Gradient Methods for Stochastic Optimization in Relative Scale

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Outline

1. Introduction
2. Problem Formulation
3. Gradient Method
4. Oracle for Maximal Eigenvector
5. Dual Averaging Method
6. Numerical Experiments
7. Application: MaxCut Problem
8. Conclusions

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Optimization in Relative Scale

Problem

$$f^* := \min_{x \in Q} f(x),$$

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

Goal: Find approximate solution $\bar{x} \in Q$ with relative accuracy $\delta \in (0, 1)$:

$$f(\bar{x}) \leq (1 + \delta) f^*.$$

Main feature: Complexity of methods does not depend on f^* (or data defining the problem).

Relative Accuracy vs Absolute Accuracy

Note:

- δ-relatively inexact solution $\iff$ ϵ-absolutely inexact solution:

$$f(\bar{x}) \leq (1+\delta) f^* \quad \iff \quad f(\bar{x}) - f^* \leq \epsilon, \qquad \epsilon := \delta f^*.$$

- However, usually we cannot achieve what we want "for free" by simply reusing existing methods and complexity results.

Example (Gradient Method). To achieve δ-relative accuracy, it needs

$$N = \frac{LR_0^2}{\epsilon} = \frac{LR_0^2}{\delta f^*}$$

iterations, where L is the Lipschitz constant of ∇f and $R_0 := \|x_0 - x^*\|$. Depending on f^*, N could be very large, even if δ is moderate!

We need special methods.

Context and Contributions

- There already exist several gradient-type methods for optimization in relative scale: (Nesterov, 2008; Nesterov, 2009; Nesterov, 2010).
- However, they all work with an exact oracle (exact computations of objective function and/or its gradient).

This work

New first-order methods with inexact stochastic oracle.

Motivating Example

Spectral Linear Regression (SLR) problem

$$\min_{x \in \mathbb{R}^d} \|A(x) - C\|, \qquad A(x) := \sum_{i=1}^{d} x_i A_i,$$

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

- Computing subgradient requires computing a pair of leading singular vectors of an $n \times m$ matrix.
- Cost of exact computation: $O(n^3) \implies$ infeasible for large n (and difficult to exploit sparsity).
- But approximate singular vectors are much more affordable: they require only a small number of matrix-vector products.
- The corresponding linear algebra methods are typically randomized, so we obtain inexact approximate subgradients.

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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

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

  where $\|h\|_B := \langle Bh, h \rangle^{1/2}$.
- We have a δ-relatively inexact stochastic subgradient oracle $\hat{g}$:

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

- The size of $\hat{g}$ is relatively bounded:

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

Example: Squared Spectral Norm

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

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

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

Relatively inexact stochastic subgradient:

$$\hat{G}(X) := 2\hat{u}\hat{u}^T X, \qquad \hat{u} \sim \text{MaxEV}(XX^T, \delta).$$

δ-relatively inexact stochastic eigenvector

Given a matrix $A \in \mathbb{S}^n_+$, compute $\hat{u} \sim \text{MaxEV}(A, \delta)$ such that

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

Relative boundedness: $\hat{G}$ is relatively bounded w.r.t. F with $L = 2$:

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

Composition with Affine Mapping

Consider

$$f(x) = F(Ax + b), \qquad x \in \mathbb{E},$$

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 $\hat{G}$ for F.
- Oracle $\hat{G}$ is uniformly relatively bounded with constant L.

Define the seminorm induced by $B = A^* B_1 A$:

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

and stochastic oracle

$$\hat{g}(x) := A^* \hat{G}(Ax + b), \qquad x \in \mathbb{E}.$$

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

$$x_0 = \operatorname*{argmin}_{x \in Q} \|Ax + b - y_0\|_{B_1}.$$

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Gradient Method with Relative Inexact Stochastic Oracle

$$\hat{g}_k \sim \hat{g}(x_k), \quad x_{k+1} = \mathrm{Prox}_{Q,B}(x_k, a_k \hat{g}_k), \qquad k \geq 0,$$

where $\mathrm{Prox}_{Q,B}(x, s) := \mathrm{argmin}_{y \in Q}\{\langle s, y\rangle + \frac{1}{2}\|y - x\|_B^2\}$, and $(a_k)_{k=0}^{\infty}$ are deterministic step sizes.

Output point: Suppose $a_k < \frac{1-\delta}{L}$ for all $k \geq 0$. Define

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

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

$$(1 - \Delta_k)\, \mathbb{E}\, f(\bar{x}_k) \leq f^*, \qquad \Delta_k := \delta + \frac{1 - \delta + 2\gamma_0 L \sum_{i=0}^{k-1} a_i^2}{1 + 2\gamma_0 \sum_{i=0}^{k-1} a_i}.$$

Choice of Stepsizes

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

$$a_k \equiv \frac{1-\delta}{\sqrt{2\gamma_0 NL(1-\delta)+L^2}+L}, \qquad k \geq 0.$$

Convergence rate:

$$\Delta_N \leq \delta + \sqrt{\frac{2L}{\gamma_0 N}} \quad \Longrightarrow \quad \Delta_N \leq 2\delta, \quad \forall N \geq N(\delta) := \frac{2L}{\gamma_0 \delta^2}$$

Note: For SLR, we have $L = 2$ and $\gamma_0 = \frac{1}{n}$, so $N(\delta) = \frac{4n}{\delta^2}$ does not depend on data defining the problem.

Constant step size based on target accuracy $\delta \in (0, \frac{2}{3})$

$$a_k \equiv \frac{\delta}{2L}, \qquad k \geq 0.$$

$\Longrightarrow$ same rate for Δ_N.

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Stochastic Oracle for Maximal Eigenvector

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

Given a matrix $A \in \mathbb{S}^n_+$, compute $\hat{u} \sim \text{MaxEV}(A, \delta)$ such that

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

How to compute $\text{MaxEV}(A, \delta)$ efficiently?

Power Method

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

$$\hat{u}_p := \frac{A^p \xi}{\|A^p \xi\|}, \qquad \xi \sim \mathrm{Unif}(\mathcal{S}^{n-1}).$$

Should be computed in a numerically stable way:

Power Method

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

Complexity: p matrix-vector products.

Main result (Kuczyński and Woźniakowski, 1992)

Suppose $n \geq 8$ and $p \geq 2$. Then,

$$\mathbb{E}\langle A\hat{u}_p, \hat{u}_p \rangle \geq (1 - \delta_p)\lambda_{\max}(A), \qquad \delta_p = 0.871 \frac{\ln n}{p}.$$

Lanczos Method

Krylov subspace: $\mathcal{K}_p(A, \xi) := \mathrm{span}(\xi, A\xi, A^2\xi, \ldots, A^p\xi)$.

Lanczos Algorithm

$$\hat{u}_p \in \mathrm{Argmax}\big\{\langle Ax, x\rangle : x \in \mathcal{K}_p(A, \xi) \cap \mathcal{S}^{n-1}\big\}, \qquad \xi \sim \mathrm{Unif}(\mathcal{S}^{n-1}).$$

Accuracy estimate (Kuczyński and Woźniakowski, 1992)

Suppose $n \geq 8$, $p \geq 3$. Then,

$$\mathbb{E}\langle A\hat{u}_p, \hat{u}_p\rangle \geq (1 - \delta_p)\lambda_{\max}(A), \qquad \delta_p = 2.575\left(\frac{\ln n}{p}\right)^2.$$

Implementing Lanczos Method

Lanczos Algorithm: $\hat{u} = \text{LanczosAlg}(A, p)$

$(T, Q) \coloneqq \text{LanczosTridiag}(A, \xi, p)$ with $\xi \sim \text{Unif}(\mathcal{S}^{n-1})$.

$\hat{x} = \text{MaxEVTridiag}(T)$.

return $\hat{u} \coloneqq Q\hat{x}$.

Lanczos Tridiagonalization: $(T, Q) = \text{LanczosTridiag}(A, \xi, p)$

$q_0 \coloneqq \xi, \quad \alpha_0 \coloneqq \langle Aq_0, q_0 \rangle, \quad r_0 \coloneqq Aq_0 - \alpha_0 q_0.$

for $k = 0, \ldots, p-1$ **do**

$\beta_k \coloneqq \|r_k\|, \quad q_{k+1} \coloneqq r_k/\beta_k, \quad \alpha_{k+1} \coloneqq \langle Aq_{k+1}, q_{k+1} \rangle.$

$r_{k+1} \coloneqq Aq_{k+1} - \alpha_{k+1} q_{k+1} - \beta_k q_k.$

return $T \coloneqq \text{Tridiag}(\alpha_0, \ldots, \alpha_p; \beta_0, \ldots, \beta_{p-1}), \quad Q \coloneqq [q_0, \ldots, q_p].$

Complexity: $p + 1$ matrix-vector products $+ O(np)$.

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Drawbacks of Previously Considered Gradient Method

In the previously considered Gradient Method, we first decide on the target relative accuracy δ we want to achieve and then use at each iteration:

- Fixed oracle accuracy $\delta' := \delta/2$.
- Constant step size $a_k \equiv \delta'/(2L)$.

Disadvantages:

- Need to know δ in advance.
- The method is essentially short-step.
- Always ask for the same high oracle accuracy.

Natural idea: Use time-varying step sizes and oracle accuracies
$\Longrightarrow$ Dual Averaging Method (same worst-case complexity).

Dual Averaging Method

$$v_{k+1} = \operatorname{argmin}_{x \in Q} \left\{ \sum_{i=1}^{k} a_i [(1-\delta_i) f(w_i) + \langle g_i, x - w_i \rangle] + \frac{\beta_k}{2} \|x - x_0\|_B^2 \right\}.$$

DualAvg $\left(x_0, L, (a_k)_{k=1}^{\infty}, (\beta_k)_{k=0}^{\infty}, (\delta_k)_{k=1}^{\infty}\right)$.

$v_0 := x_0, \quad \bar{g}_0 := 0 \ (\in \mathbb{E}^*), \quad A_0 := C_0 := 0 \ (\in \mathbb{R})$.

for $k \geq 0$ **do**

$w_{k+1} := \left(\beta_k v_k + (\beta_{k+1} - \beta_k) x_0\right) / \beta_{k+1}, \quad g_{k+1} \sim g(w_{k+1}, \delta_{k+1})$.

$A_{k+1} := A_k + a_{k+1}, \quad \bar{g}_{k+1} := (A_k \bar{g}_k + a_{k+1} g_{k+1}) / A_{k+1}$.

$v_{k+1} := \operatorname{Prox}_{Q,B}\left(x_0, \frac{A_{k+1}}{\beta_{k+1}} \bar{g}_{k+1}\right)$.

$c_{k+1} := a_{k+1}\left(1 - \delta_{k+1} - \frac{L a_{k+1}}{\beta_{k+1}}\right), \quad C_{k+1} := C_k + c_{k+1}$.

$x_{k+1} := (C_k x_k + c_{k+1} w_{k+1}) / C_{k+1}$.

Choice of parameters:

$$a_k := 1, \qquad \beta_k := \sqrt{8\gamma_0 L k} + 2L, \qquad \delta_k := \frac{L a_k}{\beta_k} = \frac{1}{\sqrt{8\gamma_0 k / L} + 2}.$$

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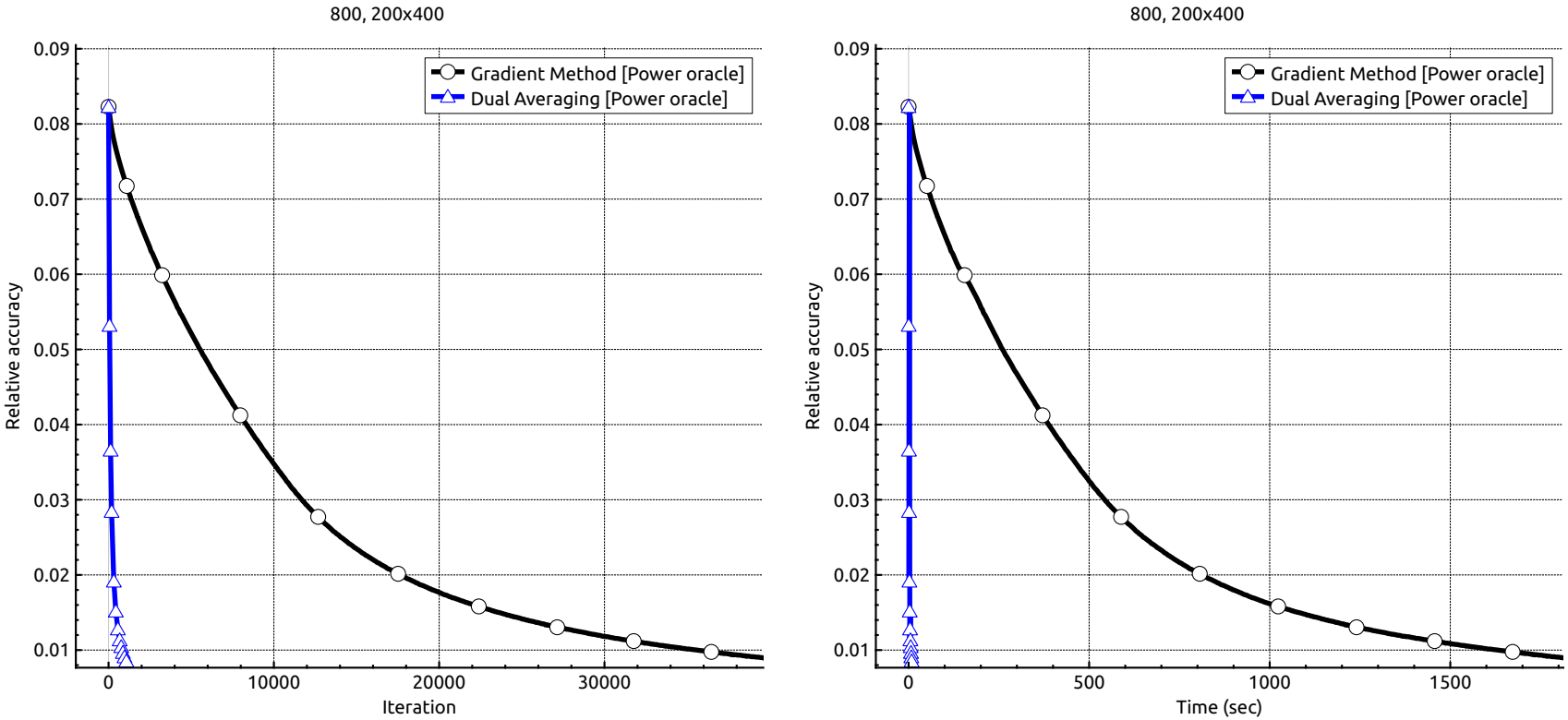
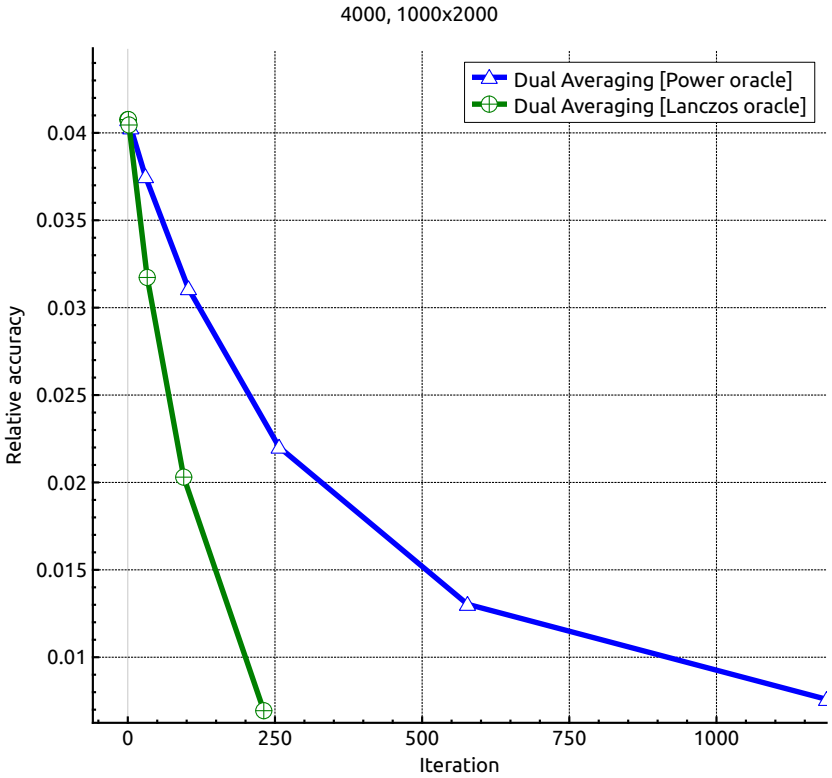
Gradient Method vs Dual Averaging

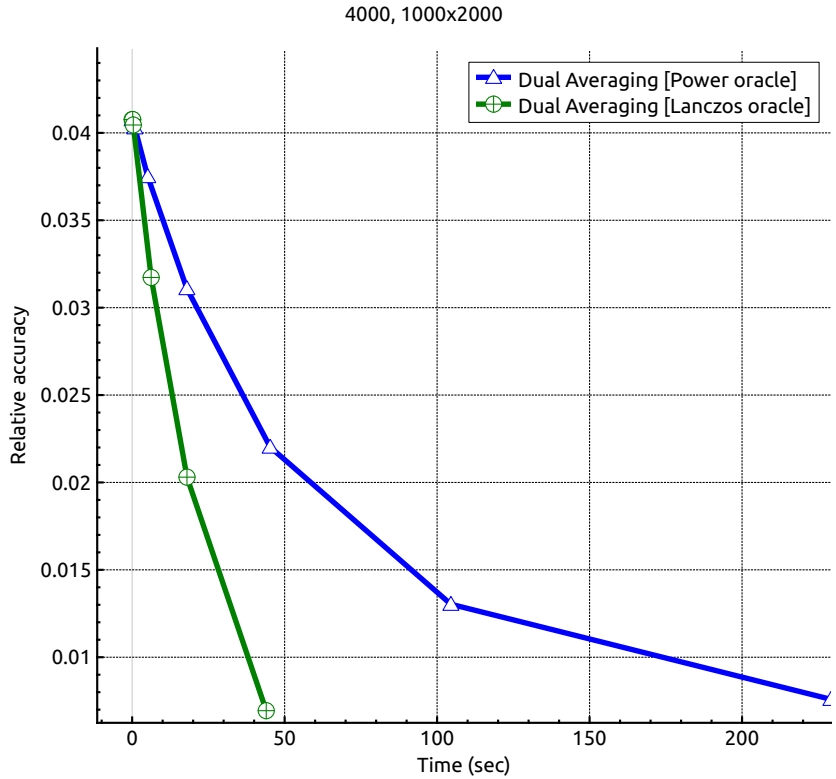
Problem: Spectral linear regression ($\delta = 0.01$ for Gradient Method).



- Dual Averaging is by *orders of magnitude* faster.
- Actual # iterations is by *orders of magnitude* smaller than the theoretical one: $N(\delta) = 8\,080\,605$.

Power Oracle vs Lanczos Oracle





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MaxCut Problem

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

MaxCut problem

$$c^* = \frac{1}{4} \max_{x \in B^n} \langle Ax, x \rangle,$$

where B^n is the boolean hypercube:

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

and $A \in \mathbb{S}_+^n$ is the Laplacian matrix of G:

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

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

SDP Relaxation

MaxCut problem:

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

SDP relaxation:

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

where $e := (1, \ldots, 1)^T \in \mathbb{R}^n$.

Accuracy of relaxation (Goemans and Williamson, 1995)

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

SDP Relaxation: Alternative Form

Problem

$$f^* = \min_{x \in Q} \left[f(x) := \lambda_{\max}\big(S(x)\big) \right], \qquad S(x) := D(x) A D(x),$$

where

$$Q := \left\{ x \in \mathbb{R}^n_{++} : \sum_{i=1}^n \frac{1}{x_i^2} \leq 1 \right\}.$$

Oracle:

$$\hat{g}(x) := 2[A(x \odot \hat{u})] \odot \hat{u} \ \left[= 2d(AD(x)\hat{u}\hat{u}^T) \right], \quad \hat{u} \sim \text{MaxEV}\big(S(x), \delta\big).$$

Choice of norm: $B = D(A)$. Then, all our assumptions are satisfied with

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

Note: Since B is diagonal, projection is cheap: $O(n)$.

Final Guarantee

We get $x_k \in Q$ with $(1-\delta)\,\mathbb{E}\, f(x_k) \leq f^*$ in at most $N(\delta)$ iterations,

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

Result

For $\hat{f}_k := (1-\delta)^{-1}\langle S(x_k)\hat{u}, \hat{u}\rangle,\ \ \hat{u} \sim \mathrm{MaxEV}\big(S(x_k), \delta\big)$, we have

$$\alpha\, \mathbb{E}\, \hat{f}_k \leq s^* \leq \mathbb{E}\, \hat{f}_k, \qquad \alpha := 0.878(1-\delta)^2.$$

Total worst-case running time:

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

Note: No need for very small δ: $\delta = 0.01 \implies \alpha \approx 0.86$ (instead of $\alpha' = 0.878$ for exact solution of SDP).

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Conclusions

Overview:

- New concept of relatively inexact stochastic subgradient.
- Arises naturally when computing inexact eigenvectors by using the Power method or the Lanczos algorithm.
- Two gradient methods for large-scale optimization in relative-scale: Gradient Method with fixed stepsize and oracle accuracy and the more practical Dual Averaging.

Paper

`https://arxiv.org/abs/2301.08352`

Thank you!

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