CPSC 540: Machine Learning

Stochastic Subgradient

Mark Schmidt

University of British Columbia

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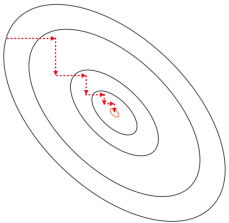
Last Time: Coordinate Optimization

- In coordinate optimization we only update one variable on each iteration.

$$w_{j_k}^{k+1} = w_{j_k}^k - \alpha_k \nabla_k f(w^k),$$



- More efficient than gradient descent if the iterations are d-times cheaper.
  - True for pairwise separable f like label propagation,

$$f(w) = \sum_{i=1}^{d} f_i(w_j) + \sum_{(i,j)\in E} f_{ij}(w_i, w_j).$$

under random choice of j_k.

Convergence Rate of Randomized Coordinate Optimization

- Last time we analyzed coordinate optimization assuming:
  - Coordinate-wise Lipschitz-continuity of ∇f and f satisfying PL inequality.
  - We choose coordinate to update j_k uniformly at random.
  - Given j_k, we take a gradient step on w_{j_k} with step-size $\alpha_k = 1/L$.

- We showed that this leads to the bound

$$\mathbb{E}[f(w^k)] - f^* \leq \left(1 - \frac{\mu}{dL}\right)^k [f(w^k) - f^*],$$

  which means we need $O\left(d\frac{L}{\mu}\log(1/\epsilon)\right)$ iterations to reach accuracy ϵ.

- If d-times cheaper, gives cost of $O\left(\frac{L}{\mu}\log(1/\epsilon)\right)$ gradient descent iterations.
  - But L is smaller for coordinate descent, so total runtime is smaller.

- For convex/non-convex functions, similar trade-off: $O(L/\epsilon)$ vs. $O(dL/\epsilon)$.

Lipschitz Sampling

- Can we do better than choosing j_k uniformly at random?
- You can go faster if you have an L_j for each coordinate:

$$|\nabla_j f(w + \gamma e_j) - \nabla_j f(w)| \leq L_j |\gamma|.$$

- Using L_{j_k} as the step-size and sampling j_k proportional to L_j gives

$$\mathbb{E}[f(w^k)] - f^* \leq \left(1 - \frac{\mu}{d\bar{L}}\right)^w [f(w^0) - f^*],$$

  where $\bar{L}$ as the average Lipschitz constant (previously we used the maximum L_j).

- For label propagation, this requires stronger assumptions on the graph structure:
  - We need expected number of edges connected to j_k to be $O(|E|/d)$.
  - This might not be true if the high-degree nodes have the highest L_j values.

Greedy Gauss-Southwell Selection Rule

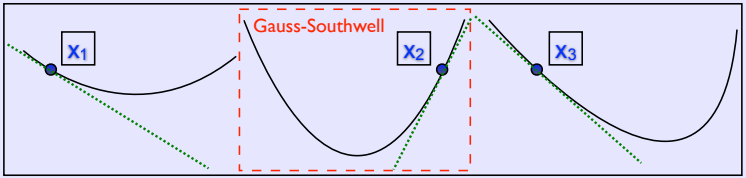
- Our bound on the progress if we choose coordinate j_k is

$$f(w^{k+1}) \leq f(w^k) - \frac{1}{2L}|\nabla_{j_k} f(w^k)|^2.$$

and the "best" j_k according to the bound is

$$j_k \in \underset{j}{\text{argmax}}\{|\nabla_j f(w^k)|\},$$

- This is called greedy selection or the Gauss-Southwell rule.



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- Can we ever find max gradient value d-times cheaper than computing gradient?
  - Yes, for pairwise-separable where maximum degree is similar to average degree.
    - Includes lattice-structured graphs, complete graphs, and Facebook graph.
  - You can efficiently track the gradient values and track the max with a max-heap.

Gauss-Southwell Selection Rule

- The progress bound under the greedy Gauss-Southwell rule is

$$f(w^{k+1}) \leq f(w^k) - \frac{1}{2L}\|\nabla f(w^k)\|_\infty^2,$$

and this leads to a faster rate of

$$f(w^k) - f^* \leq \left(1 - \frac{\mu_1}{L}\right)^k [f(w^0) - f^*],$$

where μ_1 is the PL constant in the ∞-norm

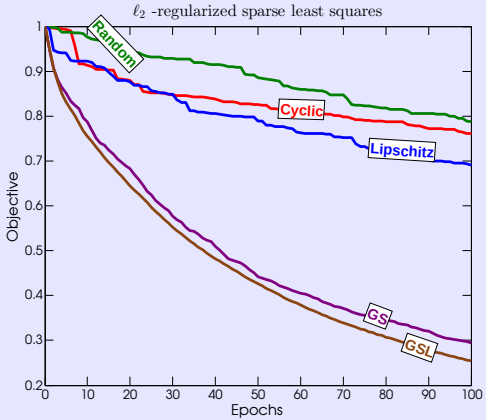
$$\mu[f(w) - f^*] \leq \frac{1}{2}\|f(w)\|_\infty^2.$$

- This is faster because $\frac{\mu}{n} \leq \mu_1 \leq \mu$ (by norm equivalences).

- If you know the L_j values, a faster rule is "Gauss-Southwell-Lipschitz".

Numerical Comparison of Coordinate Selection Rules

Comparison on problem where Gauss-Southwell has similar cost to random:



"Cyclic" goes through the j in order: bad worst-case bounds but often works well

There also exist accelerated coordinate descent methods.

Problems Suitable for Coordinate Optimization

- We now know that many problems satisfy the "d-times faster" condition.
- For example, composition of a smooth function with affine map plus separable

$$F(w) = f(Aw) + \sum_{j=1}^{d} f_j(w_j)$$

  for a matrix A, smooth function f, and potentially non-smooth f_j.
  - Includes L1-regularized least squares, logistic regression, etc.
- Key idea: you can track Aw as you go for a cost $O(n)$ instead of $O(nd)$ (bonus).
- In this setting, we get same rate as if non-smooth f_j were not there.

  (and faster than the sublinear $O(1/k)$ rate for subgradient methods)
- Recent works: coordinate optimization leads to faster PageRank methods.

Outline

Finite-Sum Optimization Problems

- Solving our standard regularized optimization problem

$$\underset{w\in\mathbb{R}^d}{\text{argmin}} \sum_{i=1}^{n} \bar{f}_i(w) \quad + \quad r(w),$$

$$\text{data fitting term} \quad + \quad \text{regularizer}$$

is a special case of solving the generic finite-sum optimization problem

$$\underset{w\in\mathbb{R}^d}{\text{argmin}} \frac{1}{n} \sum_{i=1}^{n} f_i(w),$$

where $f_i(w) = \bar{f}_i(w) + \frac{1}{n} r(w)$.

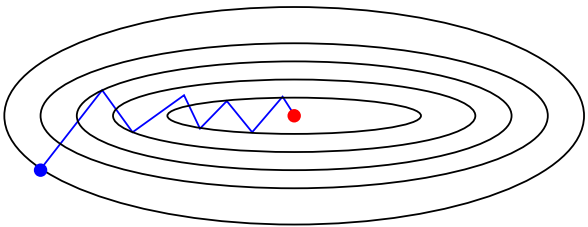
- Gradient methods are effective when d is very large.
- What if number of training examples n is very large?
  - E.g., ImageNet has ≈ 14 million annotated images.

Stochastic vs. Deterministic Gradient Methods

- We consider minimizing $f(w) = \frac{1}{n}\sum_{i=1}^{n} f_i(w)$.
- Deterministic gradient method [Cauchy, 1847]:

$$w^{k+1} = w^k - \alpha_k \nabla f(w^k) = w^k - \frac{\alpha_k}{n}\sum_{i=1}^{n} \nabla f_i(w^k).$$

  - Iteration cost is linear in n.
  - Convergence with constant α_k or line-search.



Stochastic vs. Deterministic Gradient Methods

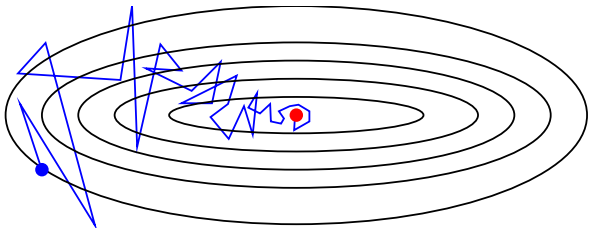
- Stochastic gradient method [Robbins & Monro, 1951]:
  - Random selection of i_k from $\{1, 2, \ldots, n\}$.

$$w^{k+1} = w^k - \alpha_k \nabla f_{i_k}(w^k).$$

  - With $p(i_k = i)$, the stochastic gradient is an unbiased estimate of gradient,

$$\mathbb{E}[\nabla f_{i_k}(w)] = \sum_{i=1}^{n} p(i_k = i) \nabla f_i(w) = \sum_{i=1}^{n} \frac{1}{n} \nabla f_i(w) = \frac{1}{n} \sum_{i=1}^{n} \nabla f_i(w) = \nabla f(w).$$

  - Iteration cost is independent of n.
  - Convergence requires $\alpha_k \to 0$.



Stochastic vs. Deterministic Gradient Methods

Stochastic iterations are n times faster, but how many iterations are needed?

- If ∇f is Lipschitz continuous then we have:

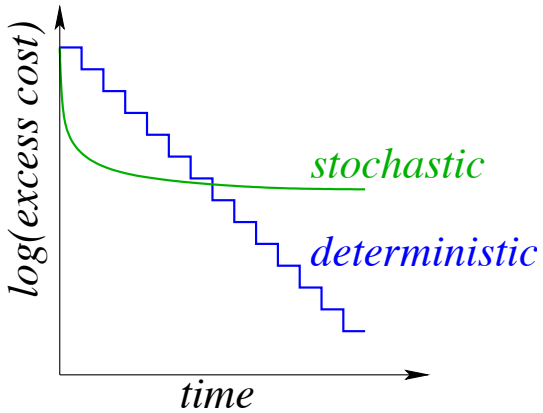
Assumption	Deterministic	Stochastic
Convex	$O(1/\sqrt{\epsilon})$	$O(1/\epsilon^2)$
Strongly	$O(\log(1/\epsilon))$	$O(1/\epsilon)$

- Stochastic has low iteration cost but slow convergence rate.
  - Sublinear rate even in strongly-convex case.
  - Bounds are unimprovable with "unbiased gradient approximation" oracle.
    - Oracle returns a g_k satisfying $\mathbb{E}[g_k] = \nabla f(w^k)$.

- Momentum and Newton-like methods do not improve rates in stochastic case.
  - Can only improve constant factors.

Stochastic vs. Deterministic Convergence Rates

Plot of convergence rates in strongly-convex case:



Stochastic will be superior for low-accuracy/time situations.

Stochastic vs. Deterministic for Non-Smooth

- The story changes for non-smooth problems.
- Consider the binary support vector machine (SVM) objective:

$$f(w) = \sum_{i=1}^{n} \max\{0, 1 - y_i(w^T x_i)\} + \frac{\lambda}{2}\|w\|^2.$$

- Rates for subgradient methods for non-smooth objectives:

Assumption	Deterministic	Stochastic
Convex	$O(1/\epsilon^2)$	$O(1/\epsilon^2)$
Strongly	$O(1/\epsilon)$	$O(1/\epsilon)$

- So for non-smooth problems:
  - Deterministic methods are not faster than stochastic method.
  - So use stochastic subgradient (iterations are n times faster).

Subgradient Method

- The basic subgradient method:

$$w^{k+1} = w^k - \alpha_k g_k,$$

  for some $g_k \in \partial f(w^k)$.
- Decreases distance to solution for small enough α_k.

- The basic stochastic subgradient method:

$$w^{k+1} = w^k - \alpha_k g_{i_k},$$

  for some $g_{i_k} \in \partial f_{i_k}(w^k)$ for some random $i_k \in \{1, 2, \dots, n\}$.

- Stochastic subgradient is n times faster with similar convergence properties.
- Decreases expected distance to solution for small enough α_k.

Outline

Convergence Rate of Stochastic Gradient Method

- We'll first show progress bound for stochastic gradient assuming ∇f is Lipschitz.
  - We'll come back to the non-smooth case.

- From the descent lemma we have

$$f(w^{k+1}) \leq f(w^k) + \nabla f(w^k)^T(w^{k+1} - w^k) + \frac{L}{2}\|w^{k+1} - w^k\|^2.$$

- Using stochastic gradient iteration $(w^{k+1} - w^k) = -\alpha_k \nabla f_{i_k}(w^k)$ gives

$$f(w^{k+1}) \leq f(w^k) - \alpha_k \nabla f(w^k)^T \nabla f_{i_k}(w^k) + \alpha_k^2 \frac{L}{2}\|\nabla f_{i_k}(w^k)\|^2.$$

Convergence Rate of Stochastic Gradient Method

- So far any choice of α_k and i_k we have

$$f(w^{k+1}) \leq f(w^k) - \alpha_k \nabla f(w^k)^T \nabla f_{i_k}(w^k) + \alpha_k^2 \frac{L}{2} \|\nabla f_{i_k}(w^k)\|^2.$$

- Let's take the expectation with respect to i_k assuming $p(i_k = i) = 1/n$,

$$\begin{aligned}\mathbb{E}[f(w^{k+1})] &\leq \mathbb{E}[f(w^k) - \alpha_k \nabla f(w^k)^T \nabla f_{i_k}(w^k) + \alpha_k^2 \frac{L}{2} \|\nabla f_{i_k}(w^k)\|^2] \\ &= f(w^k) - \alpha_k \nabla f(w^k)^T \mathbb{E}[\nabla f_{i_k}(w^k)] + \alpha_k^2 \frac{L}{2} \mathbb{E}[\|\nabla f_{i_k}(w^k)\|^2],\end{aligned}$$

  where the second line uses linearity of expectation (and α_k not depending on i_k).
- We know that $\mathbb{E}[\nabla f_{i_k}(w^k)] = \nabla f(w^k)$ (unbiased) so this gives

$$\mathbb{E}[f(w^{k+1})] \leq f(w^k) - \alpha_k \underbrace{\|\nabla f(w^k)\|^2}_{\text{good}} + \alpha_k^2 \underbrace{\frac{L}{2} \mathbb{E}[\|\nabla f_{i_k}(w^k)\|^2]}_{\text{bad}}.$$

Convergence Rate of Stochastic Gradient Method

- So a progress bound for stochastic gradient is

$$\mathbb{E}[f(w^{k+1})] \leq f(w^k) - \alpha_k \underbrace{\|\nabla f(w^k)\|^2}_{\text{good}} + \alpha_k^2 \underbrace{\frac{L}{2}\mathbb{E}[\|\nabla f_{i_k}(w^k)\|^2]}_{\text{bad}}.$$

- "Good" term looks like usual measure of progress: big gradient $\rightarrow$ big progress.
- "Bad" term is the problem: less progress if gradients are very different.
  - And now choosing $\alpha_k = 1/L$ might not be small enough.
  - But we can control badness: if α_k is small then $\alpha_k >> \alpha_k^2$.

- If we also assume PL then we get

$$\mathbb{E}[f(w^{k+1})] - f^* \leq (1 - 2\alpha_k\mu)[f(w^k) - f^*] + \alpha_k^2 \underbrace{\frac{L}{2}\mathbb{E}[\|\nabla f_{i_k}(w^k)\|^2]}_{\text{bad}}.$$

- Looks like linear convergence if far from solution and gradients are similar..
  - No progress if close to solution or have high variance in gradients.

Convergence Rate of Stochastic Subgradient Method

- The basic stochastic subgradient method:

$$w^{k+1} = w^k - \alpha g_{i_k},$$

for some $g_{i_k} \in \partial f_{i_k}(w^k)$ for some random $i_k \in \{1, 2, \dots, n\}$.

- We can't use descent lemma because f is non-differentiable.

- For convex f we can show a progress bound on distance to a w^* (bonus)

$$\mathbb{E}[\|w^{k+1} - w^*\|^2] = \underbrace{\|w^k - w^*\|^2}_{\text{old distance}} - 2\alpha_k \underbrace{g_k^T(w^k - w^*)}_{\text{good}} + \alpha_k^2 \underbrace{\mathbb{E}[\|g_{i_k}\|^2]}_{\text{bad}},$$

where g_k is a subgradient of f at w^k (good term is positive by convexity).

- Step-size α_k controls how fast we move towards solution.
- And squared step-size α_k^2 controls how much variance moves us away.

Convergence Rate of Stochastic Subgradient

- Standard assumption is that the $\mathbb{E}[\|\nabla f(w)\|^2]$ is bounded by constant B^2.

$$\mathbb{E}[\|w^{k+1} - w^*\|^2] \leq \underbrace{\|w^k - w^*\|^2}_{\text{old distance}} - 2\alpha_k \underbrace{g_k^T(w^k - w^*)}_{\text{good}} + \alpha_k^2 \underbrace{B^2}_{\text{bad}},$$

- If f is strongly-convex, then we further have that (bonus)

$$\mathbb{E}[\|w^k - w^*\|^2] \leq (1 - 2\alpha_k\mu)\|w^{k-1} - w^*\|^2 + \alpha_k^2 B^2.$$

- If α_k is *small* enough, shows distance to solution is guaranteed to decrease.

- With constant $\alpha_k = \alpha$ (with $\alpha < 2/\mu$) and applying recursively we get (bonus)

$$\mathbb{E}[\|w^k - w^*\|^2] \leq (1 - 2\alpha\mu)^k\|w^0 - w^*\|^2 + \frac{\alpha B^2}{2\mu},$$

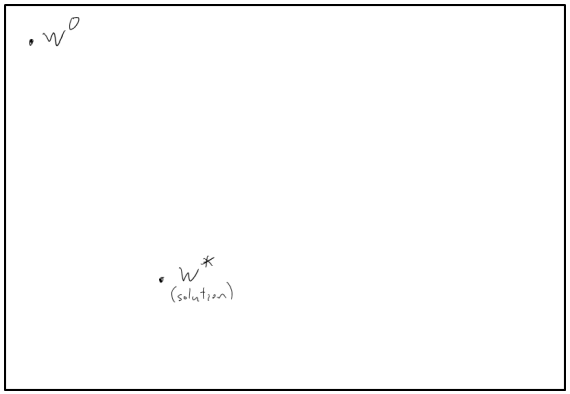
where second term bounds a geometric series.

Stochastic Gradient with Constant Step Size

- Our bound on expected distance with constant step-size:

$$\mathbb{E}[\|w^k - w^*\|^2] \leq (1 - 2\alpha\mu)^k \|w^0 - w^*\|^2 + \frac{\alpha B^2}{2\mu},$$

- First term looks like linear convergence, but second term does not go to zero.



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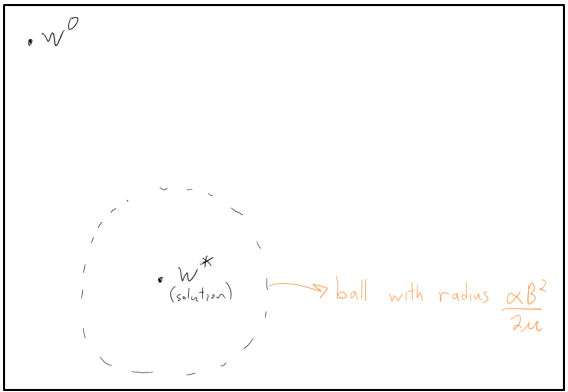

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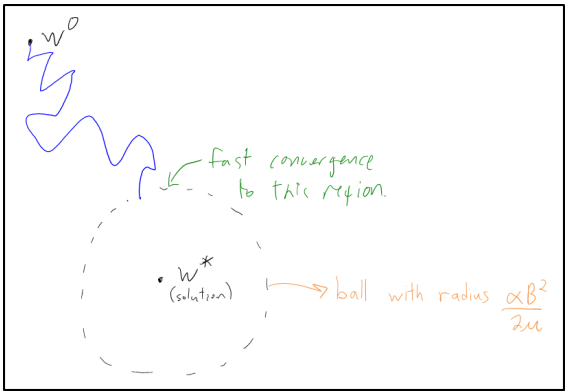

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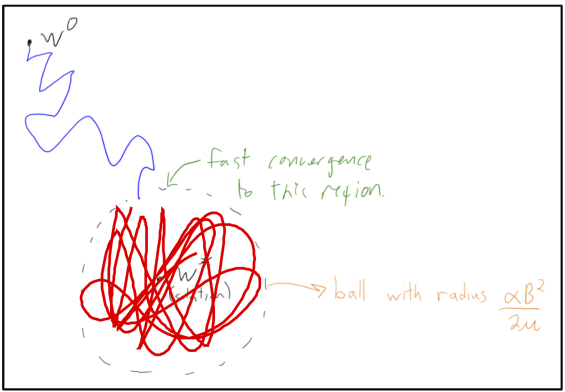


Summary

- Better coordinate selection with Lipschitz sampling or Gauss-Southwell.
- $f(Ax) + \sum_j f_j(w_j)$ structure also allows coordinate optimization.
  - Even for non-smooth f_j.
- Stochastic subgadient method: same rate as subgradient but n times cheaper.
  - Constant step-size: subgradient quickly converges to approximate solution.
- Next time: new stochastic methods with linear convergence, and the $n = \infty$ case.

Gauss-Southwell-Lipschitz

- Our bound on the progress with an L_j for each coordinate is

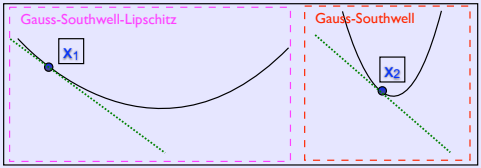
$$f(w^{k+1}) \leq f(w^k) - \frac{1}{2L_{j_k}}|\nabla_{j_k} f(w^k)|^2.$$

- The best coordinate to update according to this bound is

$$j_k \in \underset{j}{\text{argmax}} \frac{|\nabla_j f(w^k)|^2}{L_j}$$

which is called the Gauss-Southwell-Lipschitz rule.

  - "If gradients are similar, pick the one that changes more slowly".



- This is the optimal update for quadratic functions.

Problems Suitable for Coordinate Optimization

- We now know that many problems satisfy the "d-times faster" condition.
- For example, consider composition of a smooth function with affine map,

$$F(w) = f(Aw),$$

for a matrix A and a smooth function g with cost of $O(n)$.

(includes least squares and logistic regression)

- Using f' as the gradient of f, the partial derivatives have the form

$$\nabla_j F(x) = a_j^T f'(Aw).$$

- If we have Aw, this costs $O(n)$ instead of $O(nd)$ for the full gradient.
- We can track the product Aw^k as we go with $O(n)$ cost,

$$Aw^{k+1} = A(w^k + \gamma_k e_{j_k}) = \underbrace{Aw^k}_{\text{old value}} + \gamma_k \underbrace{Ae_{j_k}}_{O(n)},$$

Coordinate Optimization for Non-Smooth Objectives

- We can apply coordinate optimization for problems of the form

$$F(x) = \underbrace{f(x)}_{\text{smooth}} + \underbrace{\sum_{j=1}^{d} f_j(x_j)}_{\text{separable}},$$

where the f_j can be non-smooth.

  - This includes enforcing non-negative constraints, or using L1-regularization.

- For proximal-PL F, with coordinate-wise proximal-gradient steps we have

$$\mathbb{E}[f(w^k)] - f^* \leq \left(1 - \frac{\mu}{dL}\right)^k [f(w^0) - f^*],$$

the same convergence linear rate as if the non-smooth f_j were not there.

(and faster than the sublinear $O(1/k)$ rate for subgradient methods)

Block Coordinate Descent

- We can't apply coordinate optimization for group L1-regularization.
  - Non-smooth term is non-separable, so coordinate optimization can get stuck.
- Block coordinate optimization and block coordinate descent:
  - Update groups of variables on each iteration.
- If you choose the "blocks" to be the "groups", you can apply to group L1-regularization.
- Many problems have this "block" structure.
  - You might also use blocks to apply Newton's method to the blocks.
  - This is efficient if the block size isn't too big.

Convergence Rate of Stochastic Subgradient Method

- The basic stochastic subgradient method:

$$x^{t+1} = x^t - \alpha g_{i_t},$$

for some $g_{i_t} \in \partial f_{i_t}(x^t)$ for some random $i_t \in \{1, 2, \ldots, n\}$.

- Since function value may not decrease, we analyze distance to x^*:

$$\begin{aligned}\|x^t - x^*\|^2 &= \|(x^{t-1} - \alpha_t g_{i_t}) - x^*\|^2 \\ &= \|(x^{t-1} - x^*) - \alpha_t g_{i_t}\|^2 \\ &= \|x^{t-1} - x^*\|^2 - 2\alpha_t g_{i_t}^T (x^{t-1} - x^*) + \alpha_t^2 \|g_{i_t}\|^2.\end{aligned}$$

- Take expectation with respect to i_t:

$$\begin{aligned}\mathbb{E}[\|x^t - x^*\|^2] &= \mathbb{E}[\|x^{t-1} - x^*\|] - 2\alpha_t \mathbb{E}[g_{i_t}^T (x^{t-1} - x^*)] + \alpha_t^2 \mathbb{E}[\|g_{i_t}\|^2] \\ &= \underbrace{\|x^{t-1} - x^*\|^2}_{\text{old distance}} - 2\alpha_t \underbrace{g_t^T (x^{t-1} - x^*)}_{\text{expected progress}} + \alpha_t^2 \underbrace{\mathbb{E}[\|g_{i_t}\|^2]}_{\text{“variance”}}.\end{aligned}$$

Convergence Rate of Stochastic Subgradient

- Our expected distance given x^{t-1} is

$$\mathbb{E}[\|x^t - x^*\|^2] = \underbrace{\|x^{t-1} - x^*\|^2}_{\text{old distance}} - 2\alpha_t \underbrace{g_t^T(x^{t-1} - x^*)}_{\text{expected progress}} + \alpha_t^2 \underbrace{\mathbb{E}[\|g_{i_t}\|^2]}_{\text{"variance"}}.$$

- Step-size α_t controls how fast we move towards solution.
- But squared step-size α_t^2 controls how much variance moves us away.

- Standard assumption is that the variance is bounded by constant B^2.
- It follows from strong-convexity that (next slide),

$$g_t^T(x^{t-1} - x^*) \geq \mu\|x^{t-1} - x^*\|^2,$$

which gives

$$\begin{aligned}\mathbb{E}[\|x^t - x^*\|^2] &\leq \|x^{t-1} - x^*\|^2 - 2\alpha_t\mu\|x^{t-1} - x^*\|^2 + \alpha_t^2 B^2 \\ &= (1 - 2\alpha_t\mu)\|x^{t-1} - x^*\|^2 + \alpha_t^2 B^2.\end{aligned}$$

Strong-Convexity Inequalities for Non-Differentiable f

- A "first-order" relationship between subgradient and strong-convexity:
  - If f is μ-strongly convex then for all x and y we have
$$f(y) \geq f(x) + f'(y)^T(y-x) + \frac{\mu}{2}\|y-x\|^2,$$
for $f'(y) \in \partial f(x)$.
  - The first-order definition of strong-convexity, but with subgradient replacing gradient.
  - Reversing y and x we can write
$$f(x) \geq f(y) + f'(x)^T(x-y) + \frac{\mu}{2}\|x-y\|^2,$$
for $f'(x) \in \partial f(x)$.
  - Adding the above together gives
$$(f'(y) - f'(x)^)T(y-x)) \geq \mu\|y-x\|^2.$$
  - Applying this with $y = x^{t-1}$ and subgradient g_t and $x = x^*$ (which has $f'(x^*) = 0$ for some subgradient) gives
$$(g_t - 0)^T(x^{t-1} - x^*) \geq \mu\|x^{t-1} - x^*\|^2.$$

Convergence Rate of Stochastic Subgradient

- For full details of analyzing stochastic gradient under strong convexity, see:
  - Constant α_k: `http://circle.ubc.ca/bitstream/handle/2429/50358/stochasticGradientConstant.pdf`.
  - Decreasing α_k: `http://arxiv.org/pdf/1212.2002v2.pdf`.

- For both cases under PL, see Theorem 4 here:
  - https://arxiv.org/pdf/1608.04636v2.pdf