

First-Order Methods for Differentiable “Nonsmooth” Convex Optimization: A Tale of Frank-Wolfe and Multiplicative-Gradient

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- ① Introduction to “Standard” Gradient Methods
 - Binary Classification
 - Canonical Model: Logistic Regression
- ② “Non-Standard” Applications
- ③ Generalized Frank-Wolfe Method for Convex Composite Optimization Involving a Log-Homogeneous Barrier
 - Problem of Interest
 - Our Method
 - Computational Guarantees
 - Numerical Experiments
- ④ Generalized Multiplicative Gradient Method
 - An Interesting Story
 - AMG Method on Applications
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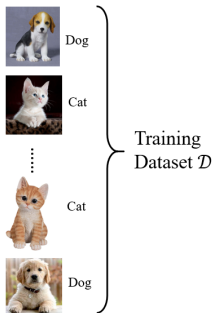
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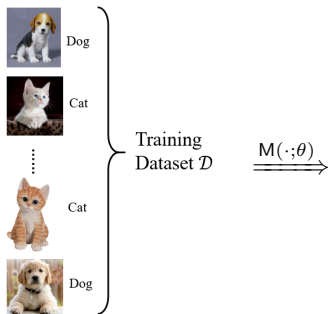
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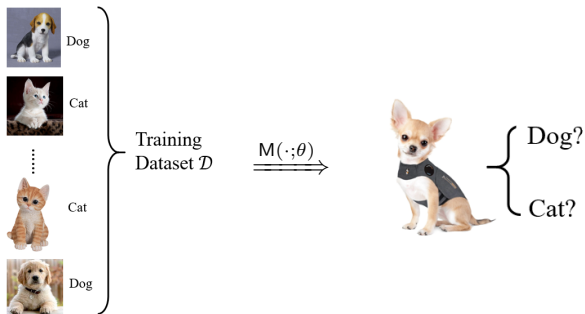
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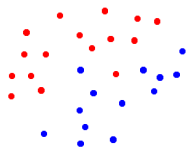
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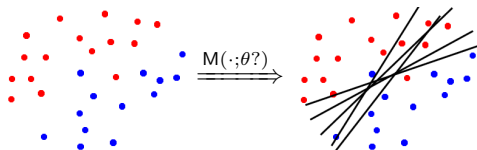
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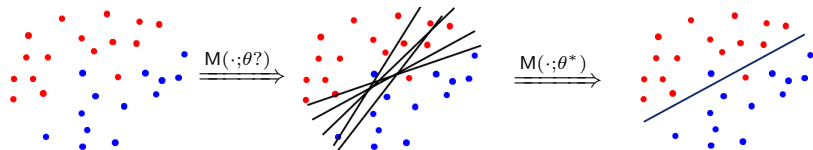
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- ▷ By “smooth”, we mean $f_{\text{LR}}(\cdot)$ has *Lipschitz gradient* on \mathbb{R}^{n+1} :

$$\|\nabla f_{\text{LR}}(\theta) - \nabla f_{\text{LR}}(\theta')\| \leq L \|\theta - \theta'\|, \quad \forall \theta, \theta' \in \mathbb{R}^{n+1} \quad (\text{LG})$$

where $L = \frac{1}{4m} \sum_{i=1}^m (\|x_i\|^2 + 1)$ is called the *smoothness parameter* of $f_{\text{LR}}(\cdot)$.

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- ▷ The smoothness parameter L appears in both *step-size* and *computational guarantees*.
- ▷ This property is also critical in ensuring sufficient decrease in line search.
- ▷ Without property, (GM) may fail both in *theory* and *practice*, and the same applies to its variants (e.g., accelerated, stochastic and coordinate versions).

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- ▷ Learning of Multivariate Hawkes Process
- ▷ Positron Emission Tomography
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Let us briefly examine several of these problems ...

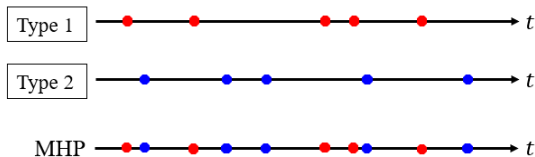
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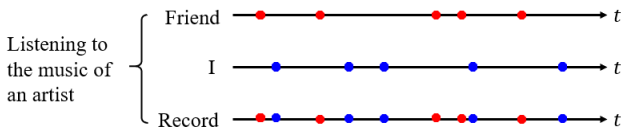
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Learning of Multivariate Hawkes Process (MHP)

- ▷ An m -dimensional MHP is a marked temporal point process that consist of m types of events, indexed by $1, \dots, m$.
- ▷ MHPs are both self-exciting and mutually-exciting.
 - Occurrence of one type of events (say type 1) increases the chance of occurrence of both *this* type of events and *other* type of events (say type 2) in the future.
- ▷ Numerous applications:
 - Seismology: Modeling earthquake aftershocks
 - Finance: Modeling limit order books
 - Analysis of social network: Modeling influences among individuals



Learning MHPs helps reveal
the network influence structure!

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where $\mathcal{H}_k := \{i \in [n] : t_i < t, u_i = k\}$, and from \mathcal{E} , we can compute

$$w_{i, l} \geq 0 \quad \text{and} \quad v_l > 0, \quad \forall i \in \mathcal{H}_k, \quad \forall l \in [m]$$

Equivalent Formulation of (MHP)

Using standard techniques, we can reformulate (MHP) to the following problem:

$$\min_x \left\{ F(x) := - \sum_{j=1}^m p_j \ln(a_j^\top x) \right\} \quad \text{s. t.} \quad x \in \Delta_n \quad (\text{PET})$$

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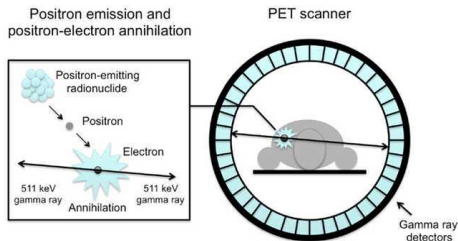
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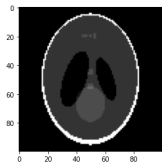
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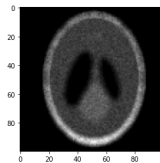
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- ▷ For all $j \in [m]$, let $p_j > 0$, $a_j \in \mathbb{R}_+^n$, $a_j \neq 0$.
- ▷ $\Delta_n := \{x \in \mathbb{R}_+^n : \sum_{i=1}^n x_i = 1\}$ is the unit simplex in \mathbb{R}^n .

Poisson Image Deblurring with TV Regularization

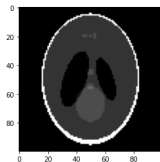


True image X

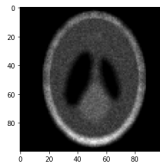


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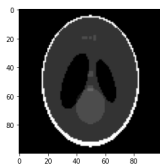
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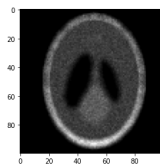
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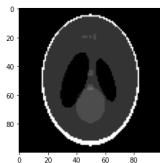
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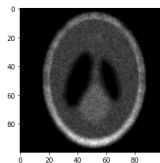
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- ▶ The observed image Y is obtained by first passing X through \mathbf{A} , and then contaminated by additive independent (entry-wise) Poisson noise.

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▷ For convenience, we

- represent the linear operator \mathbf{A} in its matrix form $A \in \mathbb{R}^{N \times N}$ ($N := mn$) and let the l -th row of A be a_l^\top for $l \in [N]$,
- let $x = \text{vec}(X) \in \mathbb{R}^N$ and $X = \text{mat}(x) \in \mathbb{R}^{m \times n}$, and similar for y and Y .

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- ▷ We seek to recover X from Y (equivalently x from y) using maximum-likelihood estimation on the TV-regularized problem:

$$\begin{aligned} \min_{x \in \mathbb{R}^N} \quad & - \sum_{l=1}^N y_l \ln(a_l^\top x) + \left(\sum_{l=1}^N a_l\right)^\top x + \lambda \text{TV}(x) \\ \text{s. t.} \quad & 0 \leq x \leq Me \end{aligned} \tag{Deblur}$$

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- ▷ (**Deblur**) has a (standard) total-variation (TV) regularization term to recover a smooth image with sharp edges. The TV term is given by

$$\text{TV}(x) := \sum_{i,j} |X_{i,j} - X_{i,j+1}| + \sum_{i,j} |X_{i,j} - X_{i+1,j}|.$$

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▷ Nesterov [Nes11] later showed that (SDP) above can be equivalently written in the dual form:

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where $A = R^\top R$ (Cholesky factorization) and $R := [r_1 \ \cdots \ r_n]$, and \mathbb{S}_+^n denotes the cone of $n \times n$ real symmetric PSD matrices.

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▷ Nesterov [Nes11] proposed his “barrier subgradient method” for solving (RBQP) with convergence rate $O(\ln(t)/\sqrt{t})$, but I will present a new gradient method with convergence rate $O(1/t)$!

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- ▷ Quantum State Tomography:
An Important problem in quantum computing and quantum information theory.

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- ▷ For each problem class, we will develop a new gradient method for tackling the problem:
 - ① A generalized Frank-Wolfe method for convex composite optimization involving a log-homogeneous barrier.
 - ② An analog of the “Multiplicative Gradient” method for convex optimization involving a log-homogeneous and gradient log-convex function.

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- ▷ $h : \mathbb{R}^n \rightarrow \mathbb{R} \cup \{+\infty\}$ is a closed and convex function, with compact domain $\mathcal{X} := \text{dom } h$
- ▷ All the applications above (except **RBQP**) fall under (**P-FW**).

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 - ① $|D^3 f(u)[w, w, w]| \leq 2\|w\|_u^3 \quad \forall u \in \text{int } \mathcal{K}, \forall w \in \mathbb{R}^m$,
 - ② $f(u_k) \rightarrow \infty$ for any $\{u_k\}_{k \geq 1} \subseteq \text{int } \mathcal{K}$ such that $u_k \rightarrow u \in \text{bd } \mathcal{K}$,
 - ③ $f(tu) = f(u) - \theta \ln(t) \quad \forall u \in \text{int } \mathcal{K}, \forall t > 0$.

where $\|w\|_u := \langle \nabla^2 f(u)w, w \rangle^{1/2}$ denotes the local norm of w at $u \in \text{int } \mathcal{K}$.

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- ▷ For some applications (e.g., PET and D-Optimal Design), the step-size can also be efficiently computed via exact line-search.
- ▷ Our algorithm does not use the special properties of the barrier or the logarithmic homogeneity of f . However, these properties are critical in deriving the computational guarantees.

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- ▷ (Iteration complexity for ε -optimality gap) Let K_ε be the number of iterations for gFW-LHSCB to obtain $\delta_k \leq \varepsilon$. Then:

$$K_\varepsilon \leq \lceil 5.3(\delta_0 + \theta + R_h) \ln(10.6\delta_0) \rceil + \left\lceil \frac{12(\theta + R_h)^2}{\varepsilon} \right\rceil .$$

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For many applications, all of the three quantities can be easily estimated, and hence the computational guarantees are known before running the algorithm.

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Numerical Experiments on Poisson Image Deblurring with TV Regularization

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- ▷ We chose the starting point $x^0 = \text{vec}(Y)$ (the vectorized noisy image), and we set $\lambda = 0.01$.

Results: Recovered Images

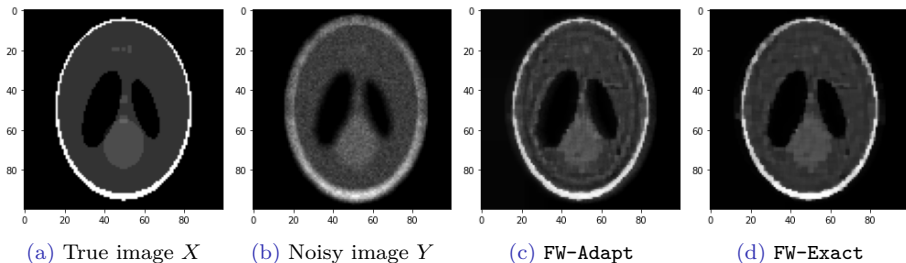
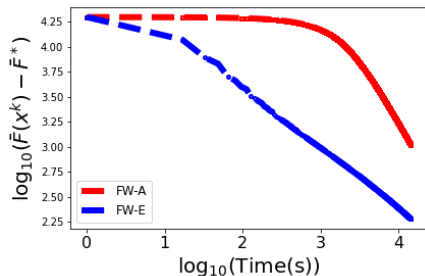
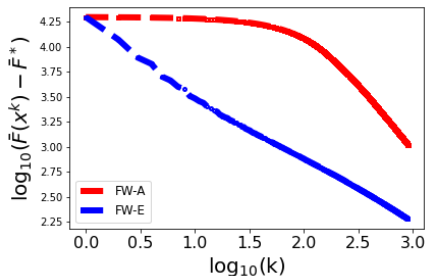


Figure 1: True, noisy and recovered Shepp-Logan phantom images.

Results: Optimality Gaps versus Time and Iterations



(a) Optimality gap versus time (in seconds)



(b) Optimality gap versus iterations

Figure 2: Comparison of optimality gaps of FW-Adapt (FW-A) and FW-Exact (FW-E) for image recovery of the Shepp-Logan phantom image.

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Motivating Example: Positron Emission Tomography

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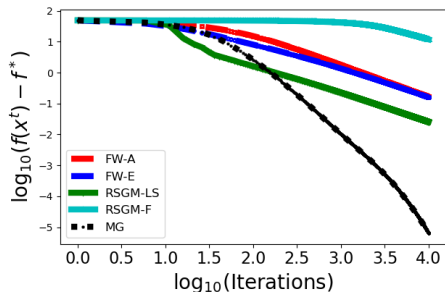
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FW-A & FW-E [Dvu20; ZF22]: Generalized FW methods for LHB (with adaptive stepsize and exact line search)

RSGM-F & RSGM-LS [BBT17; LFN18]: Relatively smooth gradient method (with fixed stepsize and backtracking line search)

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- ▷ More interestingly, there's no constant hidden in $O(\cdot)$:

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Some Deeper Questions

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These questions kept me working for half a year, and I eventually came up with some satisfactory answers to these questions ...

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- ▷ In all of these applications, the objective functions involve “ $\ln(\cdot)$ ”, and hence do not have Lipschitz-gradient on the feasible sets.

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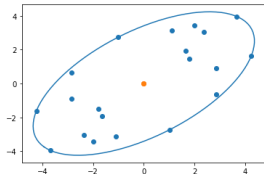
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$$\begin{aligned} \max_X \quad & F(X) := 2 \ln \left(\sum_{i=1}^n \langle X, r_i r_i^\top \rangle^{1/2} \right) \\ \text{s. t.} \quad & X \in \mathbb{S}_+^n, \langle I_n, X \rangle = 1 \end{aligned} \tag{RBQP}$$

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▷ Computational guarantee:

$$F^* - F(\bar{X}^t) \leq \ln(n)/t, \quad \forall t \geq 1 \quad \left[\bar{X}^t := (1/t) \sum_{i=0}^{t-1} X^i \right]$$

Comparison of Computational Guarantees

RSGM [BBT17; LFN18]: Relatively smooth gradient method

FW [ZF21]: Generalized FW method for LHB

GMG: Generalized Multiplicative gradient method

BSG [Nes11]: Barrier subgradient method

Table 1: Comparison of arithmetic-operations complexities
(with $x^0 = (1/n)e$ or $X^0 = (1/n)I_n$)

	RSGM	FW	GMG	BSG	Regime
PET	$O\left(\frac{mn^2}{\varepsilon} \ln\left(\frac{\ln(n)}{\varepsilon}\right)\right)$	$O\left(\frac{m^2n}{\varepsilon}\right)$	$O\left(\frac{mn \ln(n)}{\varepsilon}\right)$	$O\left(\frac{mn^2}{\varepsilon^2} \ln^2\left(\frac{n}{\varepsilon}\right)\right)$	$n = O(\exp(m))$
D-OPT	$O\left(\frac{mn^2}{\varepsilon} \ln\left(\frac{\ln(n/m)}{\varepsilon}\right)\right)$	$O\left(\frac{m^2n}{\varepsilon}\right)$	$O\left(\frac{m^2n \ln(n)}{\varepsilon}\right)$	$O\left(\frac{m^2n^2}{\varepsilon^2} \ln^2\left(\frac{n}{\varepsilon}\right)\right)$	
QST	x?	$O\left(\frac{m^2n^2}{\varepsilon}\right)$	$O\left(\frac{mn^2 \ln(n)}{\varepsilon}\right)$	$O\left(\frac{mn^3}{\varepsilon^2} \ln^2\left(\frac{n}{\varepsilon}\right)\right)$	$n = O(\exp(m))$
RBQP	x?	x?	$O\left(\frac{n^3 \ln(n)}{\varepsilon}\right)$	$O\left(\frac{n^4}{\varepsilon^2} \ln^2\left(\frac{n}{\varepsilon}\right)\right)$	

A Fun Comment From Steve

After presenting this work at U. Waterloo, Steve Vavasis commented:

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“I have been working on optimization for many years, and I have developed a mental map to categorize each talk that I have attended. *But this talk simply doesn't fit into any of the existing categories!*”

- ① Introduction to “Standard” Gradient Methods
 - Binary Classification
 - Canonical Model: Logistic Regression
- ② “Non-Standard” Applications
- ③ Generalized Frank-Wolfe Method for Convex Composite Optimization Involving a Log-Homogeneous Barrier
 - Problem of Interest
 - Our Method
 - Computational Guarantees
 - Numerical Experiments
- ④ Generalized Multiplicative Gradient Method
 - An Interesting Story
 - AMG Method on Applications
- ⑤ Concluding Remarks

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This line of research has great potential, and many problems remain open:

- ▷ Can we identify new problem classes, based on new applications arising in machine learning and data science?
- ▷ For the identified problem classes, are there faster first-order methods that can solve them?
- ▷ Lower bound on computational guarantees?

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- ▷ Besides my current research directions, I am also eager to explore the interface of optimization with other exciting topics:
 - high-dimensional statistics
 - online learning
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 - decision-making under uncertainty ...
- ▷ I also look forward to collaborating with many talented colleagues to discover new opportunities!

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