Stochastic Gradient Methods for Minimization in Relative Scale

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Outline

- Overview
- Problem Formulation
- Oracle for Maximal Eigenvector
- Stochastic Gradient Method
- 5 Application: MaxCut Problem

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Motivating Example

Spectral Linear Regression (SLR) problem

$$\min_{x \in \mathbb{R}^d} ||A(x) - C||,$$

where

$$A(x) := \sum_{i=1}^d x_i A_i,$$

and $A_1, \ldots, A_d, C \in \mathbb{R}^{n \times m}$ $(n \le m), \|\cdot\|$ is the matrix spectral norm.

Semidefinite Programming (SDP)

• SLR can be reduced to an SDP problem:

$$\begin{aligned} & \min_{x \in \mathbb{R}^d, t \in \mathbb{R}} & t \\ & \text{s.t.} & \begin{pmatrix} tI & A(x) - C \\ (A(x) - C)^T & tI \end{pmatrix} \succeq 0. \end{aligned}$$

- The SDP problem can be solved by Interior-Point methods.
- But this is expensive. Each iteration requires $O(n^3)$ time.
- Difficult to use sparsity of A_i , C.

Our Approach

Problem:
$$\phi^* := \min_{x \in \mathbb{R}^d} [\phi(x) := ||A(x) - C||].$$

• We propose randomized first-order methods that can solve this problem with relative accuracy $\delta \in (0,1)$:

$$(1-\delta)\mathbb{E}[\phi(\bar{x}_k)] \leq \phi^*.$$

• The main operation in our methods is the matrix-vector product:

$$A(x)v = \sum_{i=1}^{d} x_i(A_iv).$$

Can be evaluated in O(nnz(A)), where $nnz(A) := \sum_{i=1}^{d} nnz(A_i)$.

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Problem Formulation

Problem

$$\min_{x\in Q} f(x),$$

where $f: \mathbb{E} \to \mathbb{R}$ is a convex function and $Q \subseteq \mathbb{E}$ is a simple convex set.

Main assumptions:

• f has quadratic growth: there exists $x_0 \in Q$ and $\gamma_0 > 0$ such that

$$f(x) \ge \gamma_0 ||x - x_0||_B^2, \quad \forall x \in Q,$$

where $||h||_B := \langle Bx, x \rangle^{1/2}$.

• We have a δ -relative stochastic subgradient oracle $g(x,\xi)$:

$$f(y) \ge (1 - \delta)f(x) + \langle \mathbb{E}_{\xi}[g(x, \xi)], y - x \rangle, \qquad \forall x, y \in Q.$$

• The size of $g(x,\xi)$ is uniformly relatively bounded:

$$\mathbb{E}_{\varepsilon}[(\|g(x,\xi)\|_B^*)^2] \le 2Lf(x), \qquad \forall x \in Q.$$

Example: Squared Spectral Norm

Squared spectral norm $(n \le m)$

$$F(X) := ||X||^2 = \lambda_{\mathsf{max}}(XX^T), \qquad X \in \mathbb{R}^{n \times m}.$$

Quadratic growth: We have (w.r.t. Frobenius norm):

$$\gamma_0 = \frac{1}{n}, \qquad X_0 = 0.$$

Subgradient:

$$F'(X) = 2vv^T X, \qquad v := \text{MaxEigVec}(XX^T),$$

where $v \in \mathbb{R}^n$ is a unit leading eigenvector of XX^T :

$$(XX^T)v = \lambda_{\mathsf{max}}(XX^T)v, \qquad ||v|| = 1.$$

Relative boundedness: This subgradient is bounded w.r.t. *F*:

$$||F'(X)||_F^2 \equiv 4F(X) \implies L=2.$$

Relative Boundedness

For any function $f: \mathbb{E} \to \mathbb{R}$, define

$$F(x) \coloneqq \frac{1}{2}f^2(x).$$

Then, for any $x \in \mathbb{E}$, we have

$$\|\nabla f(x)\| \le M \quad \iff \quad \|\nabla F(x)\|^2 \le 2M^2 F(x).$$

Indeed, $\nabla F(x) = f(x)\nabla f(x)$. Hence,

$$\|\nabla F(x)\|^2 = f^2(x)\|\nabla f(x)\|^2 = 2\|\nabla f(x)\|^2 F(x).$$

Thus:

M-boundedness of $f \iff M^2$ -relative boundedness of $\frac{1}{2}f^2$.

Composition with Affine Mapping

Consider

$$f(x) = F(Ax + b),$$

where $A \colon \mathbb{E} \to \mathbb{E}_1$, $b \in \mathbb{E}_1$, and F satisfies our assumptions:

- F has quadratic growth w.r.t. $\|\cdot\|_{B_1}$ with parameters γ_0 and y_0 .
- We have δ -relative stochastic oracle $G(y, \xi)$ for F.
- Oracle $G(y,\xi)$ is uniformly relatively bounded with constant L.

Define the seminorm induced by $B = A^*B_1A$:

$$||x||_B = ||Ax||_{B_1}, \quad \forall x \in \mathbb{E}$$

and stochastic oracle

$$g(x,\xi) := A^*G(Ax + b,\xi).$$

Then, all properties are satisfied with the same constants γ_0 , L, and

$$x_0 = \underset{x \in Q}{\operatorname{argmin}} \|Ax + b - y_0\|_{\mathcal{B}}.$$

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Relative Stochastic Oracle for Spectral Norm

Computing $MaxEigVec(XX^T)$ exactly is very expensive. Instead, we would like to approximate it by a random vector:

$$\mathsf{MaxEigVec}(XX^T) \approx \mathsf{MaxEigVec}_{\delta}(XX^T, \xi).$$

Need the following subroutine:

δ -relatively inexact stochastic eigenvector ($\delta \in (0,1)$)

Given a matrix $A \in \mathbb{S}^n_+$, compute $\hat{v} \coloneqq \mathsf{MaxEigVec}_\delta(A, \xi)$ such that

$$\mathbb{E}_{\xi}\langle A\hat{v}, \hat{v} \rangle \geq (1 - \delta)\lambda_{\mathsf{max}}(A), \qquad \|\hat{v}\| = 1.$$

Then, we have a δ -relative inexact stochastic oracle:

$$G(X,\xi) := 2\hat{v}\hat{v}^T X, \qquad \hat{v} := \mathsf{MaxEigVec}_{\delta}(XX^T,\xi).$$

It is still relatively bounded:

$$||G(x,\xi)||_F^2 = 4\langle XX^T\hat{v},\hat{v}\rangle \le 4\lambda_{\max}(XX^T) = 2F(X).$$

Power Method

Let $A \in \mathbb{S}_+^n$. For an integer degree $p \ge 1$, define

$$\hat{v}_p(A,\xi) \coloneqq rac{A^p \xi}{\|A^p \xi\|}, \qquad \xi \sim \mathsf{Unif}(\mathcal{S}^{n-1}).$$

Should be computed in a numerically stable way:

Power Method

$$\hat{v}_{k+1} := \frac{A\hat{v}_k}{\|A\hat{v}_k\|}, \quad k = 0, \dots, p-1, \qquad \hat{v}_0 := \xi.$$

Complexity: p matrix-vector products.

Main result (Kuczyński and Woźniakowski, 1992)

$$\delta \leq \frac{\ln n}{p}$$
.

Lanczos Method

$$\hat{v}_p \in \underset{x \in \mathcal{K}_p \cap \mathcal{S}^{n-1}}{\operatorname{Argmax}} \langle Ax, x \rangle, \qquad \mathcal{K}_p \coloneqq \operatorname{span}(\xi, A\xi, A^2\xi, \dots, A^p\xi).$$

Accuracy estimate (Kuczyński and Woźniakowski, 1992)

For $\xi \sim \text{Unif}(\mathcal{S}^{n-1})$, we have

$$\delta \leq 3 \left(\frac{\ln n}{p}\right)^2$$
.

Implementing Lanczos Method

Lanczos tridiagonalization

Set $q_0 = 0$, $r_0 = \xi$. Iterate for $0 \le k \le p - 1$:

$$q_{k+1} = \frac{r_k}{\|r_k\|}, \qquad r_{k+1} = Aq_{k+1} - \langle Aq_{k+1}, q_{k+1} \rangle q_{k+1} - \|r_k\| q_k.$$

Result:

$$AQ_k = Q_k T_k + r_k e_k^T,$$

where $Q_k = [q_1, \ldots, q_k]$ has orthonormal columns spanning \mathcal{K}_k , $e_k \in \mathbb{R}^n$ is the kth coordinate vector, where $\mathcal{T}_k \in \mathbb{R}^{k \times k}$ is a tridiagonal matrix:

$$T_k = \mathsf{TriDiag}(\alpha_1, \ldots, \alpha_k; \beta_1, \ldots, \beta_k),$$

where $\alpha_k := \langle Aq_k, q_k \rangle$ and $\beta_k = ||r_k||$.

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Stochastic Gradient Method

Stochastic Gradient method

$$x_{k+1} = \mathsf{GradStep}_{Q,B}(x_k, a_k g_k), \qquad g_k \coloneqq g(x_k, \xi_k), \qquad k \ge 0,$$

where $a_k \ge 0$ are certainly chosen step sizes.

Gradient step: For any $x \in \mathbb{E}$ and $g \in (\ker B)^{\perp}$, denote

$$\mathsf{GradStep}_{Q,B}(x,g) \coloneqq \operatorname*{argmin}_{y \in Q} \Big\{ \langle g,y \rangle + \frac{1}{2} \|y - x\|_B^2 \Big\}.$$

(Also referred to as the "prox-mapping" by some authors.)

• When $B \succ 0$, this is the projected gradient step (w.r.t. B-norm):

$$GradStep_{Q,B}(x,g) = Proj_{Q,B}(x - B^{-1}g),$$

where $\operatorname{Proj}_{Q,B}(x) := \operatorname{argmin}_{y \in Q} \|y - x\|_B$.

• If $Q = \mathbb{E}$, point $T \coloneqq \mathsf{GradStep}_{Q,B}(x,g)$ is a solution of linear system

$$B(T-x)=-g.$$

Convergence Guarantee

Suppose a_i are deterministic step sizes and $a_i < \frac{1-\delta}{L}$.

Output point: For $c_i := a_i(1 - \delta - La_i)$, define and

$$\bar{x}_k := \frac{1}{C_k} \sum_{i=0}^{k-1} c_i x_i, \qquad C_k := \sum_{i=0}^{k-1} c_i.$$

Theorem. For any $k \ge 0$, we have

$$(1-\Delta_k)\,\mathbb{E}[f(\bar{x}_k)]\leq f^*,$$

where

$$\Delta_k := \delta + \frac{1 - \delta + 2\gamma_0 L \sum_{i=0}^{k-1} a_i^2}{1 + 2\gamma_0 \sum_{i=0}^{k-1} a_i}.$$

Choice of Stepsizes I

$$\Delta_k := \delta + \frac{1 - \delta + 2\gamma_0 L \sum_{i=0}^{k-1} a_i^2}{1 + 2\gamma_0 \sum_{i=0}^{k-1} a_i} \qquad (\geq 0).$$

General recipe

To make $\Delta_k \to \delta$, it suffices to ensure that

$$\sum_{k=0}^{\infty} a_k = \infty, \qquad \sum_{k=0}^{\infty} a_k^2 < \infty.$$

Choice of Stepsizes II

$$\Delta_k := \delta + \frac{1 - \delta + 2\gamma_0 L \sum_{i=0}^{k-1} a_i^2}{1 + 2\gamma_0 \sum_{i=0}^{k-1} a_i} \qquad (\ge 0).$$

Optimal step sizes for a fixed horizon $N \geq 1$

$$a_k = a_N^* \coloneqq \frac{1-\delta}{\sqrt{2\gamma_0 NL(1-\delta) + L^2} + L}, \qquad k \ge 0.$$

Under this choice, we have

$$\Delta_{N} \leq \delta + \sqrt{\frac{2L}{\gamma_{0}N}}.$$

In particular,

$$N \ge N(\delta) := \frac{2L}{\gamma_0 \delta^2} \implies \Delta_N \le 2\delta.$$

Choice of Stepsizes III

Constant step size based on target accuracy $\delta \in (0,1)$:

$$a_k = \frac{\delta}{2L} \implies \Delta_N \leq 2\delta, \quad \forall N \geq N(\delta).$$

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MaxCut Problem

Let G = (V, E) be an undirected weighted graph with $V = \{1, ..., n\}$ and weights $w(\{i, j\}) > 0$ for each edge $\{i, j\} \in E$.

Cut: For each vertex i = 1, ..., n, assign $x_i = \pm 1$.

Value of cut

$$c(x) = \frac{1}{2} \sum_{\{i,j\} \in E} w(\{i,j\}) (1 - x_i x_j).$$

MaxCut problem

$$c^* := \max_{x \in B^n} c(x),$$

where

$$B^n := \{x \in \mathbb{R}^n : x_i^2 = 1, i = 1, \dots, n\}.$$

Note: NP-complete! But can be efficiently approximated.

MaxCut via Laplacian Matrix

Note that

$$c(x) = \frac{1}{2} \sum_{\{i,j\} \in E} w(\{i,j\}) (1 - x_i x_j) = \frac{1}{4} \langle Ax, x \rangle,$$

where $A \in \mathbb{S}^n_+$ is the Laplacian matrix of G:

$$A_{i,j} := \begin{cases} \sum_{k: \ \{i,k\} \in E} w(\{i,k\}), & \text{if } i = j, \\ -w(\{i,j\}), & \text{if } \{i,j\} \in E, \\ 0, & \text{otherwise.} \end{cases}$$

MaxCut problem

$$4c^* = \max_{x \in B^n} \langle Ax, x \rangle.$$

SDP Relaxation

MaxCut problem:

$$s^* := \max_{x \in B^n} \langle Ax, x \rangle.$$

SDP relaxation:

$$f^* := \min_{z \in \mathbb{R}^n} \left\{ \sum_{i=1}^n z_i : A \leq D(z) \right\} = \max_{Y \in \mathbb{S}^n} \left\{ \langle A, Y \rangle : Y \succeq 0, \ d(Y) = e \right\},$$
Dual SDP relaxation

where $e \coloneqq (1, \dots, 1)^T \in \mathbb{R}^n$.

Accuracy of relaxation (Goemans and Williamson, 1995)

$$0.878 \cdot f^* \leq s^* \leq f^*$$
.

Finding the Cut

Random hyperplane algorithm (Goemans and Williamson, 1995)

- Solve Primal SDP relaxation, obtain optimal Y^* .
- ② Compute decomposition $Y^* = R^T R$, where $R \in \mathbb{R}^{m \times n}$.
- **3** Sample $u \sim \text{Unif}(S^{m-1})$.
- Compute $x^* = sign(R^T u)$.

Quality of the cut

$$\mathbb{E}_u[c(x^*)] \geq 0.878 \cdot c^*.$$

Transforming Dual Problem

We can assume that $D(A) := Diag(A_{1,1}, \dots, A_{n,n}) \succ 0$. Then,

$$f^* = \min_{z \in \mathbb{R}^n} \left\{ \sum_{i=1}^n z_i : A \leq D(z) \right\}$$

$$= \min_{z \in \mathbb{R}^n_{++}} \left\{ \sum_{i=1}^n z_i : \lambda_{\max} ([D(z)]^{-1/2} A[D(z)]^{-1/2}) \leq 1 \right\}.$$

Make change of variables $x_i = z_i^{-1/2}$. Then:

$$\begin{split} f^* &= \min_{x \in \mathbb{R}^n_{++}} \Big\{ \underbrace{\sum_{i=1}^n \frac{1}{x_i^2}}_{=:\phi(x)} : \underbrace{\lambda_{\mathsf{max}} \big(D(x) A D(x) \big) \leq 1}_{=:f(x)} \Big\} \\ &= \min_{x \in \mathbb{R}^n_{++}} [\phi(x) f(x)] = \min_{x \in \mathbb{R}^n_{++}} \{ f(x) : \phi(x) \leq 1 \}. \end{split}$$

Solving Transformed Dual

Problem

$$f^* = \min_{x \in Q} f(x), \qquad f(x) \coloneqq \lambda_{\max}(S(x)),$$

where

$$S(x) := D(x)AD(x), \qquad Q := \left\{x \in \mathbb{R}^n_{++} : \sum_{i=1}^n \frac{1}{x_i^2} \le 1\right\}.$$

Note: $f(x) = ||P(x)||^2$, where $P(x) := D(x)A^{1/2}$.

Oracle: $g(x,\xi) := 2d(AD(x)\hat{v}\hat{v}^T), \ \hat{v} := \mathsf{MaxEigVec}_{\delta}(S(x),\xi).$

Choice of norm: B = D(A).

Then, f and $g(x, \xi)$ satisfy our assumptions with

$$\gamma_0 = \frac{1}{n}$$
, $x_0 = \underset{x \in Q}{\operatorname{argmin}} ||x||_B = \operatorname{Proj}_{Q,B}(0)$, $L = 2$.

Final Guarantee I

We can get a point $\bar{x}_k \in Q$ such that

$$(1-\delta)\mathbb{E}[f(\bar{x}_k)] \leq f^*,$$

where

$$f(x) := \lambda_{\mathsf{max}}\big(S(x)\big)$$

in the following number of iterations:

$$N(\delta) = O\left(\frac{L}{\gamma_0 \delta^2}\right) = O\left(\frac{n}{\delta^2}\right).$$

Note: We cannot compute $f(\bar{x}_k)$ exactly (too expensive).

Final Guarantee II

Nevertheless, we can efficiently compute

$$\hat{f}_k := (1 - \delta)^{-1} \langle S(\bar{x}_k) \hat{v}, \hat{v} \rangle, \qquad \hat{v} := \mathsf{MaxEigVec}_{\delta} ig(S(\bar{x}_k), \xi ig)$$

such that

$$\mathbb{E}[f(\bar{x}_k)] \leq \mathbb{E}[\hat{f}_k] \leq (1-\delta)^{-2} f^*.$$

Then:

$$f^* \leq \mathbb{E}[\hat{f}_k] \leq (1-\delta)^{-2} f^*.$$

Combining this with

$$0.878 \cdot f^* \leq s^* \leq f^*$$
,

we get for the MaxCut problem:

$$\alpha \mathbb{E}[\hat{f}_k] \leq s^* \leq \mathbb{E}[\hat{f}_k],$$

where $\alpha := 0.878(1 - \delta)^2$.

Final Guarantee III

Result

We can produce \hat{f}_k such that

$$\alpha \mathbb{E}[\hat{f}_k] \leq s^* \leq \mathbb{E}[\hat{f}_k].$$

where $\alpha := 0.878(1 - \delta)^2$.

Total arithmetical complexity:

$$N(\delta) \times \underbrace{O\left(\frac{\ln n}{\sqrt{\delta}}\right)}_{\substack{\text{Number of} \\ \text{mat-vec products}}} \times \underbrace{O(|E|)}_{\substack{\text{Cost of} \\ \text{mat-vec product}}} = O\left(\frac{n|E|\ln n}{\delta^{5/2}}\right).$$

Note: We do not need a very small δ :

$$\delta = 0.05 \implies \alpha \approx 0.79,$$

 $\delta = 0.01 \implies \alpha \approx 0.86.$

Open Question

Open question: How to generate the cut corresponding to \hat{f}_k ?

Main problem: We need an approximate optimal solution Y_k for the primal SDP relaxation and its factorization

$$Y_k = R_k^T R_k$$
.

Thank you!

References



M. X. Goemans and D. P. Williamson. Improved approximation algorithms for maximum cut and satisfiability problems using semidefinite programming. *Journal of the ACM*, 42(6):1115–1145, Nov. 1995. ISSN: 0004-5411. DOI: 10.1145/227683.227684.



J. Kuczyński and H. Woźniakowski. Estimating the Largest Eigenvalue by the Power and Lanczos Algorithms with a Random Start. *SIAM Journal on Matrix Analysis and Applications*, 13(4):1094–1122, Oct. 1992. DOI: 10.1137/0613066.