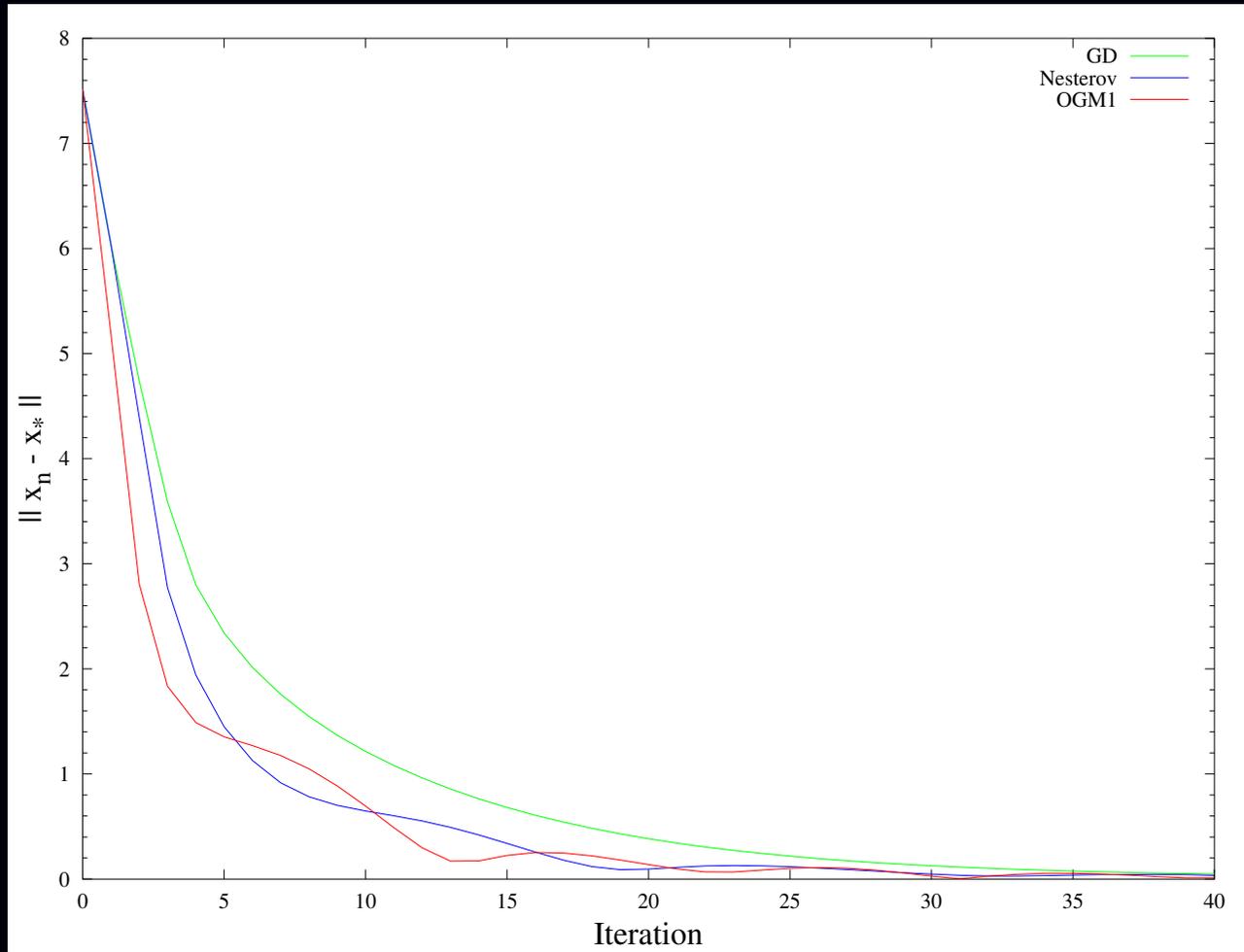
$$\implies L \triangleq \frac{1}{4} \rho \left(\sum_i \mathbf{v}_i \mathbf{v}_i' \right) + \beta \geq \max_{\mathbf{x}} \rho(\nabla^2 f(\mathbf{x}))$$

Numerical Results: logistic regression

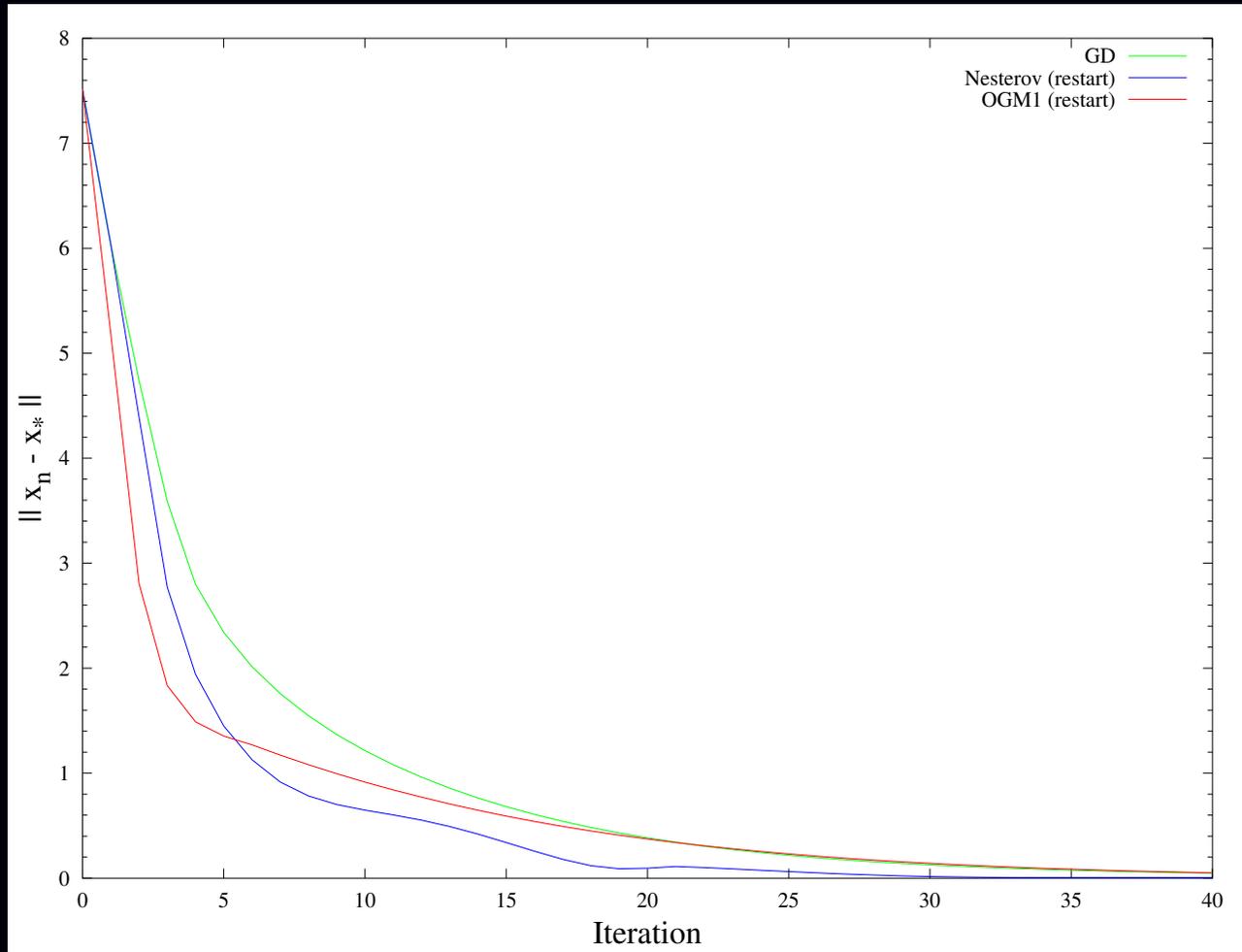


Training data, initial decision boundary (red), final decision boundary (magenta)

Numerical Results: convergence rates

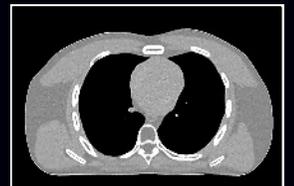
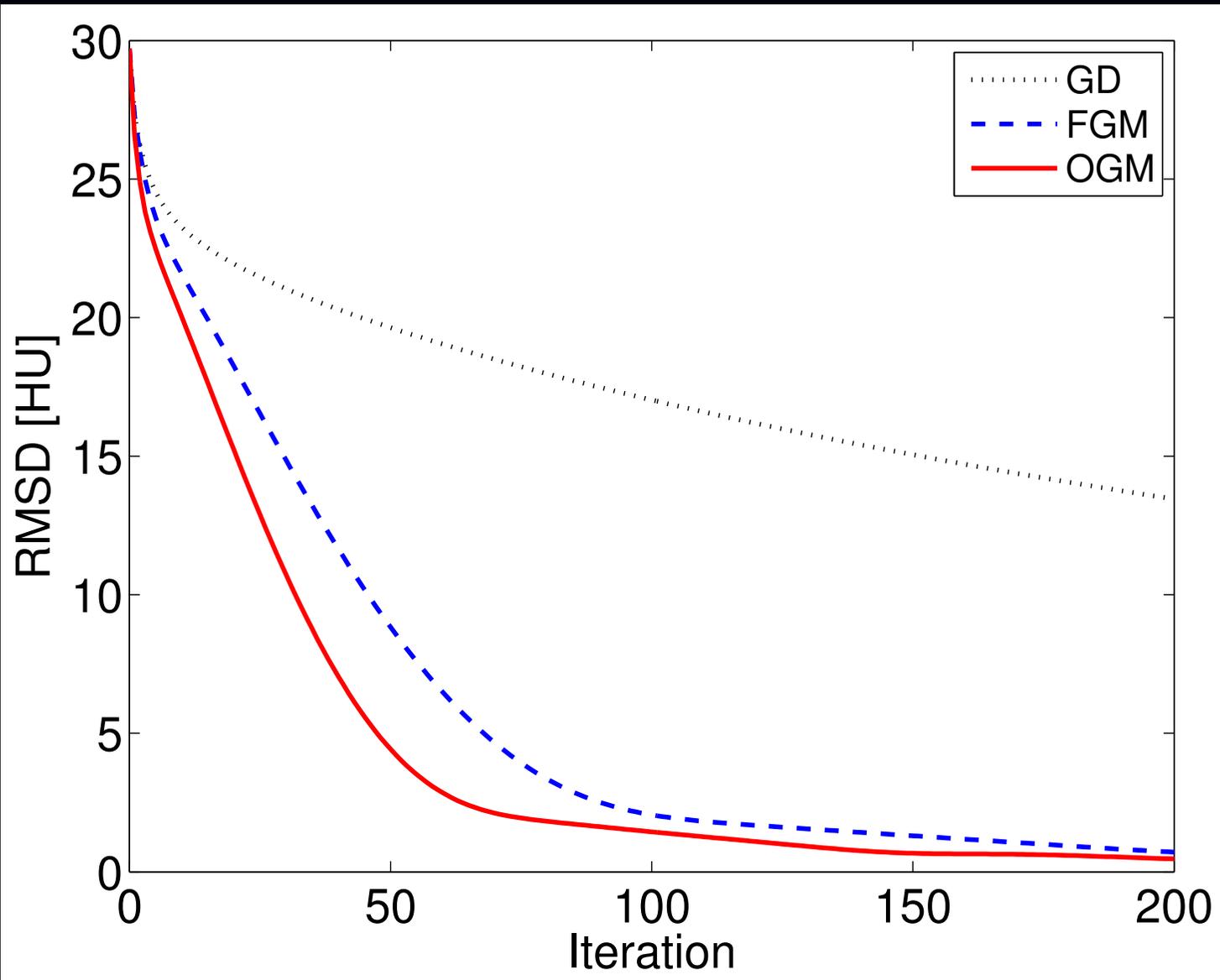


Numerical Results: adaptive restart



O'Donoghue & Candès, 2014

Low-dose 2D X-ray CT image reconstruction simulation



Summary

New optimized first-order minimization algorithm

Simple implementation akin to Nesterov's FGM

Analytical converge rate bound

Bound is $2\times$ better than Nesterov

Future work

- Constraints
- Non-smooth cost functions, *e.g.*, ℓ_1
- Tighter bounds
- Strongly convex case
- Asymptotic / local convergence rates
- Incremental gradients
- Stochastic gradient descent
- Adaptive restart
- Low-dose 3D X-ray CT image reconstruction

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