

Nonconvex Optimization for Knowledge Discovery and Data Mining



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Outline

Nonconvexity in Data Mining

Nonconvex Finite-sum Optimization

Finding First-order Stationary Points

Finding Local Minima in Nonconvex Optimization

Finding Local Minima via First-order Algorithms

Structured Nonconvex Problems

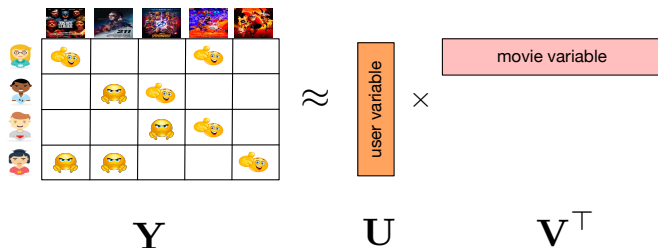
Low Rank Matrix Recovery

Robust PCA

Gaussian Graphical Models

References

Collaborative Filtering



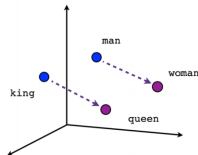
- ▶ **Matrix completion:** recover the underlying user-movie score matrix by minimizing the following objective

$$\min_{\mathbf{U}, \mathbf{V}} \frac{1}{2p} \sum_{(j,k) \in \Omega} (\mathbf{u}_{j*} \mathbf{v}_{k*}^T - Y_{jk})^2$$

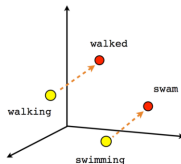
Word Embedding

- ▶ **Word2vec**: learn word embeddings by maximizing the following objective [MSC+13]

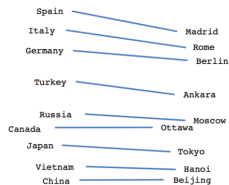
$$\log \sigma(\mathbf{u}_{w_0}^\top \mathbf{v}_{w_l}) + \sum_{i=1}^k \mathbb{E}_{w_i \sim P_n(w)} [\log \sigma(-\mathbf{u}_{w_i}^\top \mathbf{v}_{w_l})]$$



Male-Female



Verb tense



Country-Capital

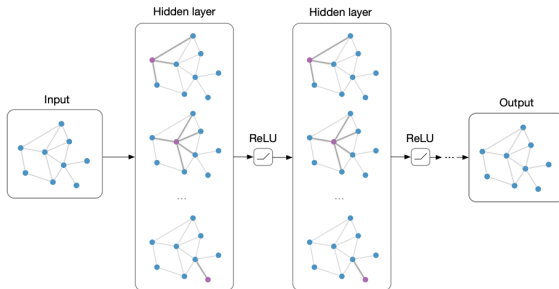
Network embedding

- ▶ **Graph convolutional network (GCN):** GCN learns network embeddings using graph-based neural network structure [KW16]

$$\mathbf{Z} = \text{softmax}(\hat{\mathbf{A}}\text{ReLU}(\dots \text{ReLU}(\hat{\mathbf{A}}\mathbf{X}\mathbf{W}^{(0)}) \dots)\mathbf{W}^{(L)}),$$

where the weight matrices are trained via solving

$$\min_{\mathbf{W}^{(0)} \dots \mathbf{W}^{(L)}} \ell(\mathbf{Z}, \mathbf{Y}).$$



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Finite-sum Optimization

- ▶ The finite-sum optimization problem:

$$\min f(\boldsymbol{\theta}) := \frac{1}{n} \sum_{i=1}^n f_i(\boldsymbol{\theta}),$$

where $f_i(\boldsymbol{\theta})$ and f are nonconvex

- ▶ For example, n can be the number of data points.

Goal: find stationary points

- ▶ First-order stationary point (FSP): $\|\nabla f(\boldsymbol{\theta})\|_2 = 0$

$$\begin{array}{ccc} \text{FSP} & & \epsilon\text{-approximate FSP} \\ \|\nabla f(\boldsymbol{\theta})\|_2 = 0 & \Rightarrow & \|\nabla f(\boldsymbol{\theta})\|_2 \leq \epsilon \end{array}$$

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Gradient Descent

Gradient Descent (GD):

$$\theta_{t+1} = \theta_t - \eta \nabla f(\theta_t)$$

- ▶ Converge to an ϵ -approximate stationary point within $O(1/\epsilon^2)$ iterations
- ▶ **Gradient complexity:** number of gradient computation in order to find an ϵ -approximate stationary point
- ▶ Gradient complexity of GD: $O(n/\epsilon^2)$

Stochastic Gradient Descent

Stochastic Gradient Descent (SGD)

$$\theta_{t+1} = \theta_t - \eta \mathbf{g}_t$$

- ▶ $\mathbf{g}_t = \nabla f_{i_t}(\theta_t)$, i_t : uniformly chosen from $\{1, \dots, n\}$
- ▶ Converge to an ϵ -approximate stationary point within $O(1/\epsilon^4)$ iterations
- ▶ Gradient complexity: $O(1/\epsilon^4)$

Adaptive Methods

Partially adaptive momentum estimation method (Padam)

[CG18]

$$\begin{aligned}\mathbf{m}_t &= \beta_1 \mathbf{m}_{t-1} + (1 - \beta_1) \mathbf{g}_t \\ \mathbf{v}_t &= \beta_2 \mathbf{v}_{t-1} + (1 - \beta_2) \mathbf{g}_t^2 \\ \hat{\mathbf{v}}_t &= \max(\hat{\mathbf{v}}_{t-1}, \mathbf{v}_t) \\ \boldsymbol{\theta}_{t+1} &= \boldsymbol{\theta}_t - \eta_t \frac{\mathbf{m}_t}{\hat{\mathbf{v}}_t^p}\end{aligned}$$

$p \in (0, 1/2]$: tuning parameter for improving generalization

- ▶ $p = 1/2$, \Rightarrow AMSGrad [RKK18]
- ▶ $p = 1/2$, $\max(\cdot)$ removed, \Rightarrow ADAM [KB14]
- ▶ $p = 1/2$, $\max(\cdot)$ removed, $\beta_1 = 0$, \Rightarrow RMSprop [HSS12]
- ▶ $p = 1/2$, $\max(\cdot)$ removed, $\beta_1 = 0$, $\mathbf{v} = 1/t \sum_{j=1}^t \mathbf{g}_j^2$, \Rightarrow AdaGrad [DHS11]

Stochastic Variance Reduced Gradient Methods

Stochastic Variance Reduced Gradient (SVRG) [JZ13]

for $t = 1, 2, \dots, T$

$$\tilde{\theta}_0 = \theta_t$$

Calculate full gradient $\mu = \nabla f(\tilde{\theta}_0)$

for $k = 0, \dots, m-1$

Randomly choose i_k from $[n]$

$$\mathbf{g}_k = \mu + \nabla f_{i_k}(\theta_k) - \nabla f_{i_k}(\tilde{\theta}_0)$$

$$\theta_{k+1} = \theta_k - \eta \mathbf{g}_k$$

end for

$$\theta_{t+1} = \tilde{\theta}_m$$

end for

- ▶ Semi-stochastic gradient: snapshot every m iterations
- ▶ Reference point, reference gradient
- ▶ Linear convergence to global minimum in strongly convex setting

Nonconvex SVRG

Nonconvex SVRG [AZH16, RHS⁺16]

for $t = 1, 2, \dots, T$

$$\tilde{\theta}_0 = \theta_t$$

Calculate full gradient $\mu = \nabla f(\tilde{\theta}_0)$

for $k = 0, \dots, m-1$

Randomly choose i_k from $[n]$

$$\mathbf{g}_k = \mu + \nabla f_{i_k}(\theta_k) - \nabla f_{i_k}(\tilde{\theta}_0)$$

$$\theta_{k+1} = \theta_k - \eta \mathbf{g}_k$$

end for

$$\theta_{t+1} = \tilde{\theta}_m$$

end for

- Gradient complexity

$$O\left(n + \frac{n^{2/3}}{\epsilon^2}\right)$$

Stochastically Controlled Stochastic Gradient

Stochastically Controlled Stochastic Gradient (SCSG) [LJCJ17]

for $t = 1, 2, \dots, T$

$$\tilde{\theta}_0 = \theta_t$$

$$\mu = 1/B \sum_{i \in \tilde{\mathcal{I}}} \nabla f_i(\tilde{\theta}), \text{ with } |\tilde{\mathcal{I}}| = B$$

Generate $m \sim \text{Geom}(B/(B+b))$

for $k = 0, \dots, m-1$

Randomly choose a subset \mathcal{I}_k of $[n]$, with $|\mathcal{I}_k| = b$

$$\mathbf{g}_k = \mu + 1/b \sum_{i \in \mathcal{I}_k} (\nabla f_i(\tilde{\theta}_k) - \nabla f_i(\theta_0))$$

$$\theta_{k+1} = \theta_k - \eta \mathbf{g}_k$$

end for

$$\theta_{t+1} = \tilde{\theta}_m$$

end for

- ▶ Mini-batch gradient in both outer loop and inner loop
- ▶ Gradient complexity $O(\min\{n^{2/3}/\epsilon^2, 1/\epsilon^{10/3}\})$
- ▶ Geometric distribution not necessary: [LL18]

Comparison on Gradient Complexity

To find an ϵ -approximate first-order stationary point:

$$\|\nabla f(\boldsymbol{\theta})\|_2 \leq \epsilon,$$

the number of stochastic gradient ∇f_i we need to compute is

Algorithm	Gradient Complexity
GD	$O(n\epsilon^{-2})$
SGD	$O(\epsilon^{-4})$
SVRG	$O(n^{2/3}\epsilon^{-2})$
SCSG	$O(\min\{n^{2/3}\epsilon^{-2}, \epsilon^{-10/3}\})$

Revisit SVRG

for $t_0 = 0, \dots, T_0 - 1$

$$\mathbf{g}_{t_0}^{(0)} = 1/B_0 \sum_{i \in \mathcal{I}_0} \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)}) \quad \Rightarrow \text{reference gradient}$$

for $t_1 = 0, \dots, T_1 - 1$

$$\mathbf{g}_{t_1}^{(1)} = 1/B_1 \sum_{i \in \mathcal{I}_1} \nabla f_i(\boldsymbol{\theta}_{t_1}^{(1)}) - \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$$

$$\mathbf{v}_t = \mathbf{g}_{t_0}^{(0)} + \mathbf{g}_{t_1}^{(1)}, \text{ where } t = t_0 T_1 + t_1$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \mathbf{v}_t$$

$$\boldsymbol{\theta}_{t_1+1}^{(1)} = \boldsymbol{\theta}_{t+1}$$

end for

$$\boldsymbol{\theta}_{t_0+1}^{(0)} = \boldsymbol{\theta}_{T_1}^{(1)} \quad \Rightarrow \text{reference point}$$

end for

- ▶ Mini-batch gradients
- ▶ Two reference points, two reference gradients
- ▶ Can more reference gradients reduce more variance?

Deeper SVRG

for $t_0 = 0, \dots, T_0 - 1$

$$\mathbf{g}_{t_0}^{(0)} = 1/B_0 \sum_{i \in \mathcal{I}_0} \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$$

for $t_1 = 0, \dots, T_1 - 1$

$$\mathbf{g}_{t_1}^{(1)} = 1/B_1 \sum_{i \in \mathcal{I}_1} \nabla f_i(\boldsymbol{\theta}_{t_1}^{(1)}) - \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$$

for $t_2 = 1, \dots, T_2 - 1$

$$\mathbf{g}_{t_2}^{(2)} = 1/B_2 \sum_{i \in \mathcal{I}_2} \nabla f_i(\boldsymbol{\theta}_{t_2}^{(2)}) - \nabla f_i(\boldsymbol{\theta}_{t_1}^{(1)})$$

$$\mathbf{v}_t = \mathbf{g}_{t_0}^{(0)} + \mathbf{g}_{t_1}^{(1)} + \mathbf{g}_{t_2}^{(2)}, \text{ where } t = t_0 T_1 T_2 + t_1 T_2 + t_2$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \mathbf{v}_t$$

$$\boldsymbol{\theta}_{t_2+1}^{(2)} = \boldsymbol{\theta}_{t+1}$$

end for

$$\boldsymbol{\theta}_{t_1+1}^{(1)} = \boldsymbol{\theta}_{T_2}^{(2)}$$

end for

$$\boldsymbol{\theta}_{t_0+1}^{(0)} = \boldsymbol{\theta}_{T_1}^{(1)}$$

end for

▷ $\mathcal{I}_0, \mathcal{I}_1, \mathcal{I}_2 \subset [n]$: batch sets with sizes B_0, B_1, B_2

Deeper SVRG

for $t_0 = 0, \dots, T_0 - 1$

$$\mathbf{g}_{t_0}^{(0)} = 1/B_0 \sum_{i \in \mathcal{I}_0} \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$$

⇒ reference gradient

for $t_1 = 0, \dots, T_1 - 1$

$$\mathbf{g}_{t_1}^{(1)} = 1/B_1 \sum_{i \in \mathcal{I}_1} \nabla f_i(\boldsymbol{\theta}_{t_1}^{(1)}) - \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$$

for $t_2 = 1, \dots, T_2 - 1$

$$\mathbf{g}_{t_2}^{(2)} = 1/B_2 \sum_{i \in \mathcal{I}_2} \nabla f_i(\boldsymbol{\theta}_{t_2}^{(2)}) - \nabla f_i(\boldsymbol{\theta}_{t_1}^{(1)})$$

$$\mathbf{v}_t = \mathbf{g}_{t_0}^{(0)} + \mathbf{g}_{t_1}^{(1)} + \mathbf{g}_{t_2}^{(2)}, \text{ where } t = t_0 T_1 T_2 + t_1 T_2 + t_2$$

$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \mathbf{v}_t$$

$$\boldsymbol{\theta}_{t_2+1}^{(2)} = \boldsymbol{\theta}_{t+1}$$

end for

$$\boldsymbol{\theta}_{t_1+1}^{(1)} = \boldsymbol{\theta}_{T_2}^{(2)}$$

end for

$$\boldsymbol{\theta}_{t_0+1}^{(0)} = \boldsymbol{\theta}_{T_1}^{(1)}$$

⇒ reference point

end for

▷ $\mathcal{I}_0, \mathcal{I}_1, \mathcal{I}_2 \subset [n]$: batch sets with sizes B_0, B_1, B_2

Stochastic Nested Variance Reduced Gradient

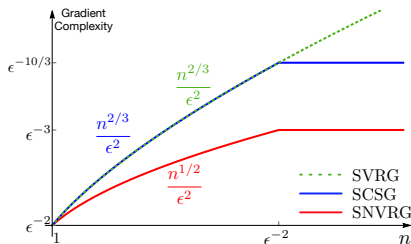
Reference point $\mathbf{x}_t^{(0)}$
Reference gradient $\mathbf{g}_t^{(0)}$
For $t_1 = 1, \dots, T_1$
Reference point $\mathbf{x}_t^{(1)}$
Reference gradient $\mathbf{g}_t^{(1)}$
.....
For $t_{K-1} = 1, \dots, T_{K-1}$
Reference point $\mathbf{x}_t^{(K-1)}$
Reference gradient $\mathbf{g}_t^{(K-1)}$
For $t_K = 1, \dots, T_K$
Reference point $\mathbf{x}_t^{(K)}$
Reference gradient $\mathbf{g}_t^{(K)}$
.....
update
$$\mathbf{x}_{t+1} = \mathbf{x}_t - \eta \sum_{i=0}^K \mathbf{g}_t^{(i)}$$

SNVRG [ZXG18c]

- ▶ Gradient complexity:

$$\tilde{O}\left(\min\left\{\frac{n^{1/2}}{\epsilon^2}, \frac{1}{\epsilon^3}\right\}\right)$$

- ▶ Comparison



Stochastic Path Integrated Differential Estimator

SPIDER [FLLZ18], (SARAH [NLST17] for convex optimization)

```
for  $t_0 = 0, \dots, T_0 - 1$   
   $\mathbf{v}_0 = 1/B_0 \sum_{i \in \mathcal{I}_0} \nabla f_i(\boldsymbol{\theta}_{t_0}^{(0)})$   
  for  $t_1 = 0, \dots, T_1 - 1$   
    Let  $t = t_0 T_1 + t_1$   
     $\mathbf{v}_t = \mathbf{v}_{t-1} + 1/B_1 \sum_{i \in \mathcal{I}_1} \nabla f_i(\boldsymbol{\theta}_t) - \nabla f_i(\boldsymbol{\theta}_{t-1})$   
     $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t - \eta \mathbf{v}_t / \|\mathbf{v}_t\|_2$   
  end for  
   $\boldsymbol{\theta}_{t_0+1}^{(0)} = \boldsymbol{\theta}_{T_1}$   
end for
```

- ▶ Recursive semi-stochastic gradient (Path Integrated)
- ▶ All the points in the inner loop are reference points
- ▶ A simplified variant without gradient normalization: SpiderBoost [WJZ⁺18]
- ▶ Gradient complexity: $O(n^{1/2}/\epsilon^2)$, the same as SNVRG

Finding a Stationary Point in Nonconvex Optimization

Algorithm	Gradient Complexity
GD	$O(n\epsilon^{-2})$
SGD [GL13]	$O(\epsilon^{-4})$
SVRG [AZH16, RHS ⁺ 16]	$O(n^{2/3}\epsilon^{-2})$
SCSG [LJCJ17]	$O(\min\{n^{2/3}\epsilon^{-2}, \epsilon^{-10/3}\})$
SPIDER [FLLZ18]	$\tilde{O}(\min\{n^{1/2}\epsilon^{-2}, \epsilon^{-3}\})$
SNVRG [ZXG18c]	$\tilde{O}(\min\{n^{1/2}\epsilon^{-2}, \epsilon^{-3}\})$

Question: can we do better?

Fundamental Limits:

Lower bound of gradient complexity for finding ϵ -approximate first-order stationary point for nonconvex smooth functions [FLLZ18, ZG19a]:

$$O\left(\frac{\sqrt{n}}{\epsilon^2}\right)$$

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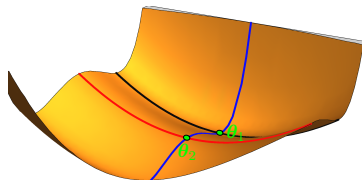
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Approximate Second-order Stationary Point



Stationary points (FSP):

- ▶ θ_1 : local minimum
- ▶ θ_2 : saddle point

- ▶ Second-order Stationary Point (SSP):

$$\|\nabla f(\boldsymbol{\theta})\|_2 = 0, \quad \lambda_{\min}(\nabla^2 f(\boldsymbol{\theta})) \geq 0$$

- ▶ $(\epsilon, \sqrt{\epsilon})$ -approximate local minimum:

$$\|\nabla f(\boldsymbol{\theta})\|_2 \leq \epsilon, \quad \lambda_{\min}(\nabla^2 f(\boldsymbol{\theta})) \geq -\sqrt{\epsilon}$$

Newton Type Methods

Incorporating Hessian information [Ben16, CP77]:

$$\theta_{t+1} = \theta_t - (\nabla^2 f(\theta_t))^{-1} \nabla f(\theta_t)$$

- ▶ Quadratic convergence in convex setting
- ▶ Hessian matrix not invertible in nonconvex setting
- ▶ $(\nabla^2 f(\theta_t))^{-1}$ not well defined

Solution: add regularizer

Cubic Regularized Newton's Methods

Minimize the cubic-regularized second-order Taylor expansion
[NP06]

$$\mathbf{h}_t = \underset{\mathbf{h} \in \mathbb{R}^d}{\operatorname{argmin}} \langle \nabla f(\boldsymbol{\theta}_t), \mathbf{h} \rangle + \frac{1}{2} \langle \nabla^2 f(\boldsymbol{\theta}_t) \mathbf{h}, \mathbf{h} \rangle + \frac{M}{6} \|\mathbf{h}\|_2^3,$$
$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \mathbf{h}_t$$

$M > 0$ is a penalty parameter

- ▶ $M = 0, \Rightarrow \mathbf{h}_t = (\nabla^2 f(\boldsymbol{\theta}_t))^{-1} \nabla f(\boldsymbol{\theta}_t)$, Newton's method
- ▶ $\|\mathbf{h}\|_2^3 \rightarrow \|\mathbf{h}\|_2^2, \Rightarrow \mathbf{h}_t = (\nabla^2 f(\boldsymbol{\theta}_t) + M\mathbf{I})^{-1} \nabla f(\boldsymbol{\theta}_t)$
- ▶ $M = 0$, constraint $\{\mathbf{h} : \|\mathbf{h}\|_2 \leq R\}$, \Rightarrow Trust Region method

Oracle Definition

- ▶ **Second Order Oracle (SO)**

Given an index i and a point θ , one SO call returns a triple:

$$[f_i(\theta), \nabla f_i(\theta), \nabla^2 f_i(\theta)]$$

- ▶ **Cubic Subproblem Oracle(CSO)**

Given a gradient vector \mathbf{g} , a Hessian matrix \mathbf{H} and a positive constant M , one CSO call returns the following minimizer

$$\mathbf{h}_{\text{sol}} = \operatorname{argmin}_{\mathbf{h} \in \mathbb{R}^d} \langle \mathbf{g}, \mathbf{h} \rangle + \frac{1}{2} \langle \mathbf{h}, \mathbf{H}\mathbf{h} \rangle + \frac{M}{6} \|\mathbf{h}\|_2^3.$$

Cubic Regularized Newton's Methods

Minimize the cubic-regularized second-order Taylor expansion
[NP06]

$$\mathbf{h}_t = \operatorname{argmin}_{\mathbf{h} \in \mathbb{R}^d} \langle \nabla f(\boldsymbol{\theta}_t), \mathbf{h} \rangle + \frac{1}{2} \langle \nabla^2 f(\boldsymbol{\theta}_t) \mathbf{h}, \mathbf{h} \rangle + \frac{M}{6} \|\mathbf{h}\|_2^3,$$
$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \mathbf{h}_t$$

$M > 0$ is a penalty parameter

- ▶ Converge to an $(\epsilon, \sqrt{\epsilon})$ -approximate local minimum within $O(\epsilon^{-3/2})$ iterations
- ▶ SO Complexity: $O(n\epsilon^{-3/2})$
- ▶ CSO Complexity: $O(\epsilon^{-3/2})$

Subsampled Cubic Regularization Method

Sub-sampled Cubic Regularization (SCR) [KL17, XRKM17]

$$\mathbf{h}_t = \operatorname{argmin}_{\mathbf{h} \in \mathbb{R}^d} \langle \mathbf{g}_t, \mathbf{h} \rangle + \frac{1}{2} \langle \mathbf{H}_t \mathbf{h}, \mathbf{h} \rangle + \frac{M}{6} \|\mathbf{h}\|_2^3,$$
$$\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \mathbf{h}_t$$

Sub-sampled gradient and Hessian matrix:

$$\mathbf{g}_t = 1/B_g \sum_{i \in \mathcal{I}_g} \nabla f_i(\boldsymbol{\theta}_t), \quad \mathbf{H}_t = 1/B_h \sum_{i \in \mathcal{I}_h} \nabla^2 f_i(\boldsymbol{\theta}_t)$$

- ▶ $\mathcal{I}_g, \mathcal{I}_h \subset [n]$ are two index sets with batch sizes B_g and B_h respectively.
- ▶ SO complexity: $O(n/\epsilon^{3/2} + 1/\epsilon^{5/2})$ no better than CR
- ▶ CSO complexity: $O(1/\epsilon^{3/2})$

Stochastic Variance-Reduced Cubic Regularization

Stochastic Variance-Reduced Cubic (SVRC) [ZXG18d]

```
for  $t_0 = 1, \dots, T_0$   
   $\tilde{\theta}_0 = \theta_t, \tilde{\mathbf{g}} = \nabla f(\tilde{\theta}_0), \tilde{\mathbf{H}} = \nabla^2 f(\tilde{\theta}_0)$   
  for  $t_1 = 0, \dots, T_1 - 1$   
     $\mathbf{h}_t = \operatorname{argmin}_{\mathbf{h}} \langle \mathbf{v}_t^{s+1}, \mathbf{h} \rangle + 1/2 \langle \mathbf{U}_t^{s+1} \mathbf{h}, \mathbf{h} \rangle + M/6 \|\mathbf{h}\|_2^3$   
     $\theta_{t+1} = \theta_t - \eta \mathbf{h}_t$   
  end for  
   $\theta_{t+1} = \tilde{\theta}_m$   
end for
```

Semi-stochastic gradient and Hessian matrix:

$$\mathbf{v}_t = \frac{1}{b_g} \sum_{i_t \in \mathcal{I}_g} \left(\nabla f_{i_t}(\theta_t) - \nabla f_{i_t}(\tilde{\theta}_0) + \tilde{\mathbf{g}} - [\nabla^2 f_{i_t}(\tilde{\theta}_0) - \tilde{\mathbf{H}}][\theta_t - \tilde{\theta}_0] \right)$$

$$\mathbf{U}_t = \frac{1}{b_h} \sum_{j_t \in \mathcal{I}_h} \left(\nabla^2 f_{j_t}(\theta_t) - \nabla^2 f_{j_t}(\tilde{\theta}_0) \right) + \tilde{\mathbf{H}},$$

Stochastic Variance-Reduced Cubic Regularization

Stochastic Variance-Reduced Cubic (SVRC) [ZXG18d]

To find an $(\epsilon, \sqrt{\epsilon})$ -approximate local minimum:

- ▶ SO complexity:

$$O\left(n + \frac{n^{4/5}}{\epsilon^{3/2}}\right)$$

- ▶ CSO complexity: $O(1/\epsilon^{3/2})$

Remarks:

- ▶ Cubic sub-problem complexity is the same as previous methods
- ▶ Second-order oracle: $(f_i(\boldsymbol{\theta}), \nabla f_i(\boldsymbol{\theta}), \nabla^2 f_i(\boldsymbol{\theta}))$
- ▶ Gradient computation: $O(d)$; Hessian matrix computation: $O(d^2) \Rightarrow$ **reduce Hessian complexity!**

Sample Efficient SVRC

Lite-SVRC: Semi-stochastic gradient and Hessian matrix:

$$\mathbf{v}_t = \frac{1}{b_g} \sum_{i_t \in \mathcal{I}_g} (\nabla f_{i_t}(\boldsymbol{\theta}_t) - \nabla f_{i_t}(\tilde{\boldsymbol{\theta}}_0) + \tilde{\mathbf{g}})$$

$$\mathbf{U}_t = \frac{1}{b_h} \sum_{j_t \in \mathcal{I}_h} (\nabla^2 f_{j_t}(\boldsymbol{\theta}_t) - \nabla^2 f_{j_t}(\tilde{\boldsymbol{\theta}}_0)) + \tilde{\mathbf{H}}$$

- ▶ The same semi-stochastic gradient used in first-order algorithms such as SVRG
- ▶ Gradient complexity $O(n/\epsilon^{3/2})$
- ▶ Hessian complexity $O(n + n^{2/3}/\epsilon^{2/3})$

Hessian Complexities of Cubic Methods

Algorithm	Gradient Complexity	Hessian Complexity
CR [NP06]	$O\left(\frac{n}{\epsilon^{3/2}}\right)$	$O\left(\frac{n}{\epsilon^{3/2}}\right)$
SCR [KL17, XRKM17]	$\tilde{O}\left(\frac{n}{\epsilon^{3/2}}\right)$	$\tilde{O}\left(\frac{n}{\epsilon^{3/2}}\right)$
SVRC [ZXG18d]	$\tilde{O}\left(n + \frac{n^{4/5}}{\epsilon^{3/2}}\right)$	$\tilde{O}\left(n + \frac{n^{4/5}}{\epsilon^{3/2}}\right)$
Lite-SVRC [ZXG18b]	$\tilde{O}\left(\frac{n}{\epsilon^{3/2}}\right)$	$\tilde{O}\left(n + \frac{n^{2/3}}{\epsilon^{3/2}}\right)$
SVRC [WZLL18]	$\tilde{O}\left(\frac{n}{\epsilon^{3/2}}\right)$	$\tilde{O}\left(n + \frac{n^{2/3}}{\epsilon^{3/2}}\right)$
SRVRC [ZG19b]	$\tilde{O}\left(\frac{n}{\epsilon^{3/2}}\right)$	$\tilde{O}\left(n + \frac{n^{1/2}}{\epsilon^{3/2}}\right)$

* $\tilde{O}(\cdot)$ hides logarithm factors.

- ▶ Gradient complexity is the same
- ▶ Variance reduced Cubic methods have Hessian complexity $O(\sqrt{n}/\epsilon^{3/2})$

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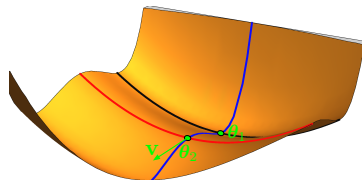
Escape Saddle Points

Cubic Regularization based algorithms (CR, SCR, SVRC, SRVRC, etc.)

- ▶ Compute $O(n + \sqrt{n}/\epsilon^{3/2})$ Hessian matrix
- ▶ $O(d^2)$ computation per Hessian matrix ☹

Gradient based algorithms (GD, SGD, SVRG, SNVRG, etc.):

- ▶ Only need to compute gradient: $O(d)$ per gradient ☺
- ▶ Converge to stationary point \Rightarrow can be a saddle point ☹



- ▶ Run SGD/SVRG
- ▶ Detect saddle point
 - ▶ Yes \Rightarrow Escape along \mathbf{v}
- ▶ Continue with SGD/SVRG

Finding Local Minima via First-order Oracles

Negative Curvature Direction (NCD): \mathbf{v} such that

$$\mathbf{v}^\top \nabla^2 f(\boldsymbol{\theta}) \mathbf{v} \leq -\sqrt{\epsilon}$$

Neon [XRY18], Neon2 [AZL18]

```
for  $t = 0, 1, \dots$ 
  if  $\|\nabla f(\boldsymbol{\theta}_t)\|_2 > \epsilon$ 
     $\boldsymbol{\theta}_{t+1} = \text{Alg}(f, \boldsymbol{\theta}_t)$  ▷ SGD/SVRG/SNVRG
  else
     $\mathbf{v}_t = \text{NCD}(f, \boldsymbol{\theta}_t)$  ▷ Negative Curvature Direction
    if  $\mathbf{v}_t$  not found
      return  $\boldsymbol{\theta}_t$  ▷  $\boldsymbol{\theta}_t$  is an SSP
    else
       $\boldsymbol{\theta}_{t+1} = \boldsymbol{\theta}_t + \eta \mathbf{v}_t$ 
end for
```

- ▶ Turn SGD/SVRG into local minimum finding algorithms
- ▶ Saddle points are rare \Rightarrow Hessian matrix computation is not often [YZG17, YXG18]

Complexity for Finding Local Minimum

Algorithm	Gradient Complexity
Pertubed GD [JGN ⁺ 17]	$O(n\epsilon^{-2})$
Neon+SGD [XRY18, AZL18]	$O(n\epsilon^{-2})$
Neon+SCSG [XRY18, AZL18]	$O(n\epsilon^{-3/2} + n^{2/3}\epsilon^{-2})$
Spider-SFO ⁺ [FLLZ18]	$\tilde{O}(n^{1/2}\epsilon^{-2})$
Neon+SNVRG [ZXG18a]	

Comparison with CR methods (SRVRC [ZG19b]):

$O(n/\epsilon^{3/2})$ gradient, $O(n^{1/2}/\epsilon^{3/2})$ Hessian

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Structured Nonconvex Problems

Nonconvex optimization with special structures:

$$\min_{\theta \in \mathbb{R}^d} f(\theta)$$

- ▶ f can have special structures: low-rankness, sparsity.
- ▶ Linear rate can be achieved!
- ▶ Global minimum can be reached!

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Low Rank Matrix Recovery

Goal: recover a low rank matrix $\mathbf{X}^* \in \mathbb{R}^{d_1 \times d_2}$ with $\text{rank}(\mathbf{X}^*) = r$.

Nonconvex optimization formulation:

$$\min_{\mathbf{U} \in \mathbb{R}^{d_1 \times r}, \mathbf{V} \in \mathbb{R}^{d_2 \times r}} \mathcal{L}_n(\mathbf{UV}^\top), \text{ subject to } \mathbf{U} \in \mathcal{C}_1, \mathbf{V} \in \mathcal{C}_2,$$

- ▶ \mathcal{L}_n is a nonconvex function based on n data observations.
- ▶ $\mathcal{C}_1, \mathcal{C}_2$: feasible sets induced by \mathbf{X}^*

Specific implications: matrix sensing, matrix completion, and one-bit matrix completion

E.g. the objective function for matrix completion

$$\min_{\mathbf{U} \in \mathbb{R}^{d_1 \times r}, \mathbf{V} \in \mathbb{R}^{d_2 \times r}} \mathcal{L}_\Omega(\mathbf{UV}^\top) := \frac{1}{2p} \sum_{(j,k) \in \Omega} (\mathbf{U}_{j*} \mathbf{V}_{k*}^\top - Y_{jk})^2$$

Alternating Projected Gradient Pursuit (Main Stage)

(\mathbf{U}, \mathbf{V}) is the solution $\Rightarrow (c\mathbf{U}, 1/c\mathbf{V})$ is the solution $\forall c \neq 0$

- ▶ Add a regularizer $\mathcal{L}_n(\mathbf{U}\mathbf{V}^\top) + \mathcal{R}(\mathbf{U}, \mathbf{V})$, e.g.

$$\mathcal{R}(\mathbf{U}, \mathbf{V}) = \|\mathbf{U}^\top \mathbf{U} - \mathbf{V}^\top \mathbf{V}\|_2^2 / 8$$

Alternating projected gradient descent:

$$\mathbf{U}^{t+1} = \mathcal{P}_{\mathcal{C}_1} \left(\mathbf{U}^t - \eta (\nabla_{\mathbf{U}} \mathcal{L}_n(\mathbf{U}^t \mathbf{V}^{t\top}) + \nabla_{\mathbf{U}} \mathcal{R}(\mathbf{U}^t, \mathbf{V}^t)) \right)$$

$$\mathbf{V}^{t+1} = \mathcal{P}_{\mathcal{C}_2} \left(\mathbf{V}^t - \eta (\nabla_{\mathbf{V}} \mathcal{L}_n(\mathbf{U}^t \mathbf{V}^{t\top}) + \nabla_{\mathbf{V}} \mathcal{R}(\mathbf{U}^t, \mathbf{V}^t)) \right),$$

- ▶ \mathcal{P} : projection operator
- ▶ For matrix completion, $\mathcal{C}_i = \{\mathbf{A} \in \mathbb{R}^{d_i \times r} \mid \|\mathbf{A}\|_{2,\infty} \leq \alpha\}$, thus the projection step is very efficient.

Singular Value Projection (Initialization Stage)

- ▶ Initialization matters: need to ensure $\mathbf{U}^0\mathbf{V}^{0\top}$ is close to \mathbf{X}^* .
- ▶ Singular Value Projection:

$$\mathbf{X}_S = \mathcal{P}_r(\mathbf{X}_{S-1} - \tau \nabla \mathcal{L}_n(\mathbf{X}_{S-1}))$$

$$[\bar{\mathbf{U}}^0, \Sigma^0, \bar{\mathbf{V}}^0] = \text{SVD}_r(\mathbf{X}_S) \text{ (after } S \text{ steps)}$$

- ▶ Initial estimator: $\mathbf{U}^0 = \bar{\mathbf{U}}^0(\Sigma^0)^{1/2}$, $\mathbf{V}^0 = \bar{\mathbf{V}}^0(\Sigma^0)^{1/2}$
- ▶ Singular value projection plus alternating projected gradient pursuit allow us to find \mathbf{X}^* in a linear convergence rate [WZG17a]

Stochastic Variance-Reduced Gradient Descent

Loss function

- ▶ $F_N(\mathbf{U}, \mathbf{V}) = \sum_{i=1}^n \mathcal{L}_i(\mathbf{U}\mathbf{V}^\top) + \mathcal{R}(\mathbf{U}, \mathbf{V})$, where
 $\mathcal{L}_i(\mathbf{U}\mathbf{V}^\top) = \sum_{j=1}^b \ell_{ij}(\mathbf{U}\mathbf{V}^\top)$

Low rank stochastic variance-reduced gradient (LRSVRG)
[WZG17a]:

for $t = 0, 1, \dots$

if $t \% m == 0$

$$\tilde{\mathbf{X}} = \mathbf{U}^t \mathbf{V}^{t\top}$$

 Randomly pick $i_t \in \{1, 2, \dots, n\}$

$$\mathbf{U}^{t+1} = \mathcal{P}_{\mathcal{C}_1} \left(\mathbf{U}^t - \eta (\nabla_{\mathbf{U}} F_{i_t}(\mathbf{U}^t, \mathbf{V}^t) - \nabla \mathcal{L}_{i_t}(\tilde{\mathbf{X}}) \mathbf{V}^t + \nabla \mathcal{L}_N(\tilde{\mathbf{X}}) \mathbf{V}^t) \right)$$

$$\mathbf{V}^{t+1} = \mathcal{P}_{\mathcal{C}_2} \left(\mathbf{V}^t - \eta (\nabla_{\mathbf{V}} F_{i_t}(\mathbf{U}^t, \mathbf{V}^t) - \nabla \mathcal{L}_{i_t}(\tilde{\mathbf{X}})^\top \mathbf{U}^t + \nabla \mathcal{L}_N(\tilde{\mathbf{X}})^\top \mathbf{U}^t) \right)$$

end for

Computational Complexity

Computational complexity for achieving ϵ accuracy

$\|\hat{\mathbf{X}} - \mathbf{X}^*\|_F \leq \epsilon$ for matrix completion

- ▶ Convex relaxation [SRJ04, CT10, RT⁺11, NW12, GHG16]:

$$O(d^3/\epsilon)$$

- ▶ Nonconvex GD [CW15, BKS16, WZG17a, ZL16, PKCS18]:

$$O(N\kappa r^3 d \log(1/\epsilon))$$

- ▶ Nonconvex LRSVRG [WZG17b]:

$$O((N + \kappa^2 b)r^3 d \log(1/\epsilon))$$

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Robust PCA

Goal: recover a low rank matrix and a sparse matrix $\mathbf{X}^*, \mathbf{S}^* \in \mathbb{R}^{d_1 \times d_2}$.

The optimization problem for robust matrix recovery:

$$\min_{\mathbf{U}, \mathbf{V}, \mathbf{S}} \mathcal{L}_n(\mathbf{UV}^\top + \mathbf{S}), \text{ subject to } \mathbf{U} \in \mathcal{C}_1, \mathbf{V} \in \mathcal{C}_2, \mathbf{S} \in \mathcal{K}$$

- ▶ \mathcal{L}_n is a nonconvex function
- ▶ $\mathcal{C}_1, \mathcal{C}_2$: feasible sets induced by \mathbf{X}^*
- ▶ \mathcal{K} : sparsity induced feasible set

Specific implications: Robust PCA, robust matrix sensing, robust one-bit matrix completion

[NNS⁺14, CW15, GWL16, YPCC16, CGJ17, ZWG18]

Double Thresholding based Algorithm (Main Stage)

- ▶ Introduce the same regularizer $\mathcal{L}_n(\mathbf{UV}^\top + \mathbf{S}) + \mathcal{R}(\mathbf{U}, \mathbf{V})$.
- ▶ Double thresholding based gradient descent:

$$\mathbf{S}^{t+1} = \mathcal{T}_\beta \circ \mathcal{H}_s(\mathbf{S}^t - \tau \nabla_{\mathbf{S}} \mathcal{L}_n(\mathbf{U}^t \mathbf{V}^{t\top} + \mathbf{S}^t))$$

$$\mathbf{U}^{t+1} = \mathcal{P}_{\mathcal{C}_1} \left(\mathbf{U}^t - \eta (\nabla_{\mathbf{U}} \mathcal{L}_n(\mathbf{U}^t \mathbf{V}^{t\top} + \mathbf{S}^t) + \nabla_{\mathbf{U}} \mathcal{R}(\mathbf{U}^t, \mathbf{V}^t)) \right)$$

$$\mathbf{V}^{t+1} = \mathcal{P}_{\mathcal{C}_2} \left(\mathbf{V}^t - \eta (\nabla_{\mathbf{V}} \mathcal{L}_n(\mathbf{U}^t \mathbf{V}^{t\top} + \mathbf{S}^t) + \nabla_{\mathbf{V}} \mathcal{R}(\mathbf{U}^t, \mathbf{V}^t)) \right)$$

- ▶ Hard thresholding operator \mathcal{H}_s : set all but the largest s elements in magnitude to zero.
- ▶ Truncation operator \mathcal{T}_β :

$$[\mathcal{T}_\theta(\mathbf{S})]_{ij} := \begin{cases} S_{ij}, & \text{if } |S_{ij}| \geq |S_{i,*}^{(\theta d_2)}| \text{ and } |S_{ij}| \geq |S_{*,j}^{(\theta d_1)}|, \\ 0, & \text{otherwise.} \end{cases}$$

Singular Value Projection with Hard Thresholding (Initialization Stage)

- ▶ Initialization matters: need to ensure initial estimators are close to \mathbf{X}^* , \mathbf{S}^*
- ▶ Singular value projection for low rank structure.
- ▶ Hard thresholding for sparse structure:

$$\mathbf{S}_{\ell+1} = \mathcal{H}_s(\mathbf{S}_\ell - \tau' \nabla_{\mathbf{S}} \mathcal{L}_n(\mathbf{X}_\ell + \mathbf{S}_\ell)).$$

- ▶ The whole algorithm can find \mathbf{X}^* and \mathbf{S}^* with a linear convergence rate [ZWG18]

Efficiency and Robustness

Fully observed Robust PCA

Algorithm	Computational Complexity	Robustness
Convex Relaxation [XCS10]	$O(d^3/\epsilon)$	$O(1/r)$
Nonconvex RPCA [NNS ⁺ 14]	$O(r^2 d^2 \log(1/\epsilon))$	$O(1/r)$
Alt RPCA [GWL16]	$O(rd^2 \log(1/\epsilon))$	$O(1/d)$
Fast RPCA [YPCC16]	$O(rd^2 \log(1/\epsilon))$	$O(1/r^{1.5})$
DT RPCA [ZWG18]	$O(rd^2 \log(1/\epsilon))$	$O(1/r)$

*Robustness means the fraction of corrupted observations

Partially observed Robust PCA

Algorithm	Sample Complexity	Computational Complexity
Fast RPCA [YPCC16]	$O(r^2 d \log d)$	$\tilde{O}(r^4 d \log d)$
PG-RMC [CGJ17]	$\tilde{O}(r^2 d \log^2 d)$	$\tilde{O}(r^3 d \log^2 d)$
DT RPCA [ZWG18]	$O(rd \log d)$	$\tilde{O}(r^3 d \log d)$

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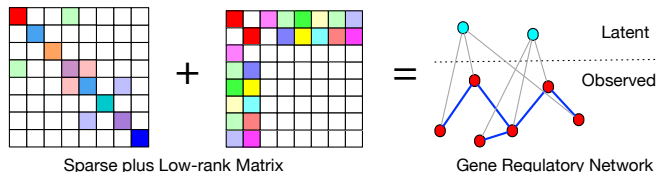
Robust PCA

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Latent Variable Gaussian Graphical Models

Latent Variable Gaussian Graphical Model (LVGGM) [XMG17]



- ▶ Data $\mathbf{X} = (\mathbf{X}^O, \mathbf{X}^L) \sim N(\mathbf{0}, \tilde{\Omega}^*) \Rightarrow \mathbf{X}^O \sim N(\mathbf{0}, \Omega^{*-1})$
- ▶ $\Omega^* = \mathbf{S}^* + \mathbf{L}^*$: sparse + low rank

Optimization problem:

$$\min_{\mathbf{S}, \mathbf{Z}} q_n(\mathbf{S}, \mathbf{Z}) = \text{tr} [\hat{\Sigma}(\mathbf{S} + \mathbf{Z}\mathbf{Z}^\top)] - \log |\mathbf{S} + \mathbf{Z}\mathbf{Z}^\top|, \quad \text{s.t. } \|\mathbf{S}\|_{0,0} \leq s,$$

- ▶ $\hat{\Sigma} = 1/n \sum_i \mathbf{X}_i \mathbf{X}_i^\top$: sample covariance matrix
- ▶ Negative log-likelihood function. Nonconvex in (\mathbf{S}, \mathbf{Z})

Latent Variable Gaussian Graphical Models

Initialization: one step SVD [YPCC16]

$$\hat{\Sigma} = \frac{1}{n} \sum_{i=1}^n \mathbf{x}_i \mathbf{x}_i^\top \Rightarrow \mathbf{S}^{(0)} = \mathcal{H}_s(\hat{\Sigma}^{-1})$$
$$\text{SVD}(\hat{\Sigma}^{-1} - \mathbf{S}^{(0)}) = \mathbf{U} \mathbf{D} \mathbf{U}^\top \Rightarrow \mathbf{Z}^{(0)} = \mathbf{U} \mathbf{D}_r^{1/2}$$

Alternating Gradient Descent (AltGD):

$$\mathbf{S}^{t+1} = \mathcal{H}_s\left(\mathbf{S}^t - \eta \nabla_{\mathbf{S}} q_n(\mathbf{S}^t, \mathbf{Z}^t)\right)$$
$$\mathbf{Z}^{t+1} = \mathbf{Z}^t - \eta' \nabla_{\mathbf{Z}} q_n(\mathbf{S}^t, \mathbf{Z}^t)$$

- ▶ \mathcal{H}_s : preserve the s largest magnitudes

Linear convergence to the true parameter up to statistical error [XMG17]

Latent Variable Gaussian Graphical Models

Setting	Method	$\ \Omega^T - \Omega^*\ _F$	Time (s)
$d = 100, r = 2, n = 2000$	PPA	0.7350 ± 0.0359	1.1610
	ADMM	0.7563 ± 0.0298	1.1120
	AltGD	0.6236 ± 0.0669	0.0250
$d = 500, r = 5, n = 10000$	PPA	0.9813 ± 0.0192	35.7220
	ADMM	1.0610 ± 0.0134	25.8010
	AltGD	0.8210 ± 0.0143	0.4800
$d = 1000, r = 8, n = 2.5 \times 10^4$	PPA	1.1639 ± 0.0179	356.7360
	ADMM	1.1869 ± 0.0254	156.5550
	AltGD	0.9021 ± 0.0244	7.4740
$d = 5000, r = 10, n = 2 \times 10^5$	PPA	1.4824 ± 0.0120	33522.0200
	ADMM	1.5012 ± 0.0240	21090.7900
	AltGD	1.3449 ± 0.0084	445.6730

More than $50\times$ speedup than convex methods!

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Summary

General finite-sum optimization

- ▶ Find an ϵ -approximate first-order stationary point
- ▶ Find an $(\epsilon, \sqrt{\epsilon})$ -approximate local minimum
- ▶ sublinear convergence rate

Structured nonconvex problems

- ▶ Low rank matrix recovery, robust PCA, latent variable Gaussian graphical models, etc.
- ▶ With a proper initialization, linear convergence to global minimum

Slides, video and other information are available on <https://sites.google.com/view/sdm2019-nonconvex>

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