A Stochastic Smoothing Algorithm for Semidefinite Programming

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Introduction

Focus on **maximum eigenvalue minimization**

$$\min_{x \in Q} \lambda_{\max}\left(A_0 + \sum_{i=1}^{m} x_i A_i\right) + c^T x$$

in the variable $x \in \mathbb{R}^m$, with $A_i \in \mathbf{S}_n$, $c \in \mathbb{R}^m$.

- The set Q is convex and simple, i.e. projections on Q can be computed with low complexity.
- We also implicitly assume that n is large while the target precision ϵ and the cost of forming $A(x) = A_0 + \sum_{i=1}^{m} x_i A_i$ remain relatively modest (e.g. A_i sparse).

Introduction

- All semidefinite programs with constant trace can be expressed in this way.
- In particular, many semidefinite relaxations of combinatorial problems fall in this setting (large n, modest precision target).
- The objective is non differentiable but can be regularized (more later).

Introduction

Solve

$$\min_{x \in Q} \lambda_{\max}\left(A(x)\right) + c^T x$$

using **projected subgradient.**

Input: A starting point $x_0 \in \mathbb{R}^m$.

1: **for** $t = 0$ to $N - 1$ **do**

2: Set

$$x_{t+1} = P_Q(x_t - \gamma \partial \lambda_{\max}(A(x))).$$

3: **end for**

Output: A point $x = (1/N)\sum_{t=1}^{N} x_t$.

- Here, $\gamma > 0$ and $P_Q(\cdot)$ is the Euclidean projection on Q.
- The number of iterations required to reach a target precision ϵ is

$$N = \frac{D_Q^2 M^2}{\epsilon^2}$$

where D_Q is the diameter of Q and $\|\partial \lambda_{\max}(A(x))\| \leq M$ on Q.

Introduction

The **cost per iteration** is the sum of

- The cost p_Q of computing the Euclidean projection on Q.
- The cost of computing $\partial\lambda_{\max}(A(x))$ which is e.g. $v_1 v_1^T$ where v_1 is a leading eigenvector of X.

Computing one leading eigenvector of a dense matrix X with relative precision ϵ, using a randomly started Lanczos method, with probability of failure $1-\delta$, costs

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

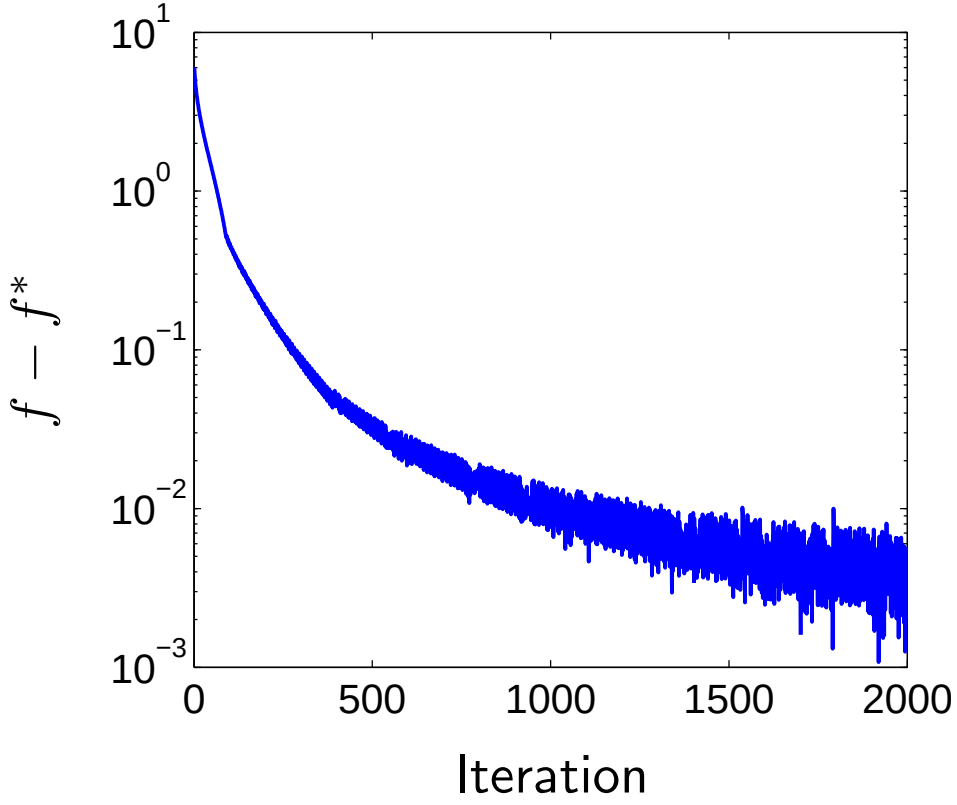
flops [Kuczynski and Wozniakowski, 1992, Th.4.2].

Introduction

Solving $\min_{X \in Q} \lambda_{\max}(A(x))$ using projected subgradient.

- Easy to implement.
- Very poor performance in practice. The $1/\epsilon^2$ dependence is somewhat punishing. . .

Example below on MAXCUT.



Introduction

[Nesterov, 2007a] We can **regularize** the objective and solve

$$\min_{x \in Q} \; f_\mu(x) \triangleq \mu \log \mathbf{Tr} \left(\exp \left(\frac{A(x)}{\mu} \right) \right)$$

for some regularization parameter $\mu > 0$ ($\exp(\cdot)$ is the **matrix** exponential here).

- If we set $\mu = \epsilon / \log n$ we get

$$\lambda_{\max}(A(x)) \leq f_\mu(x) \leq \lambda_{\max}(A(x)) + \epsilon$$

- The gradient $\nabla f_\mu(x)$ is Lipschitz continuous with constant

$$\frac{\|A\|^2 \log n}{\epsilon}$$

  where $\|A\| = \sup_{\|h\| \leq 1} \|A(h)\|_2$.

Introduction

- The number of iterations required to get an ϵ solution using the **smooth** minimization algorithm in Nesterov [1983] grows as

$$\frac{\|A\|\sqrt{\log n}}{\epsilon}\sqrt{\frac{d(x^*)}{\sigma}}$$

  where $d(\cdot)$ is strongly convex with parameter $\sigma > 0$.

- The **cost per iteration** is (usually) dominated by the cost of forming the matrix exponential

$$\exp\left(\frac{A(x)}{\mu}\right)$$

  which is $O(n^3)$ flops [Moler and Van Loan, 2003].

- Much better empirical performance.

Introduction

This means that the two classical complexity options for solving

$$\min_{X \in Q} \lambda_{\max}(A(x))$$

(assuming $A(x)$ cheap)

- **Subgradient methods**

$$O\left(\frac{D_Q^2(n^2 \log n + p_Q)}{\epsilon^2}\right)$$

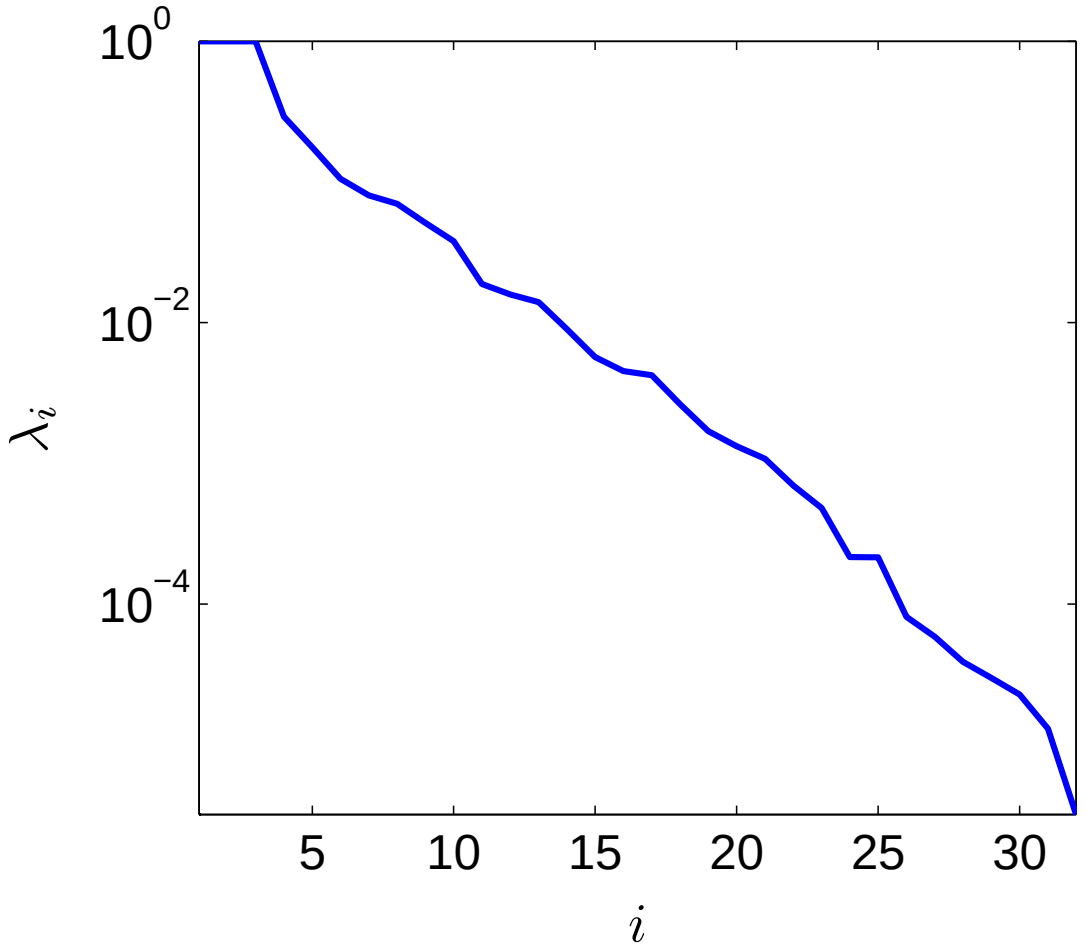
- **Smooth optimization**

$$O\left(\frac{D_Q\sqrt{\log n}(n^3 + p_Q)}{\epsilon}\right)$$

  if we pick $\|\cdot\|_2^2$ in the prox term.

Introduction

Approximate gradient is often enough. This means computing only a few leading eigenvectors.



Spectrum of $\exp((X - \lambda_{\max}(X)\mathbf{I})/0.1)$ at the MAXCUT solution.

Introduction

[d'Aspremont, 2008] Convergence guarantees using **approximate gradients**.

If $\tilde{\nabla} f(x)$ is the approximate gradient, we require

$$|\langle \tilde{\nabla} f(x) - \nabla f(x), y - z \rangle| \leq \delta \quad x, y, z \in Q,$$

hence the condition depends on the diameter of Q. For example, to solve

$$\begin{array}{ll} \text{minimize} & \lambda_{\max}(A + X) \\ \text{subject to} & |X_{ij}| \leq \rho \end{array}$$

we only compute the j largest eigenvalues of $A + X$, with j such that

$$\frac{(n-j)e^{\lambda_j}\sqrt{\sum_{i=1}^{j} e^{2\lambda_i}}}{(\sum_{i=1}^{j} e^{\lambda_i})^2} + \frac{\sqrt{n-j}\; e^{\lambda_j}}{\sum_{i=1}^{j} e^{\lambda_i}} \leq \frac{\delta}{\rho n}.$$

The impact of the **diameter** makes these conditions quite conservative.

Introduction

Other conditions (often less stringent) are detailed in [Devolder, Glineur, and Nesterov, 2011] when solving

$$\min_{x \in Q} \max_{u \in U} \Psi(x, u)$$

If u_x is an approximate solution to $\max_{u \in U} \Psi(x, u)$, we can check $V_i(u_x) \leq \delta$

$$V_1(u_x) = \max_{u \in U} \nabla_2 \Psi(x, u_x)^T (u - u_x)$$

$$V_2(u_x) = \max_{u \in U} \left\{ \Psi(x, u) - \Psi(x, u_x) + \kappa \|u - u_x\|^2 / 2 \right\}$$

$$V_3(u_x) = \max_{u \in U} \Psi(x, u) - \Psi(x, u_x)$$

where

$$V_1(u_x) \leq V_2(u_x) \leq V_3(u_x) \leq \delta$$

- The target accuracy δ on the oracle is a function of the target accuracy ϵ.
- Not clear yet if they can be tested independently of the diameter.

Introduction

- Approximate gradients reduce empirical complexity. No **a priori** bounds on iteration cost.
- More efficient to run a lot of cheaper iterations, everything else being equal.

Objectives

- Keep some of the performance of smooth methods, while lowering the cost of smoothing?
- Get a more refined understanding of the iteration complexity versus convergence speed tradeoff?

One possible solution here: **stochastic gradient approximations.**

Outline

- Introduction
- **Stochastic Smoothing**
- Maximum Eigenvalue Minimization

Stochastic Smoothing

Gaussian smoothing. Suppose $f(x) : \mathbb{R}^n \to \mathbb{R}$ is Lipschitz continuous w.r.t. the Euclidean norm, with constant μ. The function

$$g(x) = \mathbf{E}[f(x + (\sigma/\sqrt{n})u)]$$

where $u \sim \mathcal{N}(0, \mathbf{I}_n)$ and $\sigma > 0$, has a Lipschitz continuous gradient with

$$\|\nabla g(x) - \nabla g(y)\| \leq \frac{2\mu n}{\sigma}\|x - y\|.$$

Used in e.g. [Nesterov, 2011] to get explicit complexity bounds on gradient free optimization methods.

- $g(X) = \mathbf{E}[\lambda_{\max}(X + (\sigma/n)U]$ where $U \in \mathbf{S}_n$ is a symmetric matrix with standard normal upper triangle coefficients, has a Lipschitz continuous gradient with constant
$$O\left(\frac{n^{3/2}}{\sigma}\right)$$
- A smooth algorithm (if implementable) would require $O(n^{3/4})$ iterations.

Stochastic Smoothing

Gradient smoothness. Call $f(X) = \lambda_{\max}(X)$, define

$$g(X, Y) = \lim_{t \to 0} \frac{\partial^2 f(X + tY)}{\partial t^2}$$

and $L_f > 0$ such that

$$\|\nabla f(X) - \nabla g(Y)\| \leq L_f \|X - Y\|$$

we have

$$L_f = \sup_{X,Y} g(X, Y) = \sup_X \frac{1}{2(\lambda_1(X) - \lambda_2(X))}$$

The **spectral gap** controls the gradient's smoothness.

Stochastic Smoothing

Rank one updates. Suppose $D \in \mathbf{S}_n$, we have almost explicit expressions for the eigenvalue decomposition of the matrix

$$D + \sigma u u^T$$

where $u \in \mathbb{R}^n$ and $\sigma > 0$.

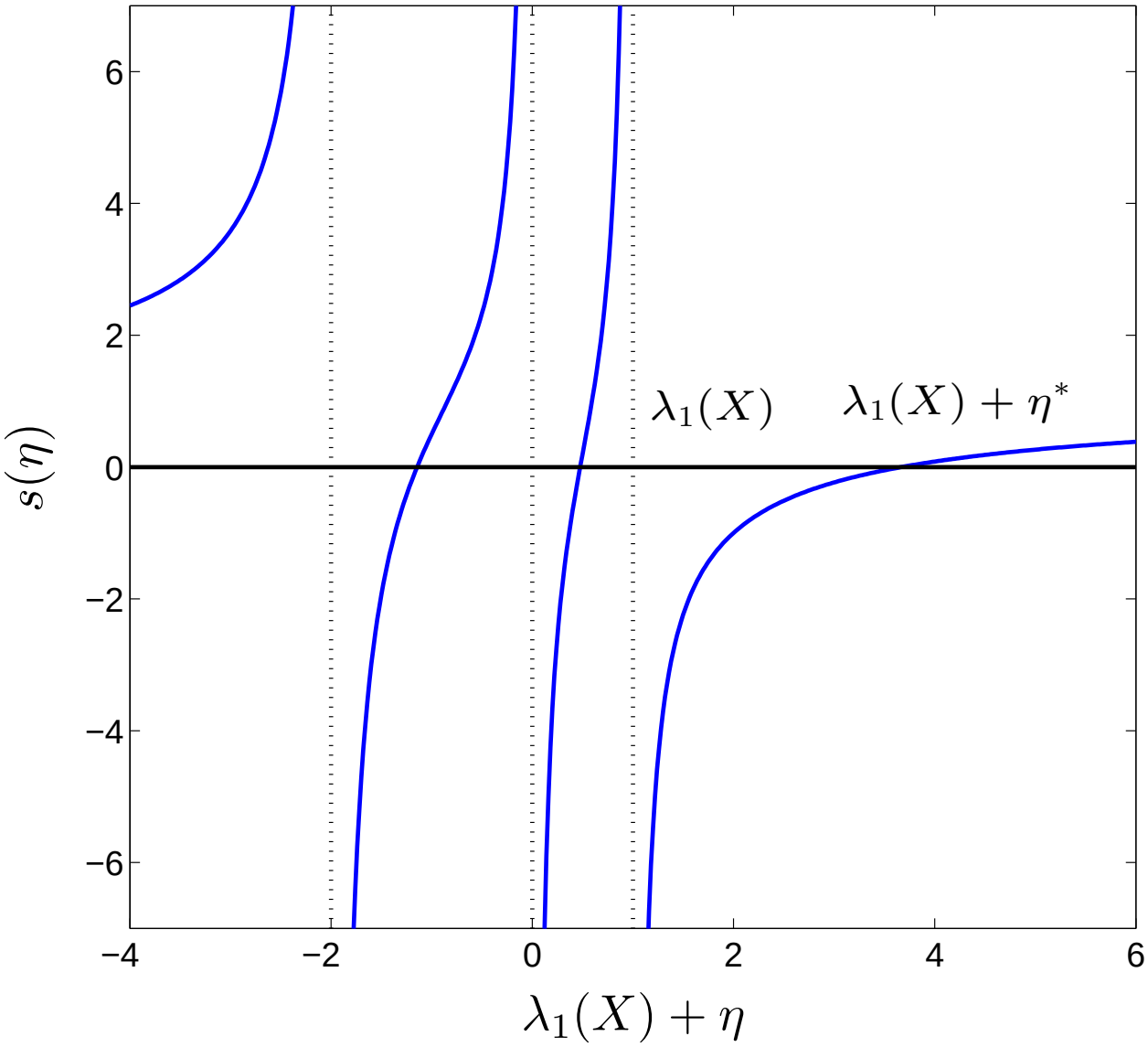
- W.l.o.g. we can assume D is diagonal (just change u).
- If we write $\lambda_1(X + \sigma u u^T) = \lambda_1(X) + \eta$, we know that

$$\eta > 0 \quad \text{if } u_i \neq 0 \text{ for } i = 1, \ldots, n$$

- The eigenvalues of X and $X + \sigma u u^T$ are **interlaced.**
- The increment η^* is the unique positive root of the **secular equation**

$$s(\eta) \triangleq \frac{1}{\sigma} - \frac{u_1^2}{\eta} - \sum_{i=2}^{n} \frac{u_i^2}{(\lambda_1(X) - \lambda_i(X)) + \eta} = 0$$

Stochastic Smoothing



Spectrum of X is $\{-2,-2,0,1\}$, fourth eigenvalue of $X+\sigma uu^T$ at -2.

Stochastic Smoothing

- The function

$$s^+(\eta) \triangleq \frac{1}{\sigma} - \frac{u_1^2}{\eta}$$

  is an upper bound on $s(\eta)$.
- This means that the root of $s^+(\eta)$ is a **lower bound** on η^* and we get

$$\eta^* \geq \frac{u_1^2}{\sigma}$$

- Together with interlacing, this yields

$$\lambda_2(X + \sigma uu^T) \leq \lambda_1(X) \leq \lambda_1(X) + \eta^* \leq \lambda_1(X + \sigma uu^T)$$

Finally, we get **a lower bound on the spectral gap**

$$\lambda_1(X + \sigma uu^T) - \lambda_2(X + \sigma uu^T) \geq \frac{u_1^2}{\sigma}$$

Stochastic Smoothing

Rank one Gaussian smoothing. Suppose we pick $u \in \mathbb{R}^n$ with i.i.d. $u_i \sim \mathcal{N}(0,1)$ and define

$$f(X) = \mathbf{E}[\lambda_{\max}(X + (\epsilon/n)uu^T)]$$

for some $\epsilon > 0$.

- Because $uu^T \succeq 0$ and $\lambda(\cdot)$ is 1-Lipschitz

$$\lambda_{\max}(X) \leq \mathbf{E}[\lambda_{\max}(X + (\epsilon/n)uu^T)] \leq \lambda_{\max}(X) + \epsilon$$

- The Gaussian distribution is rotationally invariant, so the spectral gap is bounded below by $\epsilon u_1^2/n$ where $u_1 \sim \mathcal{N}(0,1)$ hence

$$L \leq \frac{n}{\epsilon\, u_1^2}$$

Unfortunately $\mathbf{E}[1/u_1^2] = +\infty$, easy to fix. . .

Stochastic Smoothing

Max-rank one Gaussian smoothing. Suppose we pick $u_i \in \mathbb{R}^n$ with i.i.d. $u_{ij} \sim \mathcal{N}(0,1)$ and define

$$f(X) = \mathbf{E}\left[\max_{i=1,\ldots,k} \lambda_{\max}(X + (\epsilon/n)u_i u_i^T)\right]$$

- Approximation results are preserved up to a constant $c_k > 0$

$$\lambda_{\max}(X) \leq \mathbf{E}[\lambda_{\max}(X + (\epsilon/n)uu^T)] \leq \lambda_{\max}(X) + c_k\epsilon$$

- The Gaussian distribution is rotationally invariant, so the spectral gap is bounded below by

$$\max_{i=1,\ldots,k} \frac{\epsilon\, u_{i,1}^2}{n}$$

  where u_i are i.i.d. with $u_{i,1} \sim \mathcal{N}(0,1)$.
- The complexity of computing $\max_{i=1,\ldots,k} \lambda_{\max}(X + (\epsilon/n)u_i u_i^T)$ is

$$O(kn^2 \log n).$$

Stochastic Smoothing

Proposition 1

Max-rank one Gaussian smoothing. *The function*

$$f(X) = \mathbf{E}\left[\max_{i=1,\ldots,k} \lambda_{\max}(X + (\epsilon/n)u_i u_i^T)\right]$$

is smooth and the Lipschitz constant of its gradient is bounded by

$$L_f \leq \mathbf{E}\left[\frac{n}{2\epsilon}\left(\min_{i=1,\ldots,k} \frac{1}{u_{i,1}^2}\right)\right] \leq C_k \frac{n}{\epsilon}$$

where $C_k = \frac{1}{\sqrt{2}}\frac{k}{k-2}$, *is finite when* $k \geq 3$.

Coarse, numerical simulations show C_3 is around 0.75...

Stochastic Smoothing

Gradient variance. We have

$$\partial \lambda_{\max}(X) = v_1(X)v_1(X)^T$$

where $v_1(X)$ is a leading eigenvector of X.

- We have, when D is diagonal

$$v_1(D + uu^T)_i = c\frac{u_i}{\lambda_1(D + uu^T) - \lambda_i(D)}$$

  where $c > 0$ is a normalization term.

- By symmetry, when u is Gaussian, $A = \mathbf{E}[v_1(X + uu^T)v_1(X + uu^T)^T]$ is diagonal, with

$$\mathbf{E}[\mathbf{Tr}\left(v_1v_1^T - A\right)^2] = 1 - \mathbf{Tr}\, A^2,$$

  where $\mathbf{Tr}\, A = 1$ with $A_{ii} \geq 0$.

This means that $\mathbf{E}[\mathbf{Tr}\left(v_1v_1^T - A\right)^2]$ is of order 1.

Outline

- Introduction
- Stochastic Smoothing
- **Maximum Eigenvalue Minimization**

Maximum Eigenvalue Minimization

Solve **maximum eigenvalue minimization** after stochastic smoothing

$$\min_{x\in Q} \mathbf{E}\left[\max_{j=1,\ldots,3} \lambda_{\max}\left(A_0 + \sum_{i=1}^{m} x_i A_i + \frac{\epsilon}{n} u_j u_j^T\right)\right] + c^T x$$

in the variable $x \in \mathbb{R}^m$, with $A_i \in \mathbf{S}_n$, $c \in \mathbb{R}^m$ and the u_j are Gaussian.

We use an optimal stochastic minimization algorithm in [Lan, 2009] which is a generalization of the algorithm in Nesterov [1983], with increasing step size.

Maximum Eigenvalue Minimization

Optimal Stochastic Composite Optimization. The algorithm in Lan [2009] solves

$$\min_{x \in Q} \Psi(x) \triangleq f(x) + h(x)$$

with the following assumptions

- $f(x)$ has Lipschitz gradient with constant L and $h(x)$ is Lipschitz with constant M,
- we have a **stochastic oracle** $G(x, \xi_t)$ for the gradient, which satisfies

$$\mathbf{E}[G(x, \xi_t)] = g(x) \in \partial \Psi(x) \quad \text{and} \quad \mathbf{E}[\|G(x, \xi_t) - g(x)\|_*^2] \leq \sigma^2$$

After N iterations, the iterate x_{N+1} satisfies

$$\mathbf{E}\left[\Psi(x_{N+1}^{ag}) - \Psi^*\right] \leq \frac{8LD_{\omega,Q}^2}{N^2} + \frac{4D_{\omega,Q}\sqrt{4\mathcal{M}^2 + \sigma^2}}{\sqrt{N}}$$

which is optimal. Additional assumptions guarantee convergence w.h.p.

Maximum Eigenvalue Minimization

Stochastic line search.

- The bounds on variance and smoothness are very conservative.
- Line search allows to take full advantage of the smoothness of $\lambda_{\max}(X)$ outside of pathological areas.

Monotonic line search. In Lan [2009], we test

$$\begin{aligned}\Psi(x_{t+1}^{ag}, \xi_{t+1}) \quad \leq \quad & \Psi(x_t^{md}, \xi_t) + \langle G(x_t^{md}, \xi_t), x_{t+1}^{ag} - x_t^{md} \rangle \\ & + \frac{\alpha}{4\gamma_t \beta_t} \|x_{t+1}^{ag} - x_t^{md}\|^2 + 2\mathcal{M} \|x_{t+1}^{ag} - x_t^{md}\|\end{aligned}$$

while decreasing the step size monotonically across iterations.

Maximum Eigenvalue Minimization

Optimal Smooth Stochastic Minimization with Line Search.

Input: An initial point $x^{ag} = x_1 = x^w \in \mathbb{R}^n$, an iteration counter $t = 1$, the number of iterations N, line search parameters $\gamma^{min}, \gamma^{max}$, γ^d, $\gamma > 0$, with $\gamma^d < 1$.

1: Set $\gamma = \gamma^{max}$.
2: **for** $t = 1$ to N **do**
3: Define $x_t^{md} = \frac{2}{t+1} x_t + \frac{t-1}{t+1} x_t^{ag}$
4: Call the stochastic gradient oracle to get $G(x_t^{md}, \xi_t)$.
5: **repeat**
6: Set $\gamma_t = \frac{(t+1)\gamma}{2}$.
7: Compute the prox mapping $x_{t+1} = P_{x_t}(\gamma_t G(x_t^{md}, \xi_t))$.
8: Set $x_{t+1}^{ag} = \frac{2}{t+1} x_{t+1} + \frac{t-1}{t+1} x_t^{ag}$.
9: **until** $\Psi(x_{t+1}^{ag}, \xi_{t+1}) \leq$
$\Psi(x_t^{md}, \xi_t) + \langle G(x_t^{md}, \xi_t), x_{t+1}^{ag} - x_t^{md} \rangle + \frac{\alpha \gamma^d}{4\gamma} \|x_{t+1}^{ag} - x_t^{md}\|^2 + 2\mathcal{M} \|x_{t+1}^{ag} - x_t^{md}\|$
or $\gamma \leq \gamma^{min}$. If exit condition fails, set $\gamma = \gamma \gamma^d$ and go back to step 5.
10: Set $\gamma = \max\left\{\gamma^{min}, \gamma\right\}$.
11: **end for**

Output: A point x_{N+1}^{ag}.

Maximum Eigenvalue Minimization

For maximum eigenvalue minimization

- We have $\sigma \leq 1$, but we can reduce this by averaging q gradients, to control the tradeoff between smooth and non-smooth terms.
- If we set $q = \max\{1, D_Q/(\epsilon\sqrt{n})\}$ and $N = 2D_Q\sqrt{n}/\epsilon$ we get the following complexity picture

Complexity	Num. of Iterations	Cost per Iteration
Nonsmooth alg.	$O\left(\frac{D_Q^2}{\epsilon^2}\right)$	$O(p_Q + n^2 \log n)$
Smooth stochastic alg.	$O\left(\frac{D_Q\sqrt{n}}{\epsilon}\right)$	$O\left(p_Q + \max\left\{1, \frac{D_Q}{\epsilon\sqrt{n}}\right\} n^2 \log n\right)$
Smoothing alg.	$O\left(\frac{D_Q\sqrt{\log n}}{\epsilon}\right)$	$O(p_Q + n^3)$

Numerical Results

- Maximum eigenvalue minimization problem over a hypercube (sparse PCA)

$$\begin{array}{ll} \text{minimize} & \lambda_{\max}(A+X) \\ \text{subject to} & -\rho \leq X_{ij} \leq \rho, \quad \text{for } i,j=1,\ldots,n \end{array}$$

  on gene expression covariance matrix.

- We set a fixed number of outer iterations for the stochastic smoothing algorithm and record the number of iterations required by the deterministic algorithm to reach the same objective value.
- We set $q = 5$, $k = 3$ and the maximum number of iterations to $20\sqrt{n}$ in the stochastic algorithm. We also scale the Lipschitz constant by a factor 200!
- Total number of eigenvectors used as a hardware and implementation independent complexity benchmark.
- A bit unfair: complexity ratio between `eig` and (a good implementation) of `eigs` is closer to $n/300$.

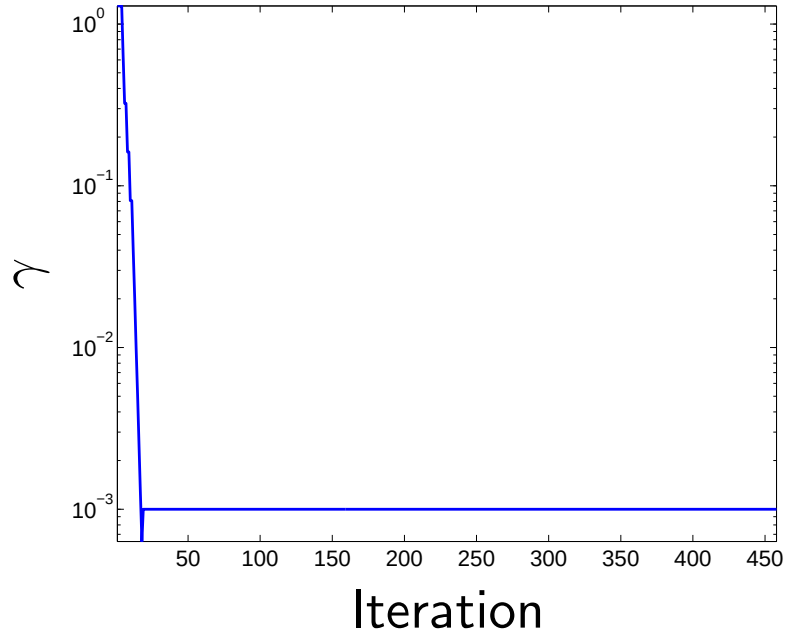
Numerical Results

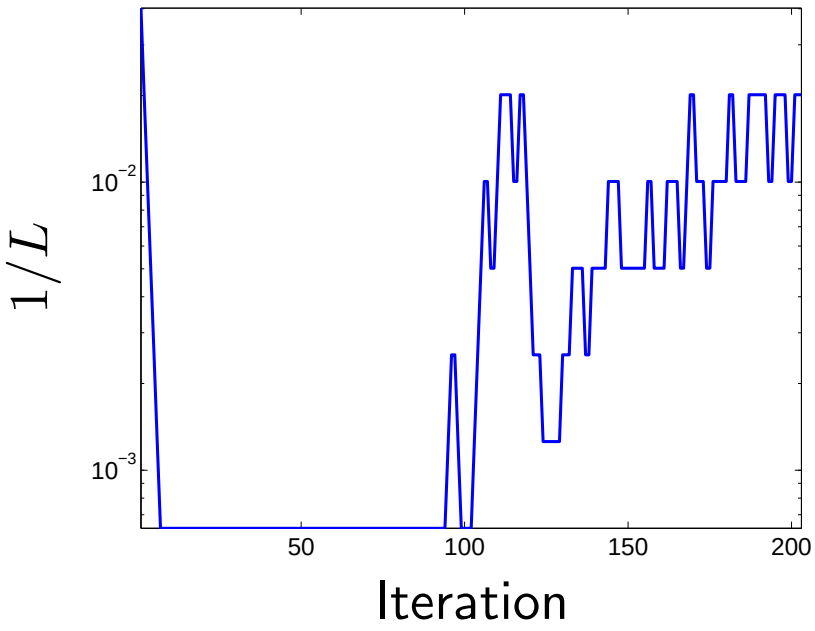
n	# Iters. (Stoch.)	# Eigvs.	# Iters. (Det.)	# Eigvs.
100	200	6 120	100	40 400
200	283	8 565	100	81 200
500	447	13 470	100	203 000

Number of iterations and total number of eigenvectors computed by the stochastic algorithm (Stoch.) and the algorithm in [Nesterov, 2007b, §4] (Det.) to reach identical objective values.

Numerical Results

- Plot the sequence of step size parameters γ for the stochastic algorithm together with the inverse Lipschitz constant $1/L$ (which controls step size) used in the deterministic smoothing algorithm.
- In the stochastic algorithm, the step size is increasing even when γ is constant.





Left: Step size scaling parameter γ for the stochastic algorithm.
Right: Inverse Lipschitz constant $1/L$ in the deterministic algorithm.

Conclusion

- Stochastic smoothing with a few eigenvalues.
- Explicit control of the iteration cost versus smoothness tradeoff.

Some open problems. . .

- Not clear how to get convergence with high probability.
- Stochastic algorithm with non monotonic step sizes?
- $\lambda_{\max}(X + VV^T)$ with $V \in \mathbb{R}^{n\times k}$ Gaussian is slightly cheaper to evaluate than the maximum of k eigenvalues $\max_{i=1,\ldots,k} \lambda_{\max}(X + (\epsilon/n)u_i u_i^T)$. It should be smooth too. . .
- The function $f(X)$ and its gradient $\nabla f(X)$ commute, hence are simultaneously diagonalizable. This means that smoothing can be seen as a spectral function. Can we write other smooth spectral functions as expectations?

*

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