Randomized Smoothing Techniques in Optimization

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Based on joint work with Peter Bartlett, Michael Jordan,
Martin Wainwright, Andre Wibisono

Stanford University

Information Systems Laboratory Seminar
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Problem Statement

Goal: solve the following problem

$$\begin{aligned} \text{minimize} \quad & f(x) \\ \text{subject to} \quad & x \in \mathcal{X} \end{aligned}$$

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Often, we will assume

$$f(x) := \frac{1}{n} \sum_{i=1}^{n} F(x; \xi_i) \quad \text{or} \quad f(x) := \mathbb{E}[F(x; \xi)]$$

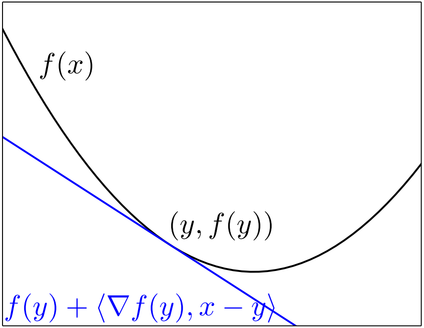
Gradient Descent

Goal: solve

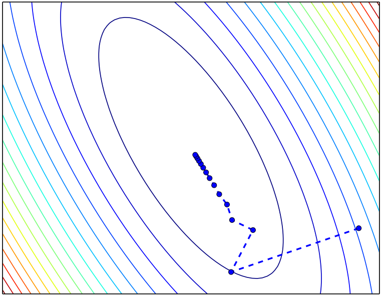
$$\text{minimize} \quad f(x)$$

Technique: go down the slope,

$$x_{t+1} = x_t - \alpha \nabla f(x_t)$$



When is optimization easy?



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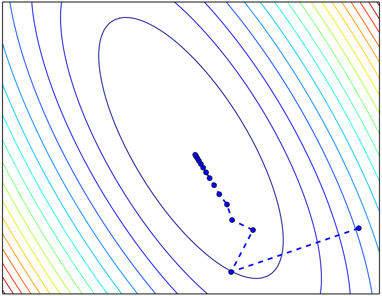

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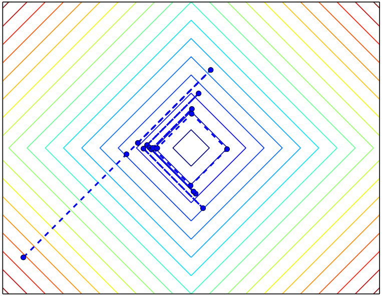

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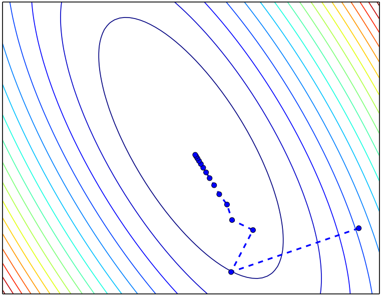

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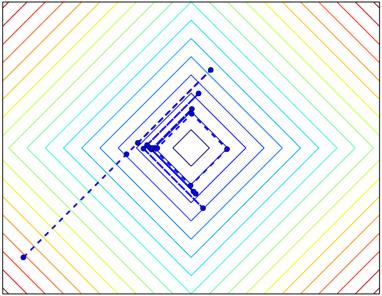

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Even harder problems:

- We cannot compute gradients $\nabla f(x)$
- Function f is non-convex and non-smooth

Example 1: Robust regression

- Data in pairs $\xi_i = (a_i, b_i) \in \mathbb{R}^d \times \mathbb{R}$
- Want to estimate $b_i \approx a_i^\top x$

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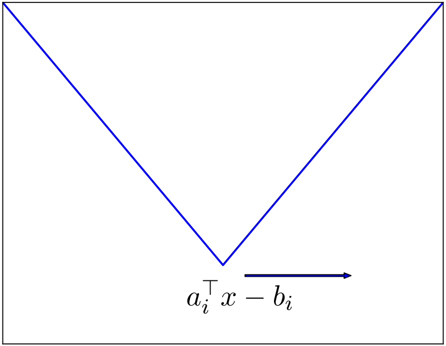
- Data in pairs $\xi_i = (a_i, b_i) \in \mathbb{R}^d \times \mathbb{R}$
- Want to estimate $b_i \approx a_i^\top x$
- To avoid outliers, minimize

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} |a_i^\top x - b_i| = \frac{1}{n}\|Ax - b\|_1$$

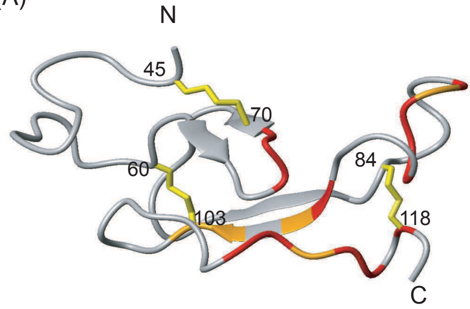


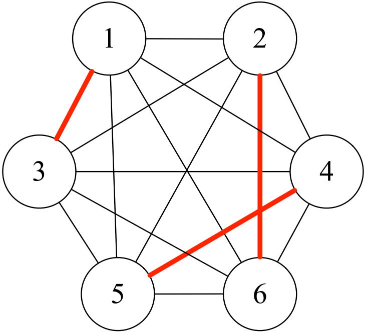
Example 2: Protein Structure Prediction

RSCCPCYWGGCPWGQNCYPEGCSGPKV

1 2 3 4 5 6

(A)

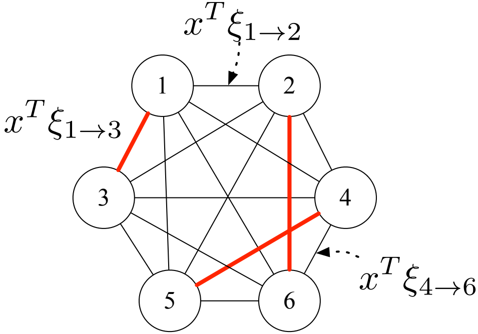




(Grace et al., PNAS 2004)

Protein Structure Prediction

Featurize edges e in graph: vector ξ_e. Labels y are *matching* in a graph, set $\mathcal{V}$ is *all matchings*.



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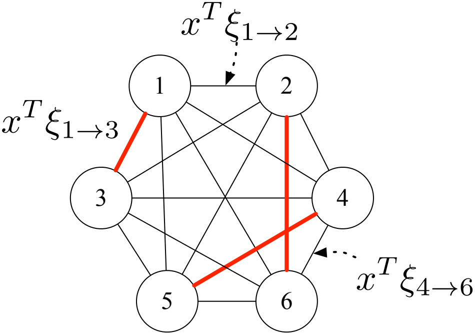

Goal: Learn weights x so that

$$\operatorname*{argmax}_{\widehat{\nu}\in\mathcal{V}} \left\{ \sum_{e\in\widehat{\nu}} \xi_e^\top x \right\} = \nu$$

i.e. learn x so maximum matching in graph with edge weights $x^\top \xi_e$ is correct

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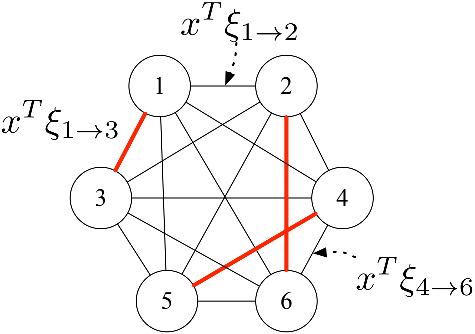

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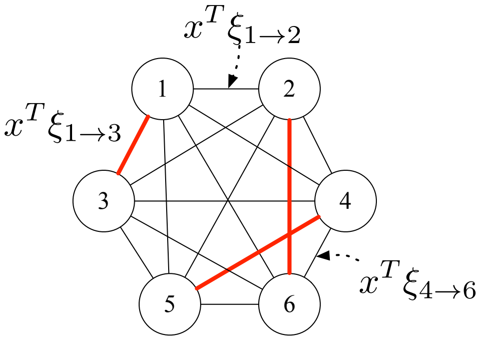

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Loss function: $L(\nu,\widehat{\nu})$ is *number of disagreements* in matchings

$$F(x;\{\xi,\nu\}) := \max_{\widehat{\nu}\in\mathcal{V}}\left(L(\nu,\widehat{\nu}) + x^\top\sum_{e\in\widehat{\nu}}\xi_e - x^\top\sum_{e\in\nu}\xi_e\right).$$

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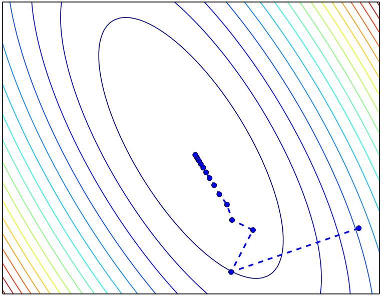

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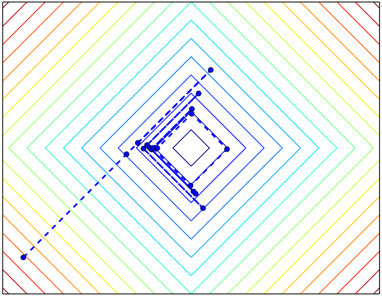

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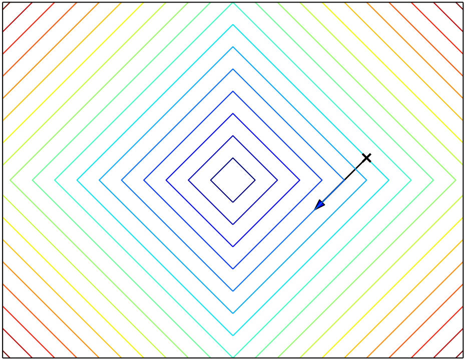
Let Z be a random variable, and for small u, look at f near points

$$f(x + uZ),$$

where u is small



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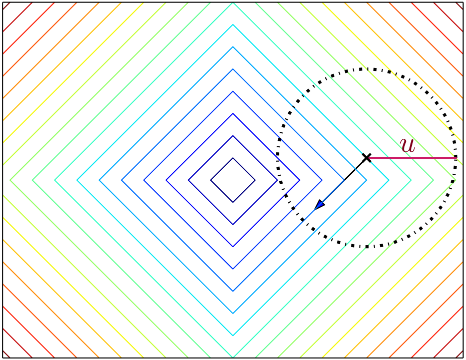

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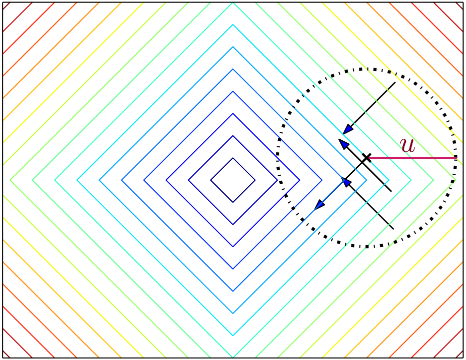

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- Smooth and non-smooth zero order stochastic and non-stochastic optimization problems

III Parallelism: really fast solutions for large scale problems [D., Bartlett, Wainwright 2013]

- Smooth and non-smooth stochastic optimization problems

Instance I: Gradient Sampling Algorithm

Problem: Solve

$$\underset{x \in \mathcal{X}}{\text{minimize}} \; f(x)$$

where f is potentially non-smooth and non-convex (but assume it is continuous and a.e. differentiable) [Burke, Lewis, Overton 2005]

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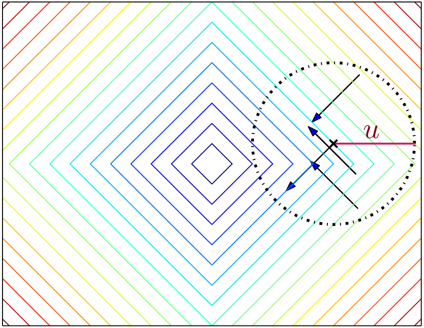
At each iteration t,

- Draw $Z_1, \ldots, Z_m$ i.i.d. $\|Z_i\| \leq 1$
- Set $g_t^i = \nabla f(x_t + u Z_i)$
- Set gradient g_t as

$$g_t = \operatorname{argmin}_g \left\{ \|g\|_2^2 : \begin{array}{c} g = \sum_i \lambda_i g_t^i \\ \lambda \geq 0, \sum_i \lambda_i = 1 \end{array} \right\}$$

- Update $x_{t+1} = x_t - \alpha g_t$, where $\alpha > 0$ chosen by line search



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Define the set

$$G_u(x) := \mathrm{Conv}\left\{ \nabla f(x') : \left\| x' - x \right\|_2 \leq u, \;\; \nabla f(x') \text{ exists} \right\}$$

Proposition (Burke, Lewis, Overton):
There exist cluster points $\bar{x}$ of the sequence x_t, and for any such cluster point,

$$0 \in G_u(\bar{x})$$

Instance II: Zero Order Optimization

Problem: We want to solve

$$\underset{x \in \mathcal{X}}{\text{minimize}} \;\; f(x) = \mathbb{E}[F(x; \xi)]$$

but we are only allowed to observe function values $f(x)$ (or $F(x; \xi)$)

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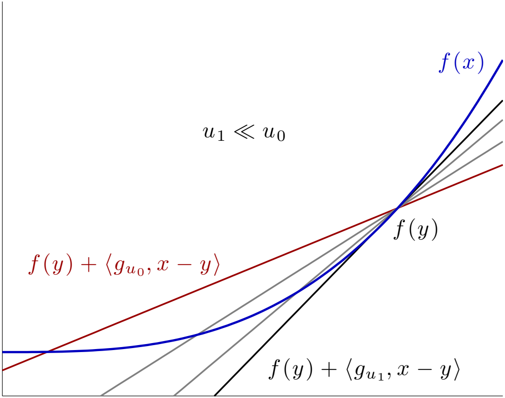
Idea: Approximate gradient by function differences

$$f'(y) \approx g_u := \frac{f(y+u) - f(y)}{u}$$



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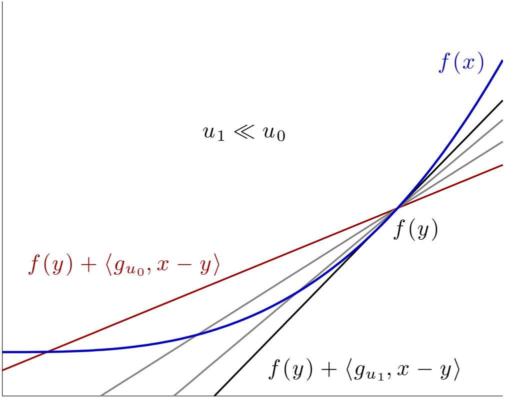

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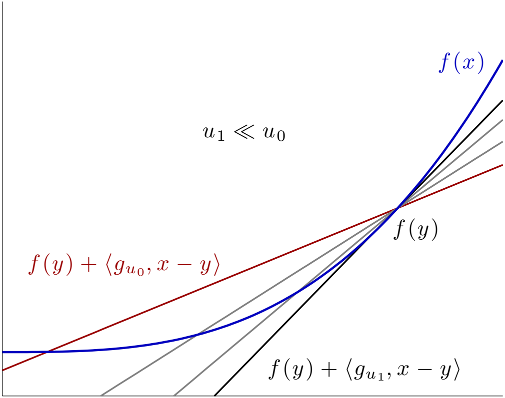
- Can randomized perturbations give insights?



Stochastic Gradient Descent

Algorithm: At iteration t

- Choose random ξ, set

$$g_t = \nabla F(x_t; \xi_i)$$

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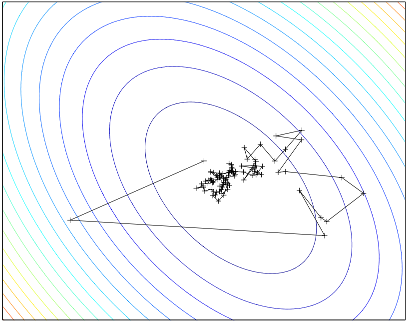

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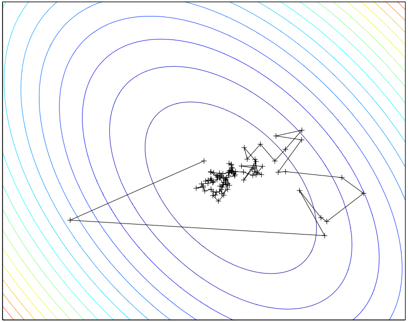

Theorem (Russians): Let $\widehat{x}_T = \frac{1}{T}\sum_{t=1}^{T} x_t$ and assume $R \geq \|x^* - x_1\|_2$, $G^2 \geq \mathbb{E}[\|g_t\|_2^2]$. Then

$$\mathbb{E}[f(\widehat{x}_T) - f(x^*)] \leq RG\frac{1}{\sqrt{T}}$$

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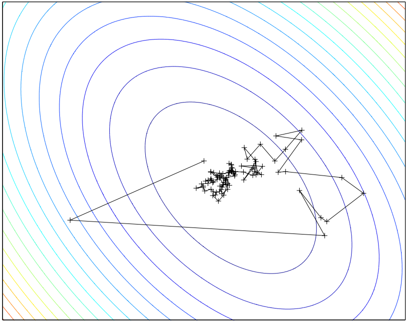

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Note: Dependence on G important

Derivative-free gradient descent

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Question: How well can we estimate gradient ∇f using only function differences? And how small is the norm of this estimate?

Derivative-free gradient descent

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Question: How well can we estimate gradient ∇f using only function differences? And how small is the norm of this estimate?

First idea gradient estimator:

- Sample $Z \sim \mu$ satisfying $\mathbb{E}_\mu[ZZ^\top] = I_{d\times d}$
- Gradient estimator at x:

$$g = \frac{f(x + uZ) - f(x)}{u} Z$$

Perform gradient descent using these g

Two-point gradient estimates

- At any point x and any direction z, for small $u > 0$

$$\frac{f(x+uz) - f(x)}{u} \approx f'(x,z) := \lim_{h \downarrow 0} \frac{f(x+hz) - f(x)}{h}$$

- If $\nabla f(x)$ exists, $f'(x,z) = \langle \nabla f(x), z \rangle$
- If $\mathbb{E}[ZZ^\top] = I$, then $\mathbb{E}[f'(x,Z)Z] = \mathbb{E}[ZZ^\top \nabla f(x)] = \nabla f(x)$

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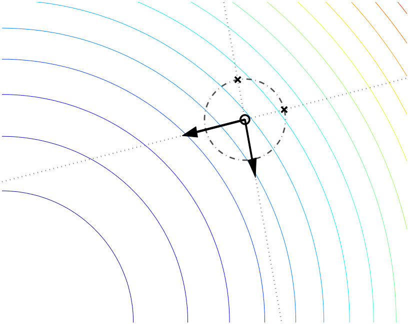
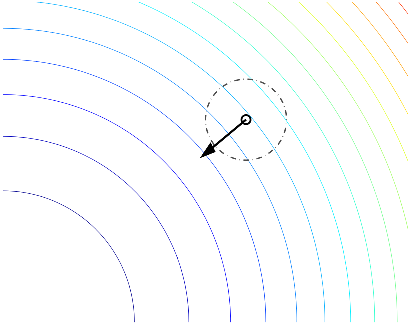


Random estimates



Average $\approx \nabla f$

Two-point stochastic gradient: differentiable functions

To solve d-dimensional problem

$$\underset{x \in \mathcal{X} \subset \mathbb{R}^d}{\text{minimize}} \; f(x) := \mathbb{E}[F(x;\xi)]$$

Algorithm: Iterate

- Draw ξ according to distribution, draw $Z \sim \mu$ with $\mathrm{Cov}(Z) = I$
- Set $u_t = u/t$ and

$$g_t = \frac{F(x_t + u_t Z;\xi) - F(x_t;\xi)}{u_t} Z$$

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Theorem (D., Jordan, Wainwright, Wibisono)**:** With appropriate α, if $R \geq \|x^* - x_1\|_2$ and $\mathbb{E}[\|\nabla F(x;\xi)\|_2^2] \leq G^2$ for all x, then

$$\mathbb{E}[f(\widehat{x}_T) - f(x^*)] \leq RG \cdot \frac{\sqrt{d}}{\sqrt{T}} + O\left(u^2 \frac{\log T}{T}\right).$$

Comparisons to knowing gradient

Convergence rate scaling

$$RG\frac{1}{\sqrt{T}} \quad \text{versus} \quad RG\frac{\sqrt{d}}{\sqrt{T}}$$

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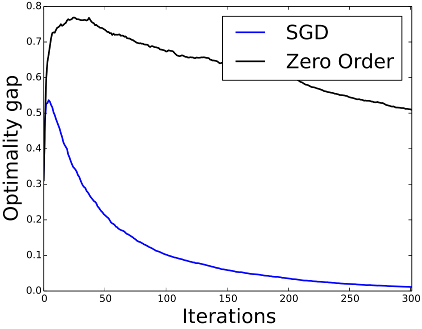

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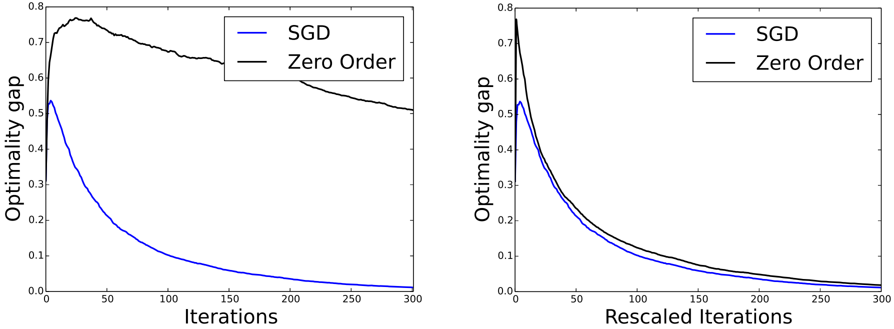

Two-point stochastic gradient: non-differentiable functions

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Example: Let $f(x) = \|x\|_2$. Then if $\mathbb{E}[ZZ^\top] = I_{d\times d}$, at $x = 0$

$$\mathbb{E}[\|(f(uZ) - 0)Z/u\|_2^2] = \mathbb{E}[\|Z\|_2^2 \, \|Z\|_2^2] \geq d^2$$

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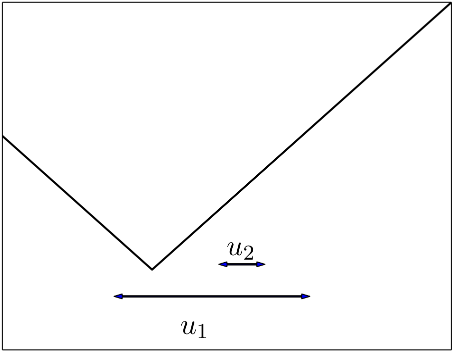
Idea: More randomization!



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Proposition (D., Jordan, Wainwright, Wibisono)**:** If Z_1, Z_2 are $N(0, I_{d\times d})$ or uniform on $\|z\|_2 \le \sqrt{d}$, then

$$g := \frac{f(x + u_1 Z_1 + u_2 Z_2) - f(x + u_1 Z_1)}{u_2} Z_2$$

satisfies

$$\mathbb{E}[g] = \nabla f_{u_1}(x) + \mathcal{O}(u_2/u_1) \quad \text{and} \quad \mathbb{E}[\|g\|_2^2] \le d\left(\sqrt{\frac{u_2}{u_1}} d + \log(2d)\right).$$

Two-point stochastic gradient: non-differentiable functions

Problem: If f is non-differentiable, "kinks" make estimates too large

Proposition (D., Jordan, Wainwright, Wibisono)**:** If Z_1, Z_2 are $N(0, I_{d\times d})$ or uniform on $\|z\|_2 \le \sqrt{d}$, then

$$g := \frac{f(x + u_1 Z_1 + u_2 Z_2) - f(x + u_1 Z_1)}{u_2} Z_2$$

satisfies

$$\mathbb{E}[g] = \nabla f_{u_1}(x) + \mathcal{O}(u_2/u_1) \quad \text{and} \quad \mathbb{E}[\|g\|_2^2] \le d\left(\sqrt{\frac{u_2}{u_1}}d + \log(2d)\right).$$

Note: If $u_2/u_1 \to 0$, scaling linear in d

Two-point sub-gradient: non-differentiable functions

To solve d-dimensional problem

$$\text{minimize } \; f(x) \quad \text{subject to } \; x \in \mathcal{X} \subset \mathbb{R}^d$$

Algorithm: Iterate

- Draw $Z_1 \sim \mu$ and $Z_2 \sim \mu$ with $\mathrm{Cov}(Z) = I$
- Set $u_{t,1} = u/t$, $u_{t,2} = u/t^2$, and

$$g_t = \frac{f(x_t + u_{t,1}Z_1 + u_{t,2}Z_2) - F(x_t + u_{t,1}Z_1)}{u_t} Z_2$$

- Update $x_{t+1} = x_t - \alpha g_t$

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Theorem (D., Jordan, Wainwright, Wibisono)**:** With appropriate α, if $R \geq \|x^* - x_1\|_2$ and $\|\partial f(x)\|_2^2 \leq G^2$ for all x, then

$$\mathbb{E}[f(\widehat{x}_T) - f(x^*)] \leq RG \cdot \frac{\sqrt{d \log d}}{\sqrt{T}} + O\left(u \frac{\log T}{T}\right).$$

Two-point sub-gradient: non-differentiable functions

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$$\underset{x \in \mathcal{X} \subset \mathbb{R}^d}{\text{minimize}} \;\; f(x) := \mathbb{E}[F(x;\xi)]$$

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Wrapping up zero-order gradient methods

- If gradients available, convergence rates of $\sqrt{1/T}$
- If only zero order information available, in smooth and non-smooth case, convergence rates of $\sqrt{d/T}$
- Time to ϵ-accuracy: $1/\epsilon^2 \mapsto d/\epsilon^2$

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$$RG\frac{\sqrt{d}}{\sqrt{T}}.$$

- **Open question:** Non-stochastic lower bounds? (Sebastian Pokutta, next week.)

Instance III: Parallelization and fast algorithms

Goal: solve the following problem

$$\begin{array}{rl} \text{minimize} & f(x) \\ \text{subject to} & x \in \mathcal{X} \end{array}$$

where

$$f(x) := \frac{1}{n}\sum_{i=1}^{n} F(x;\xi_i) \quad \text{or} \quad f(x) := \mathbb{E}[F(x;\xi)]$$

Stochastic Gradient Descent

Problem: Tough to compute

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} F(x; \xi_i).$$

Instead: At iteration t

- Choose random ξ_i, set

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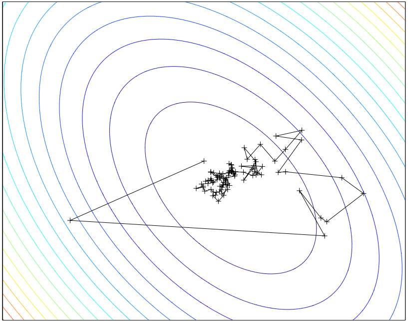
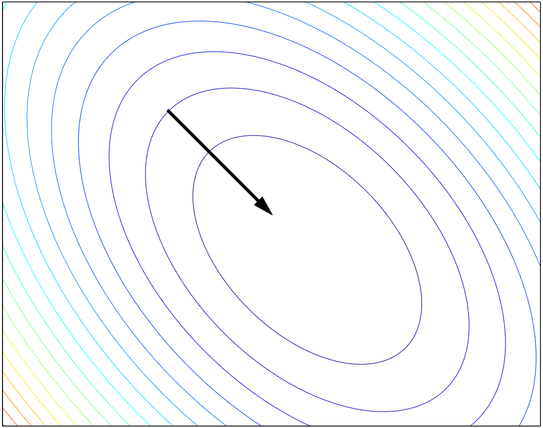


What everyone "knows" we should do

Obviously: get a lower-variance estimate of the gradient.

$$\text{Sample } g_{j,t} \text{ with } \mathbb{E}[g_{j,t}] = \nabla f(x_t) \quad \text{and use} \quad g_t = \frac{1}{m}\sum_{j=1}^{m} g_{j,t}$$



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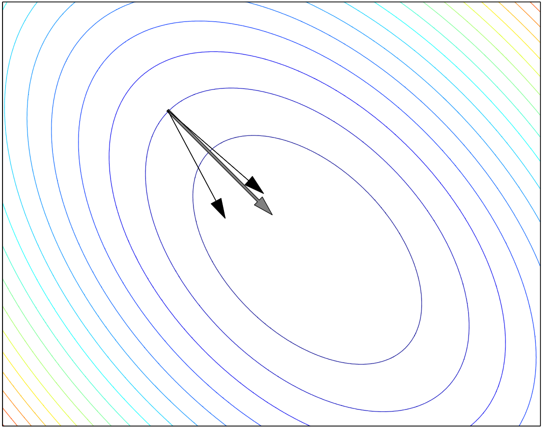

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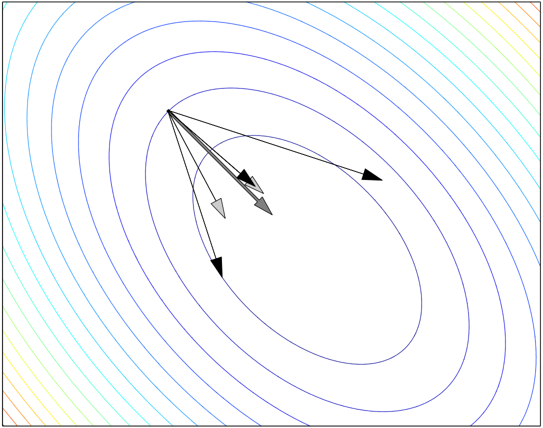

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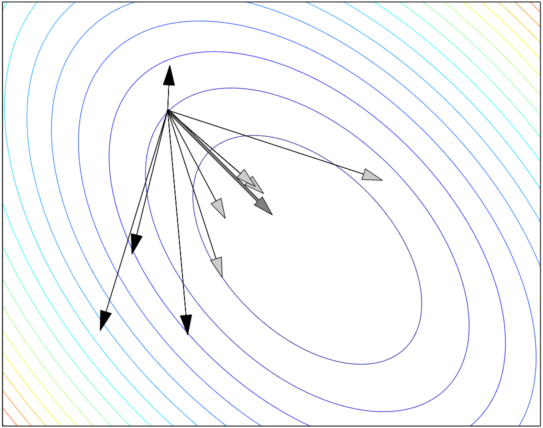

Problem: only works for smooth functions.

Non-smooth problems we care about:

- Classification

$$F(x;\xi) = F(x;(a,b)) = \left[1 - bx^\top a\right]_+$$

- Robust regression

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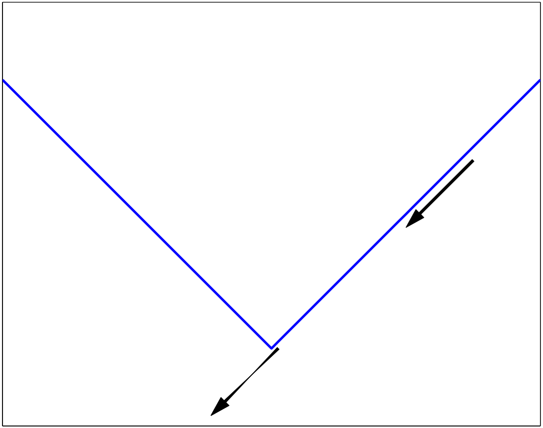
- Structured prediction (ranking, parsing, learning matchings)

$$F(x;\{\xi,\nu\}) = \max_{\widehat{\nu}\in\mathcal{V}} \left[L(\nu,\widehat{\nu}) + x^\top \Phi(\xi,\widehat{\nu}) - x^\top \Phi(\xi,\nu)\right]$$

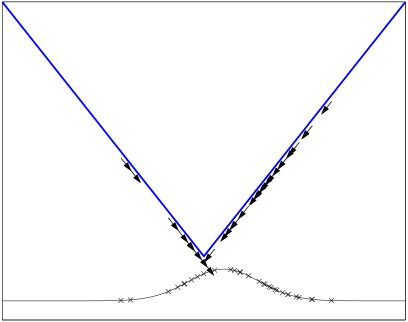
Difficulties of non-smooth

Intuition: Gradient is poor indicator of global structure



Better global estimators

Idea: Ask for subgradients from multiple points



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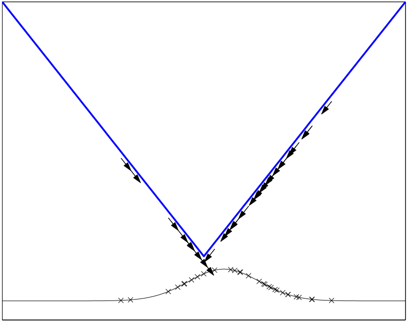
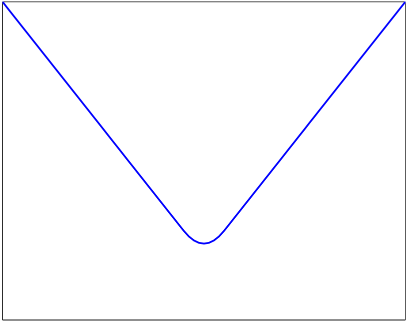




The algorithm

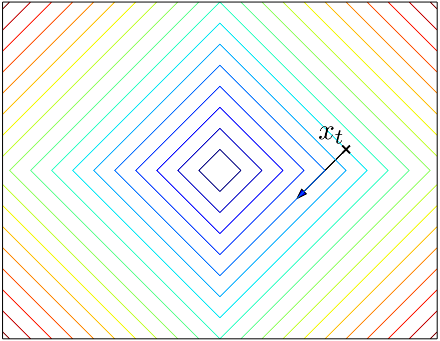
Normal approach: sample ξ at random,

$$g_{j,t} \in \partial F(x_t; \xi).$$

Our approach: add noise to x

$$g_{j,t} \in \partial F(x_t + u_t Z_j; \xi)$$

Decrease magnitude u_t over time



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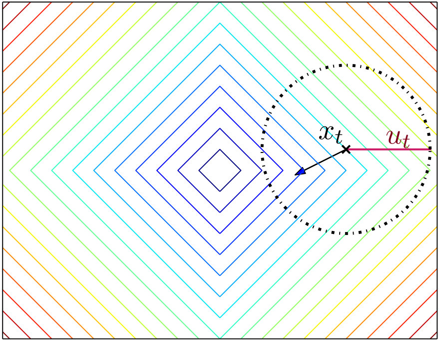

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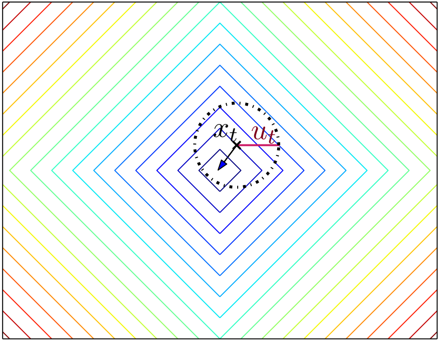

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Generalization of accelerated gradient methods (Nesterov 1983, Tseng 2008, Lan 2010). Have query point and exploration point

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III. Interpolate

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Theoretical Results

Objective:

$$\underset{x \in \mathcal{X}}{\text{minimize}} \; f(x) \quad \text{where } f(x) = \mathbb{E}[F(x;\xi)]$$

using m gradient samples for stochastic gradients.

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λ-strongly convex objectives:

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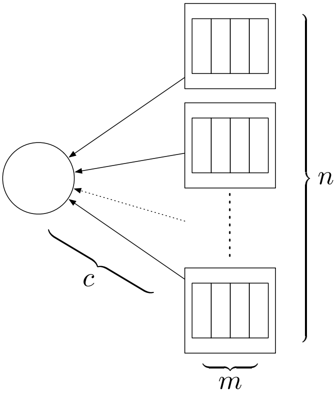
A few remarks on distributing

Convergence rate:

$$f(x_T) - f(x^*) = \mathcal{O}\left(\frac{1}{T} + \frac{1}{\sqrt{Tm}}\right)$$

- If communication is expensive, use larger batch sizes m:
  (a) Communication cost is c
  (b) n computers with batch size m
  (c) S total update steps



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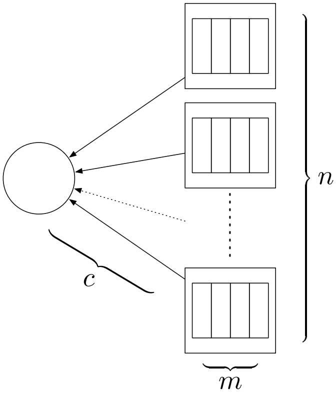
Backsolve: after $T = S(m+c)$ units of time, error is

$$\mathcal{O}\left(\frac{m+c}{T} + \frac{1}{\sqrt{Tn}} \cdot \sqrt{\frac{m+c}{m}}\right)$$

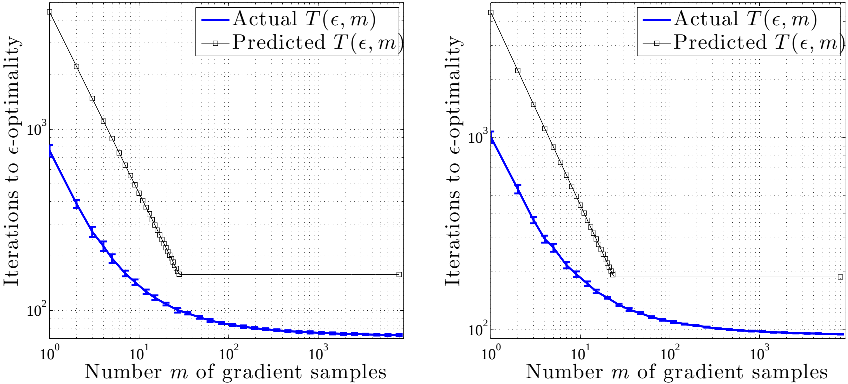


Experimental results

Iteration complexity simulations

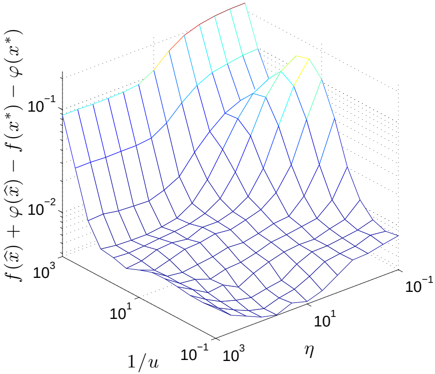
Define $T(\epsilon, m) = \min\{t \in \mathbb{N} \mid f(x_t) - f(x^*) \leq \epsilon\}$, solve robust regression problem

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} \left|a_i^\top x - b_i\right| = \frac{1}{n}\left\|Ax - b\right\|_1$$



Robustness to stepsize and smoothing

- Two parameters: smoothing parameter u, stepsize η



Plot: optimality gap after 2000 iterations on synthetic SVM problem

$$f(x) + \varphi(x) := \frac{1}{n} \sum_{i=1}^{n} \left[1 - \xi_i^\top x\right]_+ + \frac{\lambda}{2} \|x\|_2^2$$

Text Classification

Reuter's RCV1 dataset, time to ϵ-optimal solution for

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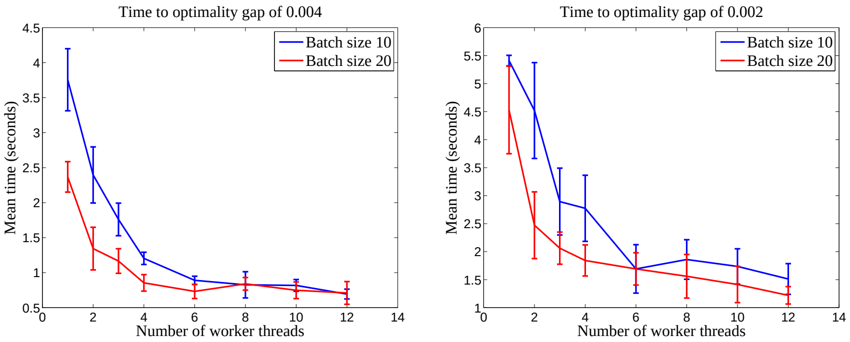

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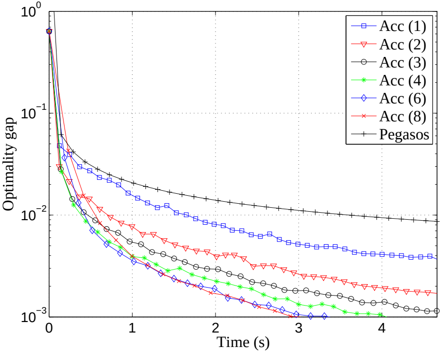
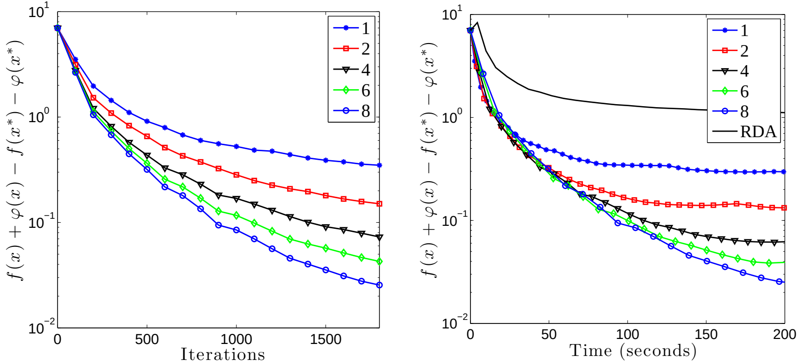


Parsing

Penn Treebank dataset, learning weights for a hypergraph parser (here x is a sentence, $y \in \mathcal{V}$ is a parse tree)

$$\frac{1}{n}\sum_{i=1}^{n} \max_{\widehat{\nu}\in\mathcal{V}} \Big[L(\nu_i, \widehat{\nu}) + x^\top \left(\Phi(\xi_i, \widehat{\nu}) - \Phi(\xi_i, \nu_i) \right) \Big] + \frac{\lambda}{2} \|x\|_2^2 \, .$$

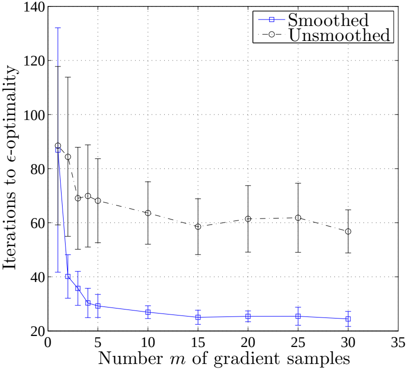


Is smoothing necessary?

Solve multiple-median problem

$$f(x) = \frac{1}{n} \sum_{i=1}^{n} \|x - \xi_i\|_1 ,$$

$\xi_i \in \{-1, 1\}^d$. Compare standard stochastic gradient:



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Thanks!

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References:

- Randomized Smoothing for Stochastic Optimization (D., Bartlett, Wainwright). *SIAM Journal on Optimization*, 22(2), pages 674–701.
- Optimal rates for zero-order convex optimization: the power of two function evaluations (D., Jordan, Wainwright, Wibisono). *arXiv:1312.2139 [math.OC]*.

Available on my webpage (`http://web.stanford.edu/~jduchi`)