Statistical Learning Models for Text and Graph Data Unconstrained Optimization Techniques

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*Contents are based on materials created by Peter Richtérik, Mark Schmidt, Francis Bach, Tianbao Yang, Rong Jin, Shenghuo Zhu, and Qihang Lin

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Reference Content

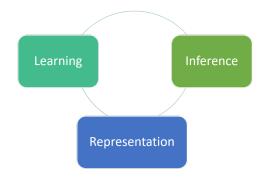
- Peter Richtérik and Mark Schmidt. ICML Tutorial on Modern Convex Optimization Methods for Large-scale Empirical Risk Minimization. https://icml.cc/2015/tutorials/2015_ICML_ ConvexOptimization_I.pdf
- Francis Bach. NIPS 2016 Tutorial on Large-Scale Optimization: Beyond Stochastic Gradient Descent and Convexity. http: //www.di.ens.fr/~fbach/fbach_tutorial_vr_nips_2016.pdf and http:

//www.di.ens.fr/~fbach/ssra_tutorial_vr_nips_2016.pdf

- Tianbao Yang, Qihang Lin, and Rong Jin. KDD Tutorial on Big Data Analytics: Optimization and Randomization. http://homepage.cs.uiowa.edu/~tyng/kdd15tutorial.html
- Tianbao Yang, Rong Jin and Shenghuo Zhu. SDM Tutorial on Stochastic Optimization for Big Data Analytics: Algorithms and Library.

http://homepage.divms.uiowa.edu/~tyng/tutorial.html

Course Organization



- Representation: language models, word embeddings, topic models, knowledge graphs
- Learning: supervised learning, semi-supervised learning, distant supervision, indirect supervision, sequence models, deep learning, optimization techniques
- Inference: constraint modeling, joint inference, search algorithms

Introduction

2 Background

Onconstrained Convex Optimization

- Gradient Based Optimization
- Stochastic Subgradient
- Finite-Sum Methods
- Non-Smooth Objectives

Optimization for Neural Networks

Introduction

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Optimization for Neural Networks

• We define a conditional log-linear model P(Y|X) as:

- \mathcal{Y} is the set of events (for language modeling, \mathcal{V})
- \mathcal{X} is the set of contexts (for n-gram language modeling, \mathcal{V}^{n-1})
- $\phi: \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^d$ is a feature vector function
- $\mathbf{w} \in \mathbb{R}^d$ are the model parameters

$$P_{\mathbf{w}}(Y = y | X = x) = \frac{\exp(\mathbf{w}^{\top} \phi(x, y))}{\sum_{y' \in \mathcal{Y}} \exp(\mathbf{w}^{\top} \phi(x, y'))}$$

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$$P_{\mathbf{w}}(Y = y | X = x) \triangleq P(Y = y | X = x, \mathbf{w})$$

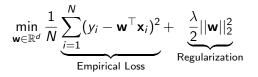
$$P_{\mathbf{w}}(Y = y | X = x) = \frac{\exp(\mathbf{w}^{\top} \phi(x, y))}{\sum_{y' \in \mathcal{Y}} \exp(\mathbf{w}^{\top} \phi(x, y'))}$$

- linear score $\mathbf{w}^{\top}\phi(x,y)$
- nonnegative $\exp(\mathbf{w}^{\top}\phi(x, y))$
- normalizer $\sum_{y' \in \mathcal{Y}} \exp(\mathbf{w}^{\top} \phi(x, y')) \triangleq Z_{\mathbf{w}}(x)$
- "Log-linear" comes from the fact that:

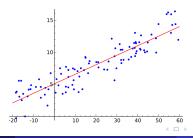
$$\log P_{\mathbf{w}}(Y = y | X = x) = \mathbf{w}^{\top} \phi(x, y) - \underbrace{\log Z_{\mathbf{w}}(x)}_{\text{constant in } y}$$

• This is an instance of the family of generalized linear models

Other Learning Problems: Least Square Regression



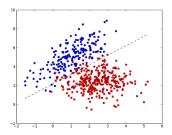
- $\mathbf{x}_i \in \mathbb{R}^d$: *d*-dimensional feature vector
- y_i: target variable
- $\mathbf{w} \in \mathbb{R}^d$: model parameters
- N: number of data points



Other Learning Problems: Classification

$$\min_{\mathbf{w}\in\mathbb{R}^d}\frac{1}{N}\sum_{i=1}^N\ell(y_i\mathbf{w}^\top\mathbf{x}_i)+\frac{\lambda}{2}||\mathbf{w}||_2^2$$

- $y_i \in \{+1, -1\}$
- Loss function $\ell(z)$, $z = y_i \mathbf{w}^\top \mathbf{x}_i$
 - SVMs: (squared) hinge loss $\ell(z) = \max(0, 1-z)^p$ where p = 1, 2
 - Logistic regression: $\ell(z) = \log(1 + exp(-z))$



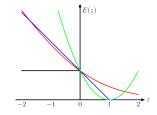
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Other Learning Problems: Logistic Regression

• Consider the case where $Y \in \{+1, -1\}$

$$P_{\mathbf{w}}(Y = +1|X = x) = \frac{\exp(\mathbf{w}^{\top}\phi(x,+1))}{\exp(\mathbf{w}^{\top}\phi(x,+1)) + \exp(\mathbf{w}^{\top}\phi(x,-1))}$$
$$= \frac{1}{1 + \exp(\mathbf{w}^{\top}(\phi(x,-1) - \phi(x,+1)))}$$
$$= \sigma(\mathbf{w}^{\top}\phi(x,+1) - \phi(x,-1))$$
$$= \sigma(\mathbf{y}\mathbf{w}^{\top}\mathbf{f}(x))$$

where $\sigma(z) = \frac{1}{1+e^{-z}}$ is logistic function



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Other Learning Problems: Feature Selection

$$\min_{\mathbf{w} \in \mathbb{R}^d} \frac{1}{N} \sum_{i=1}^N \ell(y_i \mathbf{w}^\top \mathbf{x}_i) + \lambda ||\mathbf{w}||_1$$

- ℓ_1 regularization: $||\mathbf{w}||_1 = \sum_{i=1}^d |w_i|$
- λ controls sparsity level

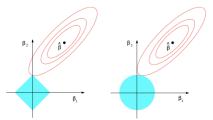


FIGURE 3.11. Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions $|\beta_1| + |\beta_2| \leq t$ and $\beta_1^2 + \beta_2^2 \leq t^2$, respectively, while the red ellipses are the contours of the least squares error function.

(Elements of Statistical Learning by Hastie, Tibshirani, and Friedman)

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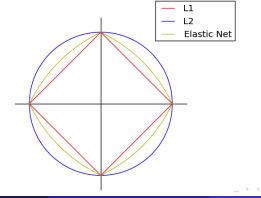
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Other Learning Problems: Feature Selection

Feature Selection using Elastic Net

$$\min_{\mathbf{w}\in\mathbb{R}^d}\frac{1}{N}\sum_{i=1}^N\ell(y_i\mathbf{w}^{\top}\mathbf{x}_i)+\lambda(||\mathbf{w}||_1+\gamma||\mathbf{w}||_2^2)$$

• Elastic net regularizer, more robust than ℓ_1 regularizer



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Why (Unconstrained) Stochastic Optimization?

Big data challenge

- Google processes 5.13B queries/day (2013)
- Twitter receives 340M tweets/day (2012)
- Facebook has 2.5 PB of user data + 15 TB/day (4/2009) (1PB=1015bytes=1000terabytes)
- eBay has 6.5 PB of user data + 50 TB/day (5/2009)
- Foundation of deep learning optimization

- Too many data points
 - Issue: can't afford go through data set many times
 - Solution: Stochastic Optimization
- High dimensional data
 - Issue: can't afford second order optimization (Newton's method)
 - Solution: first order method (i.e., gradient based method)

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Optimization for Neural Networks

• Bold letters $\mathbf{x} \in \mathbb{R}^d$ (data vector), $\mathbf{w} \in \mathbb{R}^d$ (model parameter): *d*-dimensional vectors, y_i denotes response variable of *i*th data

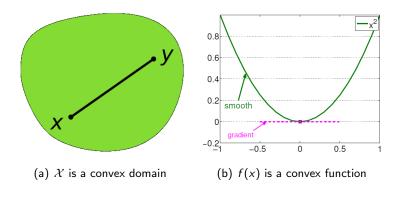
 $\bullet~ \textbf{w}, \textbf{w}' \in \mathcal{X}$ finite dimensional variable, \mathcal{X} a normed space

• Norm
$$\|\mathbf{w}\| : \mathbb{R}^d \to \mathbb{R}_+$$
, e.g.,
• ℓ_1 norm: $\|\mathbf{w}\|_1 = \sum_i |w_i|$
• ℓ_2 norm: $\|\mathbf{w}\|_2 = \sqrt{\sum_i w_i^2}$
• ℓ_∞ norm: $\|\mathbf{w}\|_\infty = \max_i |w_i|$

• Inner product
$$\langle \mathbf{w}, \mathbf{w} \rangle = \mathbf{w}^\top \mathbf{w} = \sum_{i=1}^d x_i \cdot w_i$$

Convex Optimization

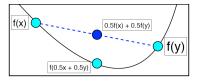
 $\mathbf{w} = \arg\min_{\mathbf{w}\in\mathcal{X}} f(\mathbf{w})$



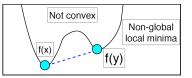
Convex Function: Three Characterizations (1)

A function f is convex if for all \mathbf{w}_x and \mathbf{w}_y we have

 $f(\alpha \mathbf{w}_{x} + (1 - \alpha)\mathbf{w}_{y}) \leq \alpha f(\mathbf{w}_{x}) + (1 - \alpha)f(\mathbf{w}_{y}), \forall \mathbf{w}_{x}, \mathbf{w}_{y} \in \mathcal{X}, \alpha \in [0, 1]$

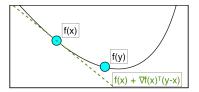


- Function is below linear interpolation between \mathbf{w}_{x} and \mathbf{w}_{y}
- Implies that all local minima are global minima



A function f is convex if for all \mathbf{w}_{x} and \mathbf{w}_{y} we have

$$f(\mathbf{w}_y) \geq f(\mathbf{w}_x) + \nabla f(\mathbf{w}_x)^{\top} (\mathbf{w}_y - \mathbf{w}_x)^{\top}$$



- The function is globally above the tangent at **w**_x (first-order condition, differentiable *f* with convex domain)
- If $\nabla f(\mathbf{w}_x) = 0$, implies \mathbf{w}_x is a global minimizer

A twice-differentiable function f is convex if for all \mathbf{w} we have

 $\nabla^2 f(\mathbf{w}) \succeq 0$

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

Convergence Measure

• Most optimization algorithms are iterative

$$\mathbf{w}_{t+1} = \mathbf{w}_t - \Delta \mathbf{w}_t$$

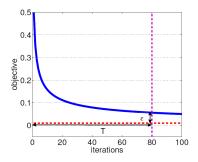
• Convergence Rate: after *T* iterations, how good is the solution

$$f(\mathbf{w}_T) - \min_{\mathbf{w} \in \mathcal{X}} f(\mathbf{w}) \le \epsilon(T)$$

 Iteration Complexity: the number of iterations T(e) needed to have

$$f(\mathbf{w}_{\mathcal{T}}) - \min_{\mathbf{w}\in\mathcal{X}} f(\mathbf{w}) \le \epsilon \quad (\epsilon \ll 1)$$

• Total Runtime = Per-iteration Cost×Iteration Complexity



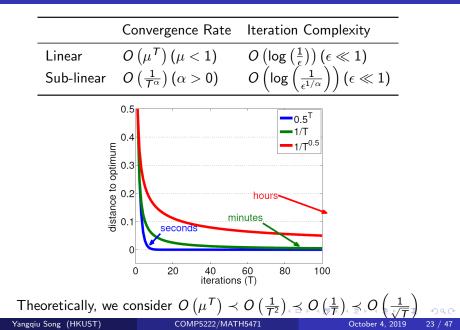
Convergence Rate: after T iterations, how good is the solution Iteration Complexity: the number of iterations $T(\epsilon)$ needed to have

• Big $O(\cdot)$ notation: explicit dependence on T or ϵ

| | Convergence Rate | Iteration Complexity |
|------------|---|---|
| Linear | $O\left(\mu^{\mathcal{T}} ight)\left(\mu < 1 ight)$ | $O\left(\log\left(rac{1}{\epsilon} ight) ight)(\epsilon\ll1)$ |
| Sub-linear | $O\left(\frac{1}{T^{\alpha}}\right)(\alpha > 0)$ | $egin{aligned} &O\left(\log\left(rac{1}{\epsilon} ight) ight)(\epsilon\ll1)\ &O\left(\log\left(rac{1}{\epsilon^{1/lpha}} ight) ight)(\epsilon\ll1) \end{aligned}$ |

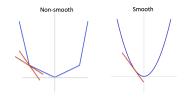
Why are we interested in Bounds?

Why Are We Interested in Bounds?

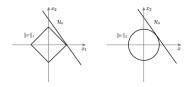


Factors that affect Iteration Complexity

• Property of function: e.g., smoothness of function



• Domain \mathcal{X} : size and geometry



• Size of problem: dimension and number of data points

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Gradient Based Optimization

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Optimization for Neural Networks

- Among only efficiently-solvable continuous problems
- You can do a lot with convex models: least squares, lasso, generlized linear models, SVMs, CRFs, etc.
- Empirically effective non-convex methods are often based on methods with good properties for convex objectives (functions are locally convex around minimizers)
- Tools from convex analysis are being extended to non-convex

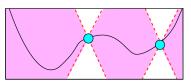
How Hard Is Real-valued Optimization?

How long to find an ϵ -optimal minimizer of a real-valued function?

 $\min_{\mathbf{w}\in\mathbb{R}^d}f(\mathbf{w})$

- General function: impossible!
- We need to make some assumptions about the function:
 - Assume f is Lipschitz-continuous: (can not change too quickly)

$$|f(\mathbf{w}) - f(\mathbf{w}')| \leq L \|\mathbf{w} - \mathbf{w}'\|$$



- After T iterations, the error of any algorithm is $O(\frac{1}{T^{1/d}})$ (and grid-search is nearly optimal)
- Optimization is hard, but assumptions make a big difference (we went from impossible to very slow)

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- We can solve convex optimization problems in polynomial-time by interior-point methods
- But these solvers require $O(d^2)$ or worse cost per iteration
 - Infeasible for applications where d may be in the billions
- Large-scale problems have renewed interest gradient methods:

$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta^t \nabla f(\mathbf{w}^t)$$

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

Logistic Regression with ℓ_2 -Norm Regularization

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

$$f(\mathbf{w}) = \sum_{i=1}^{N} \log(1 + \exp(-y_i(\mathbf{w}^{\top} \mathbf{x}_i))) + \frac{\lambda}{2} \|\mathbf{w}\|_2^2$$

- Objective f is convex
- First term is Lipschitz continuous, second term is not
- But we have

$$\mu$$
I $\preceq \nabla^2 f(\mathbf{w}) \preceq L$ *I*

for some μ and L; I is a diagonal matrix

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

Properties of Lipschitz-Continuous Gradient

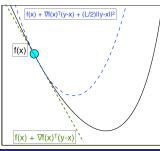
• From Taylor's theorem, for some z we have:

$$f(\mathbf{w}') = f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top} (\mathbf{w}' - \mathbf{w}) + \frac{1}{2} (\mathbf{w}' - \mathbf{w})^{\top} \nabla^2 f(\mathbf{z}) (\mathbf{w}' - \mathbf{w})$$

• Use that $\nabla^2 f(\mathbf{w}) \preceq LI$

$$f(\mathbf{w}') \leq f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top} (\mathbf{w}' - \mathbf{w}) + \frac{L}{2} \|\mathbf{w}' - \mathbf{w}\|^2$$

• Global quadratic upper bound on function value



Properties of Lipschitz-Continuous Gradient

$$f(\mathbf{w}') \leq f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top} (\mathbf{w}' - \mathbf{w}) + \frac{L}{2} \|\mathbf{w}' - \mathbf{w}\|^2$$

 Variant of gradient method if we set w^{t+1} to minimum w' value (right side gradient (w') = 0):

$$\mathbf{w}^{t+1} = \arg\min_{\mathbf{w}'} \{f(\mathbf{w}^t) + \nabla f(\mathbf{w}^t)^\top (\mathbf{w}' - \mathbf{w}^t) + \frac{L}{2} \|\mathbf{w}' - \mathbf{w}^t\|^2 \}$$

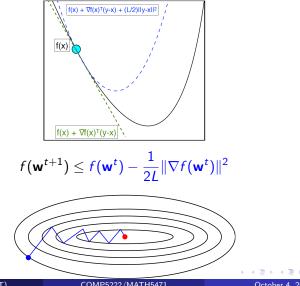
$$\Rightarrow \mathbf{w}^{t+1} = \mathbf{w}^t - \frac{1}{L} \nabla f(\mathbf{w}^t)$$

Plugging this value in:

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

Properties of Lipschitz-Continuous Gradient

Guaranteed decrease of objective



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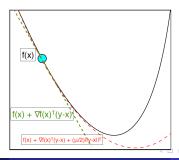
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Properties of Strong-Convexity

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

$$f(\mathbf{w}') = f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top} (\mathbf{w}' - \mathbf{w}) + \frac{1}{2} (\mathbf{w}' - \mathbf{w})^{\top} \nabla^2 f(\mathbf{z}) (\mathbf{w}' - \mathbf{w})$$

- Use that $\mu I \preceq \nabla^2 f(\mathbf{w})$ $f(\mathbf{w}) + \nabla f(\mathbf{w})^\top (\mathbf{w}' - \mathbf{w}) + \frac{\mu}{2} \|\mathbf{w}' - \mathbf{w}\|^2 \leq f(\mathbf{w}')$
- Global quadratic lower bound on function value



$$f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top}(\mathbf{w}' - \mathbf{w}) + \frac{\mu}{2} \|\mathbf{w}' - \mathbf{w}\|^2 \le f(\mathbf{w}')$$

 $\bullet\,$ Minimizing both sides in terms of w' gives

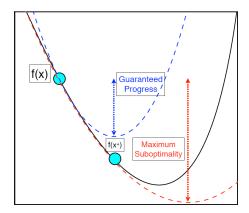
$$f(\mathbf{w}^*) \ge f(\mathbf{w}^t) - \frac{1}{2\mu} \|\nabla f(\mathbf{w}^t)\|^2$$

• Upper bound on how far we are from the solution

Linear Convergence of Gradient Descent

• We have bounds on **w**^{t+1} and **w**^{*}:

 $f(\mathbf{w}^{t+1}) \leq f(\mathbf{w}^t) - \frac{1}{2L} \|\nabla f(\mathbf{w}^t)\|^2 \qquad f(\mathbf{w}^*) \geq f(\mathbf{w}^t) - \frac{1}{2\mu} \|\nabla f(\mathbf{w}^t)\|^2$



Linear Convergence of Gradient Descent

• We have bounds on \mathbf{w}^{t+1} and \mathbf{w}^* :

 $f(\mathbf{w}^{t+1}) \leq f(\mathbf{w}^t) - \frac{1}{2L} \|\nabla f(\mathbf{w}^t)\|^2 \qquad f(\mathbf{w}^*) \geq f(\mathbf{w}^t) - \frac{1}{2\mu} \|\nabla f(\mathbf{w}^t)\|^2$

• Combine them we have:

$$f(\mathbf{w}^{t+1}) - f(\mathbf{w}^*) \le \left(1 - \frac{\mu}{L}\right) \left[f(\mathbf{w}^t) - f(\mathbf{w}^*)\right]$$

• This gives a linear convergence rate:

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

 Each iteration multiplies the error by a fixed amount (very fast if μ/L is not too close to zero)

Maximum Likelihood Logistic Regression

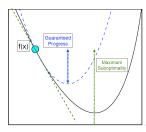
• What about maximum-likelihood logistic regression?

$$f(\mathbf{w}) = \sum_{i=1}^{N} \log(1 + \exp(-y_i(\mathbf{w}^{\top} \mathbf{x}_i)))$$

• We now only have

$$0 \preceq \nabla^2 f(\mathbf{w}) \preceq L I$$

• Convexity only gives a linear upper bound on $f(\mathbf{w}^*)$: $f(\mathbf{w}^*) \ge f(\mathbf{w}) + \nabla f(\mathbf{w})^\top (\mathbf{w}^* - \mathbf{w})$



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Maximum Likelihood Logistic Regression

• What about maximum-likelihood logistic regression?

$$f(\mathbf{w}) = \sum_{i=1}^{N} \log(1 + \exp(-y_i(\mathbf{w}^{\top} \mathbf{x}_i)))$$

We now only have

$$0 \preceq \nabla^2 f(\mathbf{w}) \preceq LI$$

• Convexity only gives a linear upper bound on $f(\mathbf{w}^*)$:

$$f(\mathbf{w}^*) \ge f(\mathbf{w}) + \nabla f(\mathbf{w})^\top (\mathbf{w}^* - \mathbf{w})$$

• If w* exists, we have the sublinear convergence rate:

$$f(\mathbf{w}^t) - f(\mathbf{w}^*) = O(1/t)$$

(compare to slower $O(\frac{1}{T^{1/d}})$ for general Lipschitz functions) Proof: http://www.stat.cmu.edu/-ryantibs/convexopt-F13/scribes/lec6.pdf • If f is convex, then $f + \lambda ||\mathbf{w}||^2$ is strongly-convex.

Gradient Method: Practical Issues

- In practice, searching for step size (line-search) is usually much faster than $\eta = 1/L$ (and doesn't require knowledge of L)
- Basic Armijo backtracking line-search:
 - 1~ Start with a large value of η
 - 2 Divide η in half until we satisfy (typically value is $\gamma = 0.0001$):

$$f(\mathbf{w}^{t+1}) \leq f(\mathbf{w}^t) - \gamma \eta \|
abla f(\mathbf{w}^t) \|^2$$

• Also, check your derivative code:

$$abla f_i(\mathbf{w}) pprox rac{f(\mathbf{w} + \delta \mathbf{e}_i) - f(\mathbf{w})}{\delta}$$

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

$$\nabla f(\mathbf{w})^{\top} \mathbf{d} \approx \frac{f(\mathbf{w} + \delta \mathbf{d}) - f(\mathbf{w})}{\delta}$$

Accelerated Gradient Method

- Is this the best algorithm under these assumptions?
- Nesterov's accelerated gradient method (Nesterov (1983)):

$$\mathbf{w}^{t+1} = \mathbf{v}^t - \eta^t \nabla f(\mathbf{v}^t), \quad \mathbf{v}^{t+1} = \mathbf{w}^t + \beta^t (\mathbf{w}^{t+1} - \mathbf{w}^t)$$

| Algorithm | Assumptions | Rate |
|-----------|-----------------|-----------------------------|
| Gradient | Convex | $O(\frac{1}{T})$ |
| Nesterov | Convex | $O(\frac{1}{T^2})$ |
| Gradient | Strongly-Convex | $O((1-\mu/L)^{\top})$ |
| Nesterov | Strongly-Convex | $O((1-\sqrt{\mu/L})^{	op})$ |

- For logistic regression and many other losses, we can get linear convergence without strong-convexity (Luo and Tseng (1993))
- Nesterovs method is much more general than linear CG
- Linear CG is much faster than Nesterov for convex quadratics
- Nonlinear CG is typically faster than Nesterov but has no complexity guarantees and sometimes fails

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- The oldest differentiable optimization method is Newton's
- Modern form uses the update

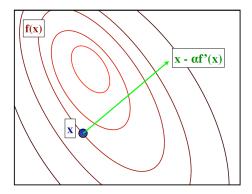
$$\mathbf{w}^{t+1} = \mathbf{w}^t - \eta \mathbf{d}$$

where \boldsymbol{d} is a solution to the system

$$abla^2 f(\mathbf{w}) \mathbf{d} =
abla f(\mathbf{w}) \ (
abla^2 f(\mathbf{w}) \succ 0)$$

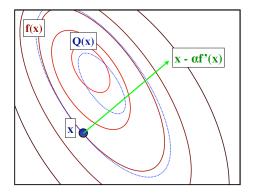
• Equivalent to minimizing the quadratic approximation:

$$f(\mathbf{w}') \approx f(\mathbf{w}) + \nabla f(\mathbf{w})^{\top} (\mathbf{w}' - \mathbf{w}) + \frac{1}{2\eta} \|\mathbf{w}' - \mathbf{w}\|_{\nabla^2 f(\mathbf{w})}^2 (\|\mathbf{w}\|_{\mathbf{H}}^2 = \mathbf{w}^{\top} \mathbf{H} \mathbf{w})$$



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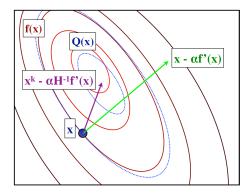
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 If ∇² f(w) is Lipschitz-continuous and ∇² f(w) ≽ µ, then close to w* Newton's method has local superlinear convergence:

$$f(\mathbf{w}^{t+1} - \mathbf{w}^*) \leq
ho^t [f(\mathbf{w}^t - \mathbf{w}^*)]$$

with $\lim_{t\to\infty} \rho^t = 0$

- Converges very fast, use it if you can!
- But requires solving $\nabla^2 f(\mathbf{w})\mathbf{d} = \nabla f(\mathbf{w})$

There are many practical variants of Newton's method:

- Modify the Hessian to be positive-definite.
- Only compute the Hessian every m iterations.
- Only use the diagonals of the Hessian.
- Quasi-Newton: Update a (diagonal plus low-rank) approximation of the Hessian (BFGS, L-BFGS).
- Hessian-free: Compute **d** inexactly using Hessian-vector products:

$$abla^2 f(\mathbf{w}) \mathbf{d} pprox \lim_{\delta o 0} rac{
abla f(\mathbf{w} + \delta \mathbf{d}) -
abla f(\mathbf{w})}{\delta}$$

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