Accelerated First-Order Methods for Exascale Simulation and Learning

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Outline

- Accelerated Residual Descent Method (ARDM)
- Accelerated Algorithms for Compressed Simulation via Deep Learning
- Generalized Stochastic Frank-Wolfe Algorithm for Loss Minimization
- Thoughts on Directions for the Program

Accelerated Residual Descent Method (ARDM)

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Accelerated methods for exascale simulation

- Numerical simulation in fluid dynamics, solid mechanics, electromagnetism, etc. leads to large nonlinear systems of equations

$$\boldsymbol{f}(\boldsymbol{u}) = \boldsymbol{0} \quad \text{with } \boldsymbol{u} \in \mathbb{R}^{10^{6-10}} \tag{1}$$

- The matrix $\partial \boldsymbol{f} / \partial \boldsymbol{u}$ exceeds the memory available in large supercomputers, therefore matrix-free methods are needed and used
- State-of-the-art massively-parallel matrix-free method for (1) is (preconditioned) forward Euler, which is analogous to gradient descent in the optimization setting
- We extend the ideas of accelerated methods for optimization to devise accelerated methods for nonlinear systems like (1)

Difference between optimization and simulation

	Matrix $\partial \boldsymbol{f} / \partial \boldsymbol{u}$	Eigenvalues of $\partial \boldsymbol{f} / \partial \boldsymbol{u}$
Optimization	Symmetric	Real
Simulation	Non-symmetric	Complex

We use linear stability theory to devise accelerated methods that are better suited to simulation (i.e., to systems with complex eigenvalues)

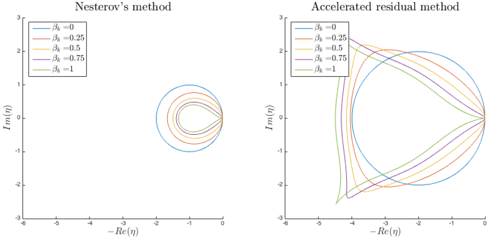


Figure: Stability regions of Nesterov's method and our accelerated residual method. β_k denotes the acceleration parameter. $\eta := \lambda\, \alpha_k$.

Accelerated Residual Descent Method

- Accelerated Nesterov's method

$$\boldsymbol{v}_k = \boldsymbol{u}_k + \beta_k(\boldsymbol{u}_k - \boldsymbol{u}_{k-1}), \tag{2a}$$

$$\boldsymbol{u}_{k+1} = \boldsymbol{v}_k - \alpha_k \boldsymbol{f}(\boldsymbol{v}_k). \tag{2b}$$

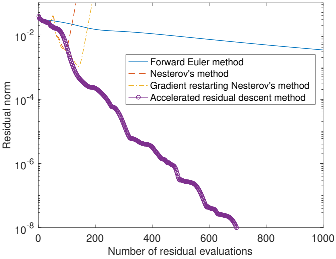
- Our method: Accelerated Residual Descent Method (ARDM)

$$\boldsymbol{v}_k = \boldsymbol{u}_k + \beta_k(\boldsymbol{u}_k - \boldsymbol{u}_{k-1}) - \alpha_k(1+\beta_k)\boldsymbol{f}(\boldsymbol{u}_k), \tag{3a}$$

$$\boldsymbol{u}_{k+1} = \boldsymbol{v}_k - \alpha_k \boldsymbol{f}(\boldsymbol{v}_k). \tag{3b}$$

Extra-term in red makes the method better suited (more robust) for simulation

Numerical results: Burgers equations



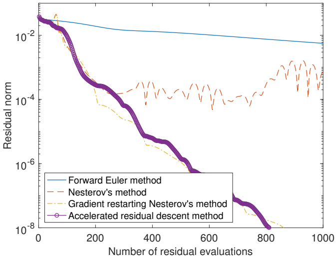


Figure: Left: No preconditioner Right: Block-Jacobi preconditioner

- Accelerated methods (Nesterov, ARDM) converge much faster than non-accelerated method (forward Euler)
- ARDM is more robust than Nesterov's method

Accelerated Algorithms for Compressed Simulation via Deep Learning

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Compressed Simulation

The numerical discretization of many problems of interest produces dynamical systesm of the form

$$\boldsymbol{x}_t = \boldsymbol{f}(\boldsymbol{x}_{t-1}), \qquad \boldsymbol{x}_t \in R^n, \quad t \in [1, \ldots, T] \tag{4}$$

$\boldsymbol{f}()$: nonlinear map

Koopman Theory

Nonlinear discrete-time system can be mapped to a linear discrete-time system of the form

$$g(\boldsymbol{x}_t) = \mathcal{K} g(\boldsymbol{x}_{t-1})$$

$\boldsymbol{g}()$: observable function of the state vector $\boldsymbol{x}$
$\mathcal{K}$: infinite-dimensional linear operator

The Koopman Invariant Subpace

If there exists a finite number of observable functions $\{g_1, \ldots, g_m\}$ that span $\mathcal{G}$ such that

$$\mathcal{K}g \in \mathcal{G}, \qquad \text{for any} \qquad g \in \mathcal{G}$$

then, $\mathcal{G}$ is an invariant subpsace and $\mathcal{K}$ becomes *finite-dimensional*
In this case, instead of solving (4) we can solve the linear problem

$$\boldsymbol{y}_t = \boldsymbol{K}\boldsymbol{y}_{t-1}, \qquad \boldsymbol{y}_t = \boldsymbol{g}(\boldsymbol{x}_t) \tag{5}$$

where $\boldsymbol{g} = [g_1, \ldots, g_m]^T$ and $\boldsymbol{K} = \boldsymbol{Y}\boldsymbol{X}^*$ with
$\boldsymbol{X} = [\boldsymbol{g}(\boldsymbol{x}_0), \ldots, \boldsymbol{g}(\boldsymbol{x}_{T-1})]$, $\boldsymbol{Y} = [\boldsymbol{g}(\boldsymbol{x}_1), \ldots, \boldsymbol{g}(\boldsymbol{x}_T)]$,
and recover

$$\boldsymbol{x}_t = \boldsymbol{g}^{-1}(\boldsymbol{y}_t)$$

Dimensionality Reduction

- Koopman theory allows for model reduction of nonlinear system (4) of dimension n to linear system (5) of dimension m.
- When $m \ll n$ we can have dimensionality reduction by several orders of magnitude.
- Challenges:
  - The construction of $\boldsymbol{K}$ requires the computation of $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_T\}$, i.e., we need to perform the full simulation (4)
  - The second challenge is to construct/recover the vector-valued observable $\boldsymbol{g}$ and its inverse $\boldsymbol{g}^{-1}$.

Learning Koopman Invariant Subspaces

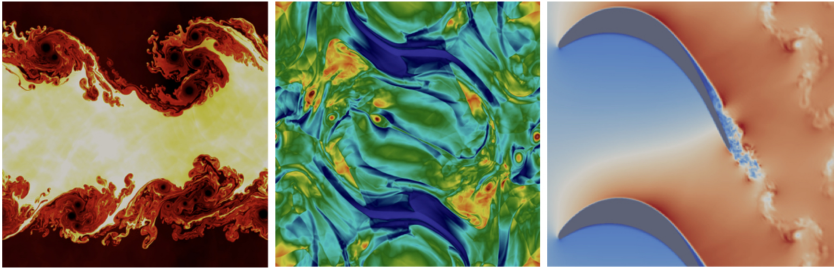
- Learn $(\boldsymbol{K}, \boldsymbol{g}, \boldsymbol{g}^{-1})$ from data $\{\boldsymbol{x}_0, \ldots, \boldsymbol{x}_p\}$ with $p \ll T$
- Training sets $\boldsymbol{X}_0 = [\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{p-1}]$ and $\boldsymbol{X}_1 = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_p]$
- Encoder Neural Net generates $\boldsymbol{X}_0 = [\boldsymbol{x}_0, \ldots, \boldsymbol{x}_{p-1}]$ and $\boldsymbol{X}_1 = [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_p]$
- Advance simulation $\hat{\boldsymbol{y}}_t = (\hat{\boldsymbol{Y}}\hat{\boldsymbol{X}}^*)\,\hat{\boldsymbol{y}}_{t-1}$
- Decoder Neural Net applies mapping $\boldsymbol{g}^{-1}$ to obtain $\{\hat{\boldsymbol{x}}_0, \ldots, \hat{\boldsymbol{x}}_p\}$
- Neural Nets are trained by solving

$$\min_{\boldsymbol{g}} L(\boldsymbol{g}; (\boldsymbol{x}_0, \ldots, \boldsymbol{x}_p)) := \|\boldsymbol{X}_0 - \hat{\boldsymbol{X}}_0(\boldsymbol{g})\|_F^2 + \|\boldsymbol{X}_1 - \hat{\boldsymbol{X}}_1(\boldsymbol{g})\|_F^2$$

where $\hat{\boldsymbol{X}}_0 = [\hat{\boldsymbol{x}}_0, \ldots, \hat{\boldsymbol{x}}_{p-1}]$ and $\hat{\boldsymbol{X}}_1 = [\hat{\boldsymbol{x}}_1, \ldots, \hat{\boldsymbol{x}}_p]$

Compressed Simulation

Plan on applying compressed simulation ideas to problems of practical interest.



High-fidelity simulations of Kelvin-Helmholtz instability (left), Orszag-Tang MHD flow (center), and turbine cascade flow (right). These simulations are performed using a high-order finite element code (DIGASO) developed by the PIs.

Generalized Stochastic Frank-Wolfe (GSFW) for Loss Minimization

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Problem of Interest

The problem of interest is the following general loss minimization problem:

$$\begin{array}{llll} P: & L_n^* = & \min_\beta & L_n(\beta) := \frac{1}{n}\sum_{j=1}^n l_j(x_j^T\beta) \\ & & \text{s.t.} & \beta \in Q \end{array}$$

$l_j(\cdot)$ is a univariate loss function that is strictly convex, differentiable, and γ-smooth:

$$|\dot{l}_j(a) - \dot{l}_j(b)| \le \gamma|a-b| \ \text{ for all } a, b \in \mathbb{R}$$

$Q \subset \mathbb{R}^p$ is a closed and bounded convex set

Define the separable loss function $L_n(s) := \frac{1}{n}\sum_{j=1}^n l_j(s_j)$

Denote $X := [x_1^T; x_2^T; \ldots; x_n^T]$. Then $s := X\beta$ and $L_n(s) = L_n(X\beta)$

Examples in Statistical and Machine Learning

- LASSO

$$\min_\beta \quad \frac{1}{2n}\sum_{j=1}^n (y_j - x_j^T\beta)^2$$

$$s.t. \quad \|\beta\|_1 \leq \delta \ ,$$

where $l_j(\cdot) = \frac{1}{2}(y_j - \cdot)^2$ and $Q = \{\beta : \|\beta\|_1 \leq \delta\}$

- Sparse Logistic Regression

$$\min_\beta \quad \frac{1}{n}\sum_{j=1}^n \ln(1+\exp(-y_j x_j^T\beta))$$

$$s.t. \quad \|\beta\|_1 \leq \delta \ ,$$

where $l_j(\cdot) = \ln(1+\exp(-y_j\cdot))$ and $Q = \{\beta : \|\beta\|_1 \leq \delta\}$

- Matrix Completion

$$\min_{\beta\in\mathbb{R}^{n\times p}} \quad \frac{1}{2|\Omega|}\sum_{(i,j)\in\Omega}(M_{i,j} - \beta_{i,j})^2$$

$$s.t. \quad \|\beta\|_* \leq \delta \ ,$$

where $l_{(i,j)}(\cdot) = \frac{1}{2}(\cdot - M_{i,j})^2$ and $Q = \{\beta : \|\beta\|_* \leq \delta\}$

- others ...

Frank-Wolfe method

$$\begin{array}{llll} \text{P:} & L_n^* = & \min_\beta & L_n(\beta) := \frac{1}{n}\sum_{j=1}^n l_j(x_j^T\beta) \\ & & \text{s.t.} & \beta \in Q \end{array}$$

Each iteration of Frank-Wolfe involves two main computations:

$$\text{compute } \nabla L_n(\beta^k)$$

and

$$\text{solve:} \quad \tilde{\beta}^k \leftarrow \arg\min_{\beta \in Q}\{\nabla L_n(\beta^k)^T\beta\}$$

The Frank-Wolfe method is an attractive first-order method to solve P:

- $O(1/\varepsilon)$ iteration bound for ε-optimal solution
- method produces "structured iterates": β^k is at most k-sparse (or rank-k) after k iterations

Stochastic Frank-Wolfe method

$$\begin{array}{llll} \text{P:} & L_n^* = & \min_\beta & L_n(\beta) := \frac{1}{n}\sum_{j=1}^n l_j(x_j^T\beta) \\ & & \text{s.t.} & \beta \in Q \end{array}$$

- gradient is $\nabla L_n(\beta^k) = \frac{1}{n}\sum_{j=1}^n \dot{l}_j(x_j^T\beta^k)x_j$
- when $n \gg 0$ it is too expensive to update $x_j^T\beta^k$ for all $j = 1, \ldots, n$ at iteration k
- Choose $j \in \mathcal{U}[1, \ldots, n]$
- $\tilde{g}^k = \dot{l}_j(x_j^T\beta^k)x_j$
- $\tilde{g}^k$ is an <u>unbiased</u> randomized estimate of $\nabla L_n(\beta^k)$
- using $\tilde{g}^k$ instead of $\nabla L_n(\beta^k)$ leads to Stochastic Frank-Wolfe methods

Comparison of Stochastic Frank-Wolfe Methods

To achieve an ε-optimal solution:

Algorithm and Reference	Number of Exact Gradient Calls	Number of Stochastic Gradient Calls	Number of Linear Optimization Oracle Calls
FW, Frank and Wolfe	$O(\frac{1}{\varepsilon})$	0	$O(\frac{1}{\varepsilon})$
SFW, Hazan and Luo	0	$O(\frac{1}{\varepsilon^3})$	$O(\frac{1}{\varepsilon})$
Online-FW, Hazan and Kale	0	$O(\frac{1}{\varepsilon^4})$	$O(\frac{1}{\varepsilon^4})$
SCGS, Lan and Zhou	0	$O(\frac{1}{\varepsilon^2})$	$O(\frac{1}{\varepsilon})$
SVRFW, Hazan and Luo	$O(\ln \frac{1}{\varepsilon})$	$O(\frac{1}{\varepsilon^2})$	$O(\frac{1}{\varepsilon})$
STORC, Hazan and Luo	$O(\ln \frac{1}{\varepsilon})$	$O(\frac{1}{\varepsilon^{1.5}})$	$O(\frac{1}{\varepsilon})$
SCGM, Mokhtari et al.	0	$O(\frac{1}{\varepsilon^3})$	$O(\frac{1}{\varepsilon^3})$
GSFW, this work	1	$O(\frac{1}{\varepsilon})$	$O(\frac{1}{\varepsilon})$

GSFW uses a biased estimate $\check{g}^k$ of $\nabla L_n(\beta^k)$

Convergence Guarantee of GSFW

Define $M := \max_{\beta \in Q} \max_{j=1,\ldots,n}\{|x_j^T \beta|\}$

Theorem: Convergence Guarantee of GSFW

For the GSFW algorithm it holds for all $k \geq 0$ that

$$\mathbb{E}\left[L_n(\bar{\beta}^k) - L_n^*\right] \;\leq\; \frac{8n\gamma M^2}{(4n+k)} + \frac{2n(2n-1)\gamma M^2}{(4n+k)(k+1)}$$

where

$$\bar{\beta}^k \;=\; \tfrac{2}{(4n+k)(k+1)} \sum_{i=0}^{k} (2n+i)\tilde{\beta}^i \;.$$

Some Thoughts on Directions for the Program

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Some Thoughts on Directions for the Program

- Optimization in the intertwined contexts of:
  - "big data"
  - data science
  - machine learning (including deep learning)
- Optimization for simulation problems in engineering design
- Machine learning (and deep learning) applied to engineering design

Thoughts on Directions for the Program, continued

- Theory: develop rigorous theoretical analyses of deep neural networks to shed light on why/when DNNs work and not work
  - DNNs do not work for all applications, it is thus important to genuinely understand their scope/limitations
- Algorithms: develop new AI/ML algorithms that are more rigorous/robust than SGD methods
  - new algorithms do not need to be more efficient than SGD
  - develop theory and performance bounds for algorithms in context of AI/ML applications

Thoughts on Directions for the Program, continued

- Applications: DNNs work well for images, textures, and languages. How about engineering design?
  - can DNNs be used to optimize engineering design or to augment optimization in engineering design?
- Data pre-processing: convolutional neural nets work well with images. For engineering applications, traditional convolutional layers may not work.
  - develop new types of pre-processing layers in DNNs for engineering design
- Big/small Data: data is often very expensive to collect in engineering design problems
  - develop new types of DNNs in this context that are intended to work well with small data

Backup for Generalized Stochastic Frank-Wolfe for Loss Minimization

Backup for

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$l_j(\cdot)$ is a univariate loss function that is strictly convex and γ-smooth:

$$|\dot{l}_j(a) - \dot{l}_j(b)| \leq \gamma|a-b| \ \text{ for all } a, b \in \mathbb{R}$$

R is a closed and bounded convex set, and $0 \in R$

Define the separable loss function $L(s) := \sum_{j=1}^n l_j(s_j)$

Denote $X := [x_1^T; x_2^T; \ldots; x_n^T]$. Then $s := X\beta$ and $L(s) = L(X\beta)$

Examples in Statistical and Machine Learning

- LASSO

$$\begin{aligned} \min_\beta \quad & \tfrac{1}{2n} \textstyle\sum_{j=1}^n (y_j - x_j^T \beta)^2 \\ s.t. \quad & \|\beta\|_1 \leq \delta \ , \end{aligned}$$

  where $l_j(\cdot) = \frac{1}{2}(y_j - \cdot)^2$ and $R = \{\beta : \|\beta\|_1 \leq \delta\}$

- Sparse Logistic Regression

$$\begin{aligned} \min_\beta \quad & \tfrac{1}{n} \textstyle\sum_{j=1}^n \ln(1 + \exp(-y_j x_j^T \beta)) \\ s.t. \quad & \|\beta\|_1 \leq \delta \ , \end{aligned}$$

  where $l_j(\cdot) = \ln(1 + \exp(-y_j \cdot))$ and $R = \{\beta : \|\beta\|_1 \leq \delta\}$

- Matrix Completion

$$\begin{aligned} \min_{\beta \in \mathbb{R}^{n \times p}} \quad & \tfrac{1}{2|\Omega|} \textstyle\sum_{(i,j) \in \Omega} (M_{i,j} - \beta_{i,j})^2 \\ s.t. \quad & \|\beta\|_* \leq \delta \ , \end{aligned}$$

  where $l_{(i,j)}(\cdot) = \frac{1}{2}(\cdot - M_{i,j})^2$ and $R = \{\beta : \|\beta\|_* \leq \delta\}$

- others ...

Frank-Wolfe and Stochastic Frank-Wolfe updates

The Frank-Wolfe method update is:

Frank-Wolfe method update

$$\text{Compute} \quad \tilde{\beta}^i \in \arg\min_{\beta \in P} \left\{ \nabla P(\beta^i)^T \beta \right\}$$

$$\beta^{i+1} \leftarrow (1-\alpha_i)\beta^i + \alpha_i \tilde{\beta}^i$$

In the traditional stochastic setting, we can only compute an (unbiased?) estimator $\tilde{g}$ of the gradient $\nabla P(\beta^i)$, and the update is

Stochastic Frank-Wolfe method update

$$\text{Compute} \quad \tilde{\beta}^i \in \arg\min_{\beta \in Q} \left\{ (\tilde{g}^i)^T \beta \right\}$$

$$\beta^{i+1} \leftarrow (1-\alpha_i)\beta^i + \alpha_i \tilde{\beta}^i$$

Stochastic Frank-Wolfe unbiased estimate of gradient

$$
\text{P:} \quad P^* = \quad \min_\beta \quad P(\beta) := \frac{1}{n}\sum_{j=1}^{n} l_j(x_j^T\beta)
$$
$$
\text{s.t.} \qquad \beta \in R
$$

- gradient is $\nabla P(\beta) = \frac{1}{n}\sum_{j=1}^{n} \dot{l}_j(x_j^T\beta)x_j$
- When n is large it is too expensive to update $x_j^T\beta$ for all $j = 1, \ldots, n$ at each iteration
- Choose $j \in \mathcal{U}[1, \ldots, n]$
- $\tilde{g} = \dot{l}_j(x_j^T\beta)x_j$
- $\tilde{g}$ is an unbiased estimate of the gradient

Stochastic Frank-Wolfe Methods

Comparison of computational complexity of recent stochastic Frank-Wolfe methods to achieve an absolute ε-optimal solution

Algorithm and Reference	Number of Exact Gradient Calls	Number of Stochastic Gradient Calls	Number of Linear Optimization Oracle Calls
FW, Frank and Wolfe	$O(\frac{1}{\varepsilon})$	0	$O(\frac{1}{\varepsilon})$
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GSFW, this work	1	$O(\frac{1}{\varepsilon})$	$O(\frac{1}{\varepsilon})$

"Substitute" Gradient

$$\text{P:} \quad P^* = \quad \min_\beta \quad P(\beta) := \frac{1}{n}\sum_{j=1}^n l_j(x_j^T\beta)$$

$$\text{s.t.} \qquad \beta \in R$$

- gradient is $\nabla P(\beta) = \frac{1}{n}\sum_{j=1}^n \dot{l}_j(x_j^T\beta)x_j$
- When n is large it is too expensive to update $x_j^T\beta$ for all $j = 1, \ldots, n$ in each iteration
- "Substitute" gradient d is computed by $d = \frac{1}{n}\sum_{j=1}^n \dot{l}_j(s_j)x_j$
- We will only update one s_j in each iteration
- d may not be an unbiased estimator of the gradient

Generalized Stochastic Frank-Wolfe Method with Substitute Gradient

Generalized Stochastic Frank-Wolfe with Substitute Gradient (GSFW)

Initialize with $\bar{\beta}^{-1} = 0$, $s^0 = 0$, and substitute gradient $d^0 = \frac{1}{n} X^T \nabla L(s^0)$, with step-size sequences $\{\alpha_i\} \in (0, 1]$, $\{\eta_i\} \in (0, 1]$.

For iterations $i = 0, 1, \ldots,$ do:

Solve l.o.o. subproblem: Compute $\tilde{\beta}^i \in \arg\min_{\beta \in R} \left\{ \left(d^i\right)^T \beta \right\}$

Choose random index: Choose $j_i \in \mathcal{U}[1, \ldots, n]$

Update s value: $s_{j_i}^{i+1} \leftarrow (1 - \eta_i) s_{j_i}^i + \eta_i (x_{j_i}^T \tilde{\beta}^i)$, and $s_j^{i+1} \leftarrow s_j^i$ for $j \neq j_i$

Update substitute gradient:

$$d^{i+1} = \frac{1}{n} X^T \nabla L(s^{i+1}) = d^i + \frac{1}{n} \left(\dot{l}_{j_i}(s_{j_i}^{i+1}) - \dot{l}_{j_i}(s_{j_i}^i) \right) x_{j_i}$$

Update primal variable: $\bar{\beta}^i \leftarrow (1 - \alpha_i) \bar{\beta}^{i-1} + \alpha_i \tilde{\beta}^i$.

(Optional Accounting:) $w^{i+1} \leftarrow \nabla L(s^{i+1})$

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Solve l.o.o. subproblem: Compute $\tilde{\beta}^i \in \arg\min_{\beta \in R} \left\{ \left(d^i\right)^T \beta \right\}$

Choose random index: Choose $j_i \in \mathcal{U}[1, \ldots, n]$

Update s value: $s_{j_i}^{i+1} \leftarrow (1-\eta_i) s_{j_i}^i + \eta_i (x_{j_i}^T \tilde{\beta}^i)$, and $s_j^{i+1} \leftarrow s_j^i$ for $j \neq j_i$

Update substitute gradient:

$$d^{i+1} = \frac{1}{n} X^T \nabla L(s^{i+1}) = d^i + \frac{1}{n} \left(\dot{l}_{j_i}(s_{j_i}^{i+1}) - \dot{l}_{j_i}(s_{j_i}^i) \right) x_{j_i}$$

Update primal variable: $\bar{\beta}^i \leftarrow (1-\alpha_i) \bar{\beta}^{i-1} + \alpha_i \tilde{\beta}^i$.

(Optional Accounting:) $w^{i+1} \leftarrow \nabla L(s^{i+1})$

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Solve l.o.o. subproblem: Compute $\tilde{\beta}^i \in \arg\min_{\beta \in R} \left\{ \left(d^i\right)^T \beta \right\}$

Choose random index: Choose $j_i \in \mathcal{U}[1, \ldots, n]$

Update s value: $s_{j_i}^{i+1} \leftarrow (1-\eta_i) s_{j_i}^i + \eta_i (x_{j_i}^T \tilde{\beta}^i)$, and $s_j^{i+1} \leftarrow s_j^i$ for $j \neq j_i$

Update substitute gradient:

$$d^{i+1} = \frac{1}{n} X^T \nabla L(s^{i+1}) = d^i + \frac{1}{n} \left(\dot{l}_{j_i}(s_{j_i}^{i+1}) - \dot{l}_{j_i}(s_{j_i}^i) \right) x_{j_i}$$

Update primal variable: $\bar{\beta}^i \leftarrow (1-\alpha_i) \bar{\beta}^{i-1} + \alpha_i \tilde{\beta}^i$.

(Optional Accounting:) $w^{i+1} \leftarrow \nabla L(s^{i+1})$

Generalized Stochastic Frank-Wolfe Method with Substitute Gradient

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Define $M := \max_{\beta \in R} \max_{j=1,\ldots,n} \{|x_j^T \beta|\}$

Theorem: Convergence Guarantee of GSFW

Consider GSFW with step-size sequences $\alpha_i = \frac{2(2n+i)}{(i+1)(4n+i)}$ and $\eta_i = \frac{2n}{2n+i+1}$ for $i = 0, 1, \ldots$. It holds for all $k \geq 0$ that

$$\mathbb{E}\left[P(\bar{\beta}^k) - P^*\right] \leq \frac{8n\gamma M^2}{(4n+k)} + \frac{2n(2n-1)\gamma M^2}{(4n+k)(k+1)} .$$

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