

# Stochastic Chebyshev Gradient Descent for Spectral Optimization

**Insu Han**<sup>1</sup>   Haim Avron<sup>2</sup>   Jinwoo Shin<sup>1</sup>

<sup>1</sup> Korea Advanced Institute of Science and Technology (KAIST)

<sup>2</sup> Tel Aviv University

NeurIPS 2018 Montréal

# Spectral Optimization

- For a scalar function  $f : \mathbb{R} \rightarrow \mathbb{R}$  and matrix  $A \in \mathbb{R}^{d \times d}$ , **spectral-sum** is defined as :

$$\Sigma_f(A) := \sum_{i=1}^d f(\lambda_i) = \text{tr}(f(A)),$$

$\lambda_1, \lambda_2, \dots, \lambda_d$  : eigenvalues of  $A$

# Spectral Optimization

- For a scalar function  $f : \mathbb{R} \rightarrow \mathbb{R}$  and matrix  $A \in \mathbb{R}^{d \times d}$ , **spectral-sum** is defined as :

$$\Sigma_f(A) := \sum_{i=1}^d f(\lambda_i) = \text{tr}(f(A)),$$

$\lambda_1, \lambda_2, \dots, \lambda_d$  : eigenvalues of  $A$

- If  $f(x) = \log x$ , it is the log-determinant
- If  $f(x) = x^{-1}$ , it is the trace of inverse
- If  $f(x) = x^p$ , it is the Schatten- $p$  norm (the nuclear norm is the case  $p = 1$ )
- if  $f(x) = x \log x$ , it is the von-Neumann entropy
- If  $f(x) = \exp(x)$ , it is the Estrada index
- If  $f(x) = \begin{cases} 1 & \text{if } x > 0 \\ 0 & \text{otherwise} \end{cases}$ , it is rank or testing positive definiteness

# Spectral Optimization

- For a scalar function  $f : \mathbb{R} \rightarrow \mathbb{R}$  and matrix  $A \in \mathbb{R}^{d \times d}$ , **spectral-sum** is defined as :

$$\Sigma_f(A) := \sum_{i=1}^d f(\lambda_i) = \text{tr}(f(A)),$$

$\lambda_1, \lambda_2, \dots, \lambda_d$  : eigenvalues of  $A$

- Goal: solve the optimization

$$\min_{\theta} \Sigma_f(A(\theta)) + g(\theta)$$

*easy to compute  $g, \nabla g$*

$A(\theta)$  is a parameterized symmetric matrix,  $g$  is a simple function.

- E.g., collaborative filtering, hyperparameter learning and etc.

# Challenges

- Gradient-based methods :

$$\theta \leftarrow \theta - \eta \nabla_{\theta} (\Sigma_f(A(\theta)) + g(\theta))$$

easy to compute

- Computing exact  $\nabla_{\theta} \Sigma_f(A(\theta))$  requires  $\mathcal{O}(d^3)$  operations,  $d$  : matrix dimension

# Challenges

- Gradient-based methods :

$$\theta \leftarrow \theta - \eta \nabla_{\theta} (\Sigma_f(A(\theta)) + g(\theta))$$

easy to compute

- Computing exact  $\nabla_{\theta} \Sigma_f(A(\theta))$  requires  $\mathcal{O}(d^3)$  operations,  $d$  : matrix dimension
- [Han et al., 2017, Dong et al., 2017] can approximate  $\nabla_{\theta} \Sigma_f(A(\theta))$  using  $\mathcal{O}(\|A\|_0)$  😊
- But, the gradient estimator is biased, which hurts stable/fast convergence of SGD 😭

# Challenges

- Gradient-based methods :

$$\theta \leftarrow \theta - \eta \nabla_{\theta} (\Sigma_f(A(\theta)) + g(\theta))$$

easy to compute

- Computing exact  $\nabla_{\theta} \Sigma_f(A(\theta))$  requires  $\mathcal{O}(d^3)$  operations,  $d$  : matrix dimension
- [Han et al., 2017, Dong et al., 2017] can approximate  $\nabla_{\theta} \Sigma_f(A(\theta))$  using  $\mathcal{O}(\|A\|_0)$  😊
- But, the gradient estimator is biased, which hurts stable/fast convergence of SGD 😭
- We propose a fast unbiased gradient estimator with convergence guarantees of SGD/SVRG

# Randomized Chebyshev Expansion

- Why biased? The prior spectral-sum approximations are **biased** on combining
  - (1) randomized trace estimator (unbiased)
  - (2) Chebyshev polynomial expansion of  $f \approx p_n$  (biased) 🥲

$$\Sigma_f(A(\theta)) = \text{tr}(f(A)) = \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top f(A) \mathbf{v}}_{\text{unbiased}}] \approx \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top p_n(A) \mathbf{v}}_{\text{biased estimator}}] \quad (\mathbf{v}: \text{random vector})$$



# Randomized Chebyshev Expansion

- Why biased? The prior spectral-sum approximations are **biased** on combining
  - (1) randomized trace estimator (unbiased)
  - (2) Chebyshev polynomial expansion of  $f \approx p_n$  (biased) 😞

$$\Sigma_f(A(\theta)) = \text{tr}(f(A)) = \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top f(A) \mathbf{v}}_{\text{unbiased}}] \approx \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top p_n(A) \mathbf{v}}_{\text{biased estimator}}] \quad (\mathbf{v}: \text{random vector})$$

- To make it unbiased, we consider the following randomized Chebyshev expansions

$$f(x) = \sum_{j=0}^{\infty} a_j T_j(x), \quad p_n(x) = \sum_{j=0}^n a_j T_j(x) \xrightarrow[\text{random sampling}]{n \sim q_n} \hat{p}_n(x) = \sum_{j=0}^n \frac{a_j}{1 - \sum_{i=0}^{j-1} q_i} T_j(x)$$

- Then,  $\mathbf{E}_n [\hat{p}_n(x)] = f(x)$  and the gradient estimator with  $\hat{p}_n$  is unbiased 😊

# Randomized Chebyshev Expansion

- Why biased? The prior spectral-sum approximations are **biased** on combining
  - (1) randomized trace estimator (unbiased)
  - (2) Chebyshev polynomial expansion of  $f \approx p_n$  (biased) 😞

$$\Sigma_f(A(\theta)) = \text{tr}(f(A)) = \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top f(A) \mathbf{v}}_{\text{unbiased}}] \approx \mathbf{E}_{\mathbf{v}}[\underbrace{\mathbf{v}^\top p_n(A) \mathbf{v}}_{\text{biased estimator}}] \quad (\mathbf{v}: \text{random vector})$$

- To make it unbiased, we consider the following randomized Chebyshev expansions

$$f(x) = \sum_{j=0}^{\infty} a_j T_j(x), \quad p_n(x) = \sum_{j=0}^n a_j T_j(x) \xrightarrow[\text{random sampling}]{n \sim q_n} \hat{p}_n(x) = \sum_{j=0}^n \frac{a_j}{1 - \sum_{i=0}^{j-1} q_i} T_j(x)$$

- Then,  $\mathbf{E}_n[\hat{p}_n(x)] = f(x)$  and the gradient estimator with  $\hat{p}_n$  is unbiased 😊
- Question: what is a good distribution  $q_n$ ?

# Optimal Degree Distribution

- An estimator with small variance leads to faster convergence.
- Problem: minimize the variance of estimator given the expected degree  $N$

$$\min_{q_n} \text{Var}_n [\hat{p}_n] \quad \text{s.t.} \quad \mathbf{E}_n[n] = N$$

# Optimal Degree Distribution

- An estimator with small variance leads to faster convergence.
- **Problem**: minimize the variance of estimator given the expected degree  $N$

$$\min_{q_n} \text{Var}_n [\hat{p}_n] \quad \text{s.t.} \quad \mathbf{E}_n[n] = N$$

**Theorem 1 [Han, Avron and Shin 2018].** The optimal degree distribution is

$$q_n^* = \begin{cases} 0 & \text{for } n < N - k \\ 1 - k(\rho - 1)\rho^{-1} & \text{for } n = N - k \\ k(\rho - 1)^2\rho^{-(n+1)} & \text{for } n > N - k \end{cases} \quad \begin{array}{l} \rho > 1 : \text{ defined by } f \\ k = \min\{N, \lfloor \frac{\rho}{\rho-1} \rfloor\} \end{array}$$

# Optimal Degree Distribution

- An estimator with small variance leads to faster convergence.
- **Problem**: minimize the variance of estimator given the expected degree  $N$

$$\min_{q_n} \text{Var}_n [\hat{p}_n] \quad \text{s.t.} \quad \mathbf{E}_n[n] = N$$

**Theorem 1 [Han, Avron and Shin 2018].** The optimal degree distribution is

$$q_n^* = \begin{cases} 0 & \text{for } n < N - k \\ 1 - k(\rho - 1)\rho^{-1} & \text{for } n = N - k \\ k(\rho - 1)^2\rho^{-(n+1)} & \text{for } n > N - k \end{cases} \quad \begin{array}{l} \rho > 1 : \text{ defined by } f \\ k = \min\{N, \lfloor \frac{\rho}{\rho-1} \rfloor\} \end{array}$$

- Under the optimal distribution, we prove the convergence guarantees of SGD/SVRG

**Theorem 2 [Han, Avron and Shin 2018].**

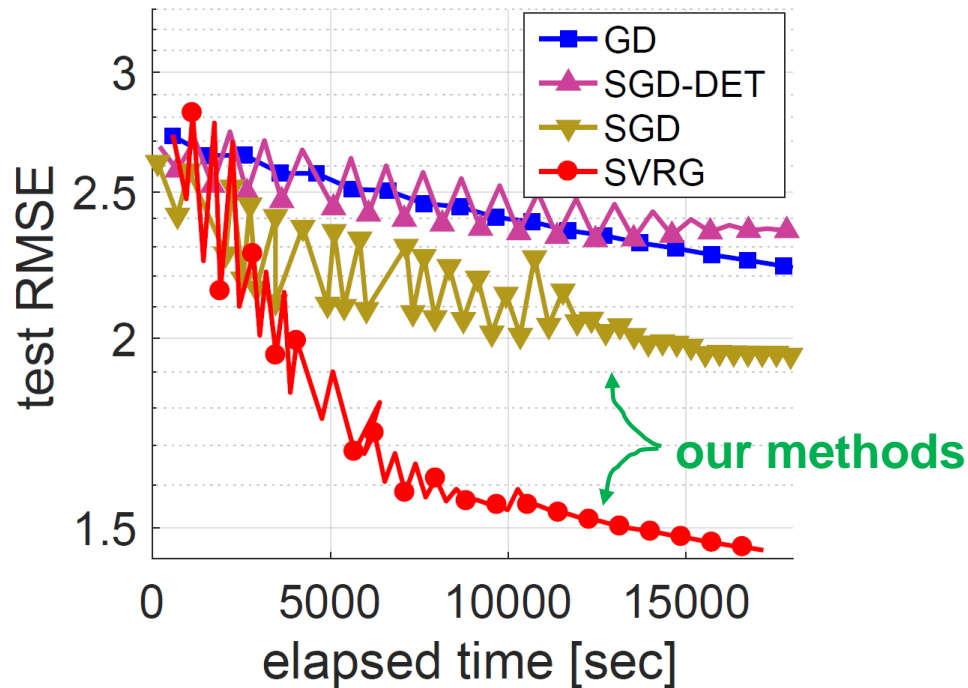
$$\mathbf{E}[\|\theta^* - \theta^{(T)}\|_2^2] \leq \frac{\mathcal{O}(1)}{T} \|\theta^* - \theta^{(0)}\|_2^2$$

$\theta^*$  : optimal

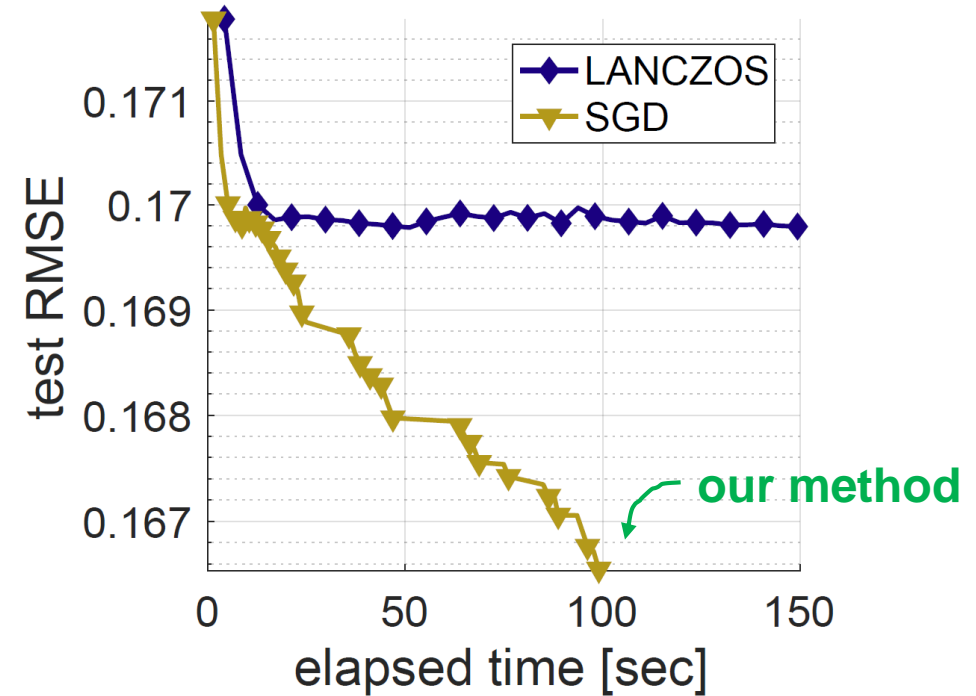
$\theta^{(T)}$  :  $\theta$  in  $T^{\text{th}}$  iteration of SGD

# Experimental Results for Two Applications

1. Matrix completion via **nuclear norm** regularization (left)
2. Gaussian process regression via **log-determinant** optimization (right)



MovieLens 10M dataset,  $f(x) = x^{1/2}$



Szeged Humid dataset,  $f(x) = \log x$

Our algorithms run at least **6 times** faster than other gradient descent methods

Thank you

# **Stochastic Chebyshev Gradient Descent for Spectral Optimization**

Key words: Matrix optimization, Randomized Chebyshev truncation, Variance minimization

**Poster # 6**

**Thursday Dec 6<sup>th</sup> 5:00 – 7:00 PM**

**@ Room 210 & 230 AB**