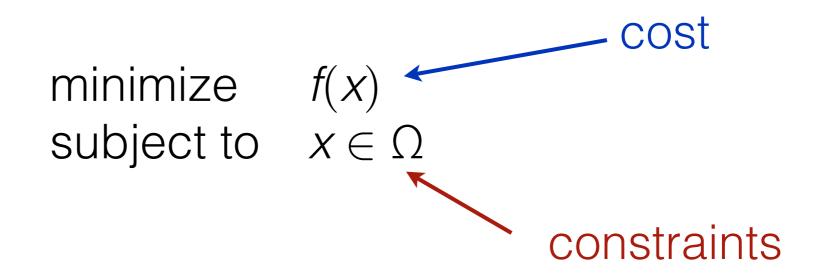
Optimization

Benjamin Recht University of California, Berkeley

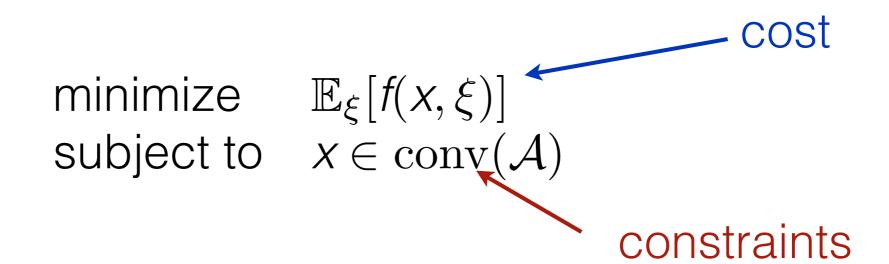
Stephen Wright University of Wisconsin-Madison

optimization



might be too much to cover in 3 hours

optimization (for big data?)

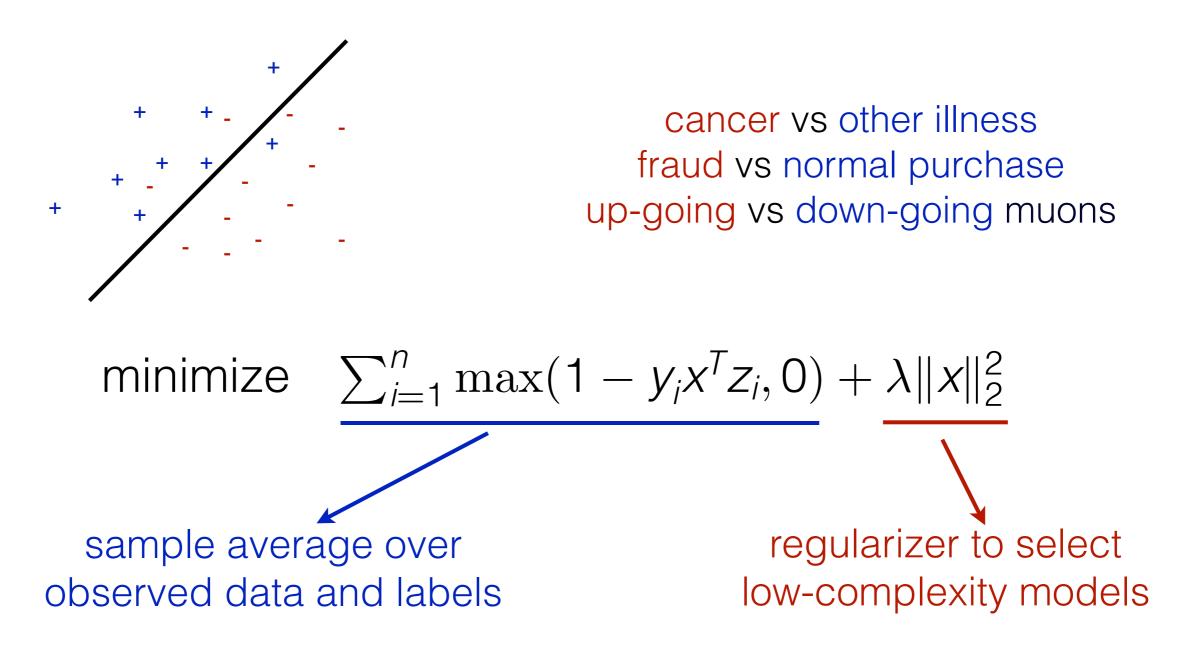


- distribution over $\boldsymbol{\xi}$ is well-behaved
- *A* is simple (low-cardinality, low-dimension, low-complexity)

minimize $\mathbb{E}_{\xi}[f(x,\xi)] + P(x)$

closely related cousin where *P* is a simple convex function

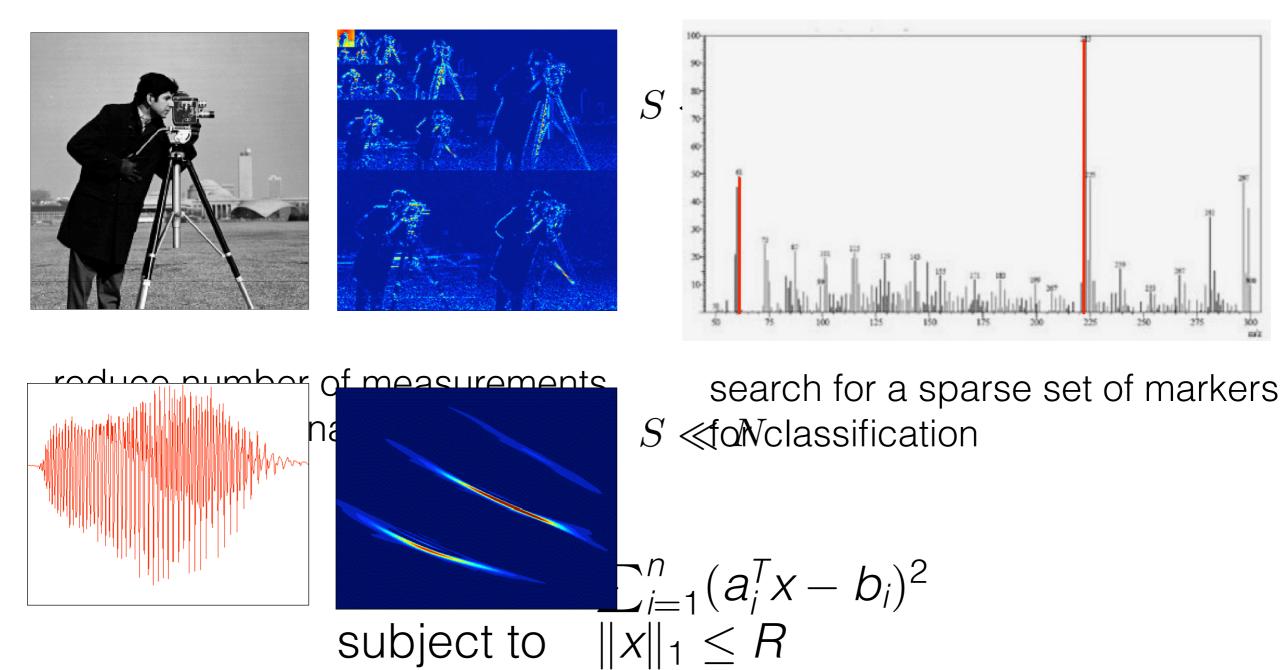
Support Vector Machines



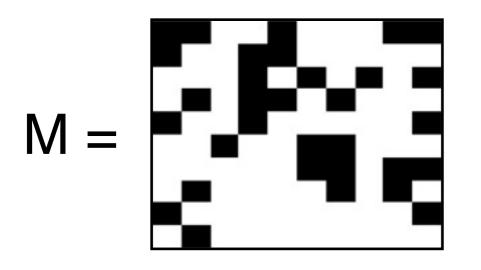
LASSO

Compressed Sensing

Sparse Modeling

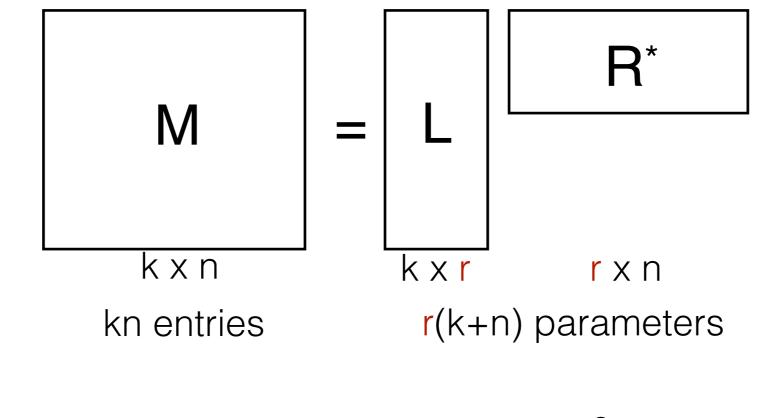


Matrix Completion



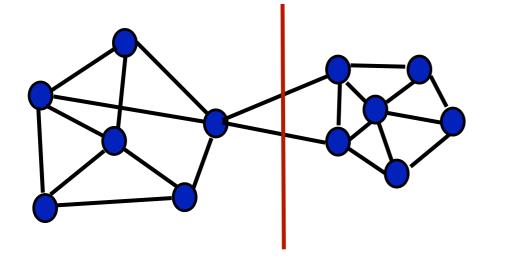
M_{ij} known for black cells M_{ij} unknown for white cells Rows index features Columns index examples Entries specified on set *E*

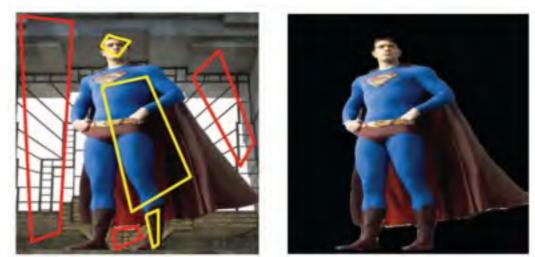
• How do you fill in the missing data?



minimize $\sum_{(u,v)\in E} (X_{uv} - M_{uv})^2 + \mu \|\mathbf{X}\|_*$

Graph Cuts



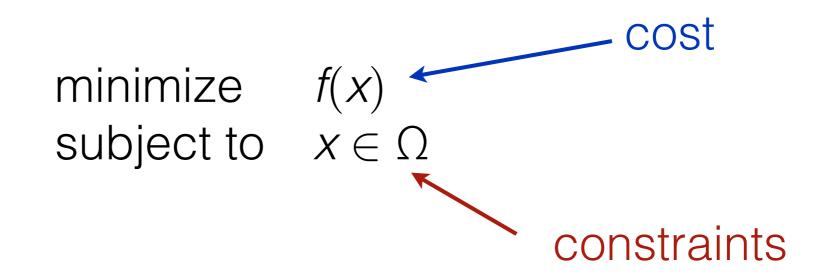


Bhusnurmath and Taylor, 2008

- Image Segmentation
- Entity Resolution
- Topic Modeling

$$\begin{array}{lll} \text{minimize} & \sum_{(u,v)\in E} |x_u - x_v| \\ \text{subject to} & x_u \in [0,1] & \text{if } u \in V \\ & x_a = 0 & \text{if } a \in A \\ & x_b = 1 & \text{if } b \in B \end{array}$$

optimization

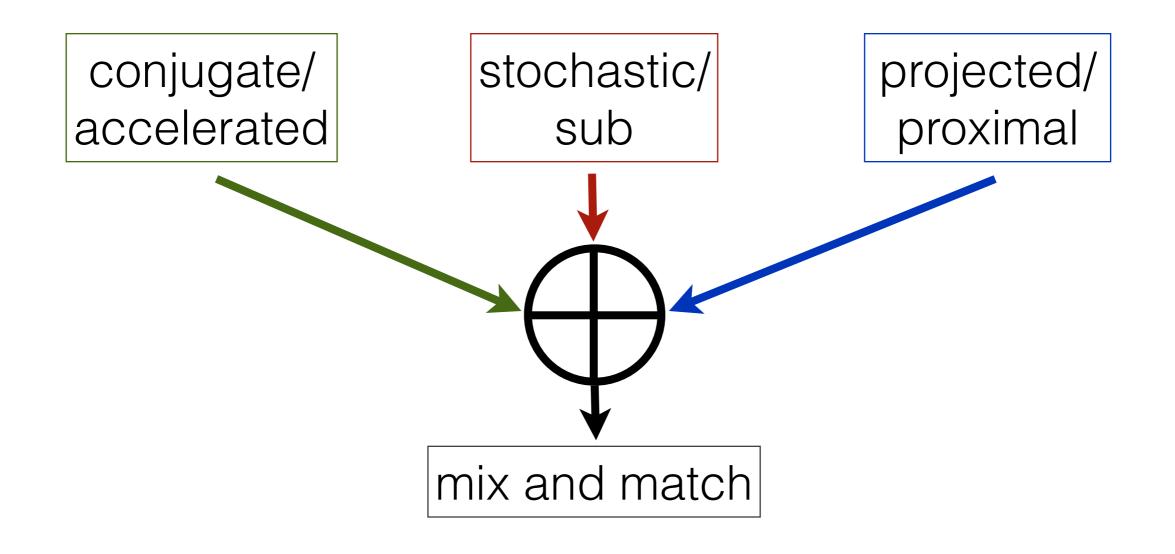


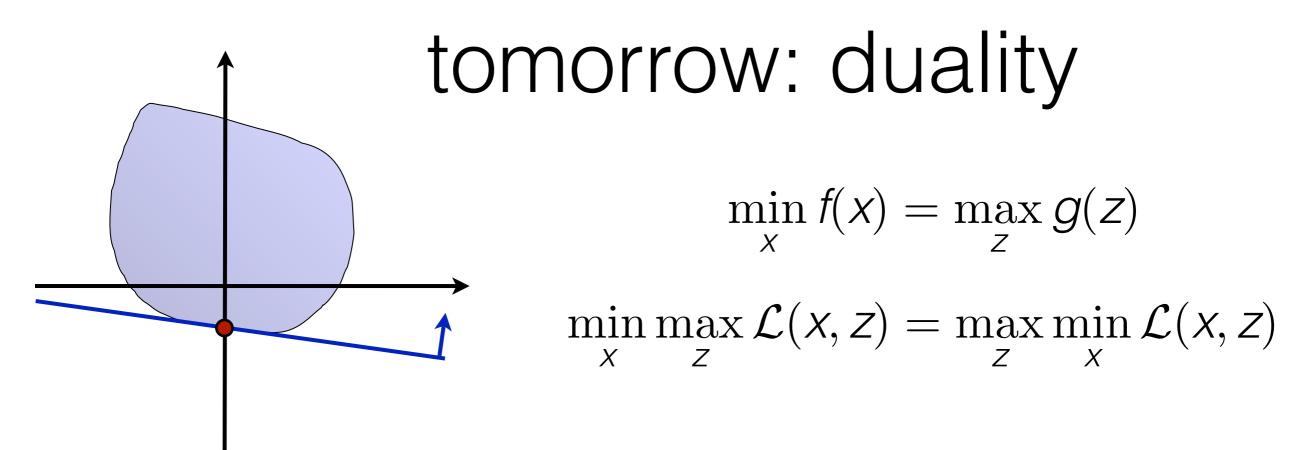
might be too much to cover in 3 hours

- optimization is *ubiquitous*
- optimization is *modular*
- optimization is *declarative*

 $x[k+1] \leftarrow x[k] + \alpha_k v[k]$

Today: gradient descent





- find problems that always lower bound the optimal value.
- puts problem in NP \(\CoNP\)
- information from one problem informs the other
- some times easier to solve one than the other
- basis of many proof techniques in data science (and tons of other areas too!)

what we'll be skipping...

- 2nd order/newton/BFGS
- interior point methods/ellipsoid methods
- active set methods, manifold identification
- branch and bound
- integrating combinatorial thinking
- derivative-free optimization
- soup of heuristics (simulated annealing, genetic algorithms, ...)
- modeling

optimality conditions

 $\begin{array}{ll} \text{minimize} & f(x) \\ \text{subject to} & x \in \mathbb{R}^n \end{array}$

Search for $\nabla f(x) = 0$

- Turns a geometric problem into an algebraic problem: solve for the point where the gradient vanishes.
- Is necessary for optimality (sufficient for convex, smooth *f*)

$$x[k+1] \leftarrow x[k] + \alpha_k v[k]$$

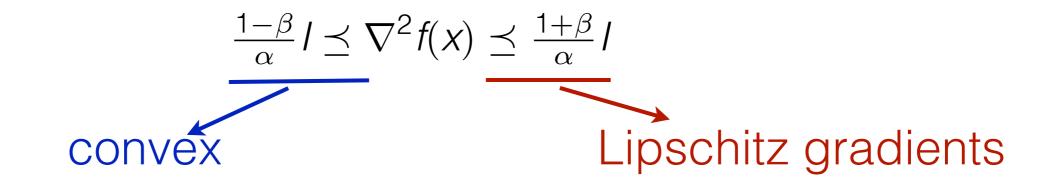
gradient descentAssume there exits an $x_* \in \mathcal{D}$
where $\nabla f(x_*) = 0$ \bigvee $x - \alpha \nabla f(x)$
is contractive on \mathcal{D}
 $||\psi(x) - \psi(z)|| \le \beta ||x - z||$ for some $0 \le \beta < 1$

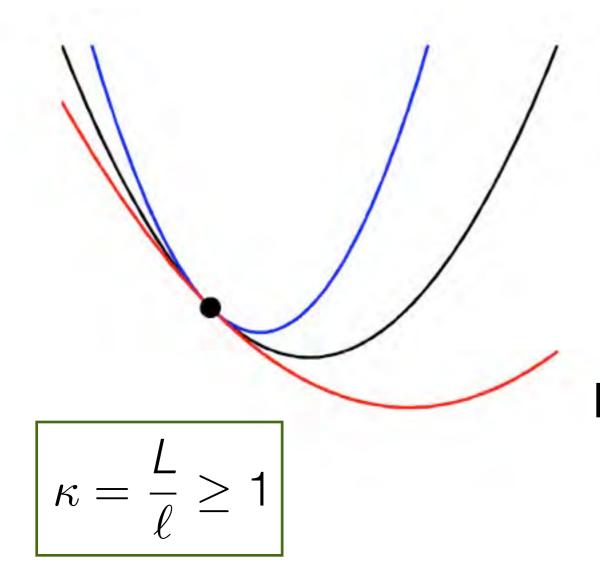
run gradient descent starting at $x[0] \in D$ $||x[k+1] - x_*|| = ||x[k] - \alpha \nabla f(x[k]) - x_*||$ $= ||\psi(x[k]) - \psi(x_*)||$ $\leq \beta ||x[k] - x_*||$ \vdots $\leq \alpha^{k+1} ||x[0] - x_*||$ \downarrow

 $\leq \beta^{k+1} \| x[0] - x_{\star} \|$ linear rate

If f is 2x differentiable, contractivity means f is convex on D

 $\frac{1}{t}\|\psi(x+t\Delta x) - \psi(x)\| \le \beta \|\Delta x\| \quad \text{for all } t > 0$





convexity $f(tx + (1 - t)z) \le tf(x) + (1 - t)f(x)$ $f(z) \ge f(x) + \nabla f(x)^{T}(z - x) + \frac{\ell}{2} ||z - x||^{2}$ strong convexity

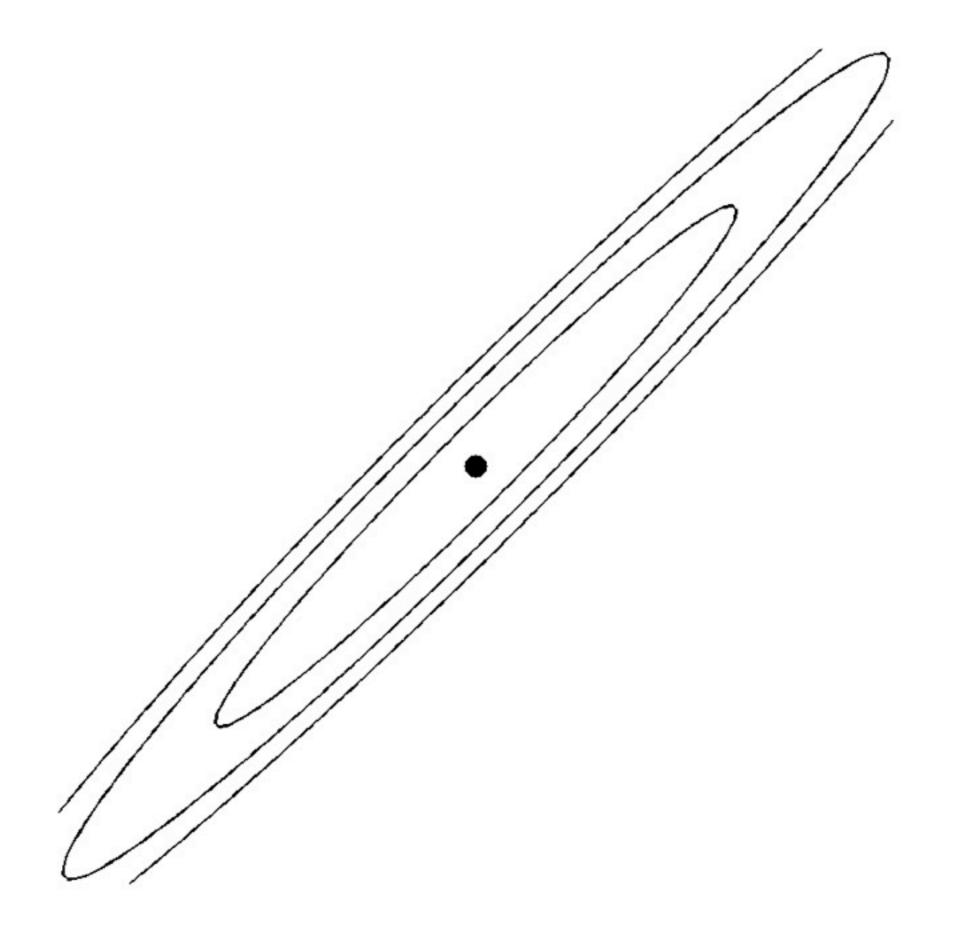
Lipschitz gradients $\|\nabla f(x) - \nabla f(z)\| \le L \|x - z\|$ $f(z) \le f(x) + \nabla f(x)^{T} (z - x) + \frac{L}{2} \|z - x\|^{2}$

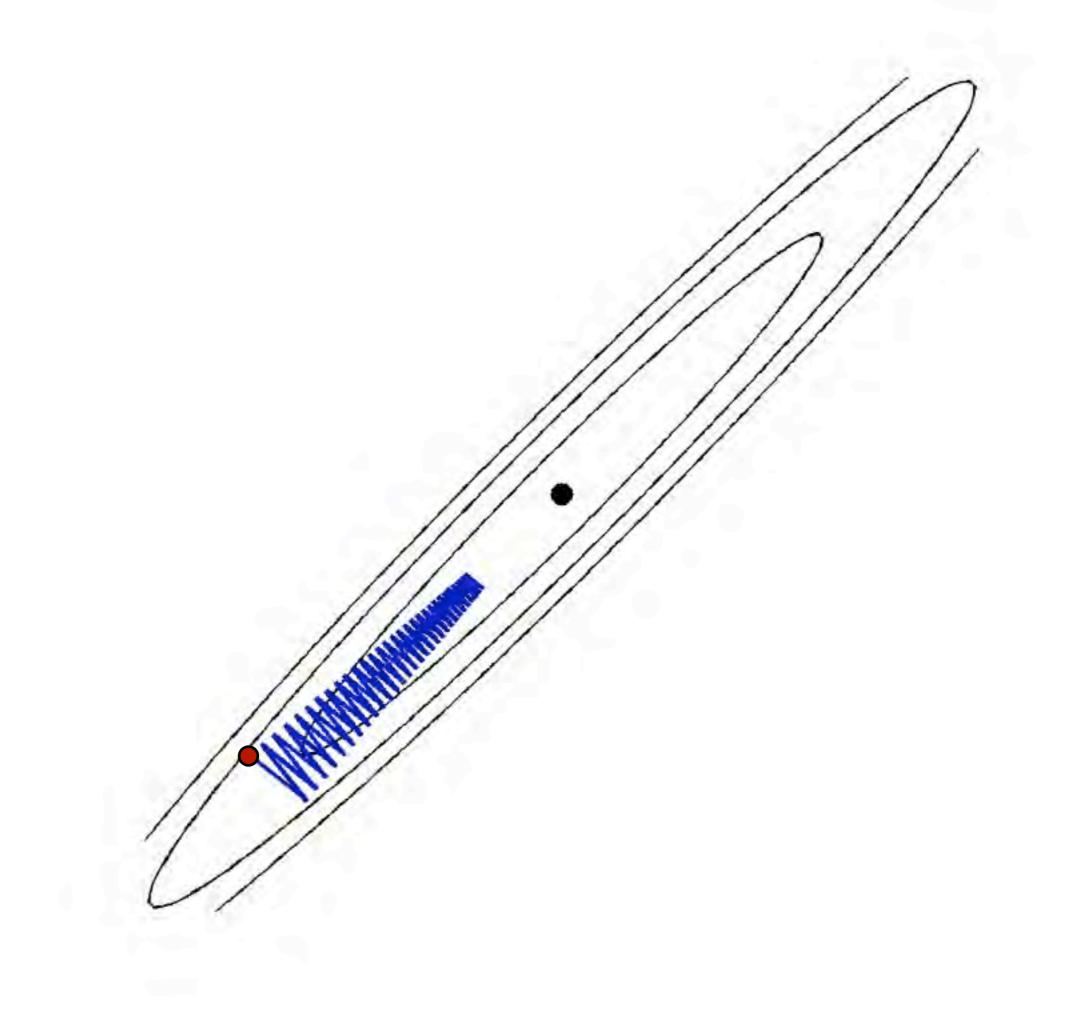
condition number of Hessian

follows from Taylor's theorem

With step size $\alpha = \frac{2}{\ell+L}$, $||x[k] - x_*|| \le \left(1 - \frac{2}{\kappa+1}\right)^{\kappa} ||x[0] - x_*||$. $f(x[k]) - f_* \le L\left(1 - \frac{2}{\kappa+1}\right)^{2\kappa} ||x[0] - x_*||^2$ Note on convergence rate With step size $\alpha = \frac{2}{\ell+L}$, $||x[k] - x_*|| \le \left(1 - \frac{2}{\kappa+1}\right)^k ||x[0] - x_*||$.

- If you don't know the exact stepsize, can we achieve the rate?
 - Exact line search: at each iteration, find the α that minimizes f(x+ α d).
 - Backtracking line search: Reduce α by constant multiple until the function value sufficiently decreases.
- Both achieve linear rate of convergence.
- More sophisticated line searches often used in practice, but none improve over this rate in the worst case.





acceleration/multistep

gradient method akin to an ODE

$$x[k+1] = x[k] - \alpha \nabla f(x[k])$$
$$\dot{x} = -\nabla f(x)$$

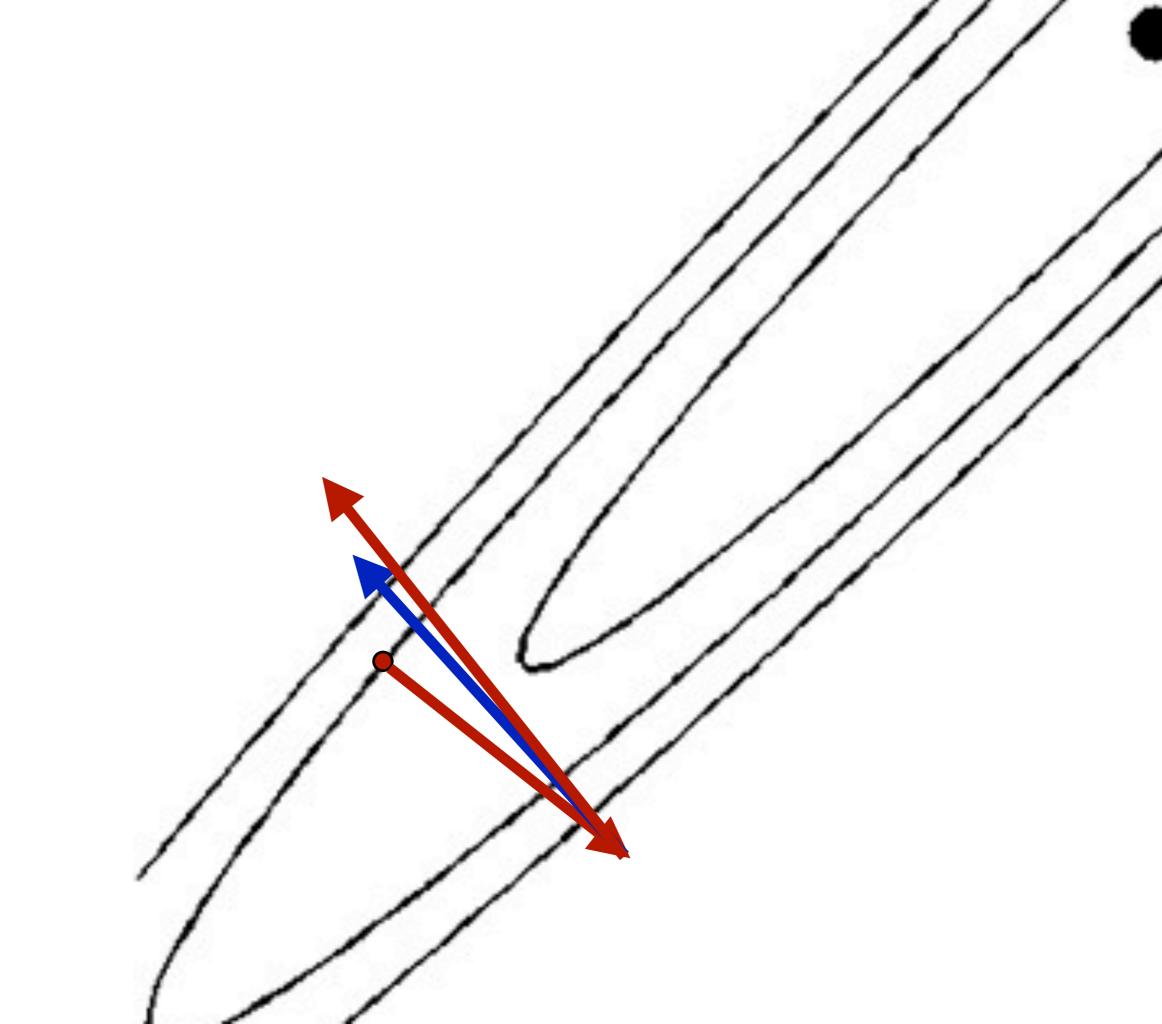
to prevent oscillation, add a second order term

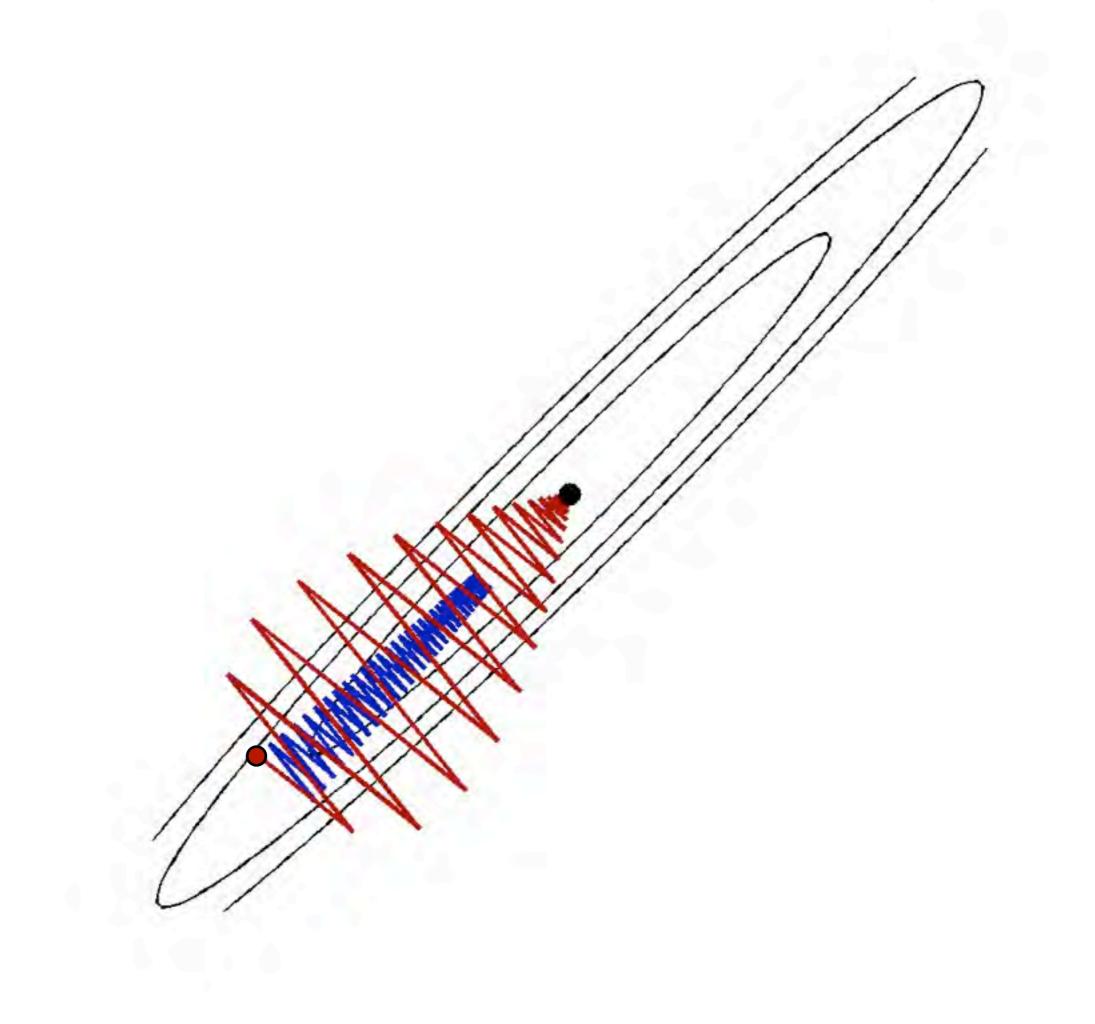
$$\ddot{x} = -b\dot{x} - \nabla f(x)$$
$$x[k+1] = x[k] - \alpha \nabla f(x[k]) + \beta(x[k] - x[k-1])$$

$$x[k+1] = x[k] + \alpha p[k]$$
$$p[k] = -\nabla f(x[k]) + \beta p[k-1]$$

heavy ball method (constant α, β)

when f is quadratic, this is Chebyshev's iterative method





analysis

$$x[k+1] = x[k] + \alpha p[k]$$
$$p[k] = -\nabla f(x[k]) + \beta p[k-1]$$

heavy ball method (constant α , β)

Analyze by defining a composite error vector:

$$W_k := \begin{bmatrix} x[k] - x_\star \\ x[k-1] - x_\star \end{bmatrix}$$

Then w[k+1] = Bw[k] + o(||w[k]||)

where
$$B := \begin{bmatrix} -\alpha \nabla^2 f(x_\star) + (1+\beta)I & -\beta I \\ I & 0 \end{bmatrix}$$

analysis (cont.)

w[k+1] = Bw[k] + o(||w[k]||)

B has the same eigenvalues as $\begin{bmatrix} -\alpha\Lambda + (1+\beta)I & -\beta I \\ I & 0 \end{bmatrix}$ $\Lambda = \operatorname{diag}(\lambda_1, \lambda_2, \dots, \lambda_n)$

where λ_i are the eigenvalues of $\nabla^2 f(x_\star)$

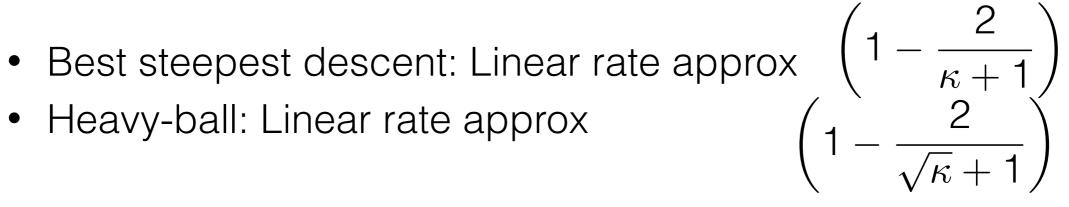
Choose α, β to explicitly minimize the max eigenvalue of B to obtain

$$\alpha = \frac{4}{L} \frac{1}{(1+1/\sqrt{\kappa})^2} \qquad \qquad \beta = \left(1 - \frac{2}{\sqrt{\kappa}+1}\right)^2.$$

Leads to linear convergence for $||x[k] - x_*||_2$ with rate approximately

$$\left(1-\frac{2}{\sqrt{\kappa}+1}\right)$$

about those rates...



• **Big difference!** To yield $||x[k] - x_*||_2 < \epsilon ||x[0] - x_*||_2$

$$\kappa \ge \frac{\kappa}{2} \log(1/\epsilon)$$
 gradient descent

$$k \ge \frac{\sqrt{\kappa}}{2} \log(1/\epsilon)$$
 heavy ball

• A factor of $\kappa^{1/2}$ difference. e.g. if $\kappa = 100$, need 10 times fewer steps.

conjugate gradients

$$x[k+1] = x[k] + \alpha_k p[k]$$
$$p[k] = -\nabla f(x[k]) + \beta_k p[k-1]$$

Choose α_k by line search (to reduce f)

Choose β_k such that p[k] is approximately conjugate to p[1], ..., p[k-1] (really only makes sense for quadratics, but whatever...)

- Does not achieve a better rate than heavy ball
- Gets around having to know parameters
- Convergence proofs very sketchy (except when f is quadratic) and need elaborate line search to guarantee local convergence.

optimal method

Nesterov's optimal method (1983,2004)

$$x[k+1] = x[k] + \alpha_k p[k]$$

$$p[k] = -\nabla f(x[k] + \beta_k (x[k] - x[k-1])) + \beta_k p[k-1]$$
because ball with extraorediant stop

heavy ball with extragradient step

$$\lambda_{k+1}^{2} = (1 - \lambda_{k+1})\lambda_{k}^{2} + \kappa^{-1}\lambda_{k+1} \qquad t_{k} = \frac{1}{2}\left(1 + \sqrt{1 + 4t_{k}^{2}}\right)$$
$$\beta_{k} = \frac{\lambda_{k}(1 - \lambda_{k})}{\lambda_{k}^{2} + \lambda_{k+1}} \qquad \beta_{k} = \frac{t_{k} - 1}{t_{k+1}} \qquad \beta_{k} = \frac{k - 1}{k + 2}$$
FISTA (Beck and Teboulle 2007)

- Recent fixes use line search to find parameters and still achieve optimal rate (modulo log factors)
- Analysis based on *estimate sequences*, using simple quadratic approximations to *f*

why "optimal?"

you can't beat the heavy ball convergence rate using only gradients and function evaluations.

$$f(x) = x_1^2 + \sum_{i=1}^{n-1} (x_i - x_{i+1})^2 + x_n^2 - 2x_1 + \mu \|x\|_2^2$$

$$\mu I \succeq \nabla^2 f(x) \succeq (4 + \mu) I$$

$$\kappa \approx 1 + \frac{4}{\mu}$$

- start at $x[0] = e_1$.
- after k steps, x[j] = 0 for j>k+1
- norm of the optimal solution on the unseen coordinates tends to $(\frac{\sqrt{\kappa}-1}{\sqrt{\kappa}+1})^{2k}$

not strongly convex ($\ell = 0$)

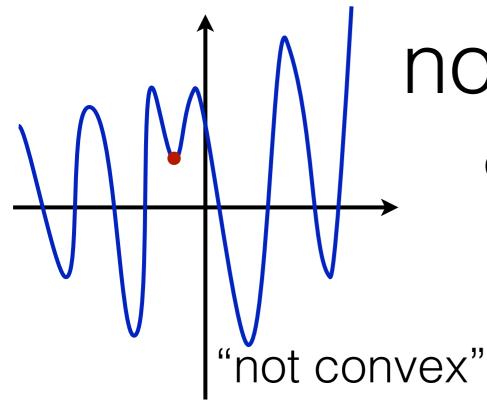
- gradient descent: $f(x[k]) f_{\star} \leq \frac{2L\|x[0] x_{\star}\|_{2}^{2}}{k + 4}$
- optimal method: $f(x[k]) f_{\star} \le \frac{4L\|x[0] x_{\star}\|_{2}^{2}}{(k+2)^{2}}$
- **Big difference!** To yield $f(x[k]) f_{\star} < \epsilon$

gradient descent

$$k \ge \frac{2L\|x[0] - x_{\star}\|_{2}^{2}}{\epsilon} - 4$$

optimal method
$$k \ge \frac{2L\|x[0] - x_{\star}\|_2}{\sqrt{\epsilon}} - 2$$

 A factor of ε^{1/2} difference. e.g. if ε=0.0001, need 100 times fewer steps.



nonconvexity

can still efficiently find a point where $\|\nabla f(x)\| \le \epsilon$ in time $O(1/\epsilon^2)$

n.b. nonconvexity really lets you model anything

$$f(x) = \sum_{i,j=1}^{d} Q_{ij} x_i^2 x_j^2 \qquad \nabla f(0) = 0 \quad \text{for all } Q$$

checking if 0 is a local minimum in NP-hard

stochastic gradient

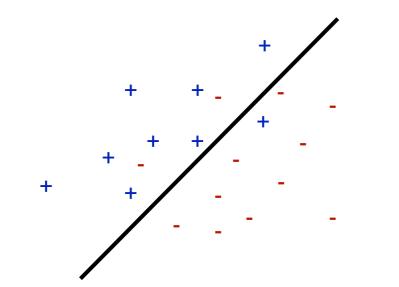
minimize $\mathbb{E}_{\xi}[f(x,\xi)]$

Stochastic Gradient Descent:

For each k, sample ξ_k and compute $x[k+1] = x[k] - \alpha_k \nabla_x f(x[k], \xi_k)$

- Robbins and Monro (1950)
- Adaptive Filtering (1960s-1990s)
- Back Propagation in Neural Networks (1980s)
- Online Learning, Stochastic Approximation (2000s)

Support Vector Machines



cancer vs other illness fraud vs normal purchase up-going vs down-going muons

minimize
$$\sum_{i=1}^{n} \max(1 - y_i x^T z_i, 0) + \lambda \|x\|_2^2$$
$$\prod_{i=1}^{n} \max(1 - y_i x^T z_i, 0) + \frac{\lambda}{n} \|x\|^2$$

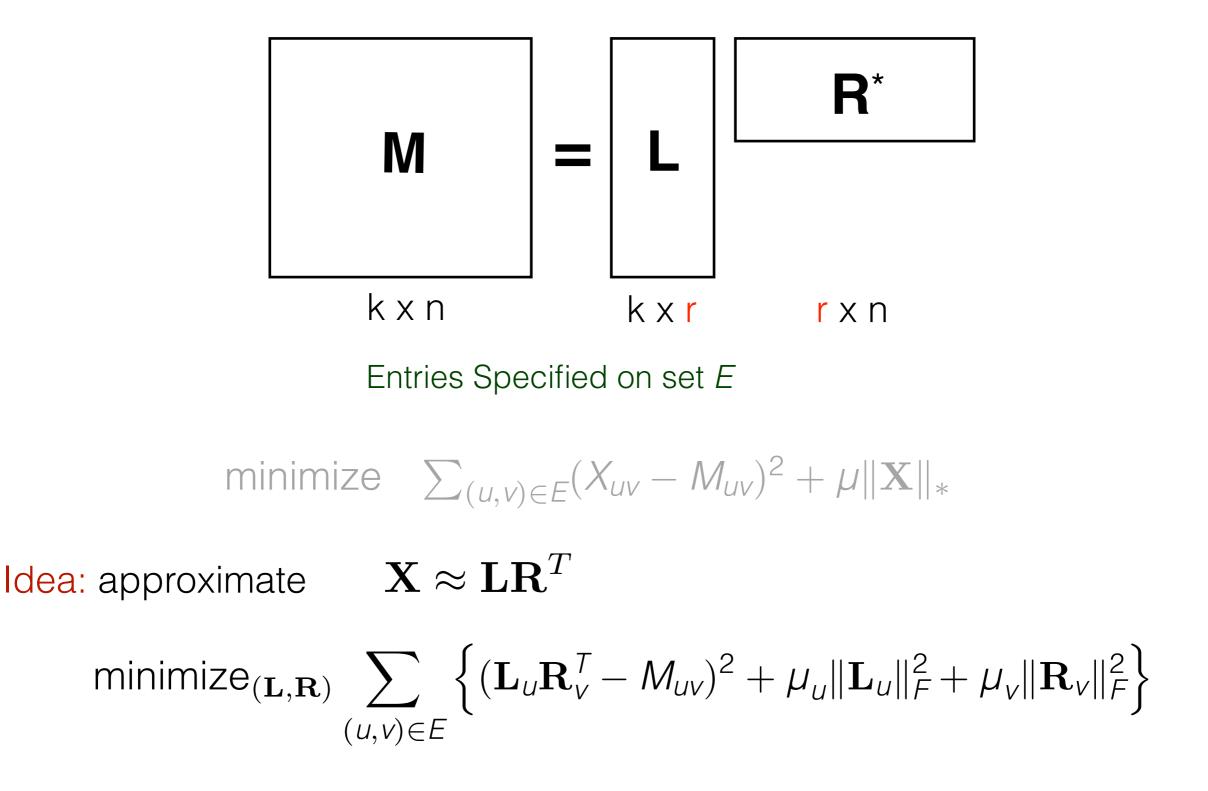
• Step 1: Pick i and compute the sign of the assignment:

$$\hat{y}_i = \operatorname{sign}(x^T Z_i)$$

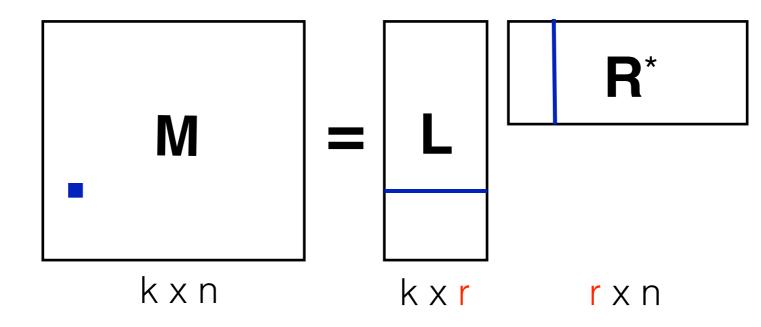
• Step 2: If $\hat{y}_i \neq y_i$,

$$x \leftarrow (1 - \frac{\alpha \lambda}{n})x + \alpha y_i Z_i$$

matrix completion



SGD code for matrix completion



$$\text{minimize}_{(\mathbf{L},\mathbf{R})} \sum_{(u,v)\in E} \left\{ (\mathbf{L}_u \mathbf{R}_v^T - M_{uv})^2 + \mu_u \|\mathbf{L}_u\|_F^2 + \mu_v \|\mathbf{R}_v\|_F^2 \right\}$$

• Step 1: Pick (u,v) and compute residual:

$$e = (\mathbf{L}_{U}\mathbf{R}_{V}^{T} - M_{UV})$$

• Step 2: Take a mixture of current model and corrected model:

$$\begin{bmatrix} \mathbf{L}_{u} \\ \mathbf{R}_{v} \end{bmatrix} \leftarrow \begin{bmatrix} (1 - \gamma \mu_{u})\mathbf{L}_{u} - \gamma e \mathbf{R}_{v} \\ (1 - \gamma \mu_{v})\mathbf{R}_{v} - \gamma e \mathbf{L}_{u} \end{bmatrix}$$

Netflix Prize

Leaderboard

Mixture of hundreds of models, including nuclear norm	Rank	Team Name No Grand Prize candidates yet	в	est Score	<u>%</u> Improver	nent	Last Submit Time
		No Progress Prize candidates yet					
	1	When Gravity and Dinosaurs Unite	1	0.8675	8.82		2008-03-01 07:03:35
	2	BellKor		0.8682	8.75	18	2008-02-28 23:40:45
	3		8	0.8708	8.47	1	2008-02-06 14:12:44
		16 2007 - RMSE = 0.0712					
	4	KorBell		0.8712	8.43		2007-10-01 23:25:23
	5			0.8720			2008-03-02 05:08:12
				0.8727	8.27		2008-03-02 08:42:29
	7			0.8729	8.25		2007-11-24 14:27:00
				0.8740	8.14		2008-02-06 12:16:40
				0.8748			2008-03-01 17:26:06
	10			0.8753			2007-10-04 04:56:45
	•		•	•		•	
	50		•	0.8897	6.49		2007-12-23 18:44:03
nuclear norm	51				6.46		2007-04-04 06:16:56
(a k a S)(D)	52	mxlg			6.45		2007-12-23 18:54:46
	53	JustWithSVD		0.8900	6.45	1	2008-02-14 16:17:54
	54	Pul-			6.45		2008-02-28 09:56:20
	55			0.8901	6.44		2008-02-29 05:53:11
		Bozo_The_Clown		0.8902	6.43		2007-09-06 17:24:48

SGD and BIG Data

minimize $\mathbb{E}_{\xi}[f(x,\xi)]$

For each k, sample ξ_k and compute $x[k+1] = x[k] - \alpha_k \nabla_x f(x[k], \xi_k)$

Ideal for big data analysis:

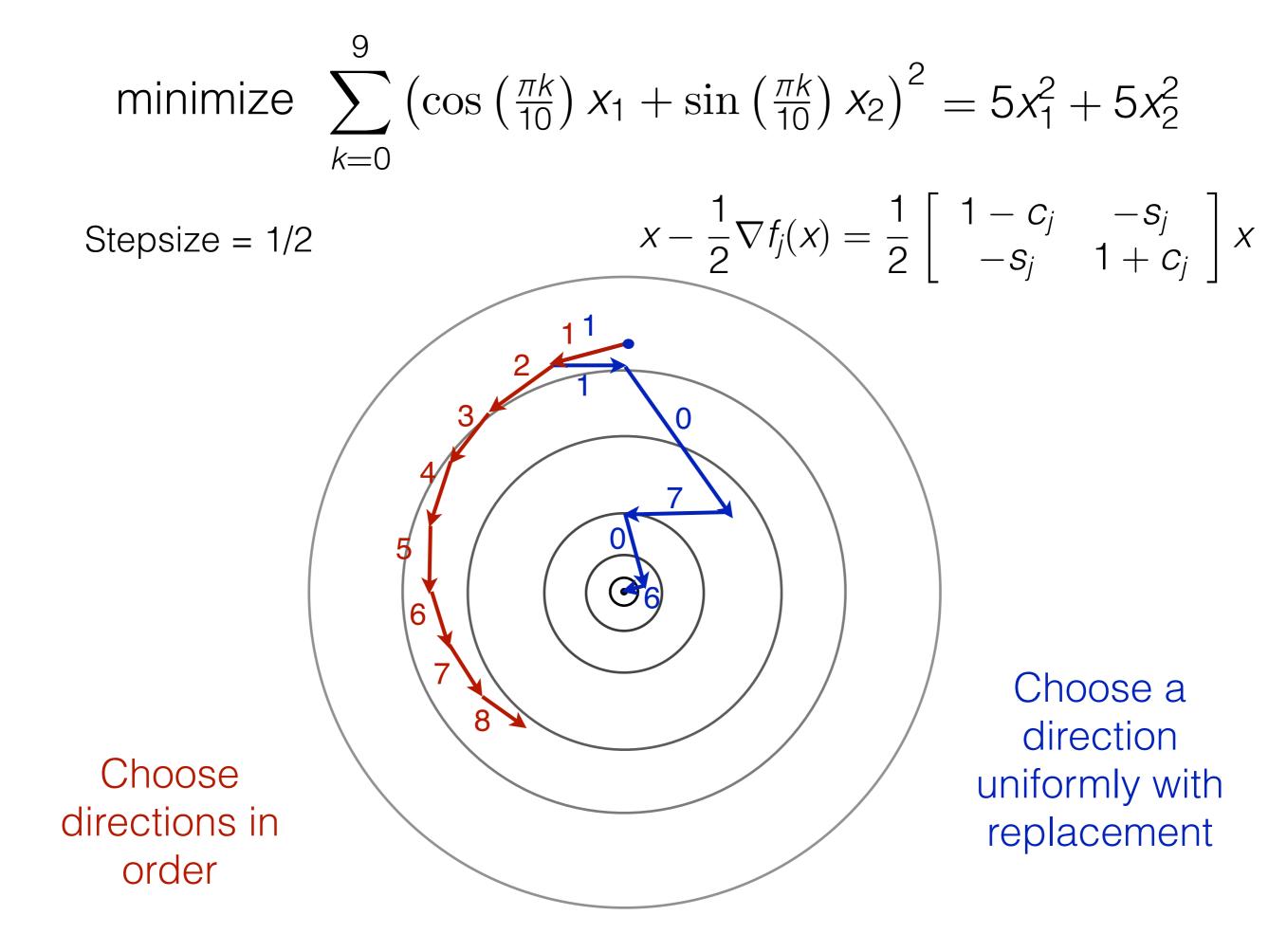


- small, predictable memory footprint
- robustness against noise in data
- rapid learning rates
- one algorithm!

Why should this work?

Example: Computing the mean minimize $\sum_{k=1}^{4} (x-k)^2$

$$\begin{aligned} x_0 &= 0 & \text{Stepsize} = 1/2k \\ x_1 &= x_0 - (x_0 - 1) = 1 \\ x_2 &= x_1 - (x_1 - 2)/2 = 1.5 \\ x_3 &= x_2 - (x_2 - 3)/3 = 2 \\ x_4 &= x_3 - (x_3 - 4)/4 = 2.5 \\ & \text{In general, if we minimize} \quad \sum_{k=1}^N (x - z_k)^2 \\ & \text{SGD returns:} \quad x_N = \frac{1}{N} \sum_{k=1}^N z_k \end{aligned}$$



convergence of sgd minimize f(x)

Assume f is strongly convex with parameter l and has Lipschitz gradients with parameter L

Assume at each iteration we sample G(x), an unbiased estimate of $\nabla f(x)$, independent of x and the past iterates

Assume $||G(x)|| \le M$ almost surely.

$$x[k+1] = x[k] - \alpha_k G_k(x[k])$$

$$\begin{aligned} \|x[k+1] - x_{\star}\|_{2}^{2} \\ &= \|x[k] - \alpha_{k}G_{k}(x[k]) - x_{\star}\|^{2} \\ &= \|x[k] - x_{\star}\|_{2}^{2} - 2\alpha_{k}(x[k] - x^{\star})^{T}G_{k}(x[k]) + \alpha_{k}^{2}\|G_{k}(x[k])\|^{2}. \end{aligned}$$

Define $a_k = \mathbb{E} \left[\|x[k] - x_{\star}\|_2^2 \right]$

 $a_{k+1} \leq a_k - 2\alpha_k \mathbb{E}[(x[k] - x^*)^T G_k(x[k])] + \alpha_k^2 M^2.$

By iterating expectation:

$$\mathbb{E}[(x[k] - x_{\star})^T G_k(x[k])] = \mathbb{E}_{G_{[k-1]}} \mathbb{E}_{G_k}[(x[k] - x_{\star})^T G_k(x[k])|G_{[k-1]}]$$
$$= \mathbb{E}[(x[k] - x_{\star})^T \nabla f(x[k])]$$

By strong convexity: $\nabla f(x[k])^T(x[k] - x_\star) \ge f(x[k]) - f(x_\star) + \frac{\ell}{2} ||x_k - x^*||^2 \ge \ell ||x_k - x^*||^2.$

$$a_{k+1} \leq (1 - 2\ell\alpha_k)a_k + \alpha_k^2 M^2$$

$$a_{k+1} \leq (1 - 2\ell\alpha_k)a_k + \alpha_k^2 M^2$$

Large steps:
$$\theta > \frac{1}{2\ell}$$
, $\alpha_k = \frac{\theta}{k}$
$$\mathbb{E}[\|x[k] - x_\star\|_2^2] \le \frac{1}{k} \cdot \max\left\{\frac{\theta^2 M^2}{2\ell\theta - 1}, \|x[0] - x_\star\|^2\right\}$$

Small steps:
$$\alpha < \frac{1}{2\ell}$$
, constant stepsize $\mathbb{E}[\|x[k] - x_{\star}\|_{2}^{2}] \leq (1 - 2\ell\alpha)^{k} \left(\|x[0] - x_{\star}\|^{2} - \frac{\alpha M^{2}}{2\ell}\right) + \frac{\alpha M^{2}}{2\ell}$ Achieves 1/k rate if run in *epochs*

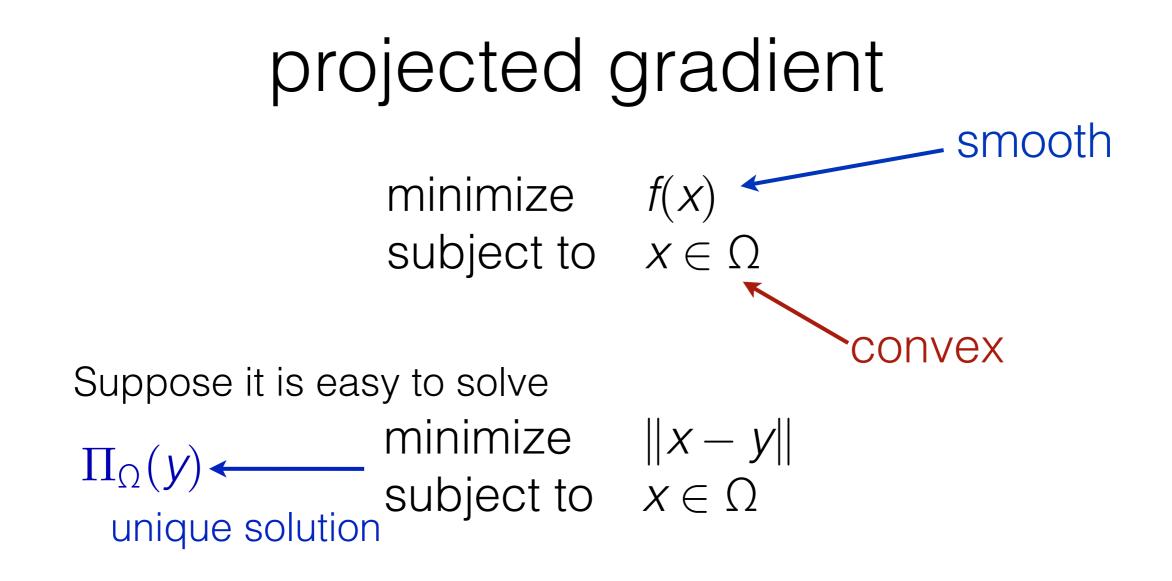
Achieves 1/k rate if run in *epochs* of diminishing stepsize

minimize_{$$x \in \mathbb{R}^d$$} $f(x) = \sum_{j=1}^N f_j(x)$

Algorithm	Time per iteration	Error after T iterations	Error after N items
Newton	O(d²N+d³)	$C_l^{2^T}$	$C_I{}^2$
Gradient	O(dN)	C_G^T	C_G
SGD	O(d) (or constant)	$\frac{C_S}{T}$	$\frac{C_S}{N}$

extensions

- non-smooth, non-strongly convex $(1/\sqrt{k})$
- non-convex (converges asymptotically)
- stochastic coordinate descent (special decomposition of *f*)
- parallelization



projected gradient method:

$$x[k+1] \leftarrow \Pi_{\Omega} \left(x[k] + \alpha_k v[k] \right)$$

$$x[k+1] \leftarrow \Pi_{\Omega} \left(x[k] + \alpha_k v[k] \right)$$

Key Lemma:
$$\|\Pi_{\Omega}(x) - \Pi_{\Omega}(z)\| \le \|x - z\|$$

Assume minimizer of $f \in \Omega$

Assume *f* is strongly convex

$$\begin{aligned} \|x[k+1] - x_{\star}\| &= \|\Pi_{\Omega}(x[k] - \alpha \nabla f(x([k])) - \Pi_{\Omega}(x_{\star})\| \\ &\leq \|x[k] - \alpha \nabla f(x[k]) - x_{\star}\| \\ &= \|\psi(x[k]) - \psi(x_{\star})\| \\ &\leq \beta \|x[k] - x_{\star}\| \\ &\leq \beta \|x[k] - x_{\star}\| \\ &\vdots \\ &\leq \beta^{k+1} \|x[0] - x_{\star}\| \end{aligned} \qquad \text{ linear rate}$$

minimize f(x) + P(x)

$$f(x) + P(x) \approx f(x[k]) + \nabla f(x[k])^{T}(x - x[k]) + \frac{1}{2\alpha} ||x - x[k]||^{2} + P(x)$$

Define
$$prox_P(x) = \arg\min_{z} \frac{1}{2} ||x - z||^2 + P(z)$$

Solving the approximation yields

$$x[k+1] = \operatorname{prox}_{\alpha_k P}(x[k] - \alpha_k \nabla f(x[k]))$$

$$proximal mapping$$

$$prox_{P}(x) = \arg \min_{Z} \frac{1}{2} ||x - z||^{2} + P(z)$$

$$P(x) = \begin{cases} 0 & x \in \Omega \\ \infty & x \notin \Omega \end{cases}$$

$$P(x) = \mu ||x||_{1}$$

$$prox_{P}(x) = \Pi_{\Omega}(x)$$

$$prox_{P}(x)_{i} = \begin{cases} x_{i} + \mu & x_{i} < -\mu \\ 0 & -\mu \leq x_{i} \leq \mu \\ x_{i} - \mu & x_{i} > \mu \end{cases}$$

P(x)

minimize f(x) + P(x)

$$f(x) + P(x) \approx f(x[k]) + \nabla f(x[k])^{T}(x - x[k]) + \frac{1}{2\alpha} ||x - x[k]||^{2} + P(x)$$

Define
$$\operatorname{prox}_{P}(x) = \arg\min_{z} \frac{1}{2} ||x - z||^{2} + P(z)$$

Solving the approximation yields

$$x[k+1] = \operatorname{prox}_{\alpha_k P}(x[k] - \alpha_k \nabla f(x[k]))$$

Key Lemma: $\| \operatorname{prox}_{P}(x) - \operatorname{prox}_{P}(y) \| \le \|x - y\|$

- immediately implies earlier analysis works for proximal gradient.
- projected gradient is a special case
- inherits rates of convergence from f (i.e., P=0)

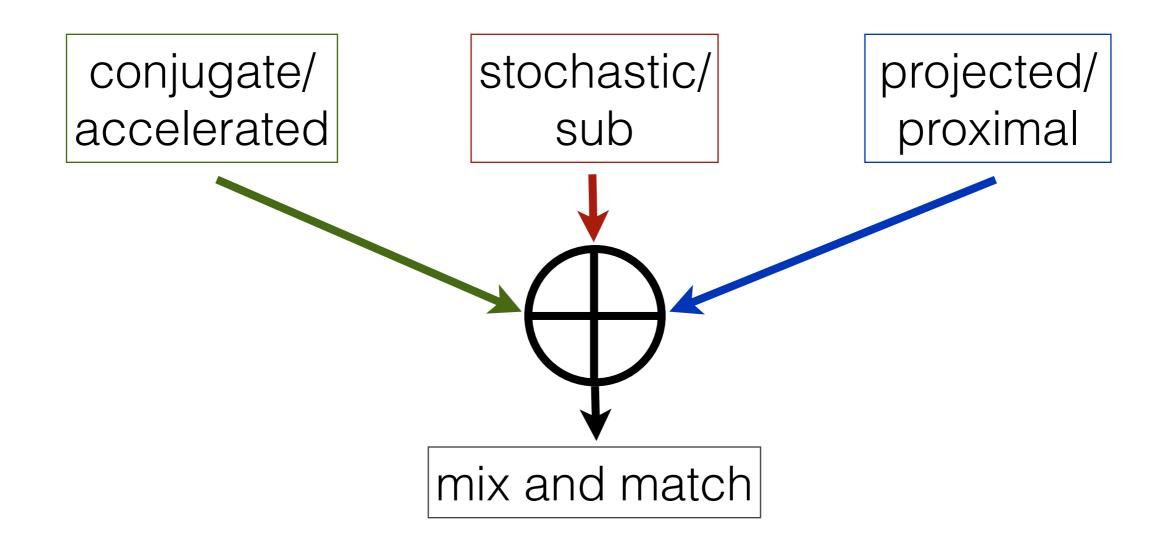
More variants

• mirror descent: use a general distance $f(x) \approx f(x_0) + \langle \nabla f(x_0), x - x_0 \rangle + \frac{1}{2\alpha} \mathcal{D}(x, x_0)$

• ADMM: combine multiple prox operators for complicated constraints.

 $x[k+1] \leftarrow x[k] + \alpha_k v[k]$

gradient descent



Everything here combines, and you get the expected rates out.