

Deterministic and Stochastic Gradient Methods for Nonsmooth Nonconvex Regularized Optimization

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Joint work with

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Nonsmooth Nonconvex Optimization

$$\min_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w}) + g_0(\mathbf{w}) + \sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w})$$

f : L -smooth func.

(∇f is Lipschitz continuous with L)

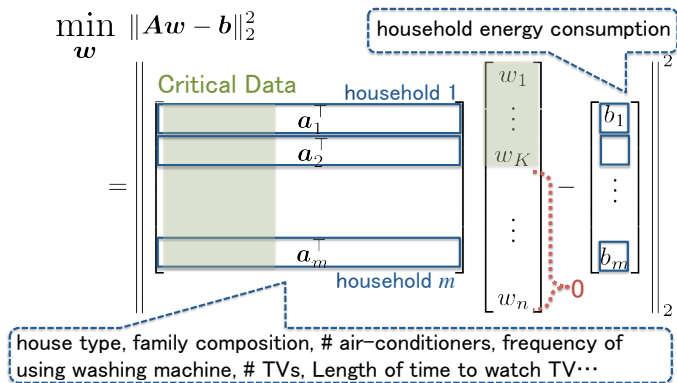
g_0, g_1, \dots, g_m : prox-friendly

($\text{prox}_{\lambda g_i}(\mathbf{w}) := \underset{\mathbf{x}}{\text{argmin}} g_i(\mathbf{x}) + \frac{1}{2\lambda} \|\mathbf{x} - \mathbf{w}\|_2^2$ is easily computed)

$f + g_0$: level-bounded

- f, g_i : can be nonconvex
- g_i : can be nonsmooth
- $\mathcal{A}_i : \mathbb{R}^n \rightarrow \mathbb{R}^{n_i}$ are linear mappings

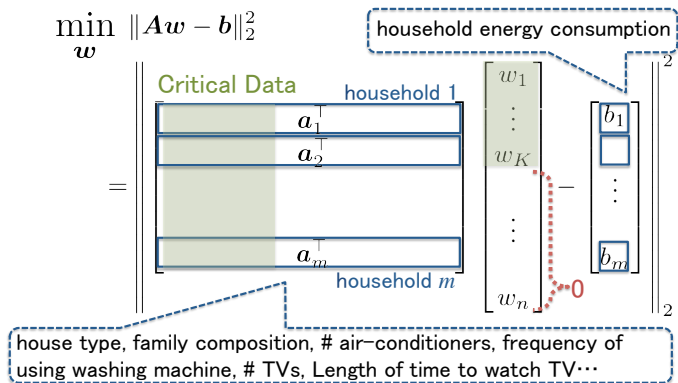
Constrained Sparse Regression Problem



under the ℓ_0 -norm const. $\|w\|_0 \leq K$ and another one $w \in C$.

$$\Rightarrow \min_w \|Aw - b\|_2^2 + \delta_{\{w: \|w\|_0 \leq K\}}(w) + \delta_C(w).$$

Constrained Sparse Regression Problem

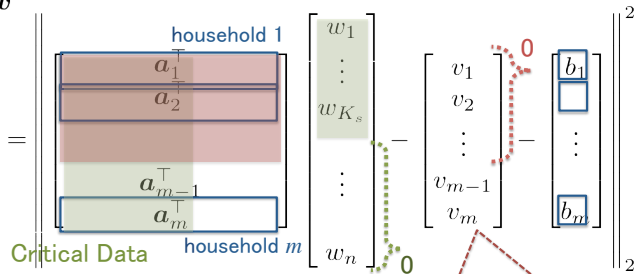


under the ℓ_0 -norm const. $\|\mathbf{w}\|_0 \leq K$ and another one $\mathbf{w} \in C$.

$$\implies \min_{\mathbf{w}} \|\mathbf{A}\mathbf{w} - \mathbf{b}\|_2^2 + \delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\mathbf{w}) + \delta_C(\mathbf{w}).$$

Simultaneous Sparse Recovery and Outlier Detection

$$\min_{\mathbf{v}, \mathbf{w}} \|\mathbf{A}\mathbf{w} - \mathbf{v} - \mathbf{b}\|_2^2$$



By taking nonzero value ($v_m = \mathbf{a}_m^\top \mathbf{w} - b_m$), the residual of sample m can be 0 \rightarrow Outlier

under two ℓ_0 -norm constraints: $\|\mathbf{v}\|_0 \leq K_o$, $\|\mathbf{w}\|_0 \leq K_s$

Nonzero elements in \mathbf{v} are regarded as outliers (the residual = 0)

Unconstrained Sparse Regularized Optimization

$$\min_{\mathbf{w}} f(\mathbf{w}) + \delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\mathbf{w})$$

Assump.: f is L -smooth func. (∇f is Lipschitz continuous with L)

- Proximal Gradient Method (PGM) iteratively solves

$$\begin{aligned} \mathbf{w}_{t+1} &= \mathbf{prox}_{\delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}} \left(\mathbf{w}_t - \frac{1}{L} \nabla f(\mathbf{w}_t) \right) \\ &= \mathbf{proj}_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}} \left(\mathbf{w}_t - \frac{1}{L} \nabla f(\mathbf{w}_t) \right), \end{aligned}$$

where the projection is easy.

Blumensath, Davies ('09), Bertimas, King & Mazumder ('16)

- PGM finds a **stationary point** of the problem.
- Weakness: When other constraints exist, projection onto the intersection of $\{\mathbf{w} : \|\mathbf{w}\|_0 \leq K\}$ and \mathcal{C} is difficult in many cases.

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Unconstrained Sparse Regularized Optimization

$$\min_{\mathbf{w} \in \mathcal{C}} f(\mathbf{w}) + \delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\mathbf{w})$$

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Two Difficulties in General Form

$$\min_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w}) + g_0(\mathbf{w}) + \sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w})$$

g_0, g_1, \dots, g_m : prox-friendly

- In general,

$$\mathbf{prox}_{g_i+g_j}(\mathbf{w}) \neq \mathbf{prox}_{g_i}(\mathbf{prox}_{g_j}(\mathbf{w})) \neq \mathbf{prox}_{g_j}(\mathbf{prox}_{g_i}(\mathbf{w})),$$

though some sufficient condition is shown in Yu (NIPS, 2013).

- $\min_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w}) + g_i(\mathcal{A}_i \mathbf{w})$ becomes difficult than $\min_{\mathbf{w} \in \mathbb{R}^n} f(\mathbf{w}) + g_i(\mathbf{w})$, because the proximal operator of $\tilde{g}_i(\mathbf{w}) := g_i(\mathcal{A}_i \mathbf{w})$ is complicated by the presence of \mathcal{A}_i .

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Examples of Nonconvex Nonsmooth Problems

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Assumption: $\mathbf{prox}_{\lambda g_i}(\mathbf{w}) := \operatorname{argmin}_{\mathbf{x}} g_i(\mathbf{x}) + \frac{1}{2\lambda} \|\mathbf{x} - \mathbf{w}\|^2$ is easy

- Sparse regularizer, e.g., $g_i(\mathbf{w}) := \|\mathbf{w}\|_1, \|\mathbf{w}\|_0$, MCP, SCAD ...
 \mathcal{A}_i can express certain structural sparsity such as $\sum_{i=2}^n |w_i - w_{i-1}|$
 \implies used in image processing for making small the horizontal or/and vertical differences between pixels
- Simple constraint $g_i(\mathbf{w}) := \delta_{\{\mathbf{w}: h_i(\mathbf{w}) \leq 0\}}(\mathbf{w})$ such as
 - ▶ $\operatorname{rank}(\mathbf{W}) \leq K_r$ ($\operatorname{rank}(\mathcal{H}(\mathbf{W})) \leq K_r$ is also possible)
 - ▶ $W_{ij} = M_{ij}, (i, j) \in \mathcal{I}$
 - ▶ $\|\operatorname{vec}(\mathbf{W})\|_0 \leq K_0$
 - ▶ $\mathbf{W} \succeq \mathbf{O}, \dots$

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- DC approach for special cases with $m = 1$ (constrained sparse opt.)
[Tono, T. & Gotoh, arXiv '17], [Gotoh, T. & Tono, MathProg '18]
- DC approach for the general problem [Liu, Pong & T., MathProg '19]
- Applications to system identification,
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Related Works

Assumption: f : L -smooth func., g_0 : prox-friendly

Deterministic approach

$$\min_{\mathbf{w}} f(\mathbf{w}) + g_0(\mathbf{w})$$

Global convergence to a stationary point when $g_0(\mathbf{w})$ is nonconvex

Wright, Nowak & Figueiredo ('09), Gong et al. ('13)

Stochastic approach

$$\min_{\mathbf{w}} h(\mathbf{w}) := \mathbb{E}_{\xi}[F(\mathbf{w}, \xi)] +$$

Non-asymptotic convergence to the *gradient mapping* (an approximation of the gradient of h) when $g_0(\mathbf{w})$ is convex

Ghadimi, Lan & Zhang, ('16), Li & Li ('18)

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Non-asymptotic convergence to an ϵ -stationary point $\bar{\mathbf{w}}$

$$\mathbb{E} [\text{dist}(0, \partial h(\bar{\mathbf{w}}))] \leq \epsilon$$

Key Idea of Our Algorithm (SDCAM)

$$\min_{\mathbf{w}} f(\mathbf{w}) + g_0(\mathbf{w}) + \underbrace{\sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w})}$$

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$$\begin{aligned} \min_{\mathbf{w}} \quad & f(\mathbf{w}) + g_0(\mathbf{w}) + \underbrace{\sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w})}_{\text{Moreau envelope func. of } g_i(\mathcal{A}_i \mathbf{w})} \\ & \geq \sum_{i=1}^m \end{aligned}$$

Moreau env.: $e_{\lambda_i} g_i(\mathbf{w}) := \min_{\mathbf{x}} g_i(\mathbf{x}) + \frac{1}{2\lambda_i} \|\mathbf{x} - \mathbf{w}\|_2^2$

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 \geq & \sum_{i=1}^m \text{Moreau envelope func. of } g_i(\mathcal{A}_i \mathbf{w}) \\
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 \end{aligned}$$

$g_i^{\lambda_i}$: convex functions

$\frac{1}{\lambda_i} \text{prox}_{\lambda_i g_i}(\mathcal{A}_i \mathbf{w}) \subseteq$ the subdifferential of the conv. func $g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w})$.

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Example of Moreau Envelope

Moreau envelope of $g_i(\mathcal{A}_i \mathbf{w}) = \frac{1}{2\lambda_i} \|\mathcal{A}_i \mathbf{w}\|_2^2 - \underbrace{g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w})}_{\text{convex}}$

Moreau envelope of $\delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\mathbf{w}) = \frac{1}{2\lambda} (\|\mathbf{w}\|_2^2 - \|\mathbf{w}\|_{2,K}^2)$

$$\|\mathbf{w}\|_0 \leq K \quad \Leftrightarrow \quad \|\mathbf{w}\|_2^2 - \|\mathbf{w}\|_{2,K}^2 = 0$$

$\|\mathbf{w}\|_{2,K}^2$: Sum of large K elements among w_i^2 , $i \in \{1, 2, \dots, n\}$

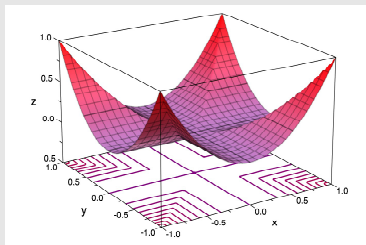
$$\begin{array}{c} \text{Sum: } \|\mathbf{w}\|_2^2 \\ \underbrace{w_{(1)}^2 \geq w_{(2)}^2 \geq \dots \geq w_{(K)}^2}_{\text{Sum: } \|\mathbf{w}\|_{2,K}^2} \geq \underbrace{w_{(K+1)}^2 \dots \geq w_{(n)}^2}_{\text{all 0}} \end{array}$$

Figs of DC representations

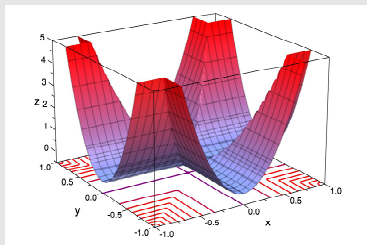
Moreau env. of $\delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\mathbf{w}) = \frac{1}{2\lambda}(\|\mathbf{w}\|_2^2 - \|\mathbf{w}\|_{2,K}^2)$: Penalty term

($\mathbf{w} \in \mathbb{R}^2$ and $K = 1$)

$$\frac{1}{2\lambda} = 1:$$



$$\frac{1}{2\lambda} = 10:$$



Moreau env. of $\delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\cdot) \xrightarrow{\lambda \rightarrow 0} \delta_{\{\mathbf{w}: \|\mathbf{w}\|_0 \leq K\}}(\cdot)$

SDCAM: Successive Difference-of-Convex Approximation Method

$$f(\mathbf{w}) + g_0(\mathbf{w}) + \sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w}) \quad [\text{Liu, Pong \& T., MathProg '19}]$$

$$\geq \left(f(\mathbf{w}) + \sum_{i=1}^m \frac{1}{2\lambda_i} \|\mathcal{A}_i \mathbf{w}\|_2^2 \right) + g_0(\mathbf{w}) - \sum_{i=1}^m g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w}) =: F^\lambda(\mathbf{w})$$

- 1 Decrease λ and ϵ . Terminate when they become almost 0.
- 2 Find an ϵ -stationary point for $\min_{\mathbf{w}} F^\lambda(\mathbf{w})$ with fixed λ .
 - Linearize $-\sum_{i=1}^m g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w})$ at \mathbf{w}_t and construct a convex subproblem
 - Solve the subproblem \Rightarrow Opt. sol: \mathbf{w}_{t+1}
 - Repeat until some termination criteria with ϵ are satisfied.

Theorem \mathbf{w}^* : accumulation point of $\{\mathbf{w}_t\}$. Under some constraint qualification, \mathbf{w}^* satisfies the first-order optimality condition:

$$\mathbf{0} \in \nabla f(\mathbf{w}^*) + \partial g_0(\mathbf{w}^*) + \sum_{i=1}^m \mathcal{A}_i^* \partial g_i(\mathcal{A}_i \mathbf{w}^*)$$

NPG_{major} for $\min_{\mathbf{w}} F^\lambda(\mathbf{w})$

We can use NPG_{major} for

Wright, Nowak & Figueiredo ('09)

$$\min_{\mathbf{w}} \underbrace{\left(f(\mathbf{w}) + \sum_{i=1}^m \frac{1}{2\lambda_i} \|\mathcal{A}_i \mathbf{w}\|_2^2 \right)}_{\text{smooth}} + \underbrace{g_0(\mathbf{w})}_{\text{prox-friendly}} - \underbrace{\sum_{i=1}^m g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w})}_{\text{convex} \rightarrow \text{linearize}}$$

In NPG_{major}, solve the t -th subproblem ($t = 0, 1, \dots$):

$$\min_{\mathbf{w} \in \mathbb{R}^n} \frac{L}{2} \|\mathbf{w} - \mathbf{w}_t\|_2^2 + \left(\nabla f(\mathbf{w}_t) + \sum_{i=1}^m \frac{1}{\lambda_i} \mathcal{A}_i^* [\mathcal{A}_i \mathbf{w}_t - \mathbf{s}_t] \right)^\top \mathbf{w} + g_0(\mathbf{w})$$

until the convergence.

$$\frac{1}{\lambda_i} \mathcal{A}_i^* \mathbf{s}_t \in \frac{1}{\lambda_i} \mathcal{A}_i^* \text{prox}_{\lambda_i g_i}(\mathcal{A}_i \mathbf{w}_t) \subseteq \mathcal{A}_i^* \partial g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w}_t)$$

The t -th Subproblem in $\text{NPG}_{\text{major}}$

In $\text{NPG}_{\text{major}}$, solve the t -th subproblem ($t = 0, 1, \dots$):

$$\begin{aligned} & \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^n} \frac{L}{2} \|\mathbf{w} - \mathbf{w}_t\|_2^2 + \left(\nabla f(\mathbf{w}_t) + \sum_{i=1}^m \frac{1}{\lambda_i} \mathcal{A}_i^* [\mathcal{A}_i \mathbf{w}_t - \mathbf{s}_t] \right)^\top \mathbf{w} + g_0(\mathbf{w}) \\ &= \operatorname{argmin}_{\mathbf{w} \in \mathbb{R}^n} \frac{L}{2} \left\| \mathbf{w} - \left(\mathbf{w}_t - \frac{1}{L} \left(\nabla f(\mathbf{w}_t) + \sum_{i=1}^m \frac{1}{\lambda_i} \mathcal{A}_i^* [\mathcal{A}_i \mathbf{w}_t - \mathbf{s}_t] \right) \right) \right\| + g_0(\mathbf{w}) \\ &\implies \mathbf{w}_{t+1} = \operatorname{prox}_{\frac{1}{L} g_0} \left(\mathbf{w}_t - \frac{1}{L} \left(\nabla f(\mathbf{w}_t) + \sum_{i=1}^m \frac{1}{\lambda_i} \mathcal{A}_i^* [\mathcal{A}_i \mathbf{w}_t - \mathbf{s}_t] \right) \right) \end{aligned}$$

$$\frac{1}{\lambda_i} \mathcal{A}_i^* \mathbf{s}_t \in \frac{1}{\lambda_i} \mathcal{A}_i^* \operatorname{prox}_{\lambda_i g_i}(\mathcal{A}_i \mathbf{w}_t) \subseteq \mathcal{A}_i^* \partial g_i^{\lambda_i}(\mathcal{A}_i \mathbf{w}_t)$$

Which Constraint Should be Approximated by Moreau Env.

Low-rank + sparse matrix completion

$$\begin{aligned} \min_{\mathbf{W} \in \mathbb{R}^{m \times n}} \quad & \frac{1}{2} \|\mathbf{W} - \mathbf{M}\|_F^2 \\ \text{s.t.} \quad & \|\text{vec}(\mathbf{W})\|_0 \leq s, \quad \text{rank}(\mathbf{W}) \leq K \end{aligned}$$

- $\mathbf{M} = \mathbf{M}_1 \mathbf{M}_2 + \sigma \mathbf{\Delta}$, where $\sigma > 0$ is a noise factor. $\mathbf{M}_1 \in \mathbb{R}^{m \times K}$, $\mathbf{M}_2 \in \mathbb{R}^{K \times n}$ and $\mathbf{\Delta}$ have i.i.d. standard Gaussian entries but $m/10$ random rows of \mathbf{M}_1 fixed to zero.
- Fix $n = 500$, $K = 10$ and $s = mn/10$ and change $\sigma \in \{.005, .010, .020\}$ and $m \in \{1000, 2000, 3000\}$.
- Decrease the param. of Moreau envelope λ as $\lambda_t = \frac{1}{10^{t+1}}$.
- Stopping criteria: (dist. of \mathbf{X}^t to each constraint) $\leq 10^{-6} \cdot \|\mathbf{X}^t\|_F$.

Which Constraint Should be Approximated by Moreau Env.

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noise	m	iter		CPU		feas.vio	
		ME. ℓ_0	ME.rank	ME. ℓ_0	ME.rank	ME. ℓ_0	ME.rank
.005	1000	41	5597	4.7	378.1	4.76e-04	1.05e-04
	2000	12	5298	4.0	647.0	6.71e-04	1.52e-04
	3000	12	4618	6.0	862.8	8.20e-04	1.89e-04
.010	1000	4508	7900	379.3	529.2	9.43e-05	2.10e-04
	2000	4453	7526	653.6	912.6	1.34e-04	3.06e-04
	3000	4428	5721	969.5	1080.6	1.64e-04	3.77e-04
.020	1000	4922	11631	413.7	769.2	1.90e-04	4.22e-04
	2000	4634	10267	675.5	1251.3	2.68e-04	6.11e-04
	3000	4580	10859	1003.5	2043.0	3.28e-04	7.55e-04

ME. ℓ_0 (or ME.rank): ℓ_0 -norm (or rank) const. is approximated

Stochastic Setting for Nonsmooth Nonconvex Optimization

Assumption: $F(\cdot, \xi)$: L -smooth func., g_0 : nonsmooth, prox-friendly
 ξ : random vector following a probability distr. P

Stochastic problem

$$\min_{\mathbf{w}} h(\mathbf{w}) := \mathbb{E}_{\xi}[F(\mathbf{w}, \xi)] + g_0(\mathbf{w})$$

or the **finite-sum problem** where the expectation is taken over an empirical distribution func.:

$$\min_{\mathbf{w}} h(\mathbf{w}) := \frac{1}{m} \sum_{i=1}^m F(\mathbf{w}, \xi_i) + g_0(\mathbf{w})$$

- Regression: $F(\mathbf{w}, \xi_i) = (\mathbf{a}_i^\top \mathbf{w} - b_i)^2$ for each data point $\xi_i := (\mathbf{a}_i, b_i)$
- Assume that data size m is huge and $g_0(\mathbf{w})$ is a regularizer, e.g., $g_0(\mathbf{w}) = \|\mathbf{w}\|_p^p$ ($p = 1, 2$), MCP, SCAD ...

SGD for Nonsmooth Nonconvex Optimization

Assumption: $F(\cdot, \xi)$: L -smooth func., g_0 : nonsmooth, prox-friendly
 ξ : random vector following a probability distr. P

Stochastic approach

$$\min_{\mathbf{w}} h(\mathbf{w}) := \mathbb{E}_{\xi}[F(\mathbf{w}, \xi)] + \underbrace{g_0(\mathbf{w})}_{\text{nonconvex}}$$

Non-asymptotic convergence to an ϵ -stationary point $\bar{\mathbf{w}}$

$$\mathbb{E} [\text{dist}(0, \partial h(\bar{\mathbf{w}}))] \leq \epsilon$$

- $g_0(\mathbf{w})$ is convex in Ghadimi, Lan & Zhang ('16), Li & Li ('18), etc.
- $g_0(\mathbf{w})$ can be nonconvex in Metel & Takeda ('19), Xu et al. ('19). A key ingredient is “Moreau envelope”.

Mini-batch Stochastic Gradient Algo. (MBSGA)

Assumption: $F(\cdot, \xi)$: L -smooth func., g_0 : nonsmooth, prox-friendly
 ξ : random vector following a probability distr. P

$$\min_{\mathbf{w}} h(\mathbf{w}) := \mathbb{E}_{\xi}[F(\mathbf{w}, \xi)] + g_0(\mathbf{w})$$

Input: $M := \lceil N^{1/4} \rceil$, $\lambda = \frac{1}{N^{1/4}}$, $\gamma = \min\{\frac{1}{L+\frac{1}{\lambda}}, \frac{1}{\sigma\sqrt{N}}\}$

$R \sim \text{uniform}\{1, \dots, N\}$

for $k = 1, \dots, R - 1$ do

- randomly generate $\{\xi_1^k, \dots, \xi_M^k\}$
- compute the approximate gradient
 $\mathbf{d}^k := \frac{1}{M} \sum_{j=1}^M \nabla F(\mathbf{w}^k, \xi_j^k) + \frac{1}{\lambda}(\mathbf{w}^k - \mathbf{s}^k)$ with $\mathbf{s}^k \in \text{prox}_{\lambda g_0}(\mathbf{w}^k)$
- compute the next iterate $\mathbf{w}^{k+1} = \mathbf{w}^k - \gamma \mathbf{d}^k$

Return \mathbf{w}^R

Convergence Results

$$\mathbb{E} [\text{dist}(0, \partial(h(\mathbf{w}^R)))] \leq O(N^{-1/4})$$

MBSGA gives an ϵ -stationary point \bar{w} in expectation, i.e.,

$$\mathbb{E} [\text{dist}(0, \partial(h(\bar{w})))] \leq \epsilon$$

less than $N = O(\epsilon^{-4})$ iterations.

Table: Comparison of **Mini-batch algorithm (MBSGA)** and **Variance reduction algorithm (VRSGA)** obtained in (b: Xu et al. ('19), a: it's arXiv)

Algorithm	Finite-sum Assumption	Gradient Call Complexity	Proximal Operator Complexity
SSDC-SPG ^a	×	$O(\epsilon^{-8})$	$O(\epsilon^{-8})$
SSDC-SVRG ^a	✓	$O(n\epsilon^{-4})$	$O(\epsilon^{-4})$
MBSGA	×	$O(\epsilon^{-5})$	$O(\epsilon^{-4})$
VRSGA	✓	$O(n^{2/3}\epsilon^{-3})$	$O(\epsilon^{-3})$
SSDC-SPG ^b	×	$O(\epsilon^{-5})$	$O(\epsilon^{-5})$
SSDC-SVRG ^b	✓	$\tilde{O}(n\epsilon^{-3})$	$\tilde{O}(\epsilon^{-3})$

Experimental Results

Application: Binary classification with smooth non-convex loss function and log-sum penalty as regularizer.

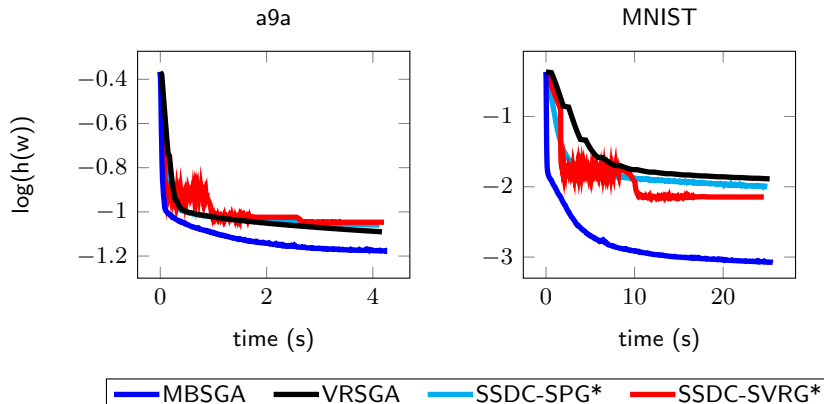


Figure: Comparison to algorithms of Xu et al. (arXiv)

Summary

$$\min_{\mathbf{w}} f(\mathbf{w}) + g_0(\mathbf{w}) + \sum_{i=1}^m g_i(\mathcal{A}_i \mathbf{w})$$

Proposed an approach using proximal operators for
 general **nonconvex nonsmooth** optimization problems
 (e.g. nonconvex sparse problems)

Application

- System identification,

[Liu, Markovsky, Pong & T., SIMAX '20]

⇒ Three rank constraints for Henkel matrices

- Sparse recovery and outlier detection

[Liu, Pong & T., COAP '19]

⇒ Sparse regularization term and ℓ_0 -norm const

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