Optimization for Machine Learning

(Lecture 2)

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MPI-IS Tübingen
Machine Learning Summer School, June 2017



Course materials

- My website (Teaching)
- Some references:
 - *Introductory lectures on convex optimization* Nesterov
 - *Convex optimization* Boyd & Vandenberghe
 - *Nonlinear programming* Bertsekas
 - Convex Analysis Rockafellar
 - Fundamentals of convex analysis Urruty, Lemaréchal
 - *Lectures on modern convex optimization* − Nemirovski
 - Optimization for Machine Learning Sra, Nowozin, Wright
 - NIPS 2016 Optimization Tutorial Bach, Sra
- Some related courses:
 - EE227A, Spring 2013, (Sra, UC Berkeley)
 - 10-801, Spring 2014 (Sra, CMU)
 - EE364a,b (Boyd, Stanford)
 - EE236b,c (Vandenberghe, UCLA)
- Venues: NIPS, ICML, UAI, AISTATS, SIOPT, Math. Prog.

Lecture Plan

- Introduction
- Recap of convexity, sets, functions
- Recap of duality, optimality, problems
- First-order optimization algorithms and techniques
- Large-scale optimization (SGD and friends)
- Directions in non-convex optimization

ML Optimization Problems

- ▶ **Data**: *n* observations $(x_i, y_i)_{i=1}^n \in \mathcal{X} \times \mathcal{Y}$
- ▶ **Prediction function**: $h(x, \theta) \in \mathbb{R}$ parameterized by $\theta \in \mathbb{R}^d$
- ► Motivating examples:
 - Linear predictions: $h(x, \theta) = \theta^{\top} \Phi(x)$ using features $\Phi(x)$
 - Neural networks: $h(x, \theta) = \theta_m^{\top} \sigma(\theta_{m-1}^{\top} \sigma(\dots \theta_2^{\top} \sigma(\theta_1^{\top} x))$
- \triangleright Estimating θ parameters is an optimization problem

$$\min_{\theta \in \mathbb{R}^d} \quad \frac{1}{n} \sum_{i=1}^n \ell(y_i, h(x_i, \theta)) + \lambda \Omega(\theta) = \frac{1}{n} \sum_{i=1}^n f_i(\theta)$$

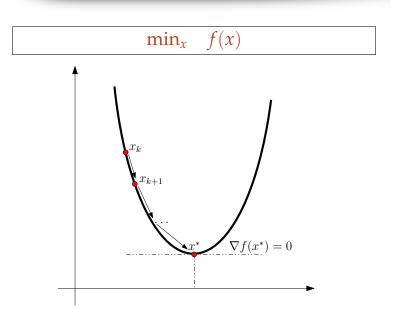
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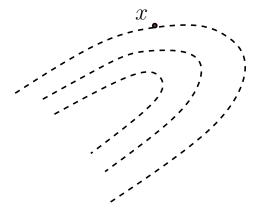
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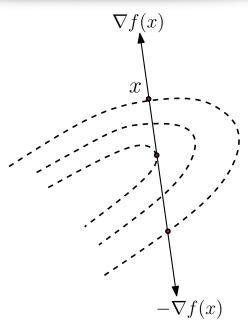
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Regression:
$$y \in \mathbb{R}$$
; **Quadratic loss**: $\ell(y, h(x, \theta)) = \frac{1}{2}(y - h(x, \theta))^2$ **Classf.**: $y \in \{\pm 1\}$; **Logistic loss**: $\ell(y, h(x, \theta)) = \log(1 + \exp(-yh(x, \theta)))$

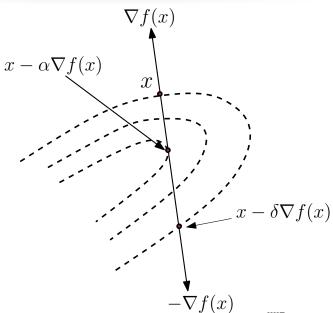
$$\min_{x} f(x)$$

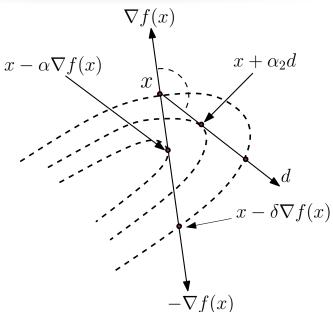












Iterative Algorithm

- 1 Start with some guess x^0 ;
- 2 For each k = 0, 1, ...
 - "Guess" α_k and d^k
 - $\mathbf{x}^{k+1} \leftarrow \mathbf{x}^k + \alpha_k d^k$
 - Check when to stop (e.g., if $\nabla f(x^{k+1}) \approx 0$)

$$x^{k+1} = x^k + \alpha_k d^k, \quad k = 0, 1, \dots$$

■ **stepsize** $\alpha_k \ge 0$, usually ensures $f(x^{k+1}) < f(x^k)$

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$$\langle \nabla f(x^k), d^k \rangle < 0$$

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Numerous ways to select α_k and d^k

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Numerous ways to select α_k and d^k

Usually (batch) methods seek monotonic descent

$$f(x^{k+1}) < f(x^k)$$

Gradient methods – direction

$$x^{k+1} = x^k + \alpha_k d^k, \quad k = 0, 1, \dots$$

- ightharpoonup Different choices of direction d^k
- Scaled gradient: $d^k = -D^k \nabla f(x^k)$, $D^k > 0$
- Newton's method: $(D^k = [\nabla^2 f(x^k)]^{-1})$
- Quasi-Newton: $D^k \approx [\nabla^2 f(x^k)]^{-1}$
- Steepest descent: $D^k = I$
- $ilde{D}$ Diagonally scaled: D^k diagonal with $D^k_{ii} pprox \left(rac{\partial^2 f(x^k)}{(\partial x_i)^2}
 ight)^{-1}$
- Discretized Newton: $D^k = [H(x^k)]^{-1}$, H via finite-diff.

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- **Diagonally scaled:** D^k diagonal with $D^k_{ii} \approx \left(\frac{\partial^2 f(x^k)}{(\partial x_i)^2}\right)^{-1}$
- Discretized Newton: $D^k = [H(x^k)]^{-1}$, H via finite-diff.
- o ...

Exercise: Verify that $\langle \nabla f(x^k), d^k \rangle < 0$ for above choices

Gradient methods – stepsize

Exact: $\alpha_k := \underset{\alpha>0}{\operatorname{argmin}} f(x^k + \alpha d^k)$

Gradient methods – stepsize

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- ► Limited min: $\alpha_k = \underset{0 < \alpha < s}{\operatorname{argmin}} f(x^k + \alpha d^k)$

Gradient methods – stepsize

- **Exact:** $\alpha_k := \underset{\alpha>0}{\operatorname{argmin}} f(x^k + \alpha d^k)$
- ► Limited min: $\alpha_k = \underset{0 \le \alpha \le s}{\operatorname{argmin}} f(x^k + \alpha d^k)$
- ► **Armijo-rule**. Given **fixed** scalars, s, β , σ with $0 < \beta < 1$ and $0 < \sigma < 1$ (chosen experimentally). Set

$$\alpha_k = \beta^{m_k} s$$
,

where we **try** $\beta^m s$ for $m = 0, 1, \dots$ until **sufficient descent**

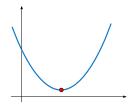
$$f(x^k) - f(x + \beta^m s d^k) \ge -\sigma \beta^m s \langle \nabla f(x^k), d^k \rangle$$

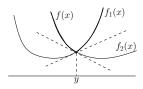
- ▶ Constant: $\alpha_k = 1/L$ (for suitable value of L)
- ▶ Diminishing: $\alpha_k \to 0$ but $\sum_k \alpha_k = \infty$.

Convergence

Assumption: Lipschitz continuous gradient; denoted $f \in C^1_L$

$$\|\nabla f(x) - \nabla f(y)\|_2 \le L\|x - y\|_2$$

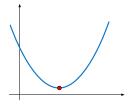


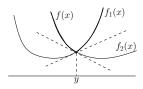


Convergence

Assumption: Lipschitz continuous gradient; denoted $f \in C_L^1$

$$\|\nabla f(x) - \nabla f(y)\|_2 \le L\|x - y\|_2$$





- Gradient vectors of closeby points are close to each other
- ♣ Objective function has "bounded curvature"
- Speed at which gradient varies is bounded

Convergence

Assumption: Lipschitz continuous gradient; denoted $f \in C^1_L$

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Lemma (Descent). Let $f \in C_L^1$. Then,

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

Theorem. Let $f \in C_L^1$ be convex, and $\{x^k\}$ is sequence generated as above, with $\alpha_k = 1/L$. Then, $f(x^{k+1}) - f(x^*) = O(1/k)$.

Remark: $f \in C_L^1$ is "good" for nonconvex too, except for $f - f^*$.

Strong convexity (faster convergence)

Assumption: Strong convexity; denote
$$f \in S^1_{L,\mu}$$
 $f(x) \ge f(y) + \langle \nabla f(y), x - y \rangle + \frac{\mu}{2} ||x - y||_2^2$

▶ A twice diff. $f : \mathbb{R}^d \to \mathbb{R}$ is convex if and only if

$$\forall x \in \mathbb{R}^d$$
, eigenvalues $\left[\nabla^2(x)\right] \geqslant 0$.

▶ A twice diff. $f: \mathbb{R}^d \to \mathbb{R}$ is μ -strongly convex if and only if

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Condition number: $\kappa := \frac{L}{\mu} \ge 1$ influences convergence speed.

Setting
$$\alpha_k = \frac{2}{\mu + L}$$
 yields linear rate $(\mu > 0)$ for gradient descent. That is, $f(x^k) - f(x^*) = O(e^{-k})$.

Strong convexity – linear rate

Theorem. If $f \in S^1_{L,\mu'}$, $0 < \alpha < 2/(L + \mu)$, then the gradient method generates a sequence $\{x^k\}$ that satisfies

$$||x^k - x^*||_2^2 \le \left(1 - \frac{2\alpha\mu L}{\mu + L}\right)^k ||x^0 - x^*||_2.$$

Moreover, if $\alpha = 2/(L + \mu)$ then

$$f(x^k) - f^* \le \frac{L}{2} \left(\frac{\kappa - 1}{\kappa + 1} \right)^{2k} ||x^0 - x^*||_2^2,$$

where $\kappa = L/\mu$ is the condition number.

Gradient methods – lower bounds

$$x^{k+1} = x^k - \alpha_k \nabla f(x^k)$$

Theorem. Lower bound I (Nesterov) For any $x^0 \in \mathbb{R}^n$, and $1 \le k \le \frac{1}{2}(n-1)$, there is a smooth f, s.t.

$$f(x^k) - f(x^*) \ge \frac{3L||x^0 - x^*||_2^2}{32(k+1)^2}$$

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Theorem. Lower bound II (Nesterov). For class of smooth, strongly convex, i.e., $S_{L,\mu}^{\infty}$ ($\mu > 0$, $\kappa > 1$)

$$f(x^k) - f(x^*) \ge \frac{\mu}{2} \left(\frac{\sqrt{\kappa} - 1}{\sqrt{\kappa} + 1} \right)^{2k} \|x^0 - x^*\|_2^2.$$

Faster methods*

Optimal gradient methods

♠ We saw efficiency estimates for the gradient method:

$$\begin{split} f \in C_L^1: & f(x^k) - f^* \leq \frac{2L\|x^0 - x^*\|_2^2}{k+4} \\ f \in S_{L,\mu}^1: & f(x^k) - f^* \leq \frac{L}{2} \left(\frac{L-\mu}{L+\mu}\right)^{2k} \|x^0 - x^*\|_2^2. \end{split}$$

Optimal gradient methods

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$$f \in S_{L,\mu}^1: \qquad f(x^k) - f^* \le \frac{L}{2} \left(\frac{L-\mu}{L+\mu}\right)^{2k} \|x^0 - x^*\|_2^2.$$

♠ We also saw lower complexity bounds

$$f \in C_L^1: \qquad f(x^k) - f(x^*) \ge \frac{3L\|x^0 - x^*\|_2^2}{32(k+1)^2}$$
$$fS_{L,\mu}^{\infty}: \qquad f(x^k) - f(x^*) \ge \frac{\mu}{2} \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^{2k} \|x^0 - x^*\|_2^2.$$

Optimal gradient methods

♠ Subgradient method upper and lower bounds

$$f(x^k) - f(x^*) \le O(1/\sqrt{k})$$

 $f(x^k) - f(x^*) \ge \frac{LD}{2(1+\sqrt{k+1})}.$

♠ Composite objective problems: proximal gradient gives same bounds as gradient methods.

Gradient with "momentum"

Polyak's method (aka heavy-ball) for $f \in S^1_{L,\mu}$

$$x^{k+1} = x^k - \alpha_k \nabla f(x^k) + \beta_k (x^k - x^{k-1})$$

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► Converges (locally, i.e., for $||x^0 - x^*||_2 \le \epsilon$) as

$$||x^{k} - x^{*}||_{2}^{2} \le \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^{2k} ||x^{0} - x^{*}||_{2}^{2},$$

for
$$\alpha_k = \frac{4}{(\sqrt{L} + \sqrt{\mu})^2}$$
 and $\beta_k = \left(\frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}\right)^2$

Nesterov's optimal gradient method

$$\min_{x} f(x)$$
, where $S_{L,\mu}^{1}$ with $\mu \geq 0$

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- 1. Choose $x^0 \in \mathbb{R}^n$, $\alpha_0 \in (0,1)$
- 2. Let $y^0 \leftarrow x^0$; set $q = \mu/L$

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- 3. k-th iteration (k > 0):
 - a). Compute intermediate update

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- c). Set $\beta_k = \alpha_k (1 \alpha_k)/(\alpha_k^2 + \alpha_{k+1})$
- d). Update solution estimate

$$y^{k+1} = x^{k+1} + \beta_k (x^{k+1} - x^k)$$

Optimal gradient method – rate

Theorem. Let $\{x^k\}$ be sequence generated by above algorithm. If $\alpha_0 \ge \sqrt{\mu/L}$, then

$$f(x^k) - f(x^*) \le c_1 \min \left\{ \left(1 - \sqrt{\frac{\mu}{L}} \right)^k, \frac{4L}{(2\sqrt{L} + c_2 k)^2} \right\},$$

where constants c_1 , c_2 depend on α_0 , L, μ .

If $\mu > 0$, select $\alpha_0 = \sqrt{\mu/L}$. The two main steps get simplified:

1. Set
$$\beta_k = \alpha_k (1 - \alpha_k) / (\alpha_k^2 + \alpha_{k+1})$$

2.
$$y^{k+1} = x^{k+1} + \beta_k(x^{k+1} - x^k)$$

$$\alpha_k = \sqrt{\frac{\mu}{L}} \qquad \beta_k = \frac{\sqrt{L} - \sqrt{\mu}}{\sqrt{L} + \sqrt{\mu}}, \qquad k \ge 0.$$

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Notice similarity to Polyak's method!

Subgradient methods

Subgradient method

$$x^{k+1} = x^k - \alpha_k g^k$$

where $g^k \in \partial f(x^k)$ is **any** subgradient

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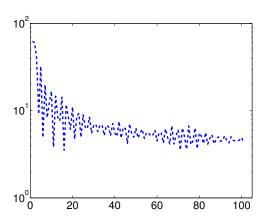
where $g^k \in \partial f(x^k)$ is **any** subgradient

Stepsize $\alpha_k > 0$ must be chosen

- ► Method generates sequence $\{x^k\}_{k>0}$
- ▶ Does this sequence converge to an optimal solution x^* ?
- ► If yes, then how fast?
- ▶ What if have constraints: $x \in \mathcal{X}$?

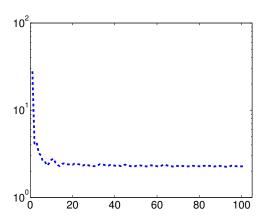
Example: Lasso problem

$$\min_{x^{k+1}} \frac{1}{2} ||Ax - b||_{2}^{2} + \lambda ||x||_{1}$$
$$x^{k+1} = x^{k} - \alpha_{k} (A^{T} (Ax^{k} - b) + \lambda \operatorname{sgn}(x^{k}))$$



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$$\min \quad \frac{1}{2} ||Ax - b||_2^2 + \lambda ||x||_1$$
$$x^{k+1} = x^k - \alpha_k (A^T (Ax^k - b) + \lambda \operatorname{sgn}(x^k))$$



(More careful implementation)

Subgradient method – stepsizes

- ▶ Constant Set $\alpha_k = \alpha > 0$, for $k \ge 0$
- ► Scaled constant $\alpha_k = \alpha/\|g^k\|_2$ ($\|x^{k+1} x^k\|_2 = \alpha$)

Subgradient method – stepsizes

- ▶ Constant Set $\alpha_k = \alpha > 0$, for $k \ge 0$
- ► Scaled constant $\alpha_k = \alpha/\|g^k\|_2$ ($\|x^{k+1} x^k\|_2 = \alpha$)
- ► Square summable but not summable

$$\sum\nolimits_k \alpha_k^2 < \infty, \qquad \sum\nolimits_k \alpha_k = \infty$$

▶ Diminishing scalar

$$\lim_{k} \alpha_k = 0, \qquad \sum_{k} \alpha_k = \infty$$

► Adaptive stepsizes (not covered)

Not a descent method! Work with best f^k so far: $f^k_{\min} := \min_{0 \le i \le k} f^i$

Exercise

Support vector machines

- ▶ Let $\mathcal{D} := \{(x_i, y_i) \mid x_i \in \mathbb{R}^n, y_i \in \{\pm 1\}\}$
- ▶ We wish to find $w \in \mathbb{R}^n$ and $b \in \mathbb{R}$ such that

$$\min_{w,b} \quad \frac{1}{2} \|w\|_2^2 + C \sum_{i=1}^m \max[0, 1 - y_i(w^T x_i + b)]$$

- ▶ Derive and implement a subgradient method
- ▶ Plot evolution of objective function
- ightharpoonup Experiment with different values of C > 0
- ▶ Plot and keep track of $f_{\min}^k := \min_{0 \le t \le k} f(x^t)$

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Can we do better in general?

Theorem. (Nesterov.) Let $\mathcal{B} = \{x \mid ||x - x^0||_2 \leq D\}$. Assume, $x^* \in \mathcal{B}$. There exists a convex function f in $C_L^0(\mathcal{B})$ (with L > 0), such that for $0 \leq k \leq n-1$, the lower-bound

$$f(x^k) - f(x^*) \ge \frac{LD}{2(1+\sqrt{k+1})},$$

holds for any algorithm that generates x^k by linearly combining the previous iterates and subgradients.

Exercise: So design problems where we can do better!

Constrained problems

Constrained optimization

$$\min \quad f(x) \qquad \text{s.t.} \quad x \in \mathcal{X}$$

Don't want to be as slow as the subgradient method

Projected subgradient method

$$x^{k+1} = P_{\mathcal{X}}(x^k - \alpha_k g^k)$$
 where $g^k \in \partial f(x^k)$ is any subgradient

► **Projection:** closest feasible point

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- ▶ Questions we may have:
 - Does it converge?
 - For which stepsizes?
 - How fast?

$$\min \quad \frac{1}{2} ||Ax - b||_2^2 + \lambda ||x||_1$$

s.t. $x \in \mathcal{X}$

► Nonnegativity $x \ge 0$ $P_{\mathcal{X}}(z) = [z]_+$ Update step: $x^{k+1} = [x^k - \alpha_k(A^T(Ax^k - b) + \lambda \operatorname{sgn}(x^k))]_+$

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▶ Linear constraints Ax = b ($A \in \mathbb{R}^{n \times m}$ has rank n)

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▶ Simplex $x^{\top}1 = 1$ and $x \ge 0$ more complex but doable in O(n), similarly ℓ_1 -norm ball

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 - low-memory
 - large-scale versions possible

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Mirror Descent

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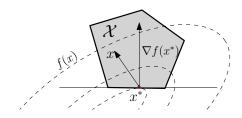
Mirror Descent

- ▶ Improvements using more information (heavy-ball, filtered subgradient, ...)
- ▶ Don't forget the dual
 - may be more amenable to optimization
 - duality gap?

What we did not cover

- ♠ Adaptive stepsize tricks
- ♠ Space dilation methods, quasi-Newton style subgrads
- Barrier subgradient method
- ♠ Sparse subgradient method
- Ellipsoid method, center of gravity, etc. as subgradient methods

$$\min \quad f(x) \quad \text{s.t. } x \in \mathcal{X}$$
$$\langle \nabla f(x^*), \ x - x^* \rangle \ge 0, \qquad \forall x \in \mathcal{X}.$$



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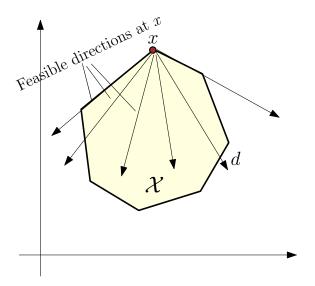
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Cone of feasible directions



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Frank-Wolfe (Conditional gradient) method

- **▲** Let $z^k \in \operatorname{argmin}_{x \in \mathcal{X}} \langle \nabla f(x^k), x x^k \rangle$
- ▲ Use different methods to select α_k

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- **▲** Let $z^k \in \operatorname{argmin}_{x \in \mathcal{X}} \langle \nabla f(x^k), x x^k \rangle$
- ▲ Use different methods to select α_k
- \spadesuit Practical when solving *linear* problem over \mathcal{X} easy
- ♠ Very popular in machine learning over recent years
- ♠ Refinements, several variants (including nonconvex)

Frequently ML problems take the regularized form

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$$f(x) := \ell(x) + r(x)$$

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Lasso, L1-LS, compressed sensing

Example: $\ell(x)$: Logistic loss, and $r(x) = \lambda ||x||_1$

L1-Logistic regression, sparse LR

Composite objective minimization

minimize
$$f(x) := \ell(x) + r(x)$$

subgradient:
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but: *f* is *smooth* plus *nonsmooth*

we should **exploit**: smoothness of ℓ for better method!

Proximal Gradient Method

$$\min \quad f(x) \quad x \in \mathcal{X}$$

Projected (sub)gradient

$$x \leftarrow P_{\mathcal{X}}(x - \alpha \nabla f(x))$$

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$$min f(x) + h(x)$$

Proximal gradient

$$x \leftarrow \operatorname{prox}_{\alpha h}(x - \alpha \nabla f(x))$$

 $prox_{\alpha h}$ denotes proximity operator for h

Why? If we can compute $prox_h(x)$ easily, prox-grad converges as fast gradient methods for smooth problems!

Proximity operator

Projection

$$P_{\mathcal{X}}(y) := \underset{x \in \mathbb{R}^n}{\operatorname{argmin}} \quad \frac{1}{2} \|x - y\|_2^2 + \mathbb{1}_{\mathcal{X}}(x)$$

Proximity operator

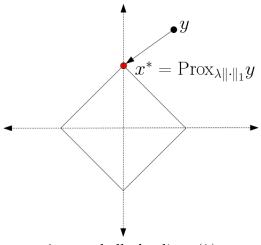
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Proximity: Replace $\mathbb{1}_{\mathcal{X}}$ by a closed convex function

$$\operatorname{prox}_{r}(y) := \underset{x \in \mathbb{R}^{n}}{\operatorname{argmin}} \quad \frac{1}{2} ||x - y||_{2}^{2} + r(x)$$

Proximity operator



 ℓ_1 -norm ball of radius $\rho(\lambda)$

Proximity operators

Exercise: Let $r(x) = ||x||_1$. Solve $\operatorname{prox}_{\lambda r}(y)$.

$$\min_{x \in \mathbb{R}^n} \quad \frac{1}{2} ||x - y||_2^2 + \lambda ||x||_1.$$

Hint 1: The above problem decomposes into n independent subproblems of the form

$$\min_{x \in \mathbb{R}} \quad \frac{1}{2}(x - y)^2 + \lambda |x|.$$

Hint 2: Consider the two cases: either x = 0 or $x \neq 0$ **Exercise:** Moreau decomposition $y = \operatorname{prox}_h y + \operatorname{prox}_{h^*} y$ (notice analogy to $V = S + S^{\perp}$ in linear algebra)

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$$x^* = \text{prox}_{\alpha h}(x^* - \alpha \nabla f(x^*)), \forall \alpha > 0$$

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How to cook-up prox-grad?

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Above fixed-point eqn suggests iteration

$$x_{k+1} = \operatorname{prox}_{\alpha_k h}(x_k - \alpha_k \nabla f(x_k))$$

Convergence*

Proximal-gradient works, why?

$$x_{k+1} = \operatorname{prox}_{\alpha_k h}(x_k - \alpha_k \nabla f(x_k))$$

 $x_{k+1} = x_k - \alpha_k G_{\alpha_k}(x_k).$

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Gradient mapping: the "gradient-like object"

$$G_{\alpha}(x) = \frac{1}{\alpha}(x - P_{\alpha h}(x - \alpha \nabla f(x)))$$

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Gradient mapping: the "gradient-like object"

$$G_{\alpha}(x) = \frac{1}{\alpha}(x - P_{\alpha h}(x - \alpha \nabla f(x)))$$

- ▶ Our lemma shows: $G_{\alpha}(x) = 0$ if and only if x is optimal
- ► So G_{α} analogous to ∇f
- ▶ If *x* locally optimal, then $G_{\alpha}(x) = 0$ (nonconvex *f*)

Assumption: Lipschitz continuous gradient; denoted $f \in C^1_L$

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- Objective function has "bounded curvature"
- Speed at which gradient varies is bounded

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Lemma (Descent). Let $f \in C_I^1$. Then,

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

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For convex f, compare with

$$f(y) \ge f(x) + \langle \nabla f(x), y - x \rangle.$$

Proof. Since $f \in C_L^1$, by Taylor's theorem, for the vector $z_t = x + t(y - x)$ we have

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$$|f(y) - f(x) - \langle \nabla f(x), y - x \rangle| = \left| \int_0^1 \langle \nabla f(z_t) - \nabla f(x), y - x \rangle dt \right|$$

$$\leq \int_0^1 |\langle \nabla f(z_t) - \nabla f(x), y - x \rangle| dt$$

Proof. Since $f \in C_L^1$, by Taylor's theorem, for the vector $z_t = x + t(y - x)$ we have

$$f(y) = f(x) + \int_0^1 \langle \nabla f(z_t), y - x \rangle dt.$$

$$\begin{array}{lcl} f(y)-f(x)-\langle \nabla f(x),\,y-x\rangle &=& \int_0^1 \langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle dt \\ |f(y)-f(x)-\langle \nabla f(x),\,y-x\rangle| &=& \left|\int_0^1 \langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle dt\right| \\ &\leq& \int_0^1 |\langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle| dt \\ &\leq& \int_0^1 \|\nabla f(z_t)-\nabla f(x)\|_2 \cdot \|y-x\|_2 dt \end{array}$$

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Add and subtract $\langle \nabla f(x), y - x \rangle$ on rhs we have

$$\begin{array}{lcl} f(y)-f(x)-\langle \nabla f(x),\,y-x\rangle &=& \int_0^1 \langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle dt \\ |f(y)-f(x)-\langle \nabla f(x),\,y-x\rangle| &=& \left|\int_0^1 \langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle dt\right| \\ &\leq& \int_0^1 |\langle \nabla f(z_t)-\nabla f(x),\,y-x\rangle| dt \\ &\leq& \int_0^1 \|\nabla f(z_t)-\nabla f(x)\|_2 \cdot \|y-x\|_2 dt \\ &\leq& L \int_0^1 t \|x-y\|_2^2 dt \\ &=& \frac{L}{2} \|x-y\|_2^2. \end{array}$$

Bounds f(y) around x with quadratic functions

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

Let
$$y = x - \alpha G_{\alpha}(x)$$
, then

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

Let $y = x - \alpha G_{\alpha}(x)$, then

$$f(y) \le f(x) - \alpha \langle \nabla f(x), G_{\alpha}(x) \rangle + \frac{\alpha^2 L}{2} \|G_{\alpha}(x)\|_2^2.$$

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

Let $y = x - \alpha G_{\alpha}(x)$, then

$$f(y) \le f(x) - \alpha \langle \nabla f(x), G_{\alpha}(x) \rangle + \frac{\alpha^2 L}{2} \|G_{\alpha}(x)\|_2^2.$$

Corollary. So if $0 \le \alpha \le 1/L$, we have

$$f(y) \le f(x) - \alpha \langle \nabla f(x), G_{\alpha}(x) \rangle + \frac{\alpha}{2} \|G_{\alpha}(x)\|_{2}^{2}.$$

$$f(y) \le f(x) + \langle \nabla f(x), y - x \rangle + \frac{L}{2} ||y - x||_2^2$$

Let $y = x - \alpha G_{\alpha}(x)$, then

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Corollary. So if $0 \le \alpha \le 1/L$, we have

$$f(y) \le f(x) - \alpha \langle \nabla f(x), G_{\alpha}(x) \rangle + \frac{\alpha}{2} ||G_{\alpha}(x)||_{2}^{2}.$$

Lemma Let $y = x - \alpha G_{\alpha}(x)$. Then, for any z we have

$$f(y) + h(y) \le f(z) + h(z) + \langle G_{\alpha}(x), x - z \rangle - \frac{\alpha}{2} \|G_{\alpha}(x)\|_{2}^{2}.$$

Exercise: Prove! (hint: f, h are convex, $G_{\alpha}(x) - \nabla f(x) \in \partial h(y)$)

We've actually shown $x' = x - \alpha G_{\alpha}(x)$ is a descent method. Write $\phi = f + h$; plug in z = x to obtain

$$\phi(x') \le \phi(x) - \frac{\alpha}{2} \|G_{\alpha}(x)\|_2^2$$
.

Exercise: Why this inequality suffices to show convergence.

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Exercise: Why this inequality suffices to show convergence. Use $z = x^*$ in corollary to obtain progress in terms of iterates:

$$\phi(x') - \phi^* \le \langle G_{\alpha}(x), x - x^* \rangle - \frac{\alpha}{2} \|G_{\alpha}(x)\|_2^2$$

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Exercise: Why this inequality suffices to show convergence. Use $z = x^*$ in corollary to obtain progress in terms of iterates:

$$\begin{split} \phi(x') - \phi^* & \leq & \langle G_{\alpha}(x), x - x^* \rangle - \frac{\alpha}{2} \|G_{\alpha}(x)\|_{2}^{2} \\ & = & \frac{1}{2\alpha} \left[2 \langle \alpha G_{\alpha}(x), x - x^* \rangle - \|\alpha G_{\alpha}(x)\|_{2}^{2} \right] \\ & = & \frac{1}{2\alpha} \left[\|x - x^*\|_{2}^{2} - \|x - x^* - \alpha G_{\alpha}(x)\|_{2}^{2} \right] \end{split}$$

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$$\sum_{i=1}^{k+1} (\phi(x_i) - \phi^*) \leq \frac{L}{2} \sum_{i=1}^{k+1} \left[\|x_i - x^*\|_2^2 - \|x_{i+1} - x^*\|_2^2 \right]$$

$$\sum_{i=1}^{k+1} (\phi(x_i) - \phi^*) \leq \frac{L}{2} \sum_{i=1}^{k+1} [\|x_i - x^*\|_2^2 - \|x_{i+1} - x^*\|_2^2]$$
$$= \frac{L}{2} [\|x_1 - x^*\|_2^2 - \|x_{k+1} - x^*\|_2^2]$$

$$\sum_{i=1}^{k+1} (\phi(x_i) - \phi^*) \leq \frac{L}{2} \sum_{i=1}^{k+1} \left[\|x_i - x^*\|_2^2 - \|x_{i+1} - x^*\|_2^2 \right]$$

$$= \frac{L}{2} \left[\|x_1 - x^*\|_2^2 - \|x_{k+1} - x^*\|_2^2 \right]$$

$$\leq \frac{L}{2} \|x_1 - x^*\|_2^2.$$

Set $x \leftarrow x_k, x' \leftarrow x_{k+1}$, and $\alpha = 1/L$. Then add

$$\sum_{i=1}^{k+1} (\phi(x_i) - \phi^*) \leq \frac{L}{2} \sum_{i=1}^{k+1} \left[\|x_i - x^*\|_2^2 - \|x_{i+1} - x^*\|_2^2 \right]$$

$$= \frac{L}{2} \left[\|x_1 - x^*\|_2^2 - \|x_{k+1} - x^*\|_2^2 \right]$$

$$\leq \frac{L}{2} \|x_1 - x^*\|_2^2.$$

Since $\phi(x_k)$ is a decreasing sequence, it follows that

$$\phi(x_{k+1}) - \phi^* \le \frac{1}{k+1} \sum_{i=1}^{k+1} (\phi(x_i) - \phi^*) \le \frac{L}{2(k+1)} \|x_1 - x^*\|_2^2.$$

This is the well-known O(1/k) rate.

▶ But for C_L^1 convex functions, optimal rate is $O(1/k^2)$!

Accelerated Proximal Gradient

$$\min \phi(x) = f(x) + h(x)$$
 Let $x^0 = y^0 \in \operatorname{dom} h$. For $k \ge 1$:
$$x^k = \operatorname{prox}_{\alpha_k h}(y^{k-1} - \alpha_k \nabla f(y^{k-1}))$$

$$y^k = x_k + \frac{k-1}{k+2}(x^k - x^{k-1}).$$

Framework due to: Nesterov (1983, 2004); also Beck, Teboulle (2009). Simplified analysis: Tseng (2008).

- Uses extra "memory" for interpolation
- Same computational cost as ordinary prox-grad
- Convergence rate theoretically optimal

$$\phi(x^k) - \phi^* \le \frac{2L}{(k+1)^2} ||x^0 - x^*||_2^2.$$

Proximal methods – cornucopia

- Douglas Rachford splitting
- ADMM (special case of DR on dual)
- Proximal-Dykstra
- Proximal methods for $f_1 + f_2 + \cdots + f_n$
- Peaceman-Rachford
- Proximal quasi-Newton, Newton
- Many other variation...