Stochastic Variance Reduced Primal Dual Algorithms for Empirical Composition Optimization

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Outline

Goal in Empirical Composition Optimization

Goal: Find θ^* such that:

$$\theta^* = \arg\min_{\theta} \frac{1}{n_X} \sum_{i=0}^{n_X-1} \phi_i\left(\frac{1}{n_{Y_i}} \sum_{j=0}^{n_{Y_i}-1} f_\theta(x_i, y_{ij}) \right) + g(\theta)$$

where,

- $(x_i, y_{ij}) \in \mathbb{R}^{m_x} \times \mathbb{R}^{m_y}$ is the (i,j)-th data sample
- $f_\theta : \mathbb{R}^{m_x} \times \mathbb{R}^{m_y} \to \mathbb{R}^\ell$ is parameterized by $\theta \in \mathbb{R}^d$
- $\phi_i : \mathbb{R}^\ell \to \mathbb{R}^+$ is a convex *merit function*
- $g(\theta)$ is a μ-strongly convex regularizer

Motivating Examples

- Unsupervised sequence classification [1]:

$$\min_{\theta}\left\{-\sum_{i=0}^{n_X-1} p_{\mathsf{LM}}(x_i)\log\left(\frac{1}{n_Y}\sum_{j=0}^{n_Y-1} f_\theta(x_i,y_j)\right)\right\}$$

  - $p_{\mathsf{LM}}:\mathbb{R}^{m_x}\to[0,1]$: Known language model
  - $f_\theta:\mathbb{R}^{m_x}\times\mathbb{R}^{m_y}\to\mathbb{R}^{\ell}$: Predicted n-gram frequency by a parameterized sequence classifier

- Risk-averse learning[2]:

$$\min_{\theta}\left\{-\frac{1}{n}\sum_{i=0}^{n-1}\langle x_i,\theta\rangle+\frac{1}{n}\sum_{i=0}^{n-1}\left(\langle x_i,\theta\rangle-\frac{1}{n}\sum_{j=0}^{n-1}\langle x_j,\theta\rangle\right)^2\right\}$$

  - $x_i\in\mathbb{R}^d$: Vector consisting of the rewards from d assets at time i
  - $\theta\in\mathbb{R}^d$: Weight vector on the d assets

[1] Y. Liu, J. Chen, & L. Deng, *Unsupervised sequence classification using sequential output statistics*, NeurIPS, 2017

[2] M.Wang, E. Fang, & H. Liu, *Stochastic compositional gradient descent: algorithms for minimizing compositions of expected-value functions*, Mathematical Programming, 2017

Challenges: Biased Gradients

- Gradient of the objective with respect to θ:

$$\frac{1}{n_X}\sum_{i=0}^{n_X-1}\left[\frac{1}{n_{Y_i}}\sum_{j=0}^{n_{Y_i}-1}\frac{\partial}{\partial\theta}f_\theta(x_i,y_{ij})\right]^{T}\left[\phi_i'\left(\frac{1}{n_{Y_i}}\sum_{j=0}^{n_{Y_i}-1}f_\theta(x_i,y_{ij})\right)\right]+\frac{\partial}{\partial\theta}g(\theta)$$

- The following "sampled stochastic gradient" is biased:

$$\left[\frac{\partial}{\partial\theta}f_\theta(x_i,y_{ij})\right]^{T}\left[\phi_i'\big(f_\theta(x_i,y_{ij})\big)\right]+\frac{\partial}{\partial\theta}g(\theta)$$

- *Cannot* directly apply SGD-like techniques

Related Work: A Special Case

- Goal: Find θ^* such that:

$$\min_\theta \frac{1}{n_X} \sum_{i=0}^{n_X-1} \phi_i\left(\frac{1}{n_Y} \sum_{j=0}^{n_Y-1} f_\theta(y_j)\right) \quad \text{vs} \quad \min_\theta \frac{1}{n_X} \sum_{i=0}^{n_X-1} \phi_i\left(\frac{1}{n_{Y_i}} \sum_{j=0}^{n_{Y_i}-1} f_\theta(x_i, y_{ij})\right)$$

- Key difference: Inner function f_θ does not depend on outside summation
- Related algorithms:
  - Compositional SGD [Wang, Fang & Liu, 2017]: Two-time-scale algorithm to deal with the two expectations separately
  - Compositional SVRG [Lian, Wang & Liu, 2017]: SVRG for compositional optimization
  - C-SAGA [Zhang & Xiao, 2019]: SAGA for compositional optimization

Our Approach: Primal Dual Formulation

For $\psi : \mathbb{R}^\ell \to \mathbb{R}$, its convex conjugate $\psi^* : \mathbb{R}^\ell \to \mathbb{R}$ is defined:

$$\psi^*(y) = \sup_{x \in \mathbb{R}^\ell} \left(\langle x, y \rangle - \psi(x) \right) \quad \overset{\text{Strong Duality}}{\Leftrightarrow} \quad \psi(x) = \sup_{y \in \mathbb{R}^\ell} \left(\langle x, y \rangle - \psi^*(y) \right)$$

Applying to our problem: Transformed min-max objective

$$\min_\theta \max_w \left\{ \underbrace{\frac{1}{n_X} \sum_{i=0}^{n_X - 1} \left[\left\langle \frac{1}{n_{Y_i}} \sum_{j=0}^{n_{Y_i}-1} f_\theta(x_i, y_{ij}), w_i \right\rangle - \phi_i^*(w_i) \right] + g(\theta)}_{L(\theta, w)} \right\}$$

- $w := \{w_0, \dots, w_{n_X - 1}\}$
- No more non-linear compositions of empirical averages
- Can sample unbiased gradients with respect to w_i's and θ
- Maximization is decoupled over w_i's

Our Algorithms: Key Ideas (I)

Dual step: Stochastic variance reduced coordinate ascent

- Batch gradient ascent for dual variables: For each $1 \leq i \leq n_X$,

$$w_i^{(k)} = \arg\min_{w_i} \left\{ -\left\langle \frac{1}{n_{Y_i}} \sum_{j=0}^{n_{Y_i}-1} f_{\theta^{(k-1)}}(x_i, y_{ij}), w_i \right\rangle + \phi_i^*(w_i) + \frac{1}{2\alpha_w} \|w_i - w_i^{(k-1)}\|^2 \right\}$$

  - Evaluating the full batch gradient is expensive
  - Updating each of the n_X variables is also expensive

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- Key Idea 1: *Exploit decoupled dual maximization* over w_i's:
  - At each iteration k, randomly sample an index i and update w_i
  - Keep other $\{w_j,\, j \neq i\}$ unchanged

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  - Keep other $\{w_j, j \neq i\}$ unchanged
- Key Idea 2: Replace the full gradient with respect w_i, with *low variance stochastic gradient*, using the SVRG technique of [Johnson & Zhang, 2013]:

$$\delta_k^w = f_{\theta^{(k-1)}}(x_{i_k}, y_{i_k j_k}) - f_{\tilde{\theta}}(x_{i_k}, y_{i_k j_k}) + \overline{f}_{i_k}(\tilde{\theta})$$

Our Algorithms: Key Ideas (II)

Primal step: Stochastic variance reduced gradient descent

- Batch gradient descent update for primal variable:

$$\theta^{(k)} = \arg\min_{\theta} \left\{ \left\langle \sum_{i=0}^{n_X - 1} \sum_{j=0}^{n_{Y_i}-1} \frac{1}{n_X n_{Y_i}} f'_{\theta^{(k-1)}}(x_i, y_{ij}) w_i^{(k)}, \theta \right\rangle + \frac{1}{2\alpha_\theta} \|\theta - \theta^{(k-1)}\|^2 \right\}$$

  - Once again, computational cost can be very large
- As before, we can use the SVRG technique to replace the full gradient with a low variance stochastic gradient:

$$\delta_k^\theta = f'_{\theta^{(k-1)}}(x_{i'_k}, y_{i'_k j'_k}) \widetilde{w}_{i'_k} - f'_{\tilde{\theta}}(x_{i'_k}, y_{i'_k j'_k}) \widetilde{w}_{i'_k} + L'_\theta(\tilde{\theta}, \widetilde{w})$$

Our Algorithms: Key Ideas (III)

Low complexity stochastic variance reduced estimator

- Stochastic Variance Reduced Gradient (SVRG) for $h(\theta) = \sum_{i=0}^{n-1} h_i(\theta)$:

$$\delta_k = h_{i_k}(\theta) - h_{i_k}(\tilde{\theta}) + h(\tilde{\theta})$$

- *Faster the reference variables $\tilde{\theta}$ and $\widetilde{w}$ are updated, lower the variance of stochastic gradient, and faster the convergence*
  - But also requires more complexity

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  - But also requires more complexity
- Trick: "Free" full batch gradient update to obtain $L'_\theta(\tilde{\theta}, w^{(k)})$
  - Key Idea 1: Use the fact that a single w_i is updated in each iteration
  - Key Idea 2: Exploit the linearity of objective in dual variables

$$L'(\tilde{\theta}, w^{(k)}) = L'(\tilde{\theta}, w^{(k-1)}) + \frac{1}{n_X} \overline{f}'_{i_k}(\tilde{\theta})\big(w_{i_k}^{(k)} - w_{i_k}^{(k-1)}\big)$$

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- Replace $L'_\theta(\tilde{\theta}, \widetilde{w})$ with $L'(\tilde{\theta}, w^{(k)})$ in naive SVRG gradient estimator

Our Algorithms: Key Ideas (IV)

Reducing the memory cost & SVRPDA - II

- Updating $L'(\tilde{\theta}, w^{(k)})$ at each iteration requires storing

$$\overline{f}_i'(\tilde{\theta}) = \sum_{j=0}^{n_{Y_i}-1} \frac{f_{\tilde{\theta}}'(x_i, y_{ij})}{n_{Y_i}}, \qquad 1 \leq i \leq n_X$$

  - Storage complexity can be very high

- Heuristic: Replace $\overline{f}_i'(\tilde{\theta})$ with sampled $f_{\tilde{\theta}}'(x_i, y_{ij})$ in update equation
- Results in low storage complexity, SVRPDA – II

Algorithm 1 SVRPDA-I

Inputs: data $\{(x_i, y_{ij}) : 0 \le i < n_X, 0 \le j < n_{Y_i}\}$; step-sizes α_θ and α_w; # inner iterations M.
Initialization: $\tilde{\theta}_0 \in \mathbb{R}^d$ and $\tilde{w}_0 \in \mathbb{R}^{\ell n_X}$.
for $s = 1, 2, \ldots$ **do**
 Set $\tilde{\theta} = \tilde{\theta}_{s-1}$, $\theta^{(0)} = \tilde{\theta}$, $\tilde{w} = \tilde{w}_{s-1}$, $w^{(0)} = \tilde{w}_{s-1}$, and compute the batch quantities (for each $0 \le i < n_X$):

$$U_0 = \sum_{i=0}^{n_X-1} \sum_{j=0}^{n_{Y_i}-1} \frac{f'_{\tilde{\theta}}(x_i, y_{ij}) w_i^{(0)}}{n_X n_{Y_i}}, \quad \overline{f}_i(\tilde{\theta}) \triangleq \sum_{j=0}^{n_{Y_i}-1} \frac{f_{\tilde{\theta}}(x_i, y_{ij})}{n_{Y_i}}, \quad \overline{f}'_i(\tilde{\theta}) = \sum_{j=0}^{n_{Y_i}-1} \frac{f'_{\tilde{\theta}}(x_i, y_{ij})}{n_{Y_i}}. \tag{11}$$

 for $k = 1$ **to** M **do**
  Randomly sample $i_k \in \{0, \ldots, n_X - 1\}$ and then $j_k \in \{0, \ldots, n_{Y_{i_k}} - 1\}$ at uniform.
  Compute the stochastic variance reduced gradient for dual update:

$$\delta_k^w = f_{\theta^{(k-1)}}(x_{i_k}, y_{i_k j_k}) - f_{\tilde{\theta}}(x_{i_k}, y_{i_k j_k}) + \overline{f}_{i_k}(\tilde{\theta}). \tag{12}$$

  Update the dual variables:

$$w_i^{(k)} = \begin{cases} \arg\min_{w_i} \Big[-\langle \delta_k^w, w_i \rangle + \phi_i^*(w_i) + \frac{1}{2\alpha_w} \| w_i - w_i^{(k-1)} \|^2 \Big] & \text{if } i = i_k \\ w_i^{(k-1)} & \text{if } i \neq i_k \end{cases}. \tag{13}$$

  Update U_k (primal batch gradient at $\tilde{\theta}$ and $w^{(k)}$) according to the following recursion:

$$U_k = U_{k-1} + \frac{1}{n_X} \overline{f}'_{i_k}(\tilde{\theta}) \big(w_{i_k}^{(k)} - w_{i_k}^{(k-1)} \big). \tag{14}$$

  Randomly sample $i'_k \in \{0, \ldots, n_X - 1\}$ and then $j'_k \in \{0, \ldots, n_{Y_{i'_k}} - 1\}$, independent of i_k and j_k, and compute the stochastic variance reduced gradient for primal update:

$$\delta_k^\theta = f'_{\theta^{(k-1)}}(x_{i'_k}, y_{i'_k j'_k}) w_{i'_k}^{(k)} - f'_{\tilde{\theta}}(x_{i'_k}, y_{i'_k j'_k}) w_{i'_k}^{(k)} + U_k. \tag{15}$$

  Update the primal variable:

$$\theta^{(k)} = \arg\min_{\theta} \Big[\langle \delta_k^\theta, \theta \rangle + g(\theta) + \frac{1}{2\alpha_\theta} \| \theta - \theta^{(k-1)} \|^2 \Big]. \tag{16}$$

 end for
 Option I: Set $\tilde{w}_s = w^{(M)}$ and $\tilde{\theta}_s = \theta^{(M)}$.
 Option II: Set $\tilde{w}_s = w^{(M)}$ and $\tilde{\theta}_s = \theta^{(t)}$ for randomly sampled $t \in \{0, \ldots, M-1\}$.
end for
Output: $\tilde{\theta}_s$ at the last outer-loop iteration.

Algorithm 1 SVRPDA-II

Inputs: data $\{(x_i, y_{ij}) : 0 \le i < n_X, 0 \le j < n_{Y_i}\}$; step-sizes α_θ and α_w; # inner iterations M.
Initialization: $\tilde{\theta}_0 \in \mathbb{R}^d$ and $\tilde{w}_0 \in \mathbb{R}^{\ell n_X}$.
for $s = 1, 2, \ldots$ **do**
  Set $\tilde{\theta} = \tilde{\theta}_{s-1}$, $\theta^{(0)} = \tilde{\theta}$, $w^{(0)} = \tilde{w}_{s-1}$, and compute the batch quantities (for each $0 \le i < n_X$):

$$U_0 = \sum_{i=0}^{n_X-1} \sum_{j=0}^{n_{Y_i}-1} \frac{f'_{\tilde{\theta}}(x_i, y_{ij}) w_i^{(0)}}{n_X n_{Y_i}}, \quad \overline{f}_i(\tilde{\theta}) \triangleq \sum_{j=0}^{n_{Y_i}-1} \frac{f_{\tilde{\theta}}(x_i, y_{ij})}{n_{Y_i}}. \tag{4}$$

  for $k = 1$ **to** M **do**
    Randomly sample $i_k \in \{0, \ldots, n_X - 1\}$ and then $j_k \in \{0, \ldots, n_{Y_{i_k}} - 1\}$ at uniform.
    Compute the stochastic variance reduced gradient for dual update:

$$\delta_k^w = f_{\theta^{(k-1)}}(x_{i_k}, y_{i_k j_k}) - f_{\tilde{\theta}}(x_{i_k}, y_{i_k j_k}) + \overline{f}_{i_k}(\tilde{\theta}). \tag{5}$$

    Update the dual variables:

$$w_i^{(k)} = \begin{cases} \arg\min_{w_i} \Big[-\langle \delta_k^w, w_i \rangle + \phi_i^*(w_i) + \frac{1}{2\alpha_w} \|w_i - w_i^{(k-1)}\|^2 \Big] & \text{if } i = i_k \\ w_i^{(k-1)} & \text{if } i \neq i_k \end{cases}. \tag{6}$$

    Update U_k according to the following recursion:

$$U_k = U_{k-1} + \frac{1}{n_X} f'_{\tilde{\theta}}(x_{i_k}, y_{i_k j''_k}) \big(w_{i_k}^{(k)} - w_{i_k}^{(k-1)} \big). \tag{7}$$

    Randomly sample $i'_k \in \{0, \ldots, n_X - 1\}$ and then $j'_k \in \{0, \ldots, n_{Y_{i'_k}} - 1\}$, independent of i_k and j_k, and compute the stochastic variance reduced gradient for primal update:

$$\delta_k^\theta = f'_{\theta^{(k-1)}}(x_{i'_k}, y_{i'_k j'_k}) w_{i'_k}^{(k)} - f'_{\tilde{\theta}}(x_{i'_k}, y_{i'_k j'_k}) w_{i'_k}^{(k)} + U_k. \tag{8}$$

    Update the primal variable:

$$\theta^{(k)} = \arg\min_{\theta} \Big[\langle \delta_k^\theta, \theta \rangle + g(\theta) + \frac{1}{2\alpha_\theta} \|\theta - \theta^{(k-1)}\|^2 \Big]. \tag{9}$$

  end for
  Option I: Set $\tilde{w}_s = w^{(k)}$ and $\tilde{\theta}_s = \theta^{(k)}$.
  Option II: Set $\tilde{w}_s = w^{(k)}$ and $\tilde{\theta}_s = \theta^{(t)}$ for randomly sampled $t \in \{0, \ldots, M-1\}$.
end for
Output: $\tilde{\theta}_s$ at the last outer-loop iteration.

Theory for Convergence

Assumptions

- $g(\theta)$ is μ-strongly convex in θ, and each ϕ_i is $1/\gamma$-smooth
- The merit functions $\phi_i(u)$ are Lipschitz with a uniform constant B_w
- $f_\theta(x_i, y_{ij})$ is B_θ-smooth in θ, and its gradients are uniformly bounded by a constant B_f
- For each given w in its domain, the function $L(\theta, w)$ is convex in θ

Main Result

After s outer-loops, to achieve error $\mathsf{E}\|\tilde{\theta}_s - \theta^*\|^2 < \epsilon$ using SVRPDA-I, total complexity required in terms of "number of oracle calls" is

$$O\big((n_X n_Y + n_X \kappa + n_X)\ln(1/\epsilon)\big)$$

Comparison with Existing Algorithms

- Our goal: $\min_\theta \frac{1}{n_X} \sum_{i=0}^{n_X-1} \phi_i\left(\frac{1}{n_{Y_i}} \sum_{j=0}^{n_{Y_i}-1} f_\theta(x_i, y_{ij})\right) + g(\theta)$

- Special case: $\min_\theta \frac{1}{n_X} \sum_{i=0}^{n_X-1} \phi_i\left(\frac{1}{n_Y} \sum_{j=0}^{n_Y-1} f_\theta(y_j)\right)$

Table: Total complexities of different stochastic composition optimization algorithms. For C-SAGA, $\alpha = 2/3$ with minibatch and $\alpha = 1$ when batch-size=1.

Methods	SVRPDA-I (Ours)	Comp-SVRG	C-SAGA	MSPBE-SVRG & MSPBE-SAGA	ASCVRG
Our problem	$(n_X n_Y + n_X \kappa) \ln \frac{1}{\epsilon}$				
Special	$(n_X + n_Y + n_X \kappa) \ln \frac{1}{\epsilon}$	$(n_X + n_Y + \kappa^3) \ln \frac{1}{\epsilon}$	$(n_X + n_Y + (n_X + n_Y)^\alpha \kappa) \ln \frac{1}{\epsilon}$		$(n_X + n_Y) \ln \frac{1}{\epsilon} + \frac{1}{\epsilon^3}$
$(n_X = 1)$	$(n_Y + \kappa) \ln \frac{1}{\epsilon}$	$(n_Y + \kappa^3) \ln \frac{1}{\epsilon}$	$(n_Y + n_Y^\alpha \kappa) \ln \frac{1}{\epsilon}$	$(n_Y + \kappa^2) \ln \frac{1}{\epsilon}$	$n_Y \ln \frac{1}{\epsilon} + \frac{1}{\epsilon^3}$

Storage Complexity of SVRPDA

Table: Storage complexity of SVRPDA-I and SVRPDA-II

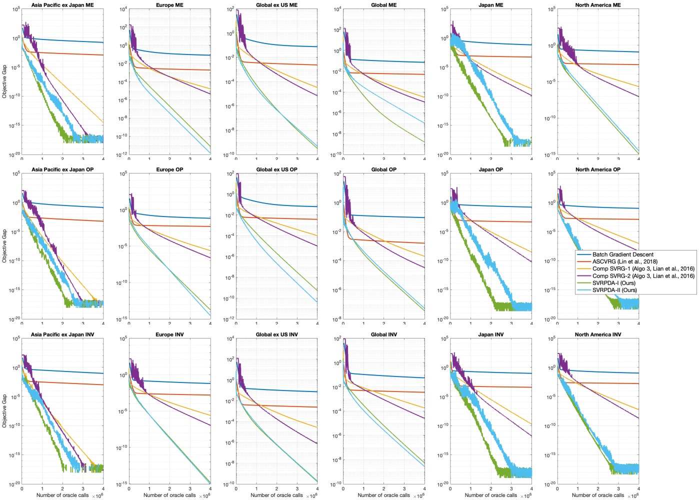
Methods	U_0	$\{\overline{f}_i\}$	$\{\overline{f}'_i\}$	$\theta^{(k)}$	$\tilde{\theta}$	$\{w_i^{(k)}\}$	δ_k^{θ}	δ_k^{w}	Total
SVRPDA-I	$O(d)$	$O(n_X \ell)$	$O(n_X d\ell)$	$O(d)$	$O(d)$	$O(n_X \ell)$	$O(d)$	$O(\ell)$	$O(n_X d\ell)$
SVRPDA-II	$O(d)$	$O(n_X \ell)$		$O(d)$	$O(d)$	$O(n_X \ell)$	$O(d)$	$O(\ell)$	$O(d+n_X \ell)$

Simulation Results: Risk Averse Learning

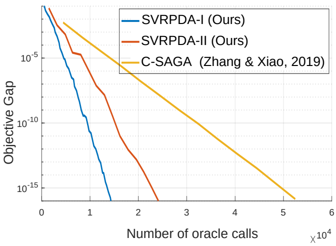
ME datasets

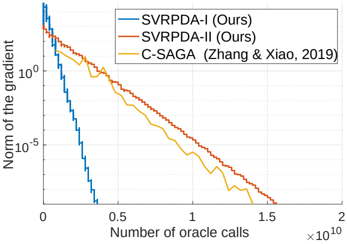
OP datasets

INV datasets



Simulation Results: MDP Policy Evaluation





Summary

- New SVRPDA algorithms are proposed to solve generic stochastic composition optimization algorithms
- Non-asymptotic bound for the error sequence was derived; Showed linear convergence of the algorithm
  - Complexity of SVRPDA was shown to be better than existing algorithms
- Experimental results showed that the algorithm outperforms all existing composition optimization algorithms
- Future work: Extensions to non-convex objectives, mini-batch SVRPDA, accelerated SVRPDA, etc.