Understanding Non-convex Optimization

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Optimization

function

$$\min_{x} \quad f(x)$$

feasible set

Variable, in R^d

$$\text{s.t.} \quad x \in \mathcal{C}$$

- In general too hard
- Convex optimization $\Longleftrightarrow$ $f(\,)$ is a convex function, $\mathcal{C}$ is convex set
- But “today’s problems”, and this tutorial, are non-convex
    - Our focus: non-convex problems that arise in machine learning

Outline of Tutorial

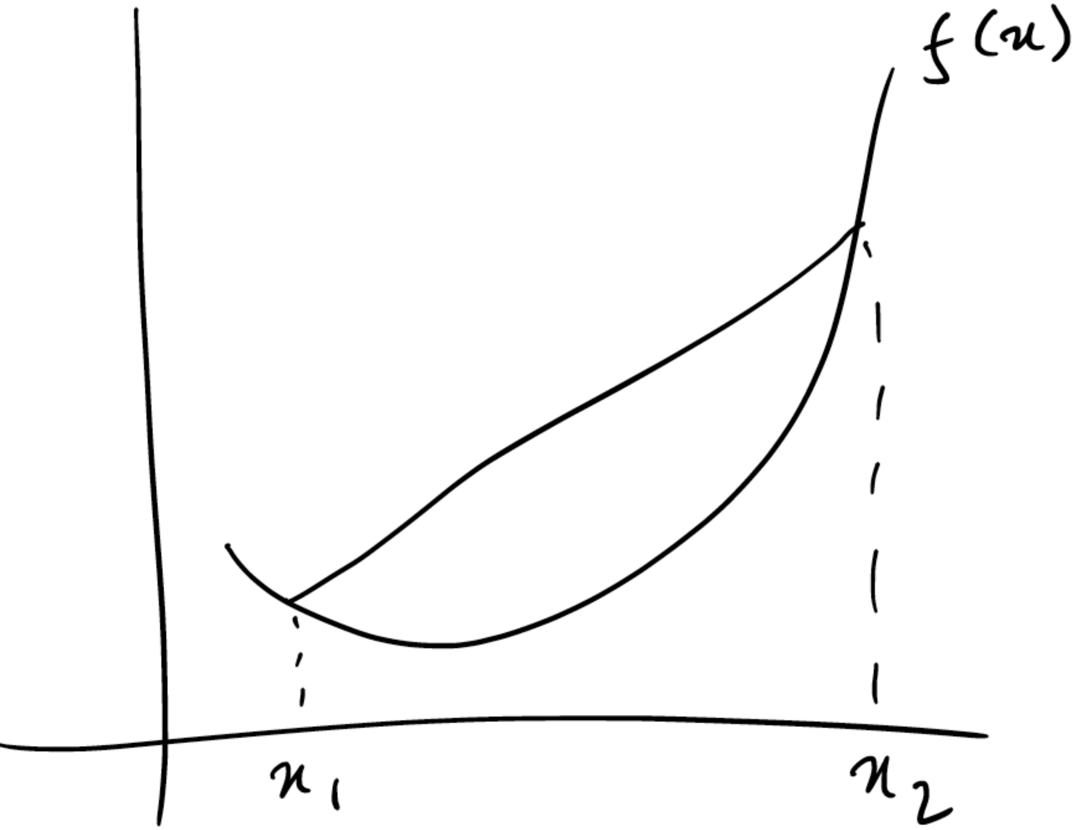
Part I (algorithms & background)

- Convex optimization (brief overview)
- Nonconvex optimization

Part II

- Example applications of nonconvex optimization
- Open directions

Convex Functions



Convex functions "lie below the line"

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2)$$

If $\nabla f(x)$ exists, convex f "lies above local linear approximation"

$$f(y) \geq \mathbf{f}(\mathbf{x}) + \nabla f(x)^T (y - x) \quad \forall y$$

- GENERAL enough to capture/model many problems
- SPECIAL enough to have **fast** "off the shelf" algorithms

low-order polynomial complexity in dimension d

Convex Optimization

$$\min_{x} \quad f(x)$$

$$\text{s.t.} \quad x \in \mathcal{C}$$

Convex function

Convex set

- **Key property of convex optimization:**

Local optimality $\Longrightarrow$ Global optimality

Proof: if x is local (but not global) opt and x^* is global, then moving from x to x^* strictly decreases f. This violates local optimality of x

- **All general-purpose methods search for locally optimal solutions**

"Black box / Oracle view" of Optimization

0^{th} order

$$x \longrightarrow \blacksquare \xrightarrow{f(x)}$$

Gradient-free

1^{st} order

$$x \longrightarrow \blacksquare \xrightarrow{\nabla f(x)}$$

Gradient Descent

2^{nd} order

$$x \longrightarrow \blacksquare \xrightarrow{\nabla^2 f(x)}$$

Newton

Stochastic 1^{st} order

$$x \longrightarrow \blacksquare \xrightarrow{g}$$

$$\mathrm{E}[g] = \nabla f(x)$$

Stochastic Gradient Descent

Non-smooth 1^{st} order

$$x \longrightarrow \blacksquare \xrightarrow{g}$$

$$\mathrm{E}[g] \in \partial f(x)$$

(Stochastic) Sub-gradient Descent

Gradients

$\nabla f(x)$ exists everywhere

For any smooth function,

- $-\nabla f(x)$ is a **local descent direction** at x
- x^* locally optimum $\Longrightarrow$ $\nabla f(x^*) = 0$

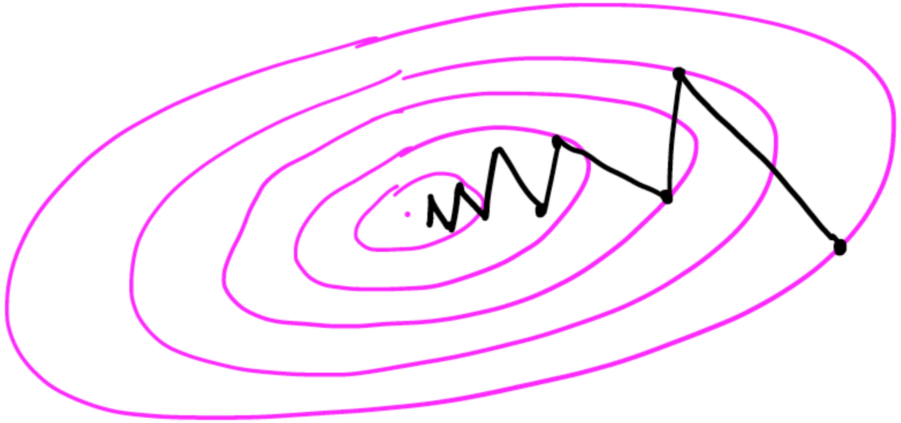
For convex functions, this means enough to search for 0-gradient points

$$x^* \text{ globally optimum} \Longleftrightarrow \nabla f(x^*) = 0$$

Gradient Descent

An iterative method to solve $\min_x \; f(x)$

$$\underbrace{x_{t+1}}_{\text{next iterate}} = \underbrace{x_t}_{\text{current iterate}} - \underbrace{\eta_t}_{\text{step size}} \underbrace{\nabla f(x_t)}_{\text{current gradient}}$$



Gradient Descent

- "Off-the shelf" method that can be applied to "any" problem
  - Only need to be able to calculate gradients (i.e. 1st order oracle)

- "Only" parameters are the step sizes η_t
  - but choosing them correctly is crucially important
  - If too small, convergence too slow. If too big, divergence / oscillation
  - The more we know about f, the better we can make this choice

Gradient Descent Convergence

$f(\cdot)$ has **β-Lipschitz gradients** if

β is a uniform bound

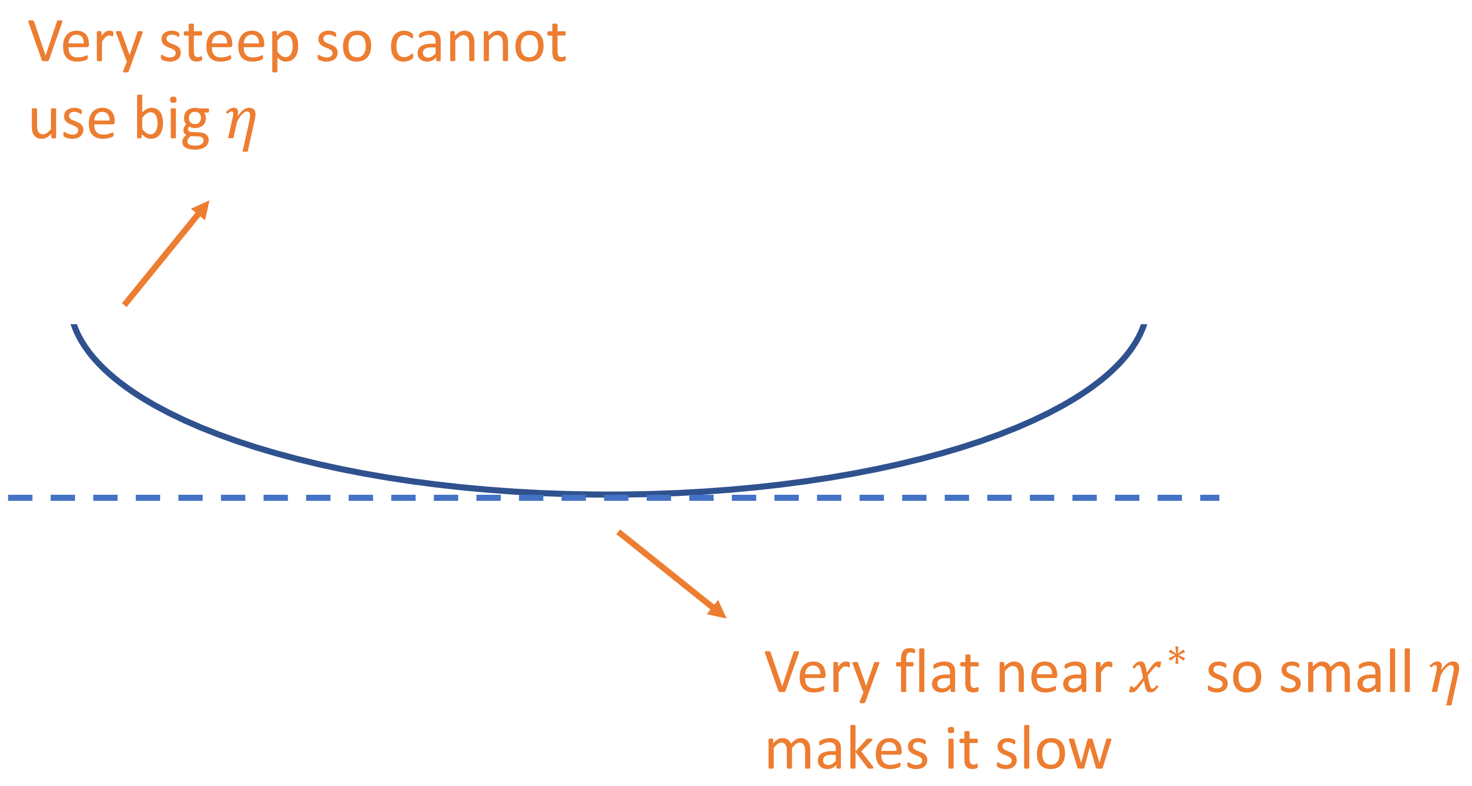
$$\|\nabla f(x) - \nabla f(y)\| \leq \beta \|x - y\| \qquad \forall x, y$$

- In this case, fixed $\boldsymbol{\eta_t = 1/\beta}$ gives

$$f(x_T) - f(x^*) \leq \epsilon \qquad \text{once} \qquad T \sim \Theta\left(\frac{1}{\epsilon}\right)$$

- This however is **not tight:** there exists a different method that is faster but only uses 1st first order oracle …

Gradient Descent Convergence



Gradient Descent Convergence

$f(\cdot)$ is **α-strongly convex** if

"cannot be too flat"

$$\|\nabla f(x) - \nabla f(y)\| \geq \alpha \|x - y\| \quad \forall x, y$$

- Now GD with fixed $\eta_t = 1/\beta$ gives

$$f(x_T) - f(x^*) \leq \epsilon \ \text{ in } \ T \sim O\left(\frac{\log(\frac{1}{\epsilon})}{-\log(1-\frac{\alpha}{\beta})}\right)$$

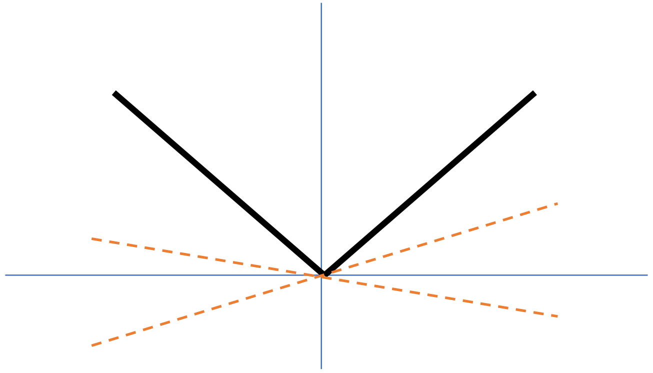
exponentially faster than
the only smooth case

Non-smooth functions

Sub-gradient of (convex) f at x is a set of “gradient like” vectors

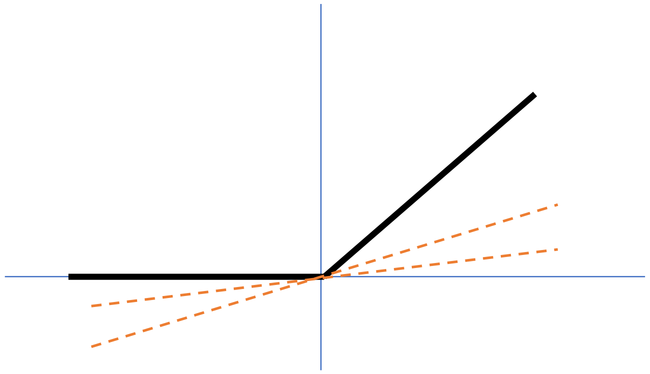
$$\{\, g \in \mathbb{R}^d: \quad f(y) \geq f(x) + g^T(y - x) \quad \forall y \,\}$$

Eg: $|x|$



$\partial f(0) = \{u: -1 \leq u \leq 1\}$

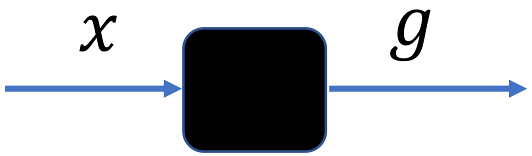
$\mathrm{relu}(x) = \max(x, 0)$



$\partial f(0) = \{u: 0 \leq u \leq 1\}$

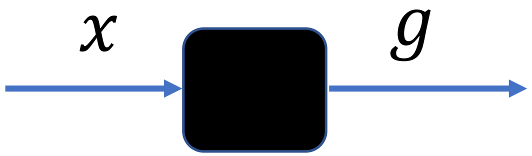
Sub-gradient Descent

Non-smooth 1^{st} order



$$g \in \partial f(x)$$

Stochastic Non-smooth 1^{st} order

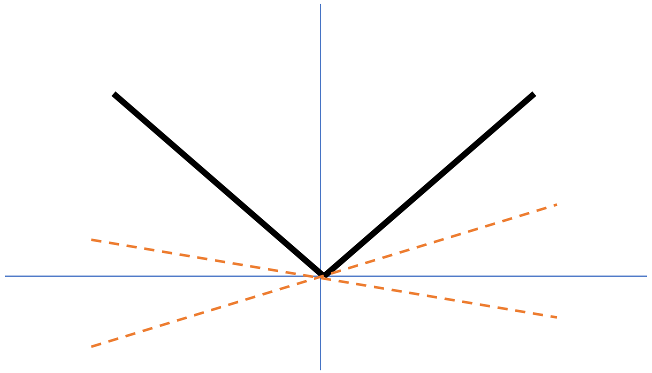


$$E[g] \in \partial f(x)$$

Sub-gradient Descent

$$x_{t+1} = x_t - \eta_t \, g_t$$

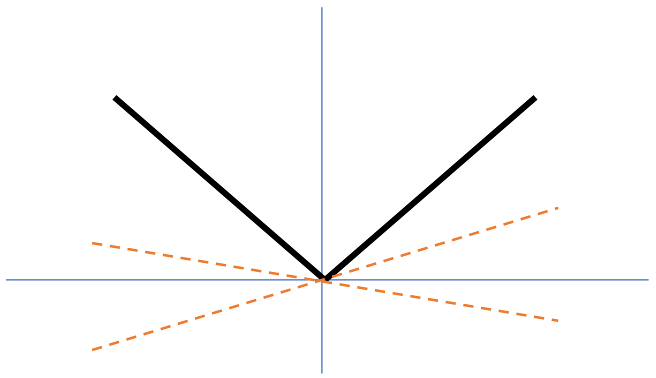
$$g_t \in \partial f(x_t)$$



Sub-gradient Descent

- Now **cannot use fixed step size** in general

η_t has to $\to 0$, else oscillations possible



E.g. for $f(x) = |x|$, subgradient $g = sign(x)$ for $x \neq 0$

$$x_+ = x - \eta\, sign(x)$$

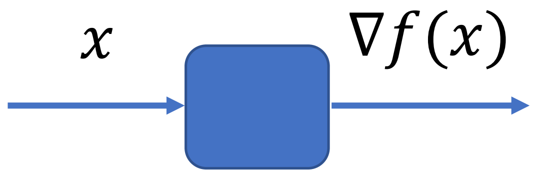
will oscillate between a and $a - \eta$
for some a that depends on initial point

Convergence slower than gradient descent because step size forced to decay:

$$f(x_T) - f(x^*) \leq \epsilon \ \text{ in } \ T \sim O(1/\epsilon^2)$$

Stochastic Gradient Descent (SGD)

Gradient Descent



But sometimes even calculating the gradient may be hard

- Large # terms

$$\min_x \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

n is large

- High dimensionality

$$\min_x \; f(x_1, \dots, x_d)$$

d is large

Stochastic Gradient Descent (SGD)

Lowering the complexity of gradient calculation via sub-sampling the sum of terms

$$x_+ = x - \eta \left(\frac{1}{n} \sum_{i=1}^{n} \nabla f_i(x) \right) \longrightarrow x_+ = x - \eta \left(\frac{1}{|\boldsymbol{B}|} \sum_{i \in \boldsymbol{B}} \nabla f_i(x) \right)$$

B is uniform subset from [n]. This is **mini-batch SGD.**

$$x_+ = x - \eta \left(\sum_{j=1}^{d} \frac{\partial f}{\partial x_j} \boldsymbol{e_j} \right) \longrightarrow x_+ = x - \eta \left(\frac{d}{|S|} \sum_{j \in S} \frac{\partial f}{\partial x_j} \boldsymbol{e_j} \right)$$

S is uniform subset from [n]. This is **block coordinate descent.**

Mini-batch SGD

Many ML problems can be reduced to optimization problems of the form

i-th sample

$$\min_x \frac{1}{n}\sum_{i=1}^{n} \boxed{l(s_i; x)} \qquad f_i(x)$$

loss function

weights

$$\nabla f(x) = \frac{1}{n}\sum_{i=1}^{n} \nabla l(s_i; x) \qquad\qquad g = \frac{1}{|B|}\sum_{i \in B} \nabla l(s_i; x)$$

"Batch or full" gradient

"Mini-batch" gradient

SGD and its Convergence Rate

g is a **Noisy Unbiased (sub) Gradient (NUS)** of $f(\cdot)$ at x if $\boldsymbol{E[g|x] \in \partial f(x)}$

In all of the cases we have seen so far, g is NUS

SGD:

$$x_{t+1} = x_t - \eta_t\, g_t$$

Suppose $\mathrm{Var}(\| g_t \| \mid x_t) \leq G_t^2$

Theorem:

$$\mathrm{E}\left[f\left(x_{\mathrm{BEST}}^{(T)}\right)\right] - f^* \leq \frac{R^2 + \sum_{t \leq T} \eta_t^2\, G_t^2}{2 \sum_{t \leq T} \eta_t}$$

Where

$$R = |x_0 - x^*|$$

SGD and its Convergence Rate

$$\mathrm{E}\left[f^{(T)}\right] - f^* \le \frac{R^2 + \sum_{t \le T} \eta_t^2 \, G_t^2}{2 \sum_{t \le T} \eta_t}$$

Idea 1: **Fixed mini-batch size** at every step

$$\Longrightarrow G_t^2 = G^2$$

$$g_t = \frac{1}{|B|} \sum_{i \in B} \nabla f_i(x_t)$$

B does not depend on t

1(a) Fixed step size $\eta_t = \eta$ gives $\mathrm{E}\left[f^{(T)}\right] - f^* \le \frac{R^2}{\eta T} + \eta G^2$

Convergence to a "ball" around the optimum at rate 1/T

SGD and its Convergence Rate

* Convergence to optimum $\Longrightarrow \eta_t$ **has to** decay with time

1(b) Best choice for trading off between two error terms: $\eta_t \sim \dfrac{1}{\sqrt{t}}$

Gives $\quad \mathrm{E}\left[f^{(T)}\right] - f^* \le O\left({}^{(R+G)}/_{\sqrt{T}}\right)$ convergence rate

- much slower compared to the $O({}^{1}/_{T})$ rate of (full) gradient descent

- dependence on n captured by G – it is $O\left(\sqrt{{}^{n}/_{|B|}}\right)$

SGD and its Convergence Rate

Fixed mini-batch size means fixed variance, which forces decaying step size and hence slow convergence

	Lipschitz f	**Strongly Convex f**
Full GD	$O(1/T)$	$O(c^T)$
Fixed-size mini-batch SGD	$O(1/\sqrt{T})$	$O(1/T)$

Variance reduction: keep step size η_t constant but decrease variance G_t as t increases

(a) By increasing size of mini-batch for some of the steps

(b) Via memory

Variance reduction in SGD

$$\min_x \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

Full GD: $x_{t+1} = x_t - \eta_t \frac{1}{n}\sum_i \nabla f_i(x_t)$ O(n) computations per iteration

SGD: $x_{t+1} = x_t - \eta_t \nabla f_{i_t}(x_t)$ O(1) computation per iteration

(but many more iterations)

random index

Stochastic Average Gradient (Schmidt, Le Roux, Bach)

current estimate for $\nabla f_n(x^{(k)})$

- Maintain $g_1^{(k)}, \dots, g_n^{(k)}$
- Initialize with one pass over all samples: $g_i^{(0)} = \nabla f_i\left(x^{(0)}\right)$

For the problem

$$\min_x \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

- At step t, pick i_t randomly (Update g's lazily)

$$g_{i_t}^{(t)} = \nabla f_{i_t}(x^{(t-1)})$$
$$g_j^{(t)} = g_j^{(t-1)} \qquad \text{for } j \neq i_t$$

- Update $x^{(k)} = x^{(k-1)} - \eta_k \frac{1}{n}\sum_{i=1}^{n} g_i^{(k)}$

Stochastic Average Gradient (SAG)

- Memory efficient implementation:

$$\frac{1}{n}\sum_{i=1}^{n} g_i^{(k)} = \frac{g_{i_k}^{(k)}}{n} - \frac{g_{i_k}^{(k-1)}}{n} + \frac{1}{n}\sum_{i=1}^{n} g_i^{(k-1)}$$

$$\Downarrow$$

$$a^{(k)} = \frac{g_{i_k}^{(k)}}{n} - \frac{g_{i_k}^{(k-1)}}{n} + a^{(k-1)}$$

- $a^{(0)}$ just accumulates $\nabla f_i(x^{(0)})$'s

Stochastic Average Gradient (SAG)

NOTE: SAG not an unbiased stochastic gradient method

- Bias = $\frac{1}{n}\sum_i \nabla f_i\left(x^{(k)}\right) - \frac{1}{n}\sum_i g_i^{(k)}$

- As $k \to \infty$, $x^{(k)} \to x^*$, so Bias $\to 0$ and variance $\to 0$ as well !

However, proving this is quite involved ….

Theorem: If each $\nabla f_i(\cdot)$ is β-Lipschitz, SAG with fixed step size has

$$\mathrm{E}\left[f^{(T)}\right] - f^* \leq \frac{cn}{T}\left[\ f^{(0)} - f^* + \beta\left\|x^{(0)} - x^*\right\|\ \right]$$

$O\left(\frac{1}{T}\right)$ convergence rate !

Stochastic Average Gradient

Theorem: If each f_i is also α-strongly convex

$$\mathrm{E}\left[f^{(T)}\right] - f^* \leq \left(1 - \frac{c_0 \alpha}{\beta}\right)^T c_1 R$$

$c_0 < 1,$ depends on n

Linear convergence
for strongly convex ..

SAG thus fixes the shortcomings of SGD wrt dependence of error on T …

… but it is biased and hence hard to prove extensions for variants like Proximal SGD …

Stochastic Variance Reduced Gradient

SVRG (Johnson and Zhang):

For epoch $t = 1, \dots, T$

$\tilde{f}_t =$ full gradient

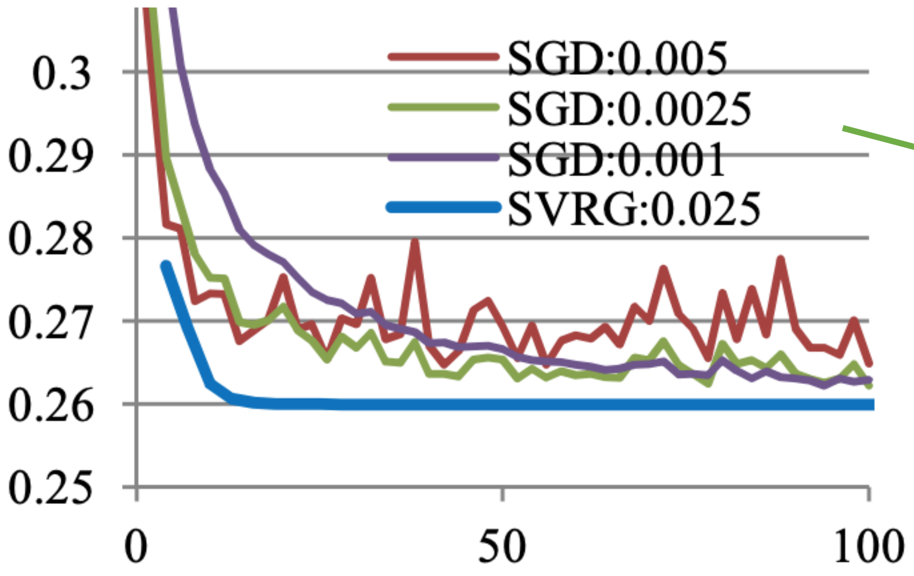
For iteration $k = 1, \dots, M$

SAG-like updates

Experiments: SVRG vs SGD (Johnson and Zhang'2013)

Multiclass logistic regression on MNIST.

Training Loss
$f(w_t)$



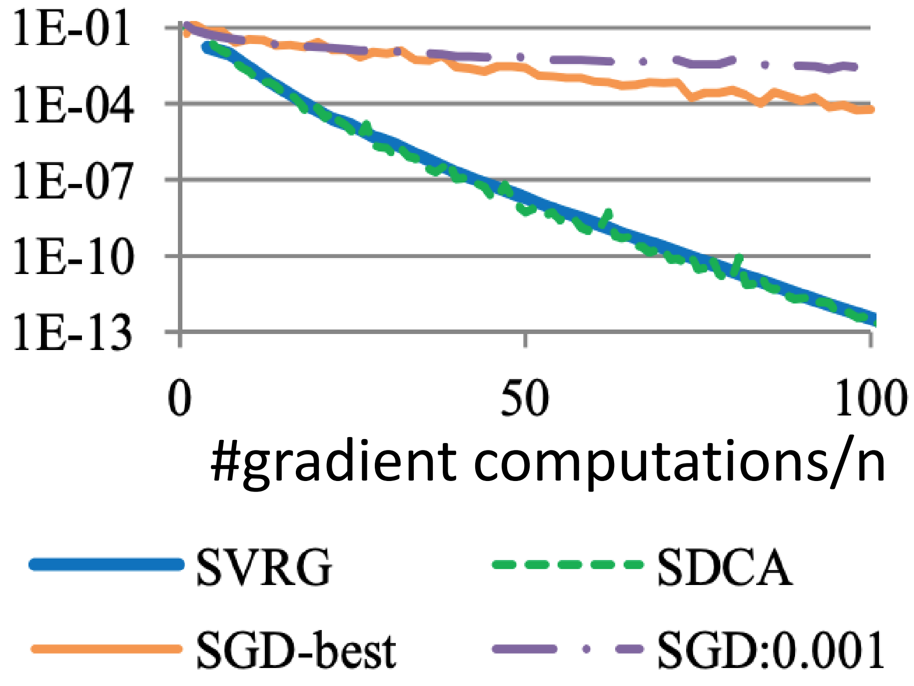
#gradient computations/n

Fixed learning rates: SVRG can use larger learning rate.

Experiments: SVRG vs SGD (Johnson and Zhang'2013)

Multiclass logistic regression on MNIST.

Training Loss Residual
$f(w_t) - f(w^*)$

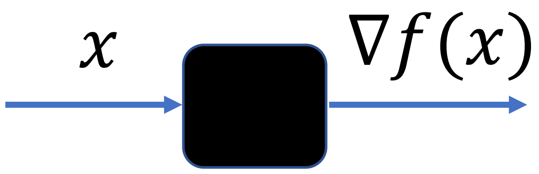


SVRG is faster than SGD with best-tuned learning rate scheduling.

Acceleration

Acceleration / Momentum

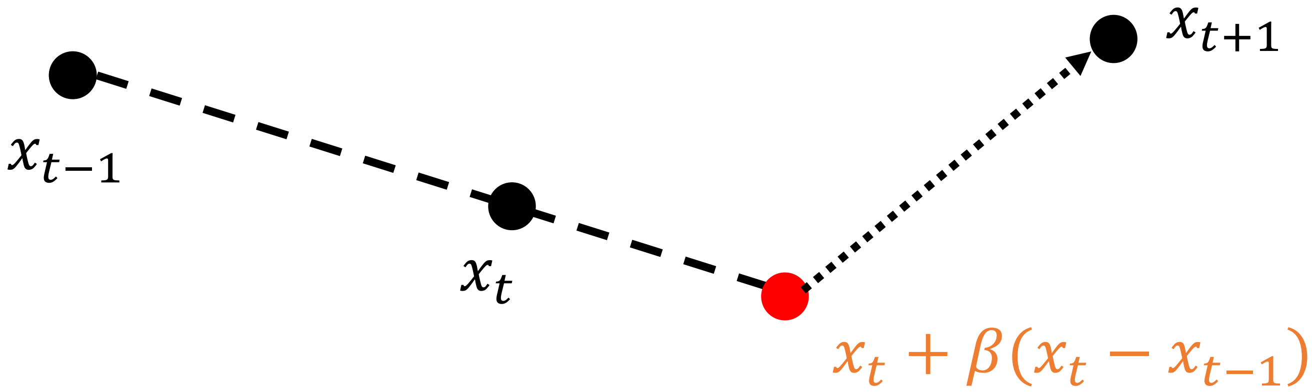
1^{st} order



Gradient descent is one algorithm that uses 1st order oracle

But it is possible to get faster rates with this oracle …

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



Can be viewed as a discretization of

$$\ddot{\boldsymbol{x}} + \tilde{\boldsymbol{\theta}}\dot{\boldsymbol{x}} + \nabla \boldsymbol{f}(\boldsymbol{x}) = \mathbf{0}$$

Convergence rates of Accelerated GD

	Smooth	Smooth & Strongly convex
Gradient Descent	$O(\frac{1}{\epsilon})$	$O(\kappa \log\left(\frac{1}{\epsilon}\right))$
Nesterov's Accelerated Gradient	$O(\frac{1}{\sqrt{\epsilon}})$	$O(\sqrt{\kappa} \log\left(\frac{1}{\epsilon}\right))$

Comparison of the convergence rates

Algorithm	Convergence rate
Subgradient	$O(\frac{1}{\epsilon^2})$
ISTA	$O(\frac{1}{\epsilon})$
FISTA	$O(\frac{1}{\sqrt{\epsilon}})$

Performance on a LASSO example.

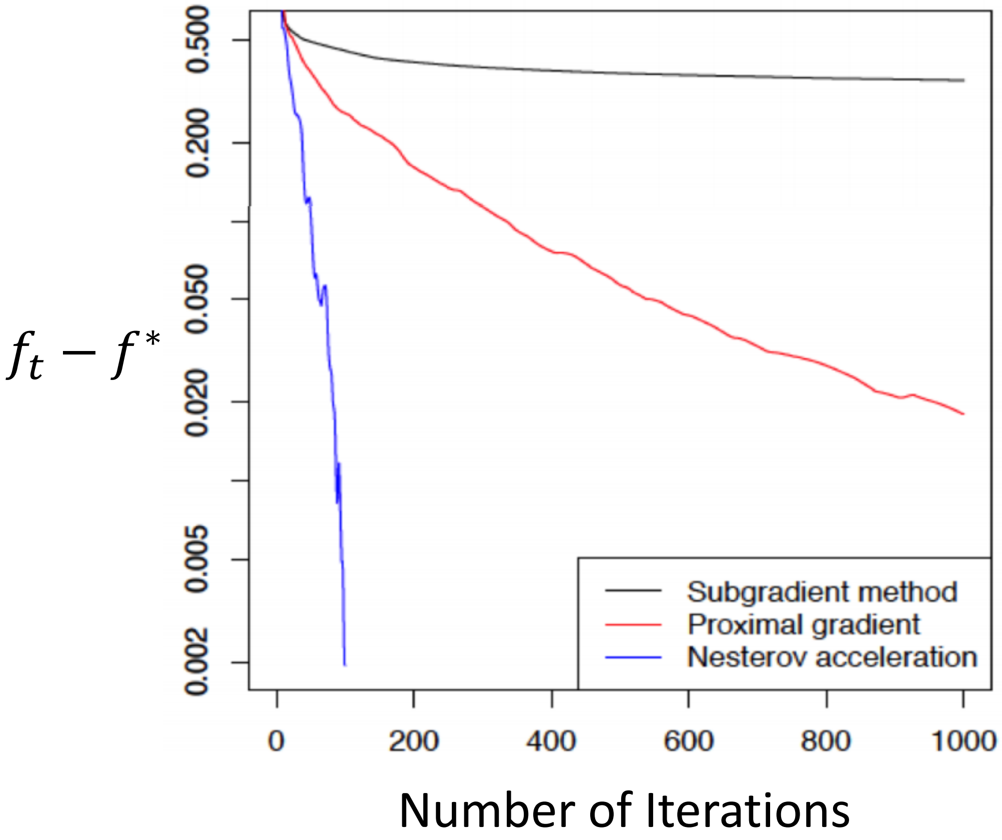


Figure taken from Tibshirani's lecture notes: http://www.stat.cmu.edu/~ryantibs/convexopt-S15/scribes/08-prox-grad-scribed.pdf

Summary of convex background

- Convex optimization can be performed efficiently
- Gradient descent (GD) is an important workhorse
- Techniques such as momentum, stochastic updates etc. can be used to speed up GD
- Well studied complexity theory with matching lower/upper bounds

Nonconvex optimization

Problem: $\min_{x} f(x)$ $f(\cdot)$: nonconvex function

Applications: Deep learning, compressed sensing, matrix completion, dictionary learning, nonnegative matrix factorization, …

Challenge: NP-hard in the worst case

Gradient descent (GD) [Cauchy 1847]

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

Question

How does it perform for non-convex functions?

Answer

Converges to first order stationary points

Definition

ϵ-First order stationary point (ϵ-FOSP) : $\|\nabla f(x)\| \leq \epsilon$

Concretely

ϵ-FOSP in $O(\epsilon^{-2})$ iterations

[Folklore]

GD for smooth functions

- **Assumption**: $f(\cdot)$ is L-smooth $\stackrel{\text{def}}{=}$ $\nabla f(\cdot)$ is L-Lipschitz

$$\|\nabla f(x) - \nabla f(y)\| \leq L \cdot \|x - y\|, \forall x, y.$$

This implies

$$f(y) \leq \underbrace{\underbrace{f(x) + \langle \nabla f(x), y - x \rangle}_{1^{\text{st}} \text{ order Taylor expansion}} + \frac{L}{2}\|x - y\|^2}_{\text{Quadratic upper bound}}, \forall x, y$$

Alternate view of GD

$$\boxed{\eta \leq \frac{1}{L}}$$

$$x_{t+1} = \operatorname{argmin}_x \underbrace{f(x_t) + \langle \nabla f(x_t), x - x_t \rangle + \frac{1}{2\eta}\|x - x_t\|^2}_{\text{Quadratic upper bound}}$$

$$f(x_{t+1}) \leq \min_x f(x_t) + \langle \nabla f(x_t), x - x_t \rangle + \frac{1}{2\eta}\|x - x_t\|^2$$
$$= f(x_t) - \frac{\eta}{2}\|\nabla f(x_t)\|^2$$

Telescoping: $f(x_T) \leq f(x_0) - \frac{\eta}{2}\sum_{t=0}^{T-1}\|\nabla f(x_t)\|^2$

Stochastic gradient descent (SGD) [Robbins, Monro 1951]

$$x_{t+1} = x_t - \eta \hat{\nabla} f(x_t); \ \mathbb{E}\left[\hat{\nabla} f(x_t)\right] = \nabla f(x_t)$$

Question

How does it perform?

Answer

Converges to first order stationary points

Definition

ϵ-First order stationary point (ϵ-FOSP) : $\|\nabla f(x)\| \leq \epsilon$

Concretely

ϵ-FOSP in $O(\epsilon^{-4})$ iterations

vs $O(\epsilon^{-2})$ for GD

Proof of convergence rate of SGD

- **<u>Assumption</u>**: $f(\cdot)$ is L-smooth $\stackrel{\text{def}}{=}$ $\nabla f(\cdot)$ is L-Lipschitz
- **<u>Assumption</u>**: $\mathbb{E}\left[\left\|\widehat{\nabla} f(x) - \nabla f(x)\right\|^2\right] \leq \sigma^2$

$$\mathbb{E}[f(x_{t+1})] \leq \mathbb{E}[f(x_t)] - \frac{\eta}{2}\mathbb{E}[\|\nabla f(x_t)\|^2] + \frac{\eta^2 L}{2}\sigma^2$$

$\eta \sim 1/\sqrt{T}$: $\qquad \frac{1}{T}\sum_{t=0}^{T-1}\mathbb{E}[\|\nabla f(x_t)\|^2] \leq O\left(\sigma/\sqrt{T}\right)$

Finite sum problems

$$f(x) = \frac{1}{n}\sum_{i=1}^{n} f_i(x)$$

- $f_i(\cdot)$ = loss on i^{th} data point; L-smooth and nonconvex
  - E.g., $f_i(\cdot) = \ell(\phi(x, a_i), b_i)$; ℓ — loss function; ϕ — model.
- Usually computing $\nabla f_i(\cdot)$ takes same amount of time for each i

GD vs SGD

ϵ — desired accuracy
n — # component functions

	# gradient calls per iteration	# iterations
GD	n	$\boldsymbol{\epsilon^{-2}}$
SGD	$\mathbf{1}$	ϵ^{-4}

Can we get best of both?

- **Main observations**:
  - Can compute exact gradients when required
  - Convergence of SGD depends on noise variance σ
- **Main idea of SVRG**: [Johnson, Zhang 2013]; [Reddi, Hefny, Sra, Poczos, Smola 2016]; [Allen-Zhu, Hazan 2016]
  - Compute full gradient in the beginning; reference point x_0
  - At x_t, $\qquad \widehat{\nabla} f(x_t) \stackrel{\text{def}}{=} \nabla f_i(x_t) - \nabla f_i(x_0) + \nabla f(x_0)$

Two potential functions

$$\sigma^2 \stackrel{\text{def}}{=} \mathbb{E}\left[\left\|\widehat{\nabla} f(x_t) - \nabla f(x_t)\right\|^2\right] \leq L\|x_0 - x_t\|^2$$

$$\mathbb{E}[f(x_{t+1})] - \mathbb{E}[f(x_t)] \leq -\frac{\eta}{2}\mathbb{E}[\|\nabla f(x_t)\|^2] + \frac{\eta^2 L}{2}\sigma^2$$

$$\|x_{t+1} - x_t\|^2 \leq \eta^2 \mathbb{E}[\|\nabla f(x_t)\|^2] + \eta^2 L\|x_0 - x_t\|^2$$

- For $t = 0, \|x_0 - x_t\|^2 = 0$.
- $\|x_0 - x_t\|^2$ can increase only if $\|\nabla f(x_t)\|^2$ is large.
- But if so, $\mathbb{E}[f(x_{t+1})]$ will decrease significantly.
- Careful combination of these two potential functions.

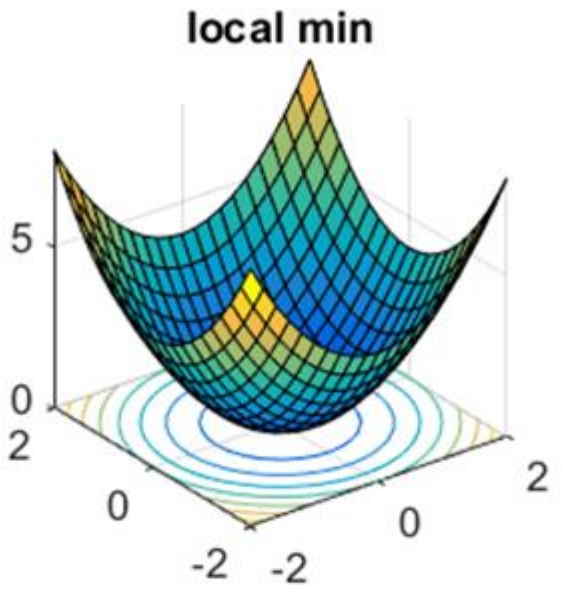
Comparison with GD/SGD

ϵ — desired accuracy
n — # component functions

	# gradient calls per iteration	# iterations
GD	n	ϵ^{-2}
SGD	1	ϵ^{-4}
SVRG	1	$n^{2/3}\epsilon^{-2}$
SNVRG (Zhou, Xu, Gu 2018) Spider (Fang, Li, Lin, Zhang 2018)	1	$n^{1/2}\epsilon^{-2} \wedge \epsilon^{-3}$

Other results: Ghadimi, Lan 2015; Allen-Zhu 2018

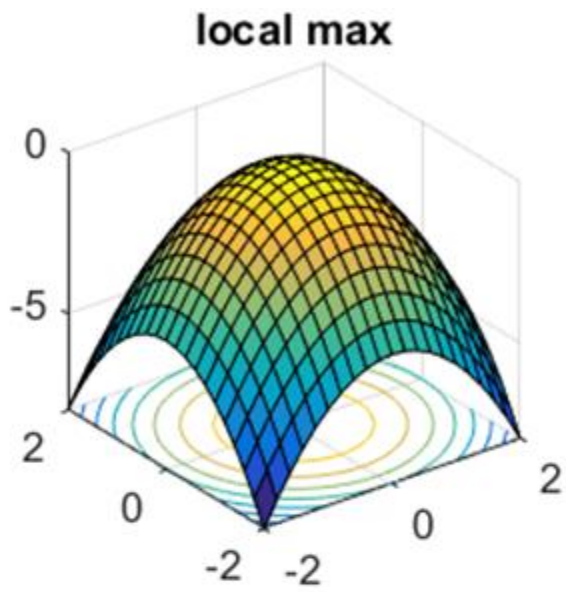
How do FOSPs look like?



Hessian PSD

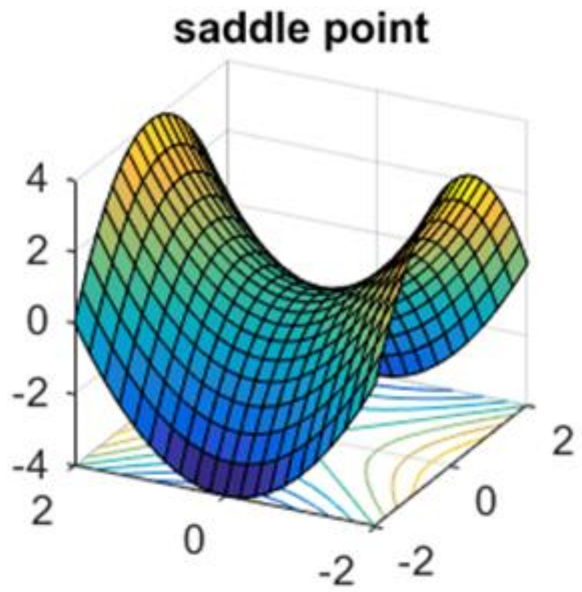
$\nabla^2 f(x) \succcurlyeq 0$

Second order stationary points (SOSP)



Hessian NSD

$\nabla^2 f(x) \preccurlyeq 0$



Hessian indefinite

$\lambda_{\min}(\nabla^2 f(x)) \leq 0$

$\lambda_{\max}(\nabla^2 f(x)) \geq 0$

FOSPs vs SOSPs in popular problems

- Very well studied
  - Matrix sensing [Bhojanapalli, Neyshabur, Srebro 2016]
  - Matrix completion [Ge, Lee, Ma 2016]
  - Robust PCA [Ge, Jin, Zheng 2017]
  - Tensor factorization [Ge, Huang, Jin, Yuan 2015]; [Ge, Ma 2017]
  - Smooth semidefinite programs [Boumal, Voroninski, Bandeira 2016]
  - Synchronization & community detection [Bandeira, Boumal, Voroninski 2016]; [Mei, Misiakiewicz, Montanari, Oliveira 2017]
  - Phase retrieval [Chen, Chi, Fan, Ma 2018]

Two major observations

- FOSPs: proliferation (exponential #) of saddle points
  - Recall FOSP $\triangleq \nabla f(x) = 0$
  - Gradient descent can get stuck near them
- SOSPs: not just local minima; as good as global minima
  - Recall SOSP $\triangleq \nabla f(x) = 0$ & $\nabla^2 f(x) \succcurlyeq 0$

<u>Upshot for these problems</u>

1. FOSP not good enough
2. Finding SOSP sufficient

How to find SOSPs?

- Cubic regularization (CR) [Nesterov, Polyak 2006]

$$x_{t+1} = \operatorname{argmin}_x \underbrace{\underbrace{f(x_t) + \langle \nabla f(x_t), x - x_t \rangle + \langle x - x_t, \nabla^2 f(x_t)(x - x_t) \rangle}_{2^{nd}\text{ order Taylor expansion}} + \frac{1}{6\eta} \|x - x_t\|^3}_{\text{Cubic upper bound}}$$

- Contrast with GD: Minimizes quadratic upper bound

GD vs CR

	Guarantee	Per Iteration cost
CR	**SOSP**	Hessian computation
GD	FOSP	**Gradient** computation

- Hessian computation is not practical for large scale applications

Can we find SOSPs using first order (gradient) methods?

GD finds SOSPs with probability 1

- [Lee, Panageas, Piliouras, Simchowitz, Jordan, Recht 2017]

$$\mathrm{Lebesguemeasure}(\{x_0 \colon \mathrm{GD\ from\ } x_0 \mathrm{\ converges\ to\ non\ SOSP}\}) = 0$$

- However, time taken for convergence could be $\Omega(d)$ [Du, Jin, Lee, Jordan, Singh, Poczos 2017]

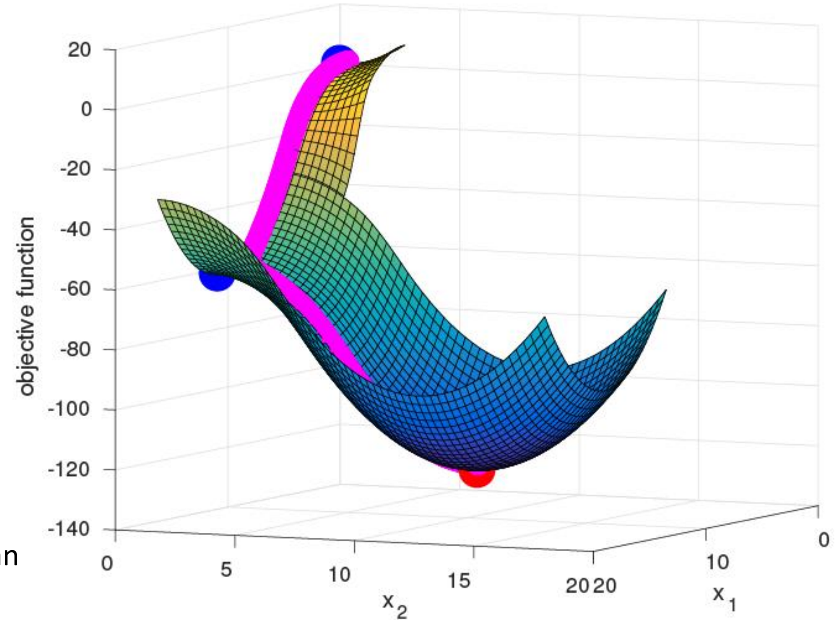


Image credit: Chi Jin & Mike Jordan

GD vs CR

	Guarantee	Per Iteration cost	# iterations
CR	**SOSP**	Hessian computation	$\boldsymbol{O}\left(\epsilon^{-1.5}\right)$
GD	**SOSP**	**Gradient** computation	$\Omega(d)$

- Convergence rate of GD too slow

Can we speed up GD for finding SOSPs?

Perturbation to the rescue!

Perturbed gradient descent (PGD)

1. **For** $t = 0,1,\cdots$ **do**
2. $x_{t+1} \leftarrow x_t - \eta \nabla f(x_t) + \xi_t$ where $\xi_t \sim Unif\left(B_0(\epsilon)\right)$

	Guarantee	Per Iteration cost	# iterations
CR	**SOSP**	Hessian computation	$\boldsymbol{O}\left(\epsilon^{-1.5}\right)$
GD	**SOSP**	**Gradient** computation	$\Omega(d)$
PGD	**SOSP**	**Gradient** computation	$\tilde{\boldsymbol{O}}\left(\epsilon^{-2}\right)$

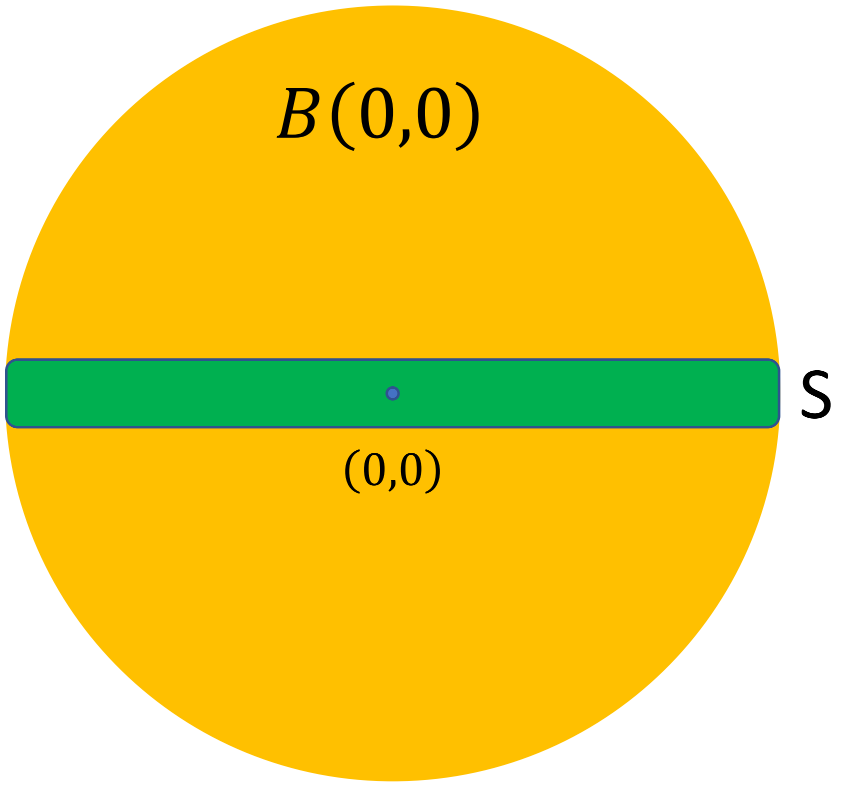
[Ge, Huang, Jin, Yuan 2015]; [Jin, Ge, Netrapalli, Kakade, Jordan 2017]

Main idea

- $S \stackrel{\text{def}}{=}$ set of points around saddle point from where gradient descent does not escape quickly
- Escape $\stackrel{\text{def}}{=}$ function value decreases significantly
- How much is $\mathrm{Vol}(S)$?
- $\mathrm{Vol}(S)$ small $\Rightarrow$ perturbed GD escapes saddle points efficiently

Two dimensional quadratic case

- $f(x) = \frac{1}{2} x^\top \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} x$
- $\lambda_{\min}(H) = -1 < 0$
- $(0,0)$ is a saddle point
- GD: $x_{t+1} = \begin{bmatrix} 1-\eta & 0 \\ 0 & 1+\eta \end{bmatrix} x_t$
- S is a thin strip, $\mathrm{Vol}(S)$ is small



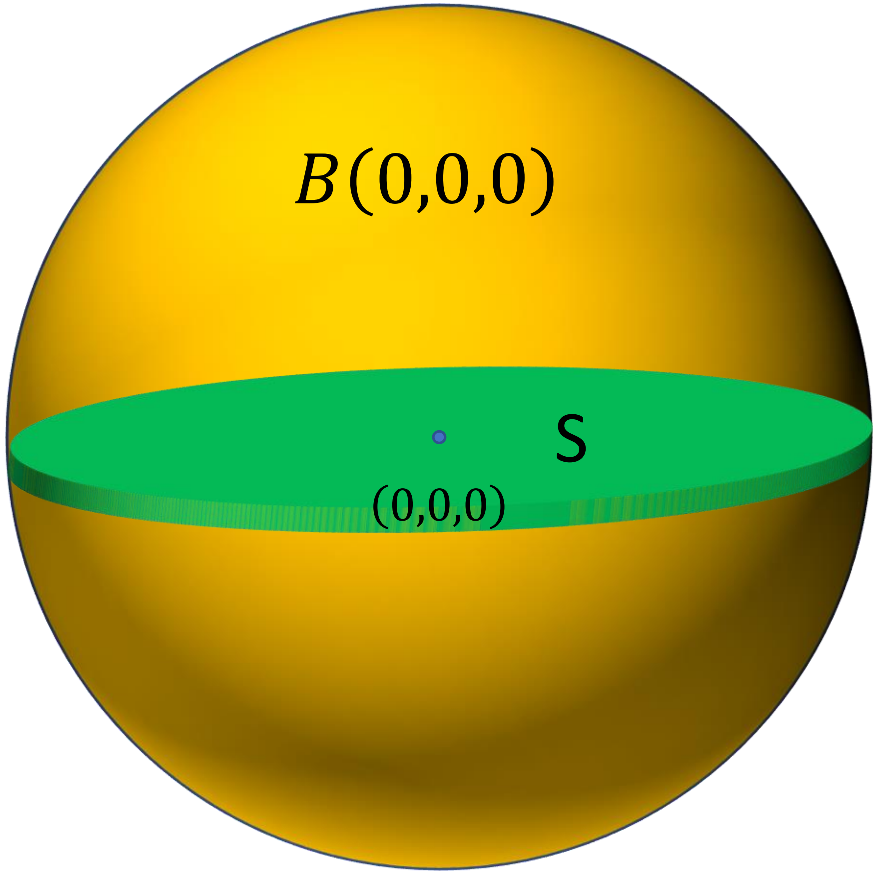
Three dimensional quadratic case

- $f(x) = \frac{1}{2} x^\top \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{bmatrix} x$

- $(0,0,0)$ is a saddle point

- GD: $x_{t+1} = \begin{bmatrix} 1-\eta & 0 & 0 \\ 0 & 1-\eta & 0 \\ 0 & 0 & 1+\eta \end{bmatrix} x_t$

- S is a thin disc, $\mathrm{Vol}(S)$ is small

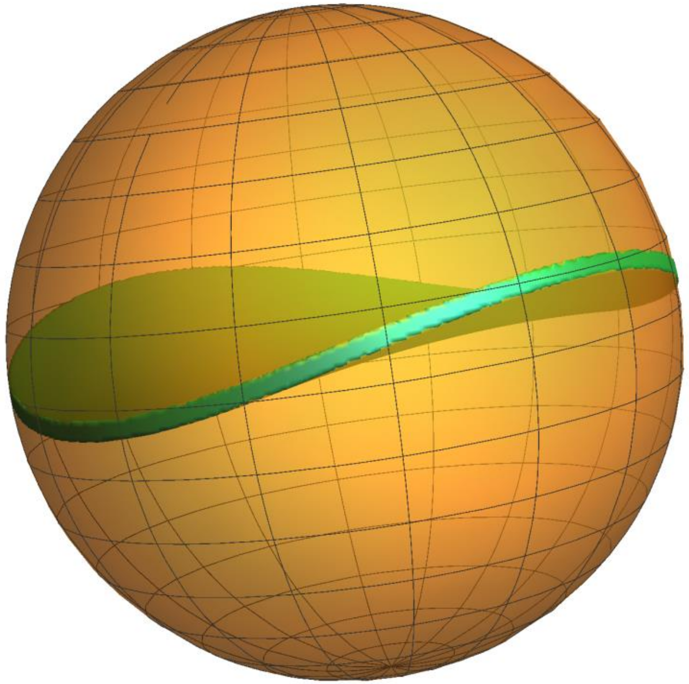


General case

<u>Key technical lemma</u>

S $\sim$ thin deformed disc

$\mathrm{Vol}(S)$ is small



Can we accelerate nonconvex GD?

	Guarantee	Per Iteration cost	# iterations
CR	**SOSP**	Hessian computation	$\boldsymbol{O}\left(\epsilon^{-1.5}\right)$
GD	**SOSP**	**Gradient** computation	$\Omega(d)$
PGD	**SOSP**	**Gradient** computation	$\tilde{O}(\epsilon^{-2})$
PAGD	**SOSP**	**Gradient** computation	$\boldsymbol{O}\left(\epsilon^{-1.75}\right)$

[Agarwal, Allen-Zhu, Bullins, Hazan, Ma 2016]

[Carmon, Duchi, Hinder, Sidford 2016, 2017]

[Jin, Netrapalli, Jordan 2018]

Differential equation view of Accelerated GD

- AGD is a discretization of the following ODE [Polyak 1965]; [Su, Candes, Boyd 2015]

$$\ddot{x} + \tilde{\theta}\dot{x} + \nabla f(x) = 0$$

- Multiplying by $\dot{x}$ and integrating from t_1 to t_2 gives us

$$f(x_{t_2}) + \frac{1}{2}\left\|\dot{x}_{t_2}\right\|^2 = f(x_{t_1}) + \frac{1}{2}\left\|\dot{x}_{t_1}\right\|^2 - \tilde{\theta}\int_{t_1}^{t_2} \|\dot{x}_t\|^2 dt$$

- Hamiltonian $f(x_t) + \frac{1}{2}\|\dot{x}_t\|^2$ decreases monotonically

After discretization

Iterate: x_t and velocity: $v_t := x_t - x_{t-1}$

- Hamiltonian $f(x_t) + \frac{1}{2\eta}\|v_t\|^2$ decreases monotonically if $f(\cdot)$ *"not too nonconvex"* between x_t and $x_t + v_t$
  - *too nonconvex* = *negative curvature*
  - Can increase if $f(\cdot)$ is *"too nonconvex"*

- If the function is *"too nonconvex"*, reset velocity or move in nonconvex direction – *negative curvature exploitation*

Can we accelerate nonconvex GD?

	Guarantee	Per Iteration cost	# iterations
CR	**SOSP**	Hessian computation	$\boldsymbol{O}\left(\epsilon^{-1.5}\right)$
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PAGD	**SOSP**	**Gradient** computation	$\boldsymbol{O}\left(\epsilon^{-1.75}\right)$

[Agarwal, Allen-Zhu, Bullins, Hazan, Ma 2016]

[Carmon, Duchi, Hinder, Sidford 2016, 2017]

[Jin, Netrapalli, Jordan 2018]

Stochastic algorithms

Perturbed SGD (PSGD)

1. **For** $t = 0,1,\ldots$ **do**
2. $x_{t+1} \leftarrow x_t - \eta \hat{\nabla} f(x_t) + \xi_t$

- Convergence rate: $O(\epsilon^{-3.5})$ [Fang, Lin, Zhang 2019]
- $O(\epsilon^{-3})$ with variance reduction [Zhou, Xu, Gu 2018]; [Fang, Li, Lin, Zhang 2018]
- **Finite sum**: $O(\epsilon^{-3} \wedge \sqrt{n}\epsilon^{-2})$

Summary of nonconvex optimization

- Local optimality for nonconvex optimization
- For many problems, SOSPs are sufficient
- Ideas such as momentum, stochastic methods, variance reduction are useful in the nonconvex setting as well
- Complexity theory still not as mature as in convex optimization

Problems where SOSPs = global optima

- Matrix sensing [Bhojanapalli, Neyshabur, Srebro 2016]
- Matrix completion [Ge, Lee, Ma 2016]
- Robust PCA [Ge, Jin, Zheng 2017]
- Tensor factorization [Ge, Huang, Jin, Yuan 2015]; [Ge, Ma 2017]
- Smooth semidefinite programs [Boumal, Voroninski, Bandeira 2016]
- Synchronization & community detection [Bandeira, Boumal, Voroninski 2016]; [Mei, Misiakiewicz, Montanari, Oliveira 2017]
- Phase retrieval [Chen, Chi, Fan, Ma 2018]

Semi-definite programs (SDPs)

$$\min_{X \in R^{n \times n}} \langle C, X \rangle \qquad s.t. \quad \langle A_i, X \rangle = b_i, 1 \le i \le m$$
$$X \succcurlyeq 0$$

- Several applications
  - Clustering (max-cut)
  - Control
  - Sum-of-squares
  - …
- Classical polynomial time solutions exist but can be slow
  - Interior-point methods
  - Ellipsoid method
  - Multiplicative weight update

Low rank solutions always exist!

- (Barvinok'95, Pataki'98): For any feasible SDP, at least one solution exists with rank $k^* \leq \sqrt{2m}$
- In several applications $m \sim n$. So $k^* \ll n$.

Burer-Monteiro: Optimize in low rank space; iterations are fast!

Burer-Monteiro approach

$$\min_{X \in R^{n \times n}} \langle C, X \rangle$$
$$s.t. \quad \langle A_i, X \rangle = b_i;\ i = 1, \cdots, m$$
$$X \succcurlyeq 0$$

$$\min_{U \in R^{n \times k}} \langle C, UU^T \rangle$$
$$s.t. \quad \langle A_i, UU^T \rangle = b_i$$

$k \sim \sqrt{m}$

n^2 dimensional problem

nk dimensional problem

Burer-Monteiro approach

$$\min_{X \in R^{n \times n}} \ \langle C, X \rangle$$
$$s.t. \quad \langle A_i, X \rangle = b_i; \ i = 1, \cdots, m$$
$$X \succcurlyeq 0$$

$$\min_{U \in R^{n \times k}} \ \langle C, UU^T \rangle$$
$$s.t. \quad \langle A_i, UU^T \rangle = b_i$$

$$k \sim \sqrt{m}$$

Penalty Version

Penalty parameter

$$\min_{U \in R^{n \times k}} f(U) = \ \langle C, UU^T \rangle + \mu \sum_i (\langle A_i, UU^T \rangle - b_i)^2$$

Nonconvex problem!

$$\min_{U \in R^{n \times k}} f(U) = \langle C, UU^T \rangle + \mu \sum_i (\langle A_i, UU^T \rangle - b_i)^2$$

Are SOSPs = global minima?

- In general, no [Bhojanapalli, Boumal, Jain, Netrapalli 2018]

Smoothed analysis

$$\min_{U \in R^{n \times k}} f(U) = \langle C + G, UU^T \rangle + \mu \sum_i (\langle A_i, UU^T \rangle - b_i)^2$$

- G: symmetric Gaussian matrix with $G_{ij} \sim N(0, \sigma^2)$
- If $k = \Omega(\sqrt{m \log 1/\epsilon})$ then with high probability

every ϵ SOSP = ϵ global optimum

[Boumal, Voroninski, Bandeira 2016]

[Bhojanapalli, Boumal, Jain, Netrapalli 2018]

Two key steps $\min_{U \in \mathbb{R}^{n \times k}} f(UU^\top)$ $f(\cdot)$ convex

1. SOSP that is rank deficient is global optimum [Burer-Monteiro 2003]

$$U \text{ SOSP and } \sigma_k(U) = 0 \Rightarrow U \text{ is a global optimum}$$

$\hookrightarrow k^{\mathrm{th}}$ largest singular value of U

2. For perturbed SDPs, with probability 1, if $k \geq \sqrt{2m}$, then

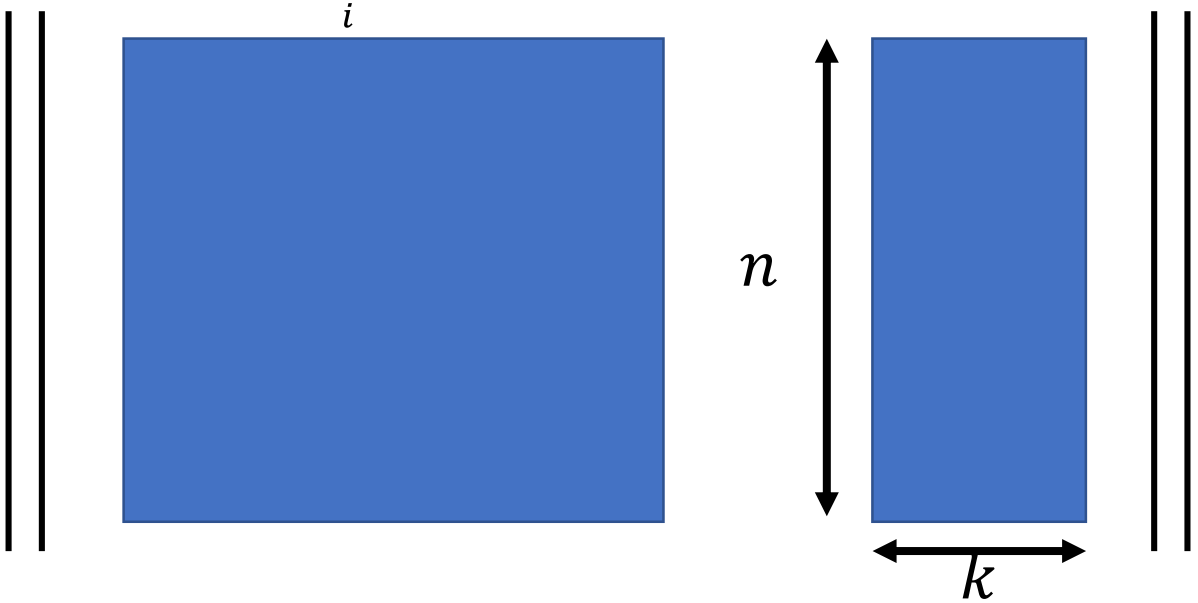
all FOSPs have $\sigma_k(U) = 0$.

ϵ-FOSP $\Rightarrow \sigma_k(U)$ is small

$$\min_{U \in R^{n \times k}} f(U) = \langle C + G, UU^T \rangle + \mu \sum_i (\langle A_i, UU^T \rangle - b_i)^2$$

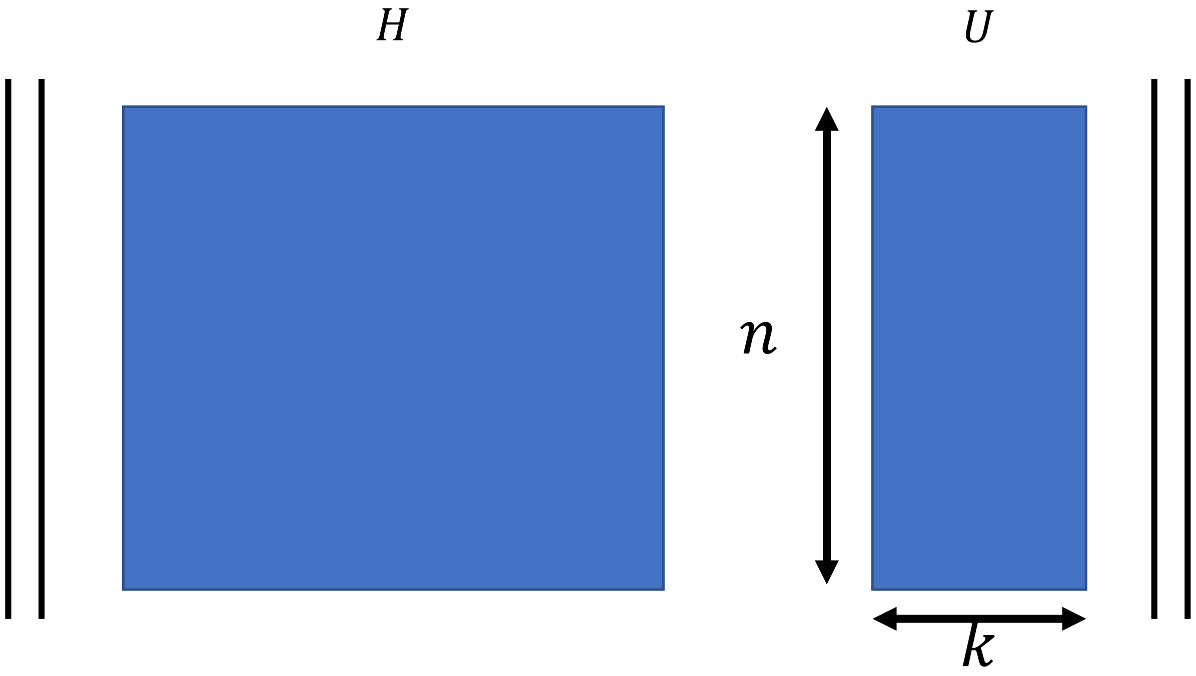
- Approximate FOSP: $\|(C + G + 2\mu \sum_i (\langle A_i, UU^\top \rangle - b_i)\, A_i) U\| \leq \epsilon$

$C + G + 2\mu \sum_i (\langle A_i, UU^\top \rangle - b_i)\, A_i$ $\quad\quad$ U



$\leq \epsilon$

Aside: Lower bound on product of matrices



$$\geq \sigma_{n-k+1}(H) \cdot \sigma_k(U)$$

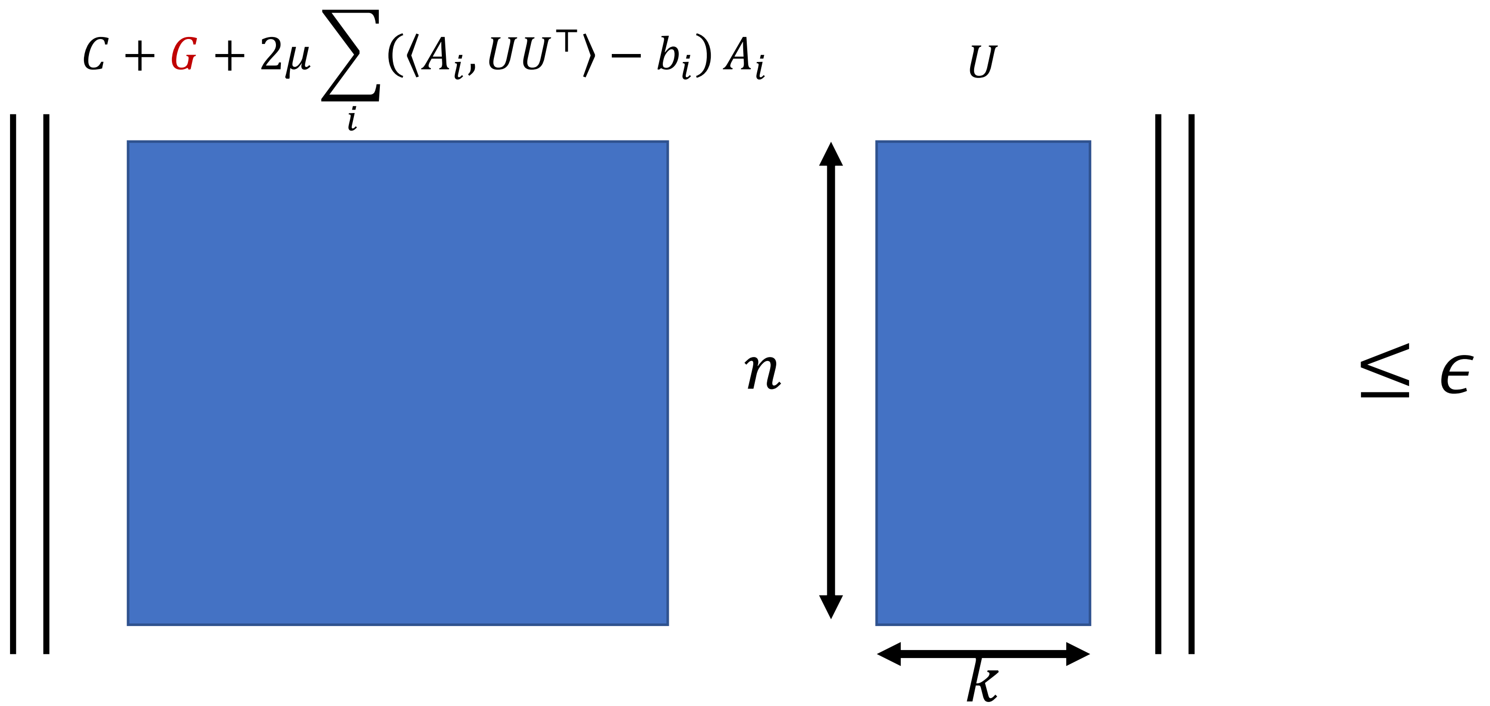
$$\boxed{\sigma_k(U) \leq \frac{\|HU\|}{\sigma_{n-k+1}(H)}}$$

FOSP $\Rightarrow \sigma_k(U)$ is small

$\sigma_{n-k+1}(C + G + 2\mu \sum_i (\langle A_i, UU^\top \rangle - b_i) A_i)$ large

$$\Downarrow$$

$\sigma_k(U)$ is small



Smallest singular values of Gaussian matrices

- $\sigma_i(G)$ denotes the i^{th} singular value of G.

$$\mathbb{P}[\sigma_n(G) = 0] = 0$$

- In general, $\sigma_{n-k}(G) \sim \frac{k}{\sqrt{n}}$.
- Can obtain large deviation bounds [Nguyen 2017]

$$\mathbb{P}\left[\sigma_{n-k}(G) < c\,\frac{k}{\sqrt{n}}\right] < \exp(-C{\color{red}k^2} + k\log n)$$

- Can extend the above to $G + {\color{blue}A}$ for any fixed matrix ${\color{blue}A}$
- In this case, ${\color{red}G} + C + 2\mu\sum_i(\langle A_i, UU^\top\rangle - b_i)\,A_i$

Summary

Several problems for which SOSPs = global optima

Convert a large convex problem into a smaller nonconvex problem

- E.g., Burer-Monteiro approach for solving SDPs
- Empirically, much faster than ellipsoid/interior point methods
- Open problem: Identify other problems which have this property

Alternating Minimization

Alternating Minimization

Applicable to a special class of problems:

those here variables can be split into two sets, i.e. $x = (u, v)$ such that

$$\min_u f(u, v) \qquad \text{feasible / “easy” for fixed } v$$

$$\min_v f(u, v) \qquad \text{feasible / “easy” for fixed } u$$

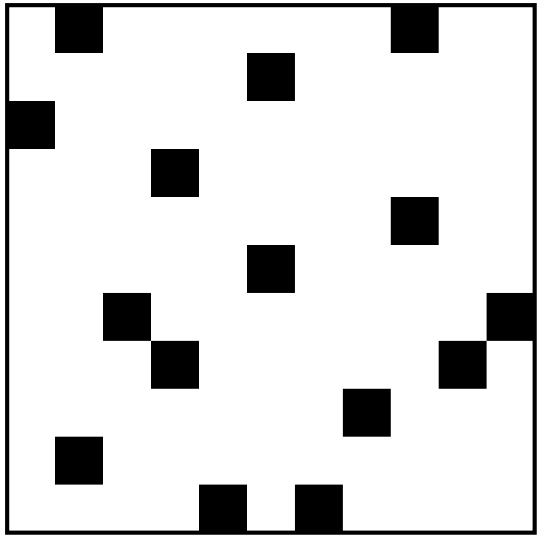
Alt-min: (initialize)

$$u_+ = \arg\min_u \; f(u, v)$$

$$v_+ = \arg\min_v \; f(u_+, v)$$

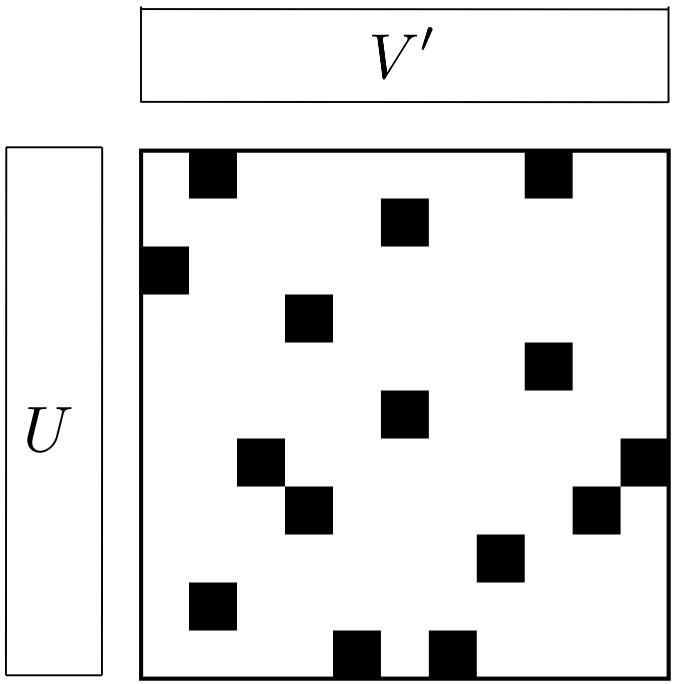
- “big” global steps, and can be much faster than “local” gradient descent
- No step size to be tuned / chosen

Matrix Completion



Find a low-rank matrix from a few (randomly sampled) elements

Matrix Completion



Find a low-rank matrix from a few (randomly sampled) elements

- Let Ω be set of sampled elements

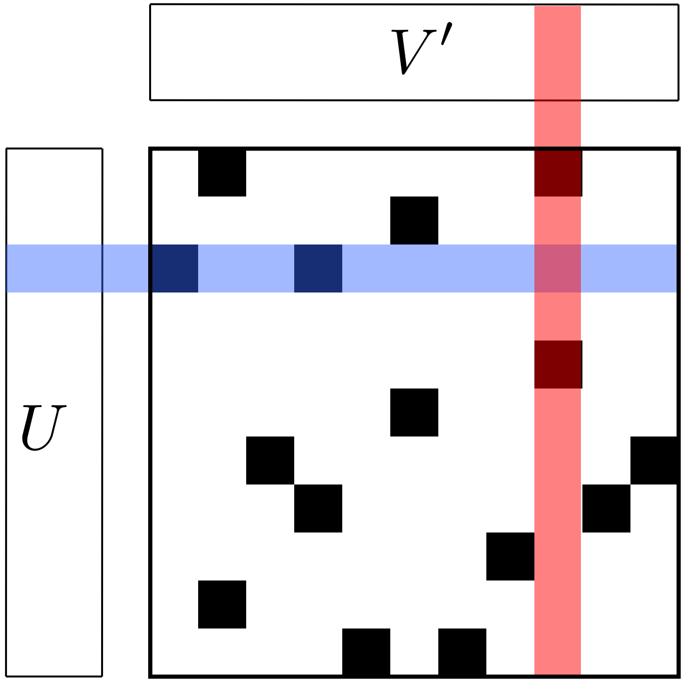
Alt min:

(1) Write as non-convex problem

$$\min_{U,V} \|\mathcal{P}_\Omega(M - UV')\|_F$$

(2) Alternately optimize U and V

AltMin for Matrix Completion



Naturally decouples into small least-squares problems

(a) For all i

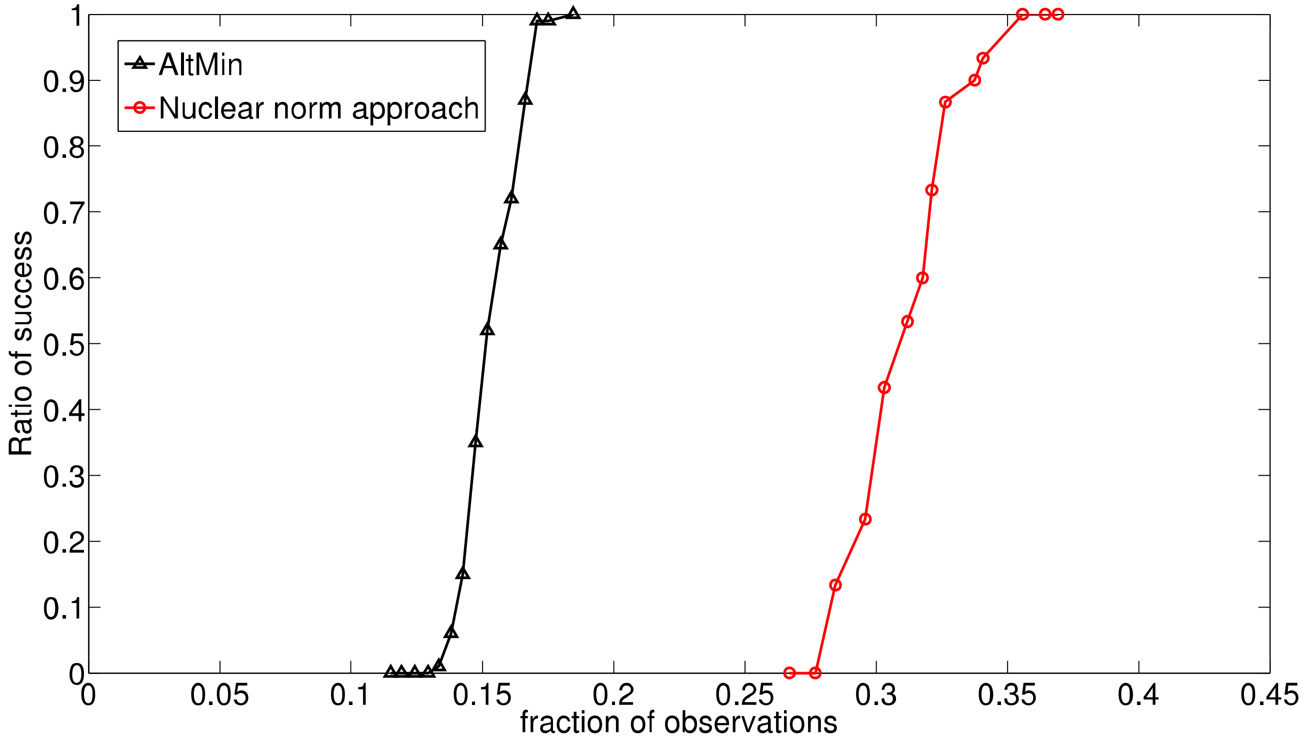
$$u_i \leftarrow \min_u \sum_{j:(i,j)\in\Omega} (m_{ij} - \langle u, v_j \rangle)^2$$

(b) For all j

$$v_j \leftarrow \min_v \sum_{i:(i,j)\in\Omega} (m_{ij} - \langle u_i, v \rangle)^2$$

Closed form, embarrassingly parallel

Matrix Completion



Empirically: AltMin needs **fewer samples** than convex methods like trace-norm minimization

- with memory as small as input and output
- very fast, parallel

Theoretically: both take $O(nr^2 \log n)$ randomly chosen samples for exact recovery of incoherent matrices

- w/ spectral initialization
- close to the lower bound of $\Omega(nr \log n)$

Mixed linear regression

Solve linear equations, except that each is either

$$y_i = \langle x_i, \beta_0^* \rangle \qquad \text{or} \qquad y_i = \langle x_i, \beta_1^* \rangle$$

Find β_1^*, β_0^* given $\{y_i, x_i\}$

Natural for modeling with latent classes

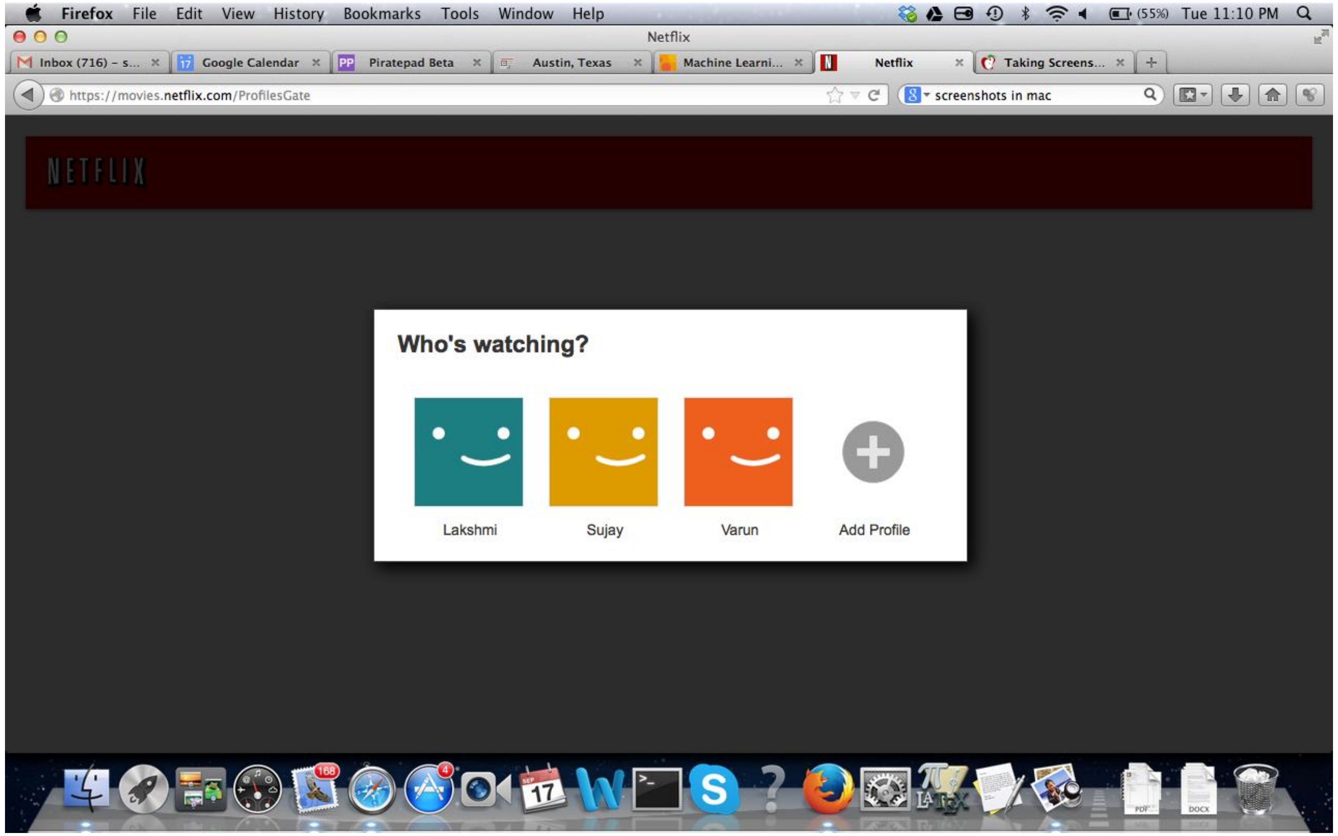
- Evolutionary biology: separating phenotypes
- Quantitative Finance: detecting regime change
- Healthcare: separating patient classes for differential treatment

Several specialized R packages (see [Grun,Leisch] for overview)

- all implement variants / optimizations of EM - **AltMin**

Mixed Linear Regression

… my netflix problem …



Mixed Linear Regression

AltMin: alternate between the z's and the $\beta' s$

$$\min_{\beta_1,\beta_0} \sum_i \min_{z_i \in \{0,1\}} \left(y_i - z_i\langle x_i, \beta_1\rangle + (1-z_i)\langle x_i, \beta_0\rangle\right)^2$$

(a) Assign each sample to the lower current error

$$\widehat{z}_i = 1 \quad \Leftrightarrow \quad (y_i - \langle x_i, \widehat{\beta}_1\rangle)^2 \, < \, (y_i - \langle x_i, \widehat{\beta}_0\rangle)^2$$

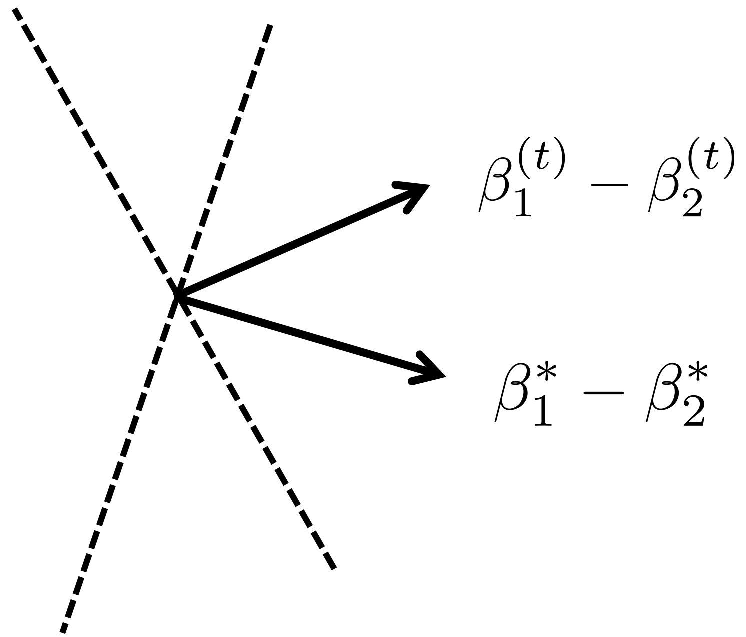
(b) Update each β from its assigned samples

$$\widehat{\beta}_1 \ \leftarrow \ \arg\min_{\beta} \sum_{i:z_i=1} (y_i - \langle x_i, \beta\rangle)^2$$

Both updates are
Simple closed forms !

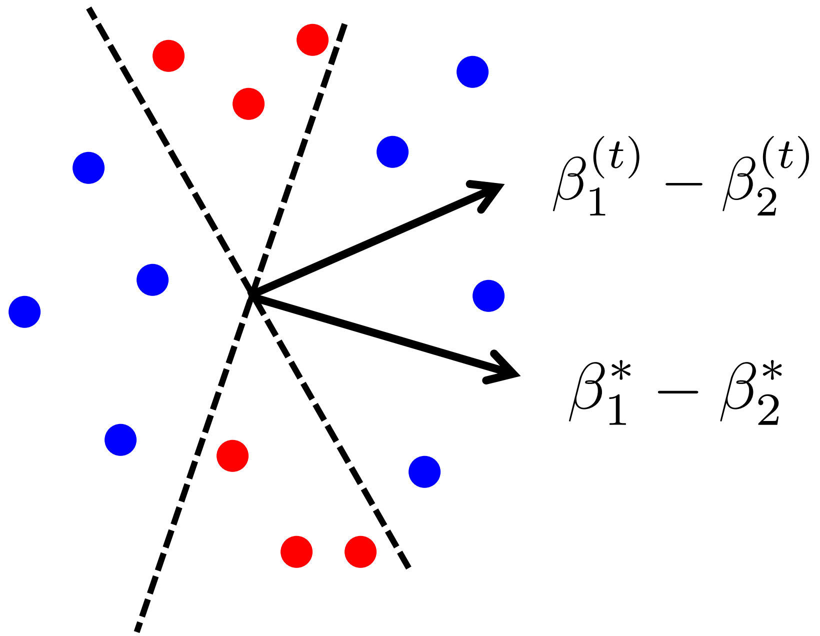
Mixed Linear Regression

Intuition: current iterate $\beta_1^{(t)}, \beta_2^{(t)}$ truth β_1^*, β_2^*



Mixed Linear Regression

Intuition: current iterate $\beta_1^{(t)}, \beta_2^{(t)}$ truth β_1^*, β_2^*



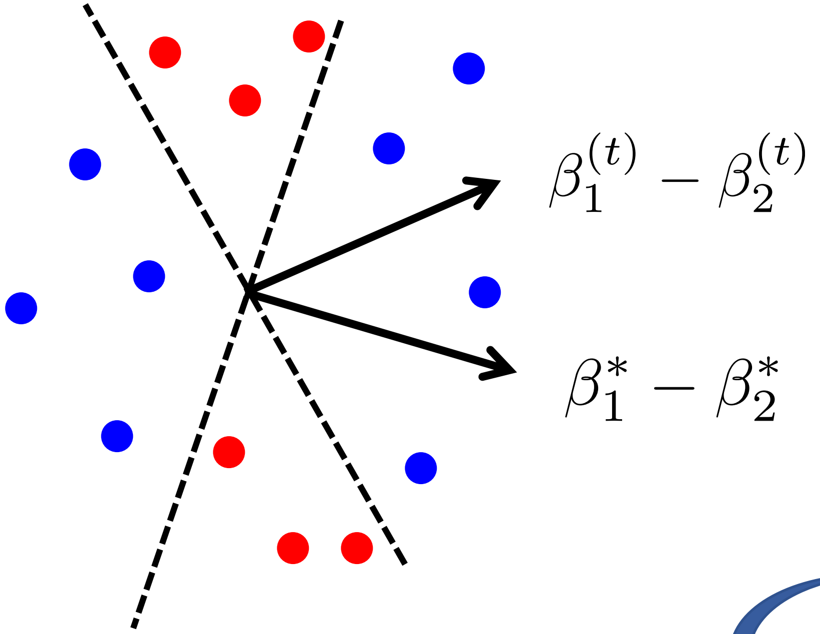
If β_1, β_2 not too far from β_1^*, β_2^*

Then **majority** points will be correctly assigned.

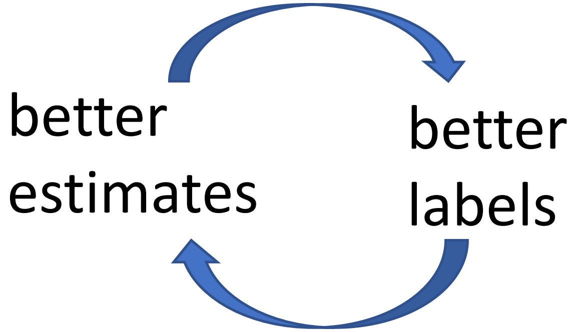
So, running least-squares on these will yield better next iterate.

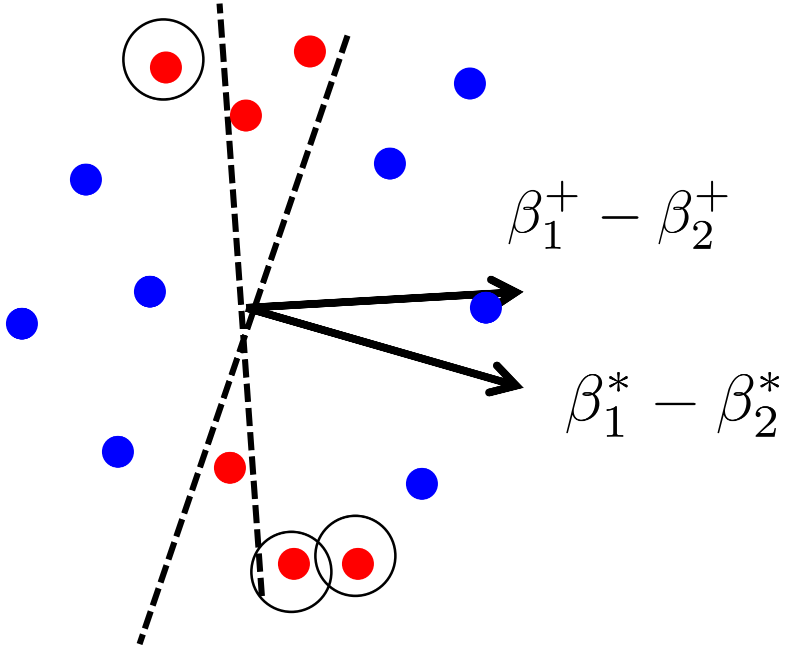
Mixed Linear Regression

Intuition: current iterate $\beta_1^{(t)}, \beta_2^{(t)}$ truth β_1^*, β_2^*



Virtuous cycle





But only once it is decent enough
… so need **initialization** …

Spectral Initialization

Matrix Completion

Take top-r eigenvectors of
sparse 0-filled matrix

Mixed linear regression

Take top 2 eigenvectors of

$$M = \sum_{i=1}^{n} y_i^2 \; x_i x_i^T$$

AltMin also successful for Phase retrieval, matrix sensing, robust PCA etc.

Open Problem: a more general theory of AltMin and its convergence …

Open problems

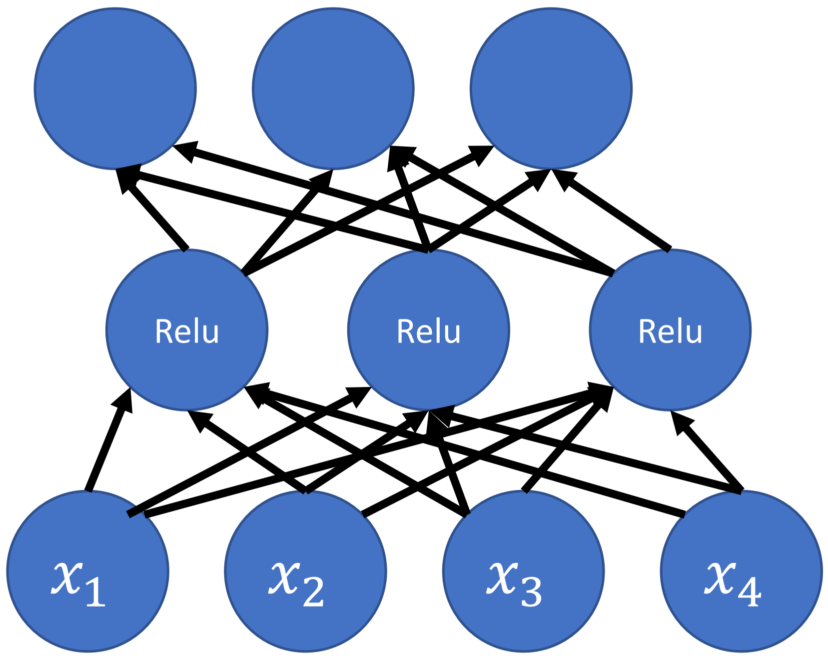
Quasi Newton methods

- First order methods that try to emulate second order methods (such as Newton method) by estimating Hessians (using gradients)
  - E.g., BFGS, L-BFGS $\nabla f(x_{k+1}) - \nabla f(x_k) \sim H(x_{k+1} - x_k)$
  - Well understood theory; widely successful for convex optimization in practice

- Nonconvex optimization
  - **Theory**: Initial results on convergence to FOSP [Wang, Ma, Goldfarb, Liu 2016]
  - **Practice**: Has not been effective so far
    - Need to design better algorithms?

Initialization

- Refers to choice of x_0; affects both optimization speed and quality of the local minimum



$$z \sim \mathcal{N}(0, \sigma_z^2)$$

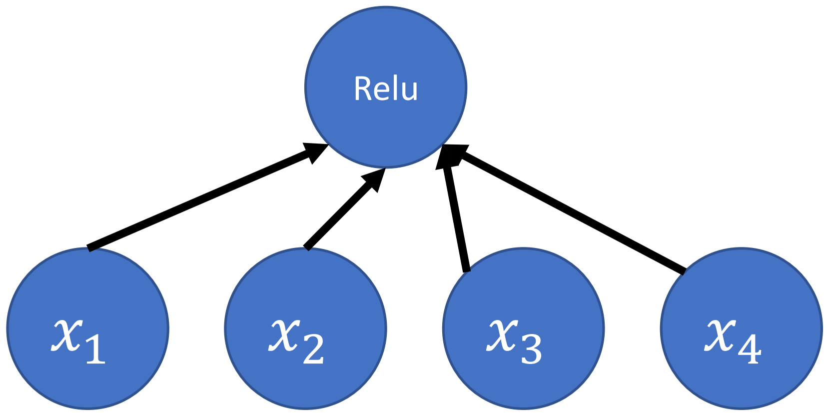
$$w \sim \mathcal{N}(0, \sigma_w^2)$$

Initialization

- Highly influential empirical works: [Glorot, Bengio 2010]; [Sutskever, Martens, Dahl, Hinton 2013]; [He, Zhang, Ren, Sun 2015]

- Main viewpoint: Gradients and activations at initialization

$$y = \mathrm{ReLU}(w^\top x)$$



$$\mathrm{Var}(y) \propto \sigma_w^2 \cdot \|x\|^2$$

- For $y \sim x_i$, choose $\sigma_w^2 \propto \frac{1}{d_{\text{in}}}$

- Training phase: not understood

Nonconvex nonconcave minimax optimization

$$\min_x \max_y f(x, y)$$

- The function to minimize $g(x) \stackrel{\text{def}}{=} \max_y f(x, y)$ defined implicitly
- Basis of generative adversarial networks (GAN) and robust training
- Notions of local optimality not well understood in the general setting
- Gradient descent ascent widely used but its convergence properties not understood

Summary

- Nonconvex optimization is the primary computational work horse in machine learning now
- Main ideas behind these algorithms come from convex optimization
- Research direction 1: Understanding statistical + optimization landscape of important nonconvex problems
    - E.g., SOSPs = global optima in matrix factorization problems
- Research direction 2: Designing faster algorithms