Smooth, Finite, and Convex Optimization

Deep Learning Summer School

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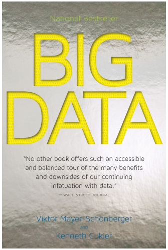
Context: Big Data and Big Models

- We are collecting data at unprecedented rates.
  - Seen across many fields of science and engineering.
  - Not gigabytes, but terabytes or petabytes (and beyond).



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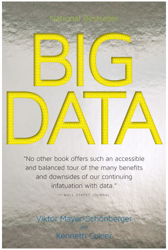

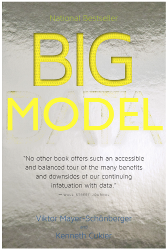

- Machine learning can use big data to fit richer models:
  - Bioinformatics.
  - Computer vision.
  - Speech recognition.
  - Product recommendation.
  - Machine translation.

Common Framework: Empirical Risk Minimization

- The most common framework is empirical risk minimization:

$$\min_{x \in \mathbb{R}^D} \frac{1}{N} \sum_{i=1}^{N} L(x, a_i, b_i) \quad + \quad \lambda r(x)$$

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

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  to conditional random fields (CRFs) and deep neural networks.
- Main practical challenges:
  - Designing/learning good features a_i.
  - Efficiently solving the problem when N or D are very large.

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    (least squares, lasso, generlized linear models, SVMs, CRFs, etc.)
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  - Tools from convex analysis are being extended to non-convex.

    (discussed in part 2)

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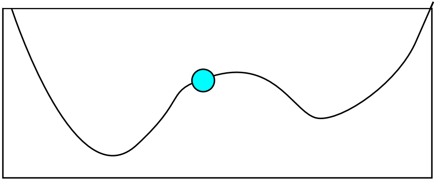

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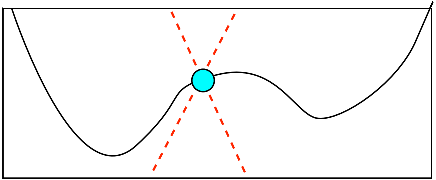

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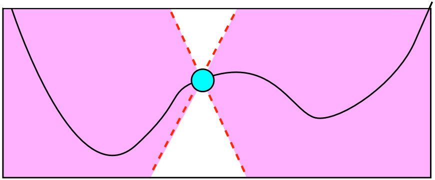

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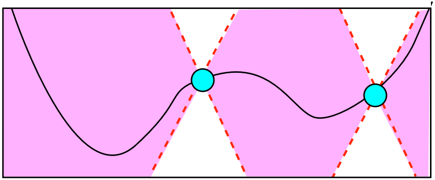

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- Optimization is hard, but assumptions make a big difference.

  (we went from impossible to very slow)

Convex Functions: Three Characterizations

A function f is convex if for all x and y we have

$$f(\theta x + (1-\theta)y) \leq \theta f(x) + (1-\theta)f(y), \quad \textit{for } \theta \in [0,1].$$

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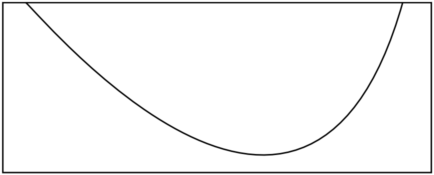

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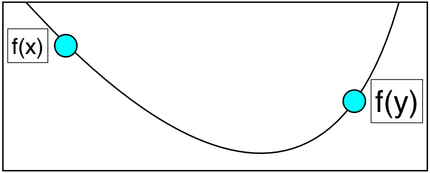

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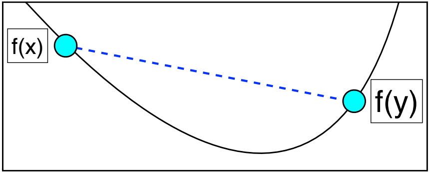

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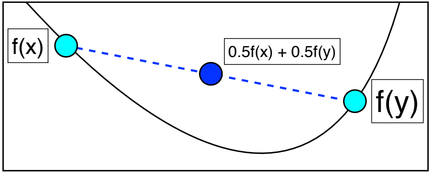

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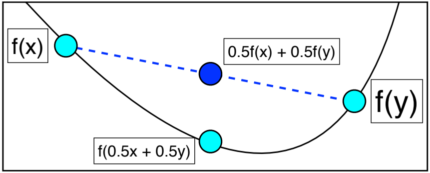

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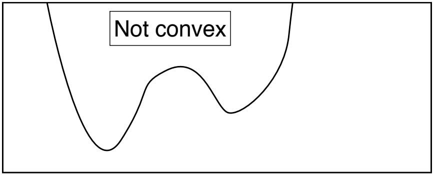

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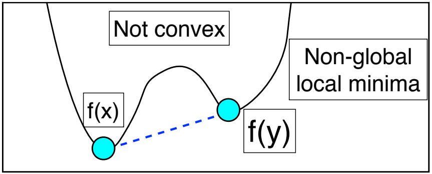

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$$f(y) \geq f(x) + \nabla f(x)^T(y-x),$$

- The function is globally above the tangent at x.

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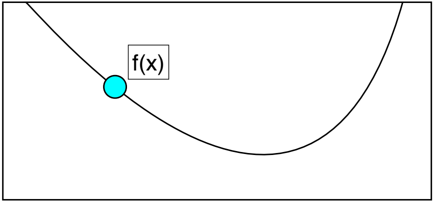

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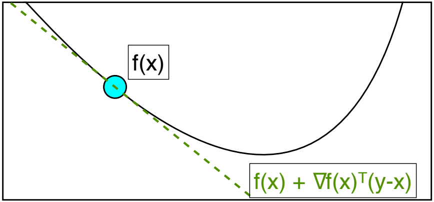

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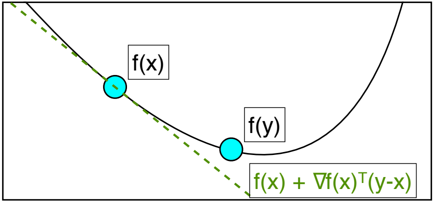

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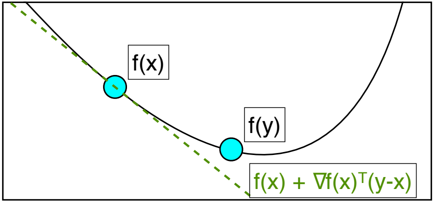

- If $\nabla f(y) = 0$, implies y is a a global minimizer.

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A twice-differentiable function f is convex if for all x we have

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

- All eigenvalues of 'Hessian' are non-negative.
- The function is *flat or curved upwards* in every direction.
- This is usually the easiest way to show a function is convex.

Examples of Convex Functions

Some simple convex functions:

- $f(x) = c$
- $f(x) = a^T x$
- $f(x) = x^T Ax$ (for $A \succeq 0$)
- $f(x) = \exp(ax)$
- $f(x) = x \log x$ (for $x > 0$)
- $f(x) = \|x\|^2$
- $f(x) = \|x\|_p$
- $f(x) = \max_i\{x_i\}$

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Some other notable examples:

- $f(x, y) = \log(e^x + e^y)$
- $f(X) = \log \det X$ (for X positive-definite).
- $f(x, Y) = x^T Y^{-1} x$ (for Y positive-definite)

Operations that Preserve Convexity

1. Non-negative weighted sum:

$$f(x) = \theta_1 f_1(x) + \theta_2 f_2(x).$$

2. Composition with affine mapping:

$$g(x) = f(Ax + b).$$

3. Pointwise maximum:

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We know that $\| \cdot \|_p$ is a norm, so it follows from (2).

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Know first term is convex, for the other terms use (3) on the two (convex) arguments, then use (1) to put it all together.

Outline

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$$x^{t+1} = x^t - \alpha_t \nabla f(x^t).$$

  - Only have $O(D)$ iteration cost!
  - But how many iterations are needed?

Logistic Regression with 2-Norm Regularization

- Let's consider logistic regression with 2-norm regularization:

$$f(x) = \sum_{i=1}^{n} \log(1 + exp(-b_i(x^T a_i))) + \frac{\lambda}{2}\|x\|^2.$$

- Objective f is convex.
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- We say that the gradient is Lipschitz-continuous.
- We say that the function is strongly-convex.

Properties of Lipschitz-Continuous Gradient

- From Taylor's theorem, for some z we have:

$$f(y) = f(x) + \nabla f(x)^T (y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(z)(y - x)$$

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- Use that $\nabla^2 f(z) \preceq LI$.

$$f(y) \leq f(x) + \nabla f(x)^T(y-x) + \frac{L}{2}\|y-x\|^2$$

- *Global quadratic upper bound on function value.*

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$$f(y) = f(x) + \nabla f(x)^T(y-x) + \frac{1}{2}(y-x)^T\nabla^2 f(z)(y-x)$$

- Use that $\nabla^2 f(z) \preceq LI$.

$$f(y) \leq f(x) + \nabla f(x)^T(y-x) + \frac{L}{2}\|y-x\|^2$$

- *Global quadratic upper bound on function value.*
- Set x^{t+1} to minimum y value:

$$x^{t+1} = x^t - \frac{1}{L}\nabla f(x^t).$$

- Plugging this value in:

$$f(x^{t+1}) \leq f(x^t) - \frac{1}{2L}\|\nabla f(x^t)\|^2.$$

- Guaranteed decrease of objective with $\alpha_t = 1/L$.

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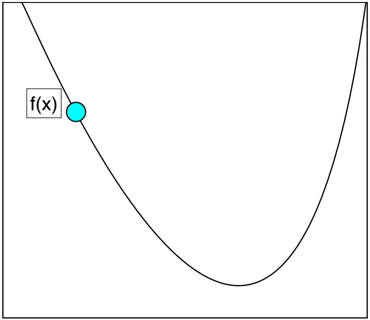

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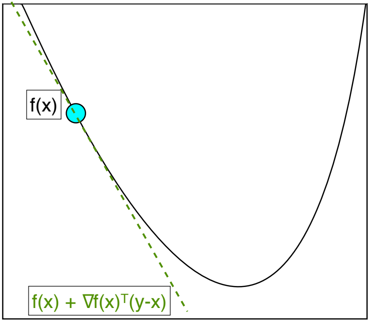

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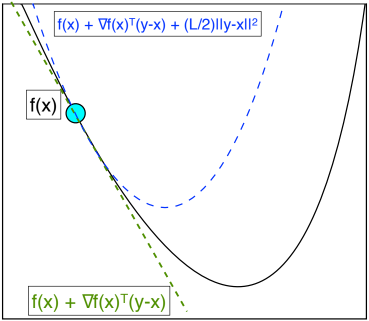

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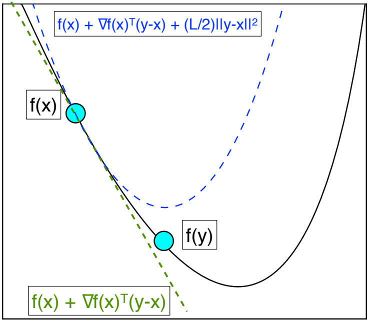

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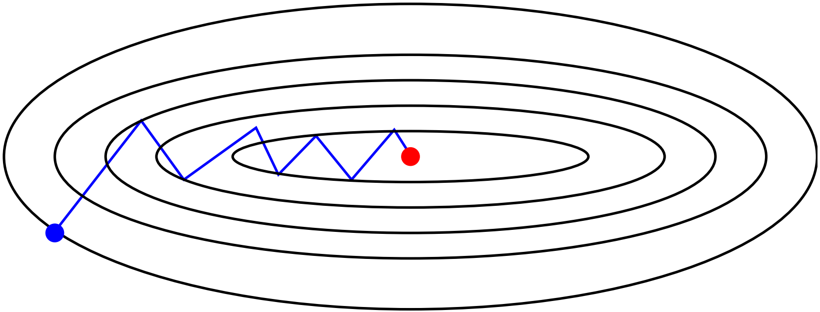

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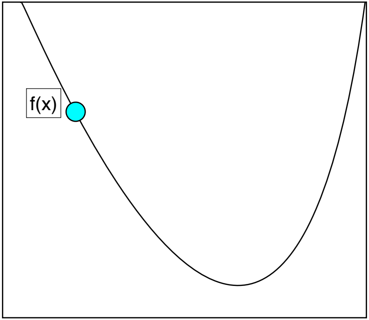

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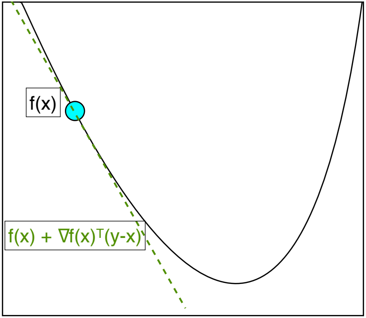

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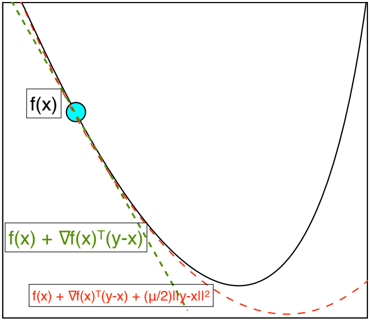

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- Minimize both sides in terms of y:

$$f(x^*) \geq f(x) - \frac{1}{2\mu}\|\nabla f(x)\|^2.$$

- Upper bound on how far we are from the solution.

Linear Convergence of Gradient Descent

- We have bounds on x^{t+1} and x^*:

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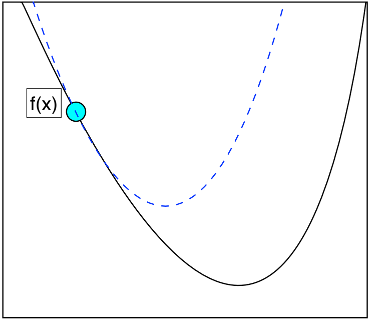

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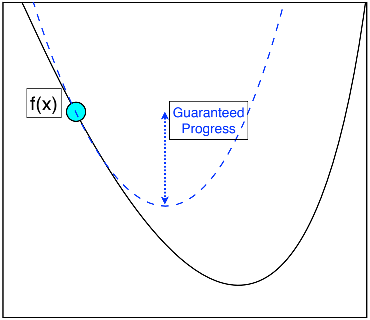

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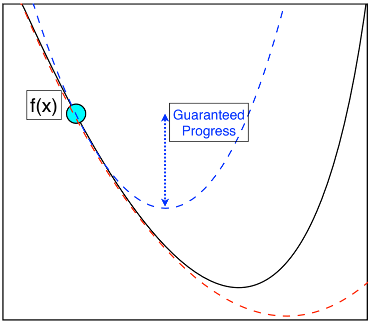

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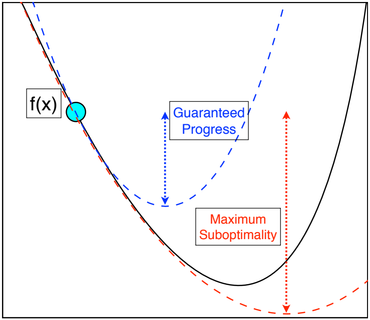

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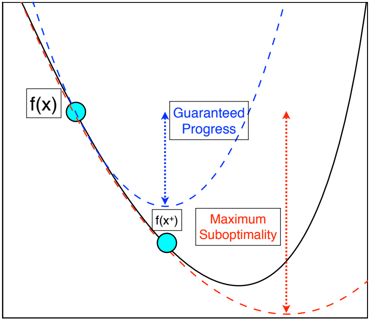

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- This gives a linear convergence rate:

$$f(x^t) - f(x^*) \leq \left(1 - \frac{\mu}{L}\right)^t [f(x^0) - f(x^*)]$$

- Each iteration multiplies the error by a fixed amount.
- Dimension-independent, and very fast if $\frac{\mu}{L} \approx 1$.

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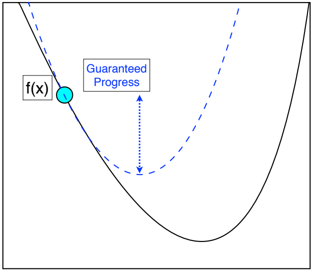

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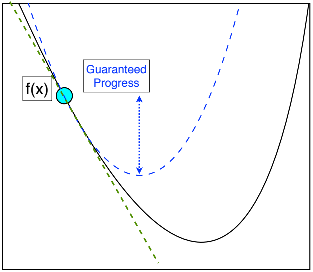

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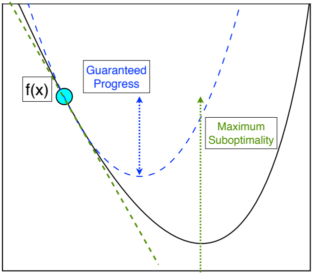

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- If f is convex, then $f + \lambda\|x\|^2$ is strongly-convex.

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- Also, check your derivative code!

$$\nabla_i f(x) \approx \frac{f(x + \delta e_i) - f(x)}{\delta}$$

- For large-scale problems you can check a random direction d:

$$\nabla f(x)^T d \approx \frac{f(x + \delta d) - f(x)}{\delta}$$

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- Similar to heavy-ball/momentum and conjugate gradient.
- Rates are nearly-optimal for dimension-independent algorithm.
- For logistic regression and many other losses, we can get linear convergence without strong-convexity [Luo & Tseng, 1993].

Newton's Method

- Newton's method is a second-order strategy.

(also called IRLS for functions of the form $f(Ax)$)

- Modern form uses the update

$$x^{t+1} = x^t - \alpha_t d_t,$$

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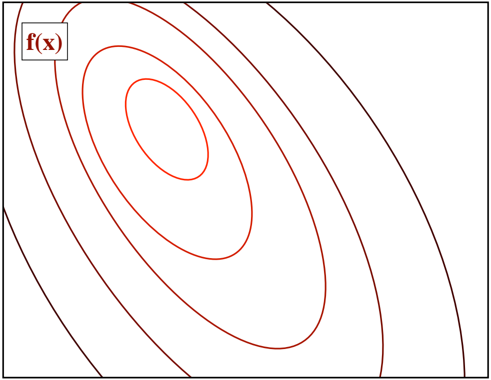
- We can generalize the Armijo condition to

$$f(x^{t+1}) \leq f(x^t) + \gamma \alpha \nabla f(x^t)^T d.$$

- Has a natural step length of $\alpha = 1$.

  (always accepted when close to a minimizer)

Newton's Method



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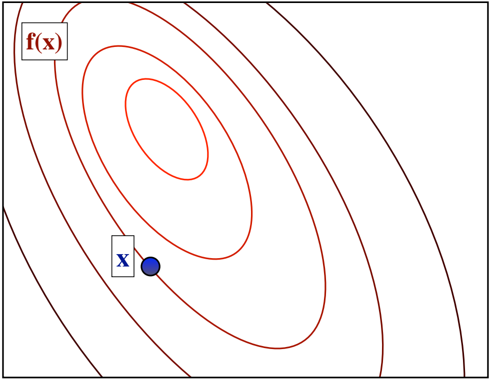

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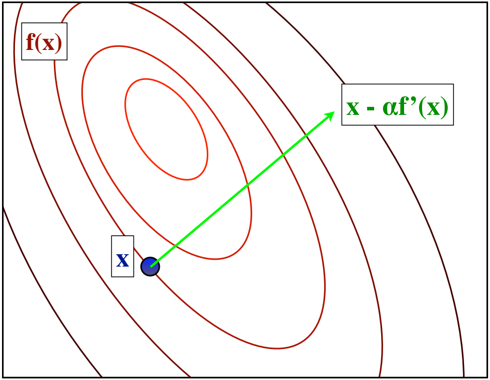

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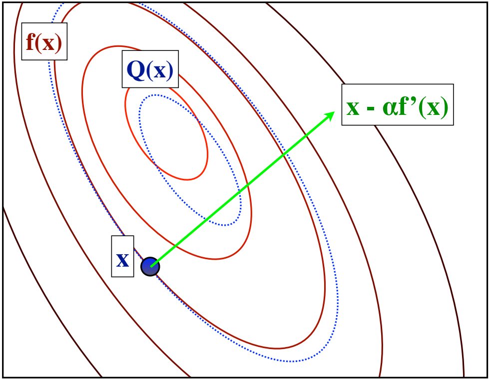

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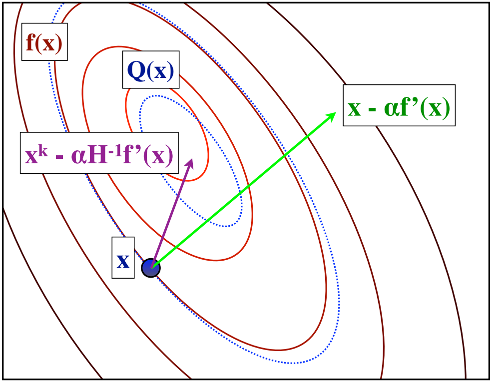

Convergence Rate of Newton's Method

- If $\nabla^2 f(x)$ is Lipschitz-continuous and $\nabla^2 f(x) \succeq \mu$, then close to x^* Newton's method has local superlinear convergence:

$$f(x^{t+1}) - f(x^*) \leq \rho_t[f(x^t) - f(x^*)],$$

  with $\lim_{t\to\infty} \rho_t = 0$.
- Converges very fast, use it if you can!

Convergence Rate of Newton's Method

- If $\nabla^2 f(x)$ is Lipschitz-continuous and $\nabla^2 f(x) \succeq \mu$, then close to x^* Newton's method has local superlinear convergence:

$$f(x^{t+1}) - f(x^*) \leq \rho_t[f(x^t) - f(x^*)],$$

  with $\lim_{t\to\infty} \rho_t = 0$.
- Converges very fast, use it if you can!
- But requires solving $\nabla^2 f(x^t)d^t = \nabla f(x^t)$.
- Variant called cubic regularization has global rates.

Newton's Method: Practical Issues

There are practical large-scale Newton-like methods:

- Only use the diagonals of the Hessian.
- Barzilai-Borwein: Choose a step-size that acts like the Hessian over the last iteration:

$$\alpha = \frac{(x^{t+1} - x^t)^T(\nabla f(x^{t+1}) - \nabla f(x^t))}{\|\nabla f(x^{t+1}) - f(x^t)\|^2}$$

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- Quasi-Newton: Update a (diagonal plus low-rank) approximation of the Hessian (L-BFGS).
- Hessian-free: Compute d inexactly using Hessian-vector products:
$$\nabla^2 f(x)d = \lim_{\delta \to 0} \frac{\nabla f(x + \delta d) - \nabla f(x)}{\delta}$$

Another related method is nonlinear conjugate gradient.

Numerical Comparison

Result after 25 evaluations of limited-memory solvers on 2D rosenbrock:

---

x1 = 0.0000, x2 = 0.0000 (starting point)
x1 = 1.0000, x2 = 1.0000 (optimal solution)

---

x1 = 0.8725, x2 = 0.7569 (minimize.m by C. Rasmussen)
x1 = 0.3654, x2 = 0.1230 (minFunc with steepest descent)
x1 = 0.4974, x2 = 0.2452 (minFunc with cyclic steepest descent)
x1 = 0.8756, x2 = 0.7661 (minFunc with spectral gradient descent)
x1 = 0.5840, x2 = 0.3169 (minFunc with Hessian-free Newton)
x1 = 0.7478, x2 = 0.5559 (minFunc with preconditioned Hessian-free Newton)
x1 = 1.0010, x2 = 1.0020 (minFunc with conjugate gradient)
x1 = 0.7907, x2 = 0.6256 (minFunc with scaled conjugate gradient)
x1 = 0.9794, x2 = 0.9491 (minFunc with preconditioned conjugate gradient)
x1 = 1.0000, x2 = 1.0000 (minFunc with limited-memory BFGS - default)

Outline

Big-N Problems

- Recall the regularized empirical risk minimization problem:

$$\min_{x \in \mathbb{R}^D} \frac{1}{N} \sum_{i=1}^{N} L(x, a_i, b_i) \quad + \quad \lambda r(x)$$

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

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- Gradient methods are effective when D is very large.
- What if number of training examples N is very large?
  - E.g., ImageNet has more than 14 million annotated images.

Stochastic vs. Deterministic Gradient Methods

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  - Gives unbiased estimate of true gradient,

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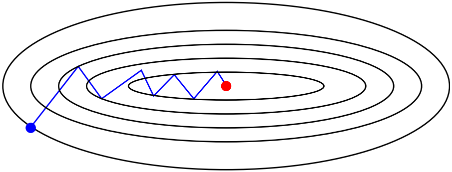

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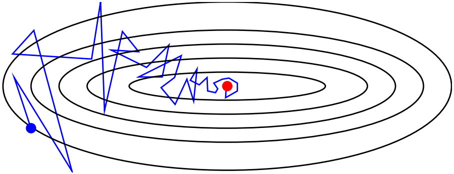

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Strongly	$O((1-\sqrt{\mu/L})^t)$	$O(1/t)$

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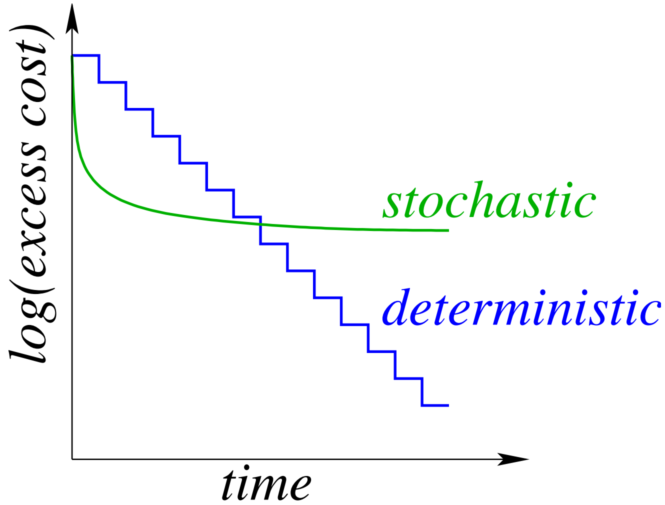
  - Bounds are unimprovable if only unbiased gradient available.
- E.g., Momentum/acceleration does not improve rate:
  - In fact, for convergence of SG the momentum must go to zero.

[Tseng, 1998]

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 objective:

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

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- Other black-box methods (cutting plane) are not faster.
- For non-smooth problems:
  - Deterministic methods are not faster than stochastic method.
  - So use stochastic subgradient (iterations are n times faster).

Sub-Gradients and Sub-Differentials

Recall that for *differentiable* convex functions we have

$$f(y) \geq f(x) + \nabla f(x)^T(y - x), \forall x, y.$$

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- At differentiable x:
  - Only subgradient is $\nabla f(x)$.
- At non-differentiable x:
  - We have a set of subgradients.
  - Called the sub-differential, $\partial f(x)$.
- Note that $0 \in \partial f(x)$ iff x is a global minimum.

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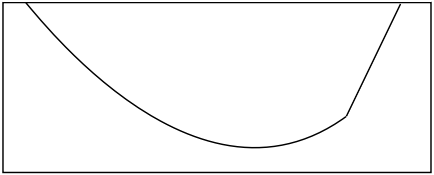

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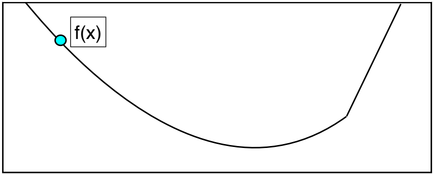

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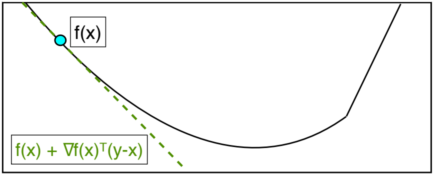

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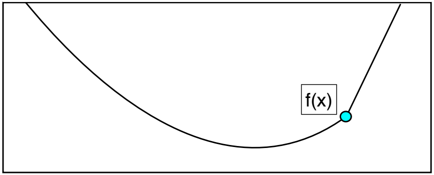

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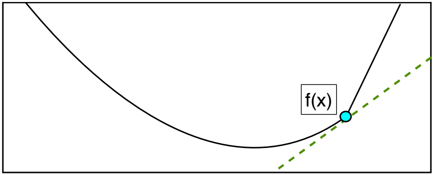

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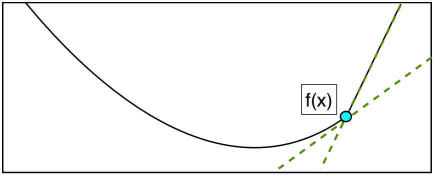

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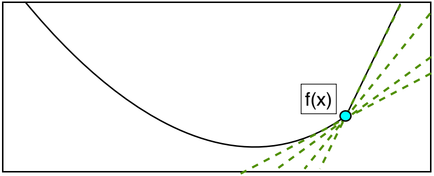

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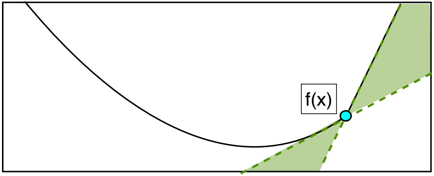

Sub-Differential of Absolute Value and Max Functions

- Sub-differential of absolute value function:

$$\partial|x| = \begin{cases} 1 & x > 0 \\ -1 & x < 0 \\ [-1, 1] & x = 0 \end{cases}$$

(sign of the variable if non-zero, anything in $[-1, 1]$ at 0)

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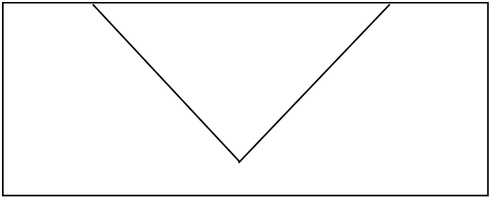

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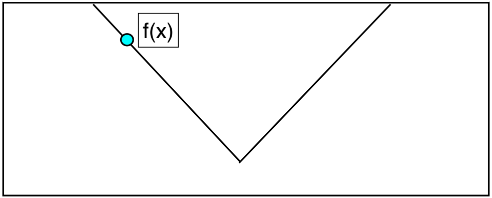

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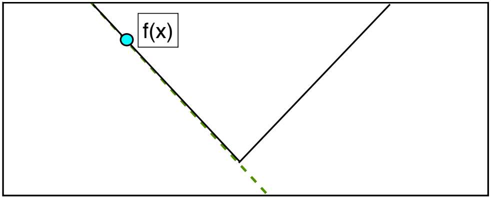

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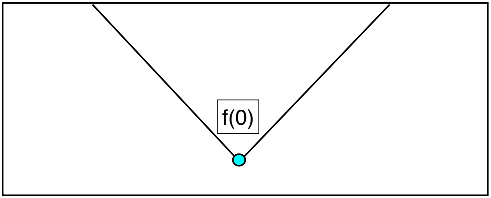

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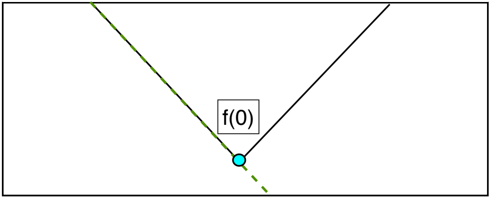

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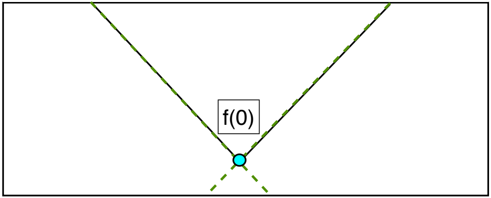

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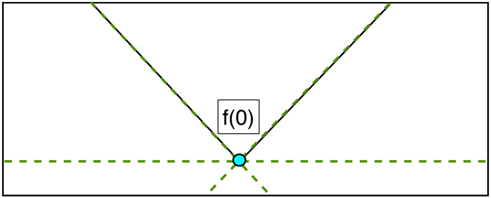

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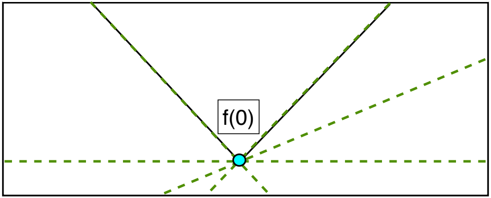

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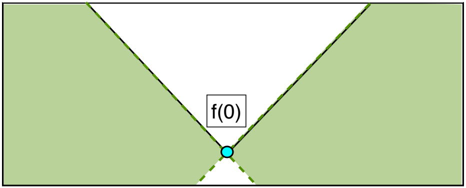

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(any convex combination of the gradients of the argmax)

Subgradient and Stochastic Subgradient methods

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- But $\|x^{t+1} - x^*\| \leq \|x^t - x^*\|$ for small enough α.
- For convergence, we require $\alpha \rightarrow 0$.
- The basic stochastic subgradient method:

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for some $d_t \in \partial f_{i_t}(x^t)$ for some random $i_t \in \{1, 2, \dots, N\}$.

Stochastic Subgradient Methods in Practice

- The theory says to use a method like this:

$$i_t = \mathrm{rand}(1, 2, \ldots, N), \quad \alpha_t = \frac{1}{\mu t}$$

$$x^{t+1} = x^t - \alpha_t f_{i_t}'(x^t).$$

  - $O(1/t)$ for smooth objectives.
  - $O(\log(t)/t)$ for non-smooth objectives.

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$$i_t = \mathrm{rand}(1, 2, \ldots, N), \quad \alpha_t = \frac{1}{\mu t}$$

$$x^{t+1} = x^t - \alpha_t f'_{i_t}(x^t).$$

  - $O(1/t)$ for smooth objectives.
  - $O(\log(t)/t)$ for non-smooth objectives.
- Except for some special cases, you should not do this.
  - Initial steps are huge: usually $\mu = O(1/N)$ or $O(1/\sqrt{N})$.
  - Later steps are tiny: $1/t$ gets small very quickly.
  - Convergence rate is not robust to mis-specification of μ.
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  - No adaptation to 'easier' problems than worst case.
- Tricks that can improve theoretical and practical properties:
  1. Use smaller initial step-sizes, that go to zero more slowly.
  2. Take a (weighted) average of the iterations or gradients:

$$\bar{x}_t = \sum_{i=1}^{t} \omega_t x_t, \quad \bar{d}_t = \sum_{i=1}^{t} \delta_t d_t.$$

Speeding up Stochastic Subgradient Methods

Works that support using large steps and averaging:

- Rakhlin et al. [2011], LaCoste-Julien et al. [2013]
  - Averaging later iterations achieves $O(1/t)$ in non-smooth case.
  - Averaging by iteration number achieves same.
- Nesterov [2007], Xiao [2010]:
  - Gradient averaging improves constants ('dual averaging').
  - Finds non-zero variables with sparse regularizers.
- Bach & Moulines [2011]:
  - $\alpha_t = O(1/t^\beta)$ for $\beta \in (0.5, 1)$ more robust than $\alpha_t = O(1/t)$.

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- Nedic & Bertsekas [2000]:
  - Constant step size ($\alpha_t = \alpha$) achieves rate of

$$\mathbb{E}[f(x^t)] - f(x^*) \leq (1 - 2\mu\alpha)^t (f(x^0) - f(x^*)) + O(\alpha).$$

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- Polyak & Juditsky [1992]:
  - In smooth case, iterate averaging is asymptotically optimal.
  - Achieves same rate as optimal stochastic Newton method.

Stochastic Newton Methods?

- Should we use accelerated/Newton-like stochastic methods?
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- Should we use accelerated/Newton-like stochastic methods?
  - These do not improve the convergence rate.
- But some positive results exist.
  - Ghadimi & Lan [2010]:
    - Acceleration can improve dependence on L and μ.
    - Improves performance at start or if noise is small.
  - Duchi et al. [2010]:
    - Newton-like AdaGrad method,

$$x^{t+1} = x^t + \alpha D \nabla f_{i_t}(x^t), \quad \text{with } D_{jj} = \sqrt{\sum_{k=1}^{t} \|\nabla_j f_{i_k}(x^t)\|}.$$

    - improves regret bounds but not optimization error.
  - Bach & Moulines [2013]:
    - Newton-like method achieves $O(1/t)$ without strong-convexity. (under extra self-concordance assumption)

Outline

Big-N Problems

- Recall the regularized empirical risk minimization problem:

$$\underbrace{\min_{x \in \mathbb{R}^D} \frac{1}{N}\sum_{i=1}^{N} L(x, a_i, b_i)}_{\text{data fitting term}} \quad + \quad \underbrace{\lambda r(x)}_{\text{regularizer}}$$

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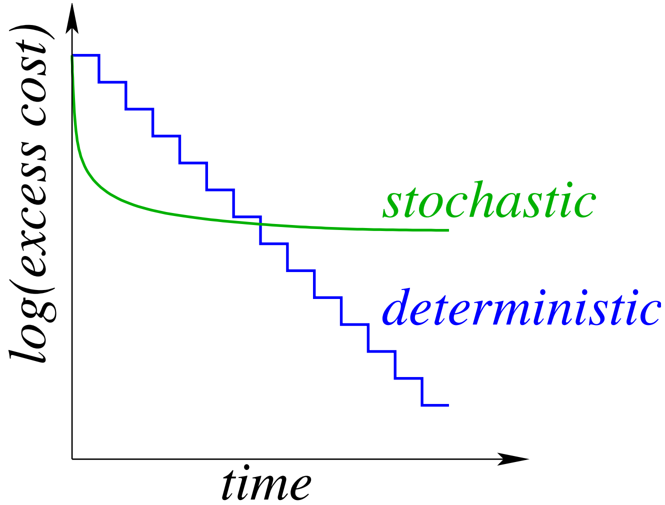
- For minimizing finite sums, can we design a better method?

Motivation for Hybrid Methods



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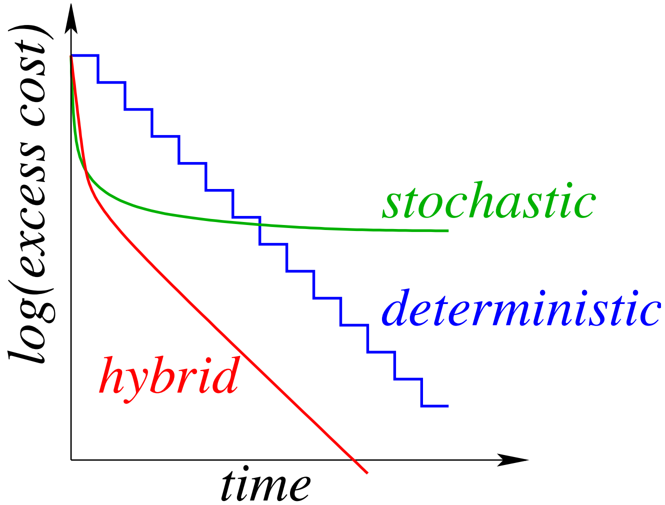

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- A common variant is to use larger sample $\mathcal{B}^t$,

$$\frac{1}{|\mathcal{B}^t|}\sum_{i\in\mathcal{B}^t}\nabla f_i(x^t) \approx \frac{1}{N}\sum_{i=1}^{N}\nabla f_i(x^t).$$

Approach 1: Batching

- The SG method with a sample $\mathcal{B}^t$ uses iterations

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- We can choose $|\mathcal{B}^t|$ to achieve a linear convergence rate:
  - Early iterations are cheap like SG iterations.
  - Later iterations can use a Newton-like method.

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  - Assumes gradients of non-selected examples don't change.
  - Assumption becomes accurate as $||x^{t+1} - x^t|| \to 0$.

Convergence Rate of SAG

- If each f_i' is $L-$continuous and f is strongly-convex, with $\alpha_t = 1/16L$ SAG has

$$\mathbb{E}[f(x^t) - f(x^*)] \leqslant \left(1 - \min\left\{\frac{\mu}{16L}, \frac{1}{8N}\right\}\right)^t C,$$

where

$$C = [f(x^0) - f(x^*)] + \frac{4L}{N}\|x^0 - x^*\|^2 + \frac{\sigma^2}{16L}.$$

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- Linear convergence rate but only 1 gradient per iteration.
  - For well-conditioned problems, constant reduction per pass:

$$\left(1 - \frac{1}{8N}\right)^N \leq \exp\left(-\frac{1}{8}\right) = 0.8825.$$

  - For ill-conditioned problems, almost same as deterministic method (but N times faster).

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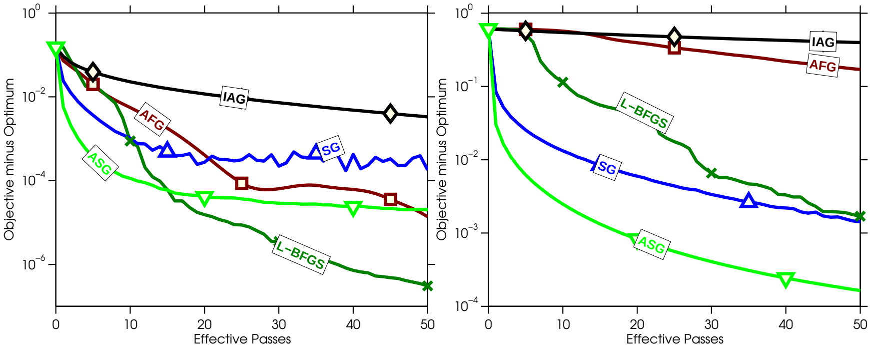
  - SAG: $O(\max\{N, \frac{L}{\mu}\}\log(1/\epsilon))$.

Comparing Deterministic and Stochatic Methods

- quantum ($n = 50000$, $p = 78$) and rcv1 ($n = 697641$, $p = 47236$)



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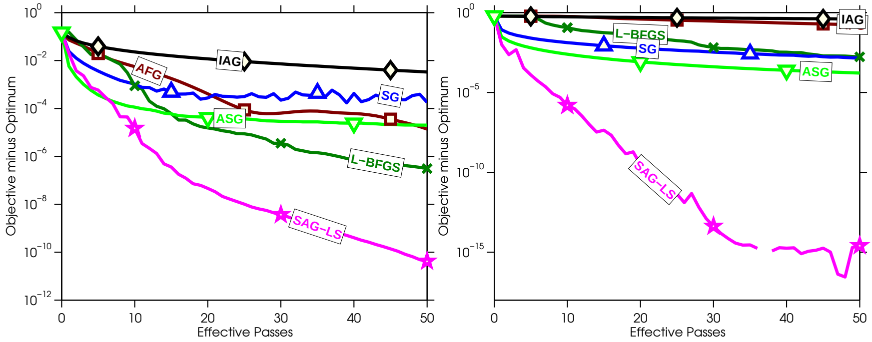

Other Linearly-Convergent Stochastic Methods

- Subsequent stochastic algorithms with linear rates:
  - Stochastic dual coordinate ascent [Shalev-Schwartz & Zhang, 2013]
  - Incremental surrogate optimization [Mairal, 2013].
  - Stochastic variance-reduced gradient (SVRG) [Johnson & Zhang, 2013, Konecny & Richtarik, 2013, Mahdavi et al., 2013, Zhang et al., 2013]
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  - SAGA [Defazio et al., 2014]
- SVRG has a much lower memory requirement (later in talk).
- There are also non-smooth extensions (last part of talk).

SAG Implementation Issues

- Basic SAG algorithm:
  - while(1)
  - Sample i from $\{1, 2, \ldots, N\}$.
  - Compute $f_i'(x)$.
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  - Adaptive non-uniform sampling [Schmidt et al., 2013].

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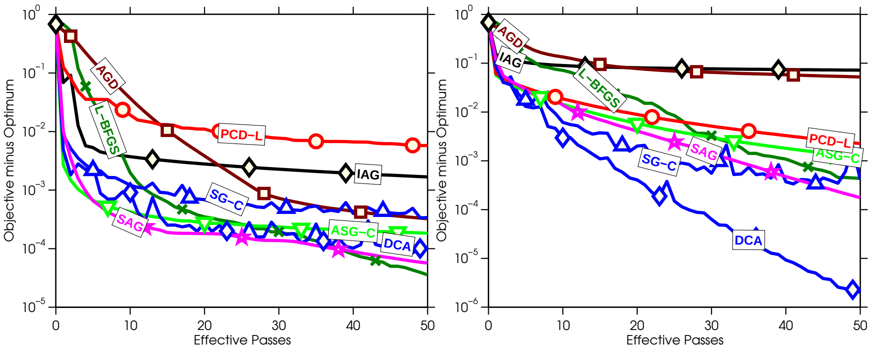
  - Adaptively estimate L_i as you go. (see paper/code).
  - Slowly learns to ignore well-classified examples.

SAG with Adaptive Non-Uniform Sampling

- protein ($n = 145751$, $p = 74$) and sido ($n = 12678$, $p = 4932$)



- Datasets where SAG had the worst relative performance.

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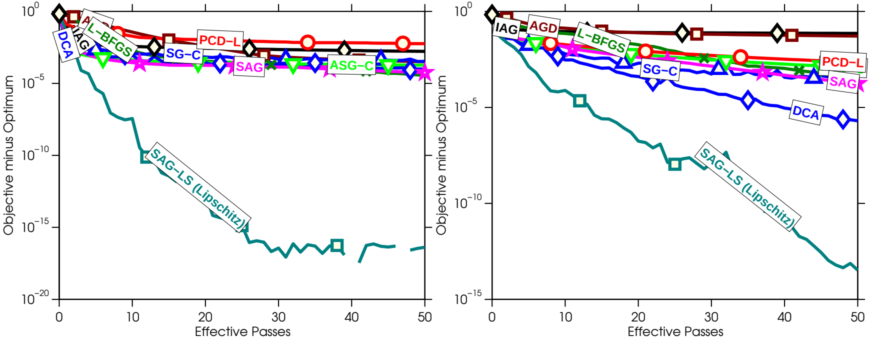

- Adaptive non-uniform sampling helps a lot.

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  3. Increase convergence rate.
     (classic SG methods: only changes constant)
- Convergence rate depends on L for mini-batches:
  - $L(\mathcal{B}) \leq L(i)$, possibly by up to $|\mathcal{B}|$.
  - Allows bigger step-size, $\alpha = 1/L(\mathcal{B})$.
  - Place examples in batches to make $L(\mathcal{B})$ small.

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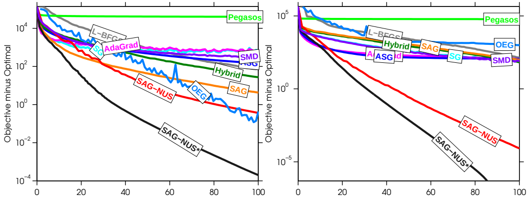

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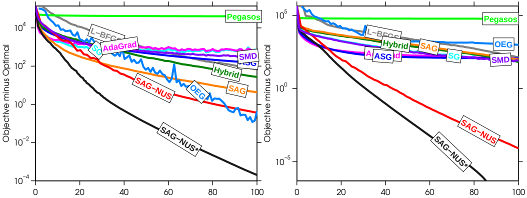

(optical character and named-entity recognition tasks)

- If the above don't work, use SVRG...

Stochastic Variance-Reduced Gradient

SVRG algorithm:

- Start with x_0
- for $s = 0, 1, 2 \ldots$
  - $d_s = \frac{1}{N} \sum_{i=1}^{N} f_i'(x_s)$
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    - Randomly pick $i_t \in \{1, 2, \ldots, N\}$
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Practical issues similar to SAG (acceleration versions, automatic step-size/termination, handles sparsity/regularization, non-uniform sampling, mini-batches).

Summary

Summary of Part 1:

- Part 1: Convex functions have special properties that allow us to efficiently minimize them.
- Part 2: Gradient-based methods allow scaling with dimensionality of problem.
- Part 3: Stochastic-gradient methods allow scaling with number of training examples, at cost of slower convergence rate.
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What is coming in Part 2:

- Can we beat subgradient methods for non-smooth problems?
- How do these optimization errors related to the test error?
- What can we say about non-convex problems?