CPSC 540: Machine Learning

Subgradients and Projected Gradient

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Admin

- Auditting/registration:
  - Today is last day to add/drop.
- Assignment 1:
  - 1 late day to hand in tonight, 2 late days for Wednesday.
- No tutorial this week.

Last Time: Iteration Complexity

- We discussed the iteration complexity of an algorithm for a problem class:
  - "How many iterations t before we guarantee an accuracy ϵ"?

- Iteration complexity of gradient descent when ∇f is Lipschitz continuous:

Assumption	Iteration Complexity	Quantity
Non-Convex	$t = O(1/\epsilon)$	$\min_{k=0,2,\ldots,t-1} \|\nabla f(w^k)\|^2 \leq \epsilon$
Convex	$t = O(1/\epsilon)$	$f(w^t) - f^* \leq \epsilon$
Strongly-Convex	$t = O(\log(1/\epsilon))$	$f(w^t) - f^* \leq \epsilon$

- Adding L2-regularization to a convex function gives a strongly-convex function.
  - So L2-regularization can make gradient descent converge much faster.

Nesterov Acceleration (Strongly-Convex Case)

- We showed that gradient descent for strongly-convex functions has

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

- Applying accelerated gradient methods to strongly-convex gives

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

  which is a faster linear convergence rate
  $(\alpha_k = 1/L, \beta_k = (\sqrt{L} - \sqrt{\mu})/(\sqrt{L} + \sqrt{\mu}))$.

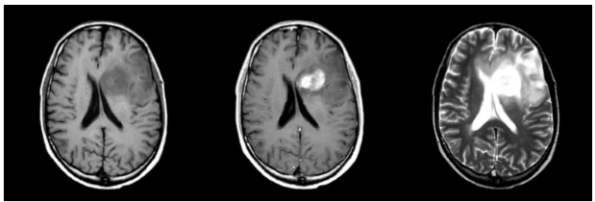
- This nearly acheives optimal possible dimension-independent rate.

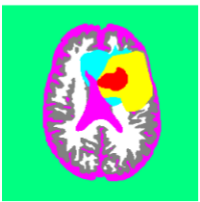
Newton and Newton-Like Algorithms

- Alternately, Newton's method achieves superlinear convergence rate.
  - Under strong-convexity and using both ∇f and $\nabla^2 f$ being Lipschitz.
  - But unfortunately this gives a superlinear iteration cost.
- There are linear-time approximations to Newton (see bonus):
  - Barzilai-Borwein step-size for gradient descent (findMin.jl).
  - Limited-memory Quasi-Newton methods like L-BFGS.
  - Hessian-free Newton methods (uses conjugate gradient to compute Newton step).
- Work amazing for many problems, but don't achieve superlinear convergence.

Motivation: Automatic Brain Tumour Segmentation

- Task: identifying tumours in multi-modal MRI data.

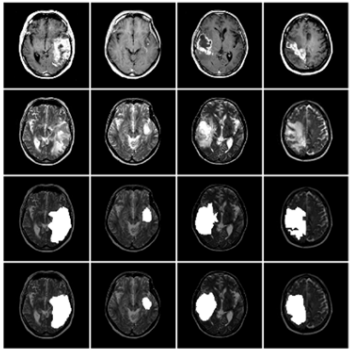


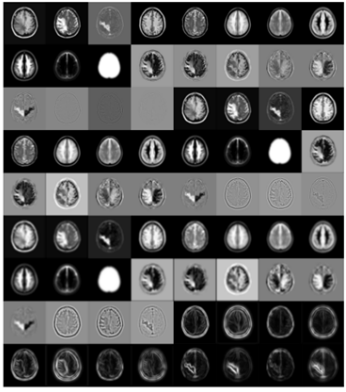


- Applications:
  - Image-guided surgery.
  - Radiation target planning.
  - Quantifying treatment response.
  - Discovering growth patterns.

Motivation: Automatic Brain Tumour Segmentation

- Formulate as supervised learning:
  - Pixel-level classifier that predicts "tumour" or "non-tumour".
  - Features: convolutions, expected values (in aligned template), and symmetry.
    - All at multiple scales.





Motivation: Automatic Brain Tumour Segmentation

- Logistic regression was among most effective models, with the right features.
- But if you used all features, it overfit.
  - We needed feature selection.

- Classical approach:
  - Define some score: AIC, BIC, cross-validation error, etc.
  - Search for features that optimize score:
    - Usually NP-hard, so we use greedy: forward selection, backward selection,...
  - In brain tumour application, even greedy methods were too slow.
    - Just one image gives 8 million training examples.

Feature Selection

- General feature selection problem:
  - Given our usual X and y, we'll use x_j to represent column j:

$$X = \begin{bmatrix} | & | & & | \\ x_1 & x_2 & \cdots & x_d \\ | & | & & | \end{bmatrix}, \quad y = \begin{bmatrix} | \\ y \\ | \end{bmatrix}.$$

  - We think some features/columns x_j are irrelevant for predicting y.
- We want to fit a model that uses the "best" set of features.

- One of most important problems in ML/statistics, but very very messy.
  - In 340 we saw how difficult it is to define what "relevant" means.

L1-Regularization

- A popular appraoch to feature selection we saw in 340 is L1-regularization:

$$F(w) = f(w) + \lambda \|w\|_1.$$

- Advantages:
  - Fast: can apply to large datasets, just minimizing one function.
    - Convex if f is convex.
  - Reduces overfitting because it simultaneously regularizes.
- Disadvantages:
  - Prone to false positives, particularly if you pick λ by cross-validation.
  - Not unique: there may be infinite solutions.

- There exist many extensions:
  - "Elastic net" adds L2-regularization to make solution unique.
  - "Bolasso" applies this on bootstrap samples to reduce false positives.
  - Non-convex regularizers reduce false positives but are NP-hard.

L1-Regularization

- Key property of L1-regularization: if λ is large, solution w^* is sparse:
  - w^* has many values that are exactly zero.

- How setting variables to exactly 0 performs feature selection in linear models:

$$\hat{y}^i = w_1 x_1^i + w_2 x_2^i + w_3 x_3^i + w_4 x_4^i + w_5 x_5^i.$$

- If $w = \begin{bmatrix} 0 & 0 & 3 & 0 & -2 \end{bmatrix}^\top$ then:

$$\begin{aligned} \hat{y}^i &= 0x_1^i + 0x_2^i + 3x_3^i + 0x_4^i + (-2)x_5^i \\ &= 3x_3^i - 2x_5^i. \end{aligned}$$

- Features $\{1, 2, 4\}$ are not used in making predictions: we "selected" $\{2, 5\}$.
  - To understand why variables are set to exactly 0, we need the notion of subgradient.

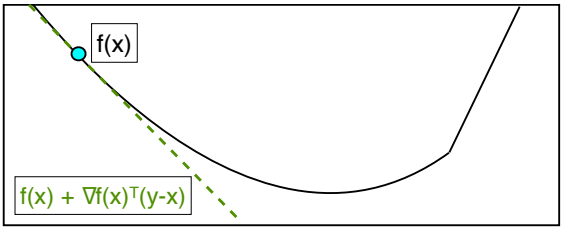
Sub-Gradients and Sub-Differentials

Differentiable convex functions are always above tangent,

$$f(v) \geq f(w) + \nabla f(w)^\top (v - w), \forall w, v.$$

A vector d is a subgradient of a convex function f at w if

$$f(v) \geq f(w) + d^\top (v - w), \forall v.$$



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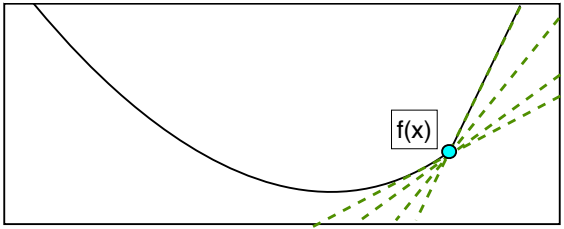


Sub-Gradients and Sub-Differentials Properties

- We can have a set of subgradients called the sub-differential, $\partial f(w)$.
  - Subdifferential is all the possible "tangent" lines.

- For convex functions:
  - Sub-differential is always non-empty (except some weird degenerate cases).
  - At differentiable w, the only subgradient is the gradient.
  - At non-differentiable w, there will be a convex set of subgradients.

  - We have $0 \in \partial f(w)$ iff w is a global minimum.
    - This generalizes the condition that $\nabla f(w) = 0$ for differentiable functions.

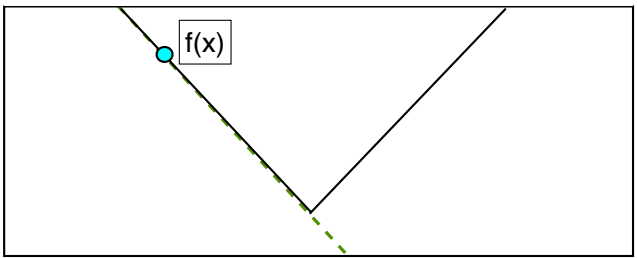
- For non-convex functions:
  - "Global" subgradients may not exist for every w.
  - Instead, we define subgradients "locally" around current w.
    - This is how you define "gradient" of ReLU function in neural networks.

Example: Sub-Differential of Absolute Function

- Sub-differential of absolute value function:

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

  - "Sign of the variable if it's non-zero, anything in $[-1, 1]$ if it's zero."



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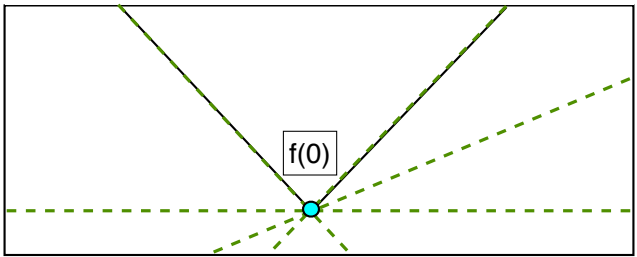


Sub-Differential of Common Operations

- Two convenient rules for calculating subgradients of convex functions:
  - Sub-differential of max is all convex combinations of argmax gradients:

$$\partial \max\{f_1(x), f_2(x)\} = \begin{cases} \nabla f_1(x) & f_1(x) > f_2(x) \\ \nabla f_2(x) & f_2(x) > f_1(x) \\ \underbrace{\theta \nabla f_1(x) + (1-\theta)\nabla f_2(x)}_{\text{for all } 0 \leq \theta \leq 1} & f_1(x) = f_2(x) \end{cases}$$

    - This rules gives sub-differential of absolute value, using that $|\alpha| = \max\{\alpha, -\alpha\}$.

  - Sub-differential of sum is all sum of subgradients of individual functions:

$$\partial(f_1(x) + f_2(x)) = d_1 + d_2 \quad \text{for any} \quad d_1 \in \partial f_1(x), d_2 \in \partial f_2(x).$$

  - Sub-differential of composition with affine function works like the chain rule:

$$\partial f_1(Aw) = A^\top \partial f_1(z), \quad \text{where} \quad z = Aw,$$

    and we also have $\partial \alpha f(w) = \alpha \partial f(w)$ for $\alpha > 0$.

Why does L1-Regularization but not L2-Regularization give Sparsity?

- Consider L2-regularized least squares,

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|^2.$$

- Element j of the gradient at $w_j = 0$ is given by

$$\nabla_j f(w) = x_j^\top \underbrace{(Xw - y)}_{r} + \lambda 0.$$

- For $w_j = 0$ to be a solution, we need $0 = \nabla_j f(w^*)$ or that

$$0 = x_j^\top r^* \quad \text{where } r^* = Xw^* - y \text{ for the solution } w^*$$

that column j is orthogonal to the final residual.

  - This is possible, but it is very unlikely (probability 0 for random data).
  - Increasing λ doesn't help.

Why does L1-Regularization but not L2-Regularization give Sparsity?

- Consider L1-regularized least squares,

$$f(w) = \frac{1}{2}\|Xw - y\|^2 + \frac{\lambda}{2}\|w\|_1.$$

- Element j of the subdifferential at $w_j = 0$ is given by

$$\partial_j f(w) \equiv x_j^\top \underbrace{(Xw - y)}_{r} + \lambda \underbrace{[-1, 1]}_{\partial|w_j|}.$$

- For $w_j = 0$ to be a solution, we need $0 \in \partial_j f(w^*)$ or that

$$\begin{aligned} 0 &\in x_j^T r^* + \lambda[-1, 1] && \text{or equivalently} \\ -x_j^T r^* &\in \lambda[-1, 1] && \text{or equivalently} \\ |x_j^\top r^*| &\leq \lambda, \end{aligned}$$

that column j is "close to" orthogonal to the final residual.

  - So features j that have little to do with y will often lead to $w_j = 0$.
  - Increasing λ makes this more likely to happen.

Outline

1 L1-Regularization and Sub-Gradients

2 Projected-Gradient Methods

Solving L1-Regularization Problems

- How can we minimize non-smooth L1-regularized objectives?

$$\underset{w \in \mathbb{R}^d}{\text{argmin}} \frac{1}{2}\|Xw - y\|^2 + \lambda\|w\|_1.$$

- Use our trick to formulate as a quadratic program?
  - $O(d^2)$ or worse.
- Make a smooth approximation to the L1-norm?
  - Destroys sparsity (we'll again just have one subgradient at zero).

- Use a subgradient method?

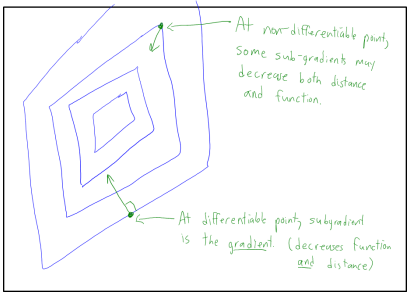
Subgradient Method

- The basic subgradient method:

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

for some $g_k \in \partial f(w^k)$.

- This can increase the objective even for small α_k.
  - Though for convex f the distance to solutions decreases:
    - $\|w^{k+1} - w^*\| < \|w^k - w^*\|$ for small enough α_k.



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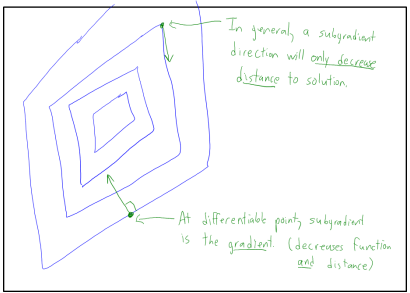

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- This can increase the objective even for small α_k.
  - Though for convex f the distance to solutions decreases:
    - $\|w^{k+1} - w^*\| < \|w^k - w^*\|$ for small enough α_k.

- The subgradients g_k don't necessarily converge to 0 as we approach a w^*.
  - If we are at a solution w^*, we might move away from it.
  - So as in stochastic gradient, we need decreasing step-sizes like

$$\alpha_k = O(1/k), \quad \text{or} \quad \alpha_k = O(1/\sqrt{k}),$$

in order to converge.
  - This destroys performance.

Convergence Rate of Subgradient Methods

- Subgradient methods are slower than gradient descent:

Assumption	Gradient	Subgradient	Quantity
Convex	$O(1/\epsilon)$	$O(1/\epsilon^2)$	$f(w^t) - f^* \leq \epsilon$
Strongly-Convex	$O(\log(1/\epsilon))$	$O(1/\epsilon)$	$f(w^t) - f^* \leq \epsilon$

- Other subgradient-based methods are not faster.
  - There are matching lower bounds in dimension-independent setting.
  - Includes cutting plane and bundle methods.

- Also, acceleration doesn't improve subgradient rates.
  - We do NOT go from $O(1/\epsilon^2)$ to $O(1/\epsilon)$ by adding momentum.

- Smoothing f and applying gradient descent doesn't help.
  - May need to have $L = 1/\epsilon$ in a sufficiently-accurate smooth approximation.
  - However, if you smooth and accelerate you can close the gaps a bit (bonus).

The Key to Faster Methods

- How can we achieve the speed of gradient descent on non-smooth problems?
  - Make extra assumptions about the function/algorithm f.

- For L1-regularized least squares, we'll use that the objective has the form

$$F(w) = \underbrace{f(w)}_{\text{smooth}} + \underbrace{r(w)}_{\text{"simple"}},$$

  that it's the sum of a smooth function and a "simple" function.
  - We'll define "simple" later, but simple functions can be non-smooth.

- Proximal-gradient methods have rates of gradient descent for such problems.
  - A generalization of projected gradient methods.

Projected-Gradient for Non-Negative Constraints

- We used projected gradient in 340 for NMF to find non-negative solutions,

$$\underset{w \geq 0}{\text{argmin}}\, f(w).$$

- In this case the algorithm has a simple form,

$$w^{k+1} = \max\{0, \underbrace{w^k - \alpha_k \nabla f(w^k)}_{\text{gradient descent}}\},$$

  where the $\max$ is taken element-wise.
  - "Do a gradient descent step, set negative values to 0."

- An obvious algorithm to try, and works as well as unconstrained gradient descent.

A Broken "Projected-Gradient" Algorithms

- Projected-gradient addresses problem of minimizing smooth f over a convex set $\mathcal{C}$,

$$\operatorname*{argmin}_{w \in \mathcal{C}} f(w).$$

- As another example, we often want w to be a probability,

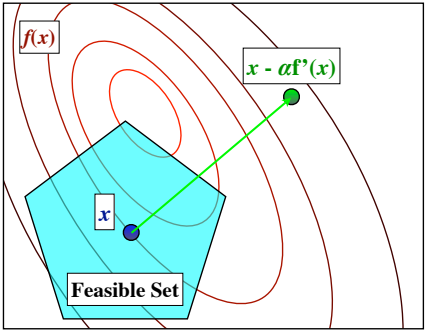
$$\operatorname*{argmin}_{w \geq 0,\ 1^\top w = 1} f(w),$$

- Based on our "set negative values to 0" intuition, we might consider this:
  1. Perform an unconstrained gradient descent step.
  2. Set negative values to 0 and divide by the sum.

- This algorithms does NOT work.
  - But it can be fixed if we use the projection onto the set in Step 2...

Projected-Gradient

$$w^{k+\frac{1}{2}} = \underbrace{w^k - \alpha_k \nabla f(w^k)}_{\text{gradient step}}, \quad w^{k+1} \in \underbrace{\underset{v \in \mathcal{C}}{\text{argmin}} \, \|v - w^{k+\frac{1}{2}}\|}_{\text{projection step}}.$$



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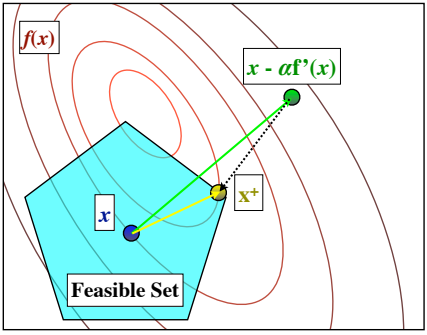


Summary

- L1-regularization: feature selection as convex optimization.
- Subgradients: generalize gradients for non-smooth convex functions.
- Subgradient method: optimal but very-slow general non-smooth method.
- Projected-gradient allows optimization with simple constraints.

- Next time: going beyond L1-regularization to "structured sparsity".

Complexity of Minimizing Strongly-Convex Functions

- For strongly-convex functions:
  - Sub-gradient methods achieve optimal rate of $O(1/\epsilon)$.
  - If ∇f is Lipschitz continuous, we've shown that gradient descent has $O(\log(1/\epsilon))$.

- Nesterov's algorithms improves this from $O(\frac{L}{\mu}\log(1/\epsilon))$ to $O(\sqrt{\frac{L}{\mu}}\log(1/\epsilon))$.
  - Corresponding to linear convergence rate with $\rho = (1 - \sqrt{\frac{\mu}{L}})$.
  - This is close to the optimal dimension-independent rate of $\rho = \left(\frac{\sqrt{L}-\sqrt{\mu}}{\sqrt{L}+\sqrt{\mu}}\right)^2$.

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

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

where d^k is a solution to the system

$$\nabla^2 f(x^k) d^k = \nabla f(x^k).$$

(Assumes $\nabla^2 f(x^k) \succ 0$)

- Equivalent to minimizing the quadratic approximation:

$$f(y) \approx f(x^k) + \nabla f(x^k)^\top (y - x^k) + \frac{1}{2\alpha_k}(y - x^k)\nabla^2 f(x^k)(y - x^k).$$

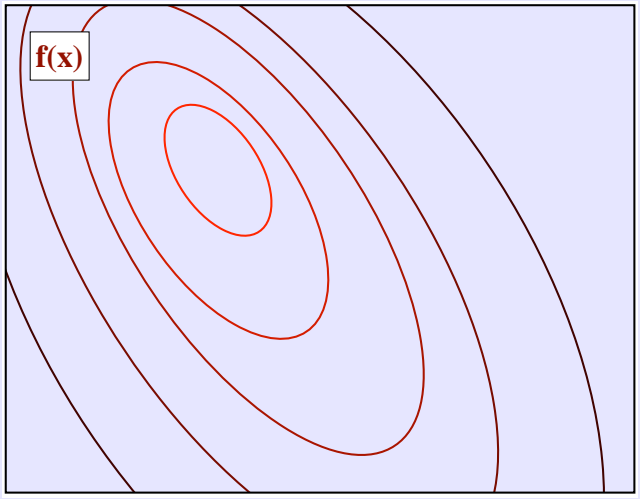
- We can generalize the Armijo condition to

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

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

(always accepted when close to a minimizer)

Newton's Method



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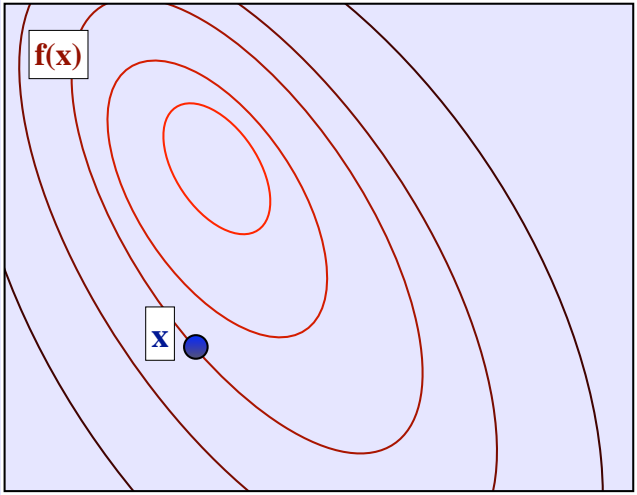

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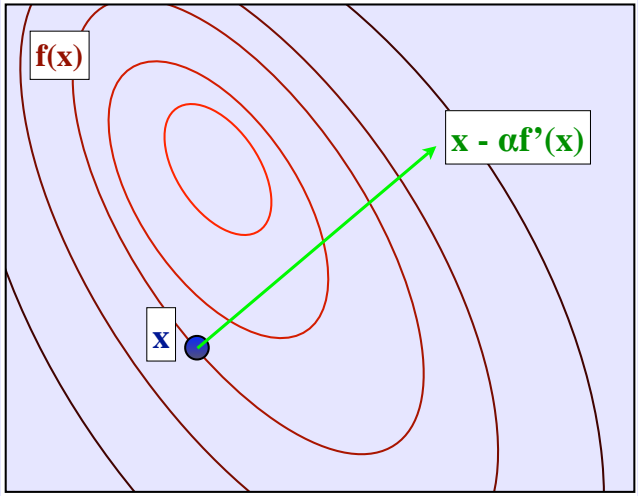

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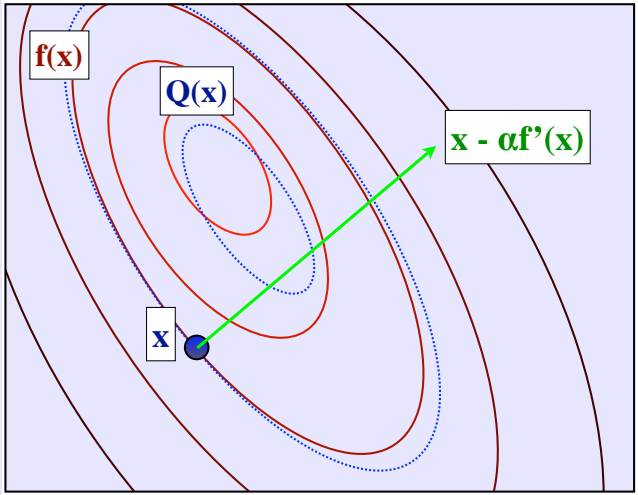

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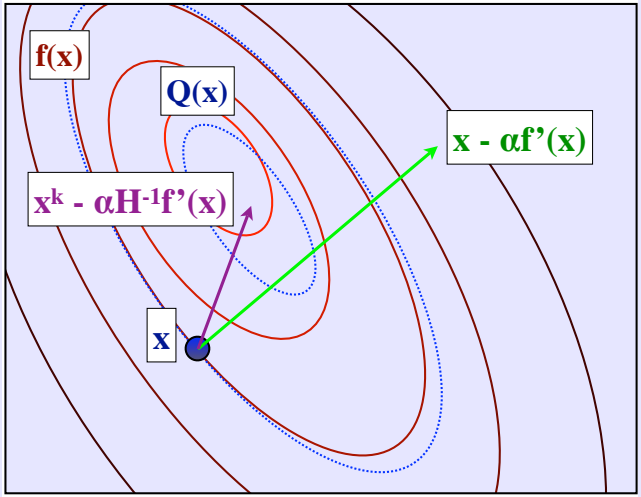


Convergence Rate of Newton's Method

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

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

  with $\lim_{k\to\infty} \rho_k = 0$.
- Converges very fast, use it if you can!
- But Newton's method is expensive if dimension d is large:
  - Requires solving $\nabla^2 f(x^k) d^k = \nabla f(x^k)$.
- "Cubic regularization" of Newton's method gives global convergence rates.

Practical Approximations to Newton's Method

- Practical Newton-like methods (that can be applied to large-scale problems):
  - Diagonal approximation:
    - Approximate Hessian by a diagonal matrix D (cheap to store/invert).
    - A common choice is $d_{ii} = \nabla^2_{ii} f(x^k)$.
    - This sometimes helps, often doesn't.
  - Limited-memory quasi-Newton approximation:
    - Approximates Hessian by a diagonal plus low-rank approximation B^k,

$$B^k = D + UV^k,$$

      which supports fast multiplication/inversion.
    - Based on "quasi-Newton" equations which use differences in gradient values.

$$(\nabla f(x^k) - \nabla f(x^{k-1})) = B^\top (x^k - x^{k-1}).$$

    - A common choice is L-BFGS.

Practical Approximations to Newton's Method

- Practical Newton-like methods (that can be applied to large-scale problems):
  - Barzilai-Borwein approximation:
    - Approximates Hessian by the identity matrix (as in gradient descent).
    - But chooses step-size based on least squares solution to quasi-Newton equations.

$$\alpha_{k+1} = -\alpha_k \frac{v^k \nabla f(x^k)}{\|v^k\|^2}, \quad \text{where} \quad v^k = \nabla f(x^k) - \nabla f(x^{k-1}).$$

    - Works better than it deserves to (*findMin.jl*).
    - We don't understand why it works so well.

Practical Approximations to Newton's Method

- Practical Newton-like methods (that can be applied to large-scale problems):
  - Hessian-free Newton:
    - Uses conjugate gradient to approximately solve Newton system.
    - Requires Hessian-vector products, but these cost same as gradient.
    - If you're lazy, you can numerically approximate them using

$$\nabla^2 f(x^k)d \approx \frac{\nabla f(x^k + \delta d) - \nabla f(x^k)}{\delta}.$$

    - If f is analytic, can compute exactly by evaluating gradient with complex numbers.

(look up "complex-step derivative")

- A related appraoch to the above is non-linear conjugate gradient.

Numerical Comparison with minFunc

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 = 0.3654, x2 = 0.1230 (minFunc with gradient descent)
x1 = 0.8756, x2 = 0.7661 (minFunc with Barzilai-Borwein)
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 non-linear conjugate gradient)
x1 = 1.0000, x2 = 1.0000 (minFunc with limited-memory BFGS - default)

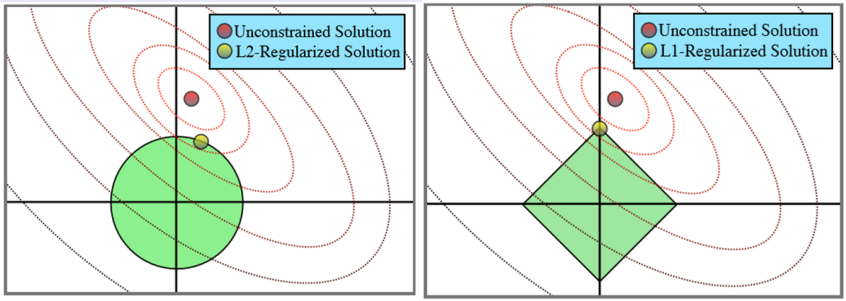
Superlinear Convergence in Practice?

- You get local superlinear convergence if:
  - Gradient is Lipschitz-continuous and f is strongly-convex.
  - Function is in $\mathcal{C}^2$ and Hessian is Lipschitz continuous.
  - Oracle is second-order and method asymptotically uses Newton's direction.
- But the practical Newton-like methods don't achieve this:
  - Diagonal scaling, Barzilai-Borwein, and L-BFGS don't converge to Newton.
  - Hessian-free uses conjugate gradient which isn't superlinear in high-dimensions.
- Full quasi-Newton methods achieve this, but require $\Omega(d^2)$ memory/time.

L1-Regularization vs. L2-Regularization

- Another view on sparsity of L2- vs. L1-regularization using our constraint trick:

$$\underset{w\in\mathbb{R}^d}{\text{argmin}}\ f(w)+\lambda\|w\|_p \quad \Leftrightarrow \quad \underset{w\in\mathbb{R}^d,\tau\in\mathbb{R}}{\text{argmin}}\ f(w)+\lambda\tau \text{ with } \tau \geq \|w\|_p.$$



- Notice that L2-regularization has a rotataional invariance.
  - This actually makes it more sensitive to irrelevant features.

Does Smoothing Help?

- Nesterov's smoothing paper gives a way to take a non-smooth convex f and number ϵ, then it constructs a new function f_ϵ such that

$$f(w) \leq f_\epsilon(w) \leq f(w) + \epsilon,$$

so that minimizing $f_\epsilon(w)$ gets us within ϵ of the optimal solution.
  - And further that $f_\epsilon(w)$ is differentiable with $L = O(1/\epsilon)$.

- If we apply gradient descent to the smooth function, we get

$$t = \underbrace{O(L/\epsilon)}_{\text{smoothed problem}} = \underbrace{O(1/\epsilon^2)}_{\text{original problem}},$$

for convex functions (same speed as subgradient).
- For strongly-convex functions we get

$$t = O(L \log(1/\epsilon)) = O((1/\epsilon)\log(1/\epsilon)),$$

which is actually worse than the best subgradient methods by a log factor.

Does Smoothing Help?

- Nesterov's smoothing paper gives a way to take a non-smooth convex f and number ϵ, then it constructs a new function f_ϵ such that

$$f(w) \leq f_\epsilon(w) \leq f(w) + \epsilon,$$

so that minimizing $f_\epsilon(w)$ gets us within ϵ of the optimal solution.
  - And further that $f_\epsilon(w)$ is differentiable with $L = O(1/\epsilon)$.

- If we apply accelerated gradient descent to the smooth function, we get

$$t = O(\sqrt{L/\epsilon}) = O(1/\epsilon),$$

which is faster than subgradient methods.
(same speed as unaccelerated gradient descent)
- For strongly-convex functions the accelerated method gets

$$t = O(\sqrt{L}\log(1/\epsilon)) = O((1/\sqrt{\epsilon})\log(1/\epsilon)),$$

which is faster than subgradient methods (but not linear converence).

What is the best subgradient?

- We considered the deterministic subgradient method,

$$x^{t+1} = x^t - \alpha_t g_t, \text{ where } g_t \in \partial f(x^t),$$

  under any choice of subgradient.

- But what is the "best" subgradient to use?
  - Convex functions have directional derivatives everywhere.
  - Direction $-g_t$ that minimizes directional derivative is minimum-norm subgradient,

$$g^t = \underset{g \in \partial f(x^t)}{\text{argmin}} \; ||g||$$

  - This is the steepest descent direction for non-smooth convex optimization problems.

  - You can compute this for L1-regularization, but not many other problems.
  - Used in best deterministic L1-regularization methods, combined with Newton.