Newton's Method

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Last time: KKT conditions

Recall that for the problem

$$\begin{array}{ll} \min\limits_{x} & f(x) \\ \text{subject to} & h_i(x) \leq 0,\ i = 1, \ldots m \\ & \ell_j(x) = 0,\ j = 1, \ldots r \end{array}$$

the KKT conditions are

- $0 \in \partial\left(f(x) + \sum_{i=1}^{m} u_i h_i(x) + \sum_{j=1}^{r} v_j \ell_j(x) \right)$ (stationarity)
- $u_i \cdot h_i(x) = 0$ for all i (complementary slackness)
- $h_i(x) \leq 0,\ \ell_j(x) = 0$ for all i, j (primal feasibility)
- $u_i \geq 0$ for all i (dual feasibility)

These are necessary for optimality (of a primal-dual pair $x^\star$ and $u^\star, v^\star$) under strong duality, and always sufficient

Last time: duality usage and correspondences

Given a function $f : \mathbb{R}^n \to \mathbb{R}$, we define its conjugate $f^* : \mathbb{R}^n \to \mathbb{R}$,

$$f^*(y) = \max_x \; y^T x - f(x)$$

Properties and examples:

- Conjugate f^* is always convex (regardless of convexity of f)
- When f is a norm, f^* is the indicator of the dual norm unit ball
- When f is closed and convex, $x \in \partial f^*(y) \iff y \in \partial f(x)$
- Non-smooth f creates constraints in f^*.
- Use duality to prove "support recovery" in lasso.

Relationship to duality (also called Fenchel duality):

$$\text{Primal :} \quad \min_x \; f(x) + g(x)$$

$$\text{Dual :} \quad \max_u \; -f^*(u) - g^*(-u)$$

Recap: First Order Optimization

	Gradient descent	**Subgrad method**	**Prox grad descent**	**Stochastic grad descent**
Criterion	smooth f	any f	smooth + simple, $f = g + h$	smooth + simple, $f = g + h$
Constraints	projection onto constraint set	projection onto constraint set	constrained prox operator	projection onto constraint set
Opti parameters	fixed step size ($t \leq 1/L$) or line search	diminishing step sizes	fixed step size ($t \leq 1/L$) or line search	fixed or diminishing step sizes, mini-batch size
Iteration cost	cheap (compute gradient)	cheap (compute subgradient)	moderately cheap (evaluate prox)	very cheap (compute stochastic gradient)
Rate	$O(1/\epsilon)$ (acceleration: $O(1/\sqrt{\epsilon})$, strong convexity: $O(\log(1/\epsilon))$)	$O(1/\epsilon^2)$	$O(1/\epsilon)$ (acceleration: $O(1/\sqrt{\epsilon})$, strong convexity: $O(\log(1/\epsilon))$)	$O(1/\epsilon^2)$, but practically converges rapidly at the start

Can we do better than first order methods?

- Better convergence rate?
- Better overall complexity (for some problems)?
- Better dependence on problem-specific quantities (e.g. smoothness parameter L and strong convexity parameter m)?

Newton's method

Given unconstrained, smooth convex optimization

$$\min_x \; f(x)$$

where f is convex, twice differentable, and $\mathrm{dom}(f) = \mathbb{R}^n$. Recall that gradient descent chooses initial $x^{(0)} \in \mathbb{R}^n$, and repeats

$$x^{(k)} = x^{(k-1)} - t_k \cdot \nabla f(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

In comparison, Newton's method repeats

$$x^{(k)} = x^{(k-1)} - \left(\nabla^2 f(x^{(k-1)})\right)^{-1} \nabla f(x^{(k-1)}), \quad k = 1, 2, 3, \ldots$$

Here $\nabla^2 f(x^{(k-1)})$ is the Hessian matrix of f at $x^{(k-1)}$

Newton's method interpretation

Recall the motivation for gradient descent step at x: we minimize the quadratic approximation

$$f(y) \approx f(x) + \nabla f(x)^T (y - x) + \frac{1}{2t}\|y - x\|_2^2$$

over y, and this yields the update $x^+ = x - t\nabla f(x)$

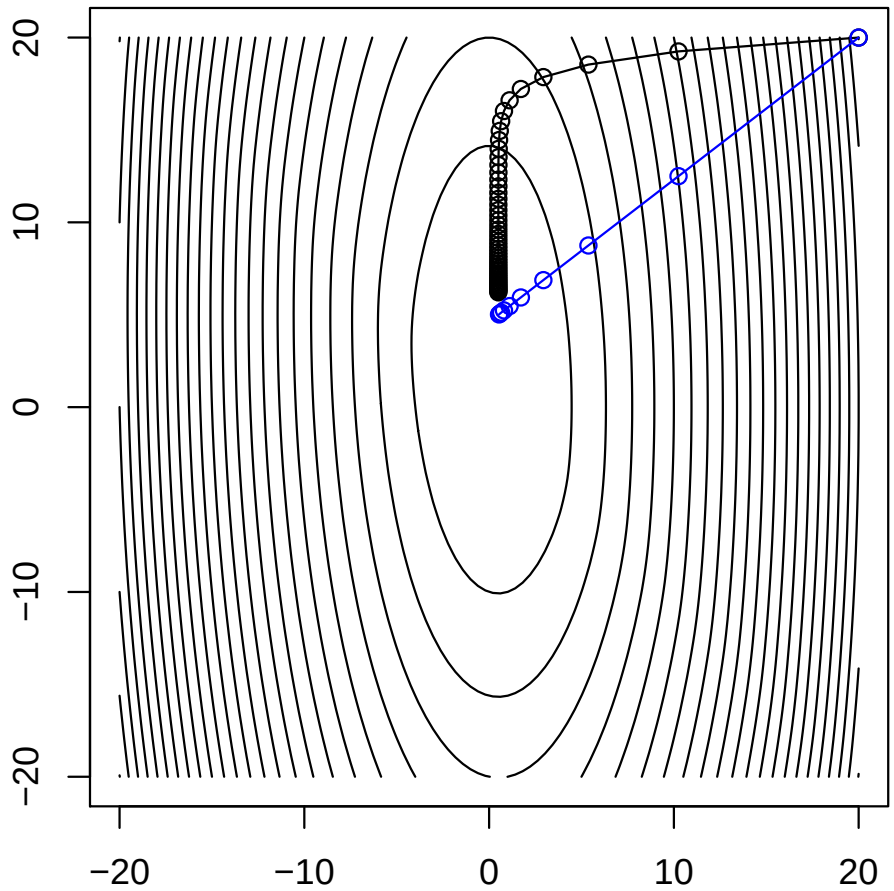
Newton's method uses in a sense a better quadratic approximation

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

and minimizes over y to yield $x^+ = x - (\nabla^2 f(x))^{-1} \nabla f(x)$

Consider minimizing $f(x) = (10x_1^2 + x_2^2)/2 + 5\log(1 + e^{-x_1 - x_2})$
(this must be a nonquadratic ... why?)

We compare gradient descent (black) to Newton's method (blue), where both take steps of roughly same length



Outline

Today:

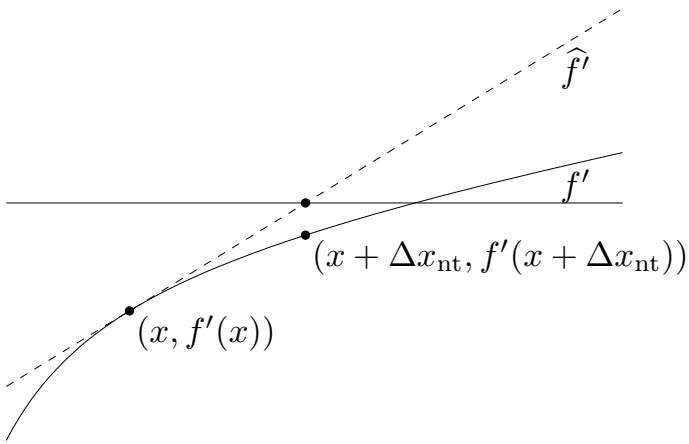
- Interpretations and properties
- Backtracking line search
- Convergence analysis
- Equality-constrained Newton
- Quasi-Newton preview

Linearized optimality condition

Aternative interpretation of Newton step at x: we seek a direction v so that $\nabla f(x+v) = 0$. Let $F(x) = \nabla f(x)$. Consider linearizing F around x, via approximation $F(y) \approx F(x) + DF(x)(y-x)$, i.e.,

$$0 = \nabla f(x+v) \approx \nabla f(x) + \nabla^2 f(x) v$$

Solving for v yields $v = -(\nabla^2 f(x))^{-1} \nabla f(x)$



(From B & V page 486)

History: work of Newton (1685) and Raphson (1690) originally focused on finding roots of polynomials. Simpson (1740) applied this idea to general nonlinear equations, and minimization by setting the gradient to zero

Affine invariance of Newton's method

Important property Newton's method: affine invariance. Given f, nonsingular $A \in \mathbb{R}^{n \times n}$. Let $x = Ay$, and $g(y) = f(Ay)$. Newton steps on g are

$$\begin{aligned} y^+ &= y - \big(\nabla^2 g(y)\big)^{-1} \nabla g(y) \\ &= y - \big(A^T \nabla^2 f(Ay) A\big)^{-1} A^T \nabla f(Ay) \\ &= y - A^{-1} \big(\nabla^2 f(Ay)\big)^{-1} \nabla f(Ay) \end{aligned}$$

Hence

$$Ay^+ = Ay - \big(\nabla^2 f(Ay)\big)^{-1} \nabla f(Ay)$$

i.e.,

$$x^+ = x - \big(\nabla^2 f(x)\big)^{-1} f(x)$$

So progress is independent of problem scaling; recall that this is not true of gradient descent

Newton decrement

At a point x, we define the Newton decrement as

$$\lambda(x) = \left(\nabla f(x)^T \left(\nabla^2 f(x)\right)^{-1} \nabla f(x)\right)^{1/2}$$

This relates to the difference between $f(x)$ and the minimum of its quadratic approximation:

$$\begin{aligned} & f(x) - \min_y \left(f(x) + \nabla f(x)^T (y-x) + \frac{1}{2}(y-x)^T \nabla^2 f(x)(y-x)\right) \\ &= f(x) - \left(f(x) - \frac{1}{2}\nabla f(x)^T \left(\nabla^2 f(x)\right)^{-1} \nabla f(x)\right) \\ &= \frac{1}{2}\lambda(x)^2 \end{aligned}$$

Therefore can think of $\lambda^2(x)/2$ as an approximate upper bound on the suboptimality gap $f(x) - f^\star$

Detour: Steepest Descent

Let $\|\cdot\|$ be a norm, the associated steepest descent algorithm iterates

$$x^+ = x + tv$$

where

$$v = \underset{w:\|w\|\leq 1}{\operatorname{argmin}} \nabla f(x)^T w$$

- When $\|\cdot\| = \|\cdot\|_2$, $v = -\nabla f(x)/\|\nabla f(x)\|_2$ — gradient descent.
- When $\|\cdot\| = \|\cdot\|_1$, $v = -\operatorname{sign}(\nabla f(x)_{i^*})\mathbf{e}_{i^*}$, where $i^* = \operatorname{argmax}_i |\nabla f(x)_i|$ — greedy coordinate descent.
- When $\|\cdot\| = \|\cdot\|_\infty$, $v = -\operatorname{sign}(\nabla f(x))$ — sign gradient descent.

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What is the "right" norm to use?

Newton's method as "adaptive" steepest descent

Take $\|\cdot\|$ to be $\|\cdot\|_{\nabla^2 f(x)}$,

$$\tilde{v} = \underset{w:\|w\|_{\nabla^2 f(x)} \leq 1}{\operatorname{argmin}} \nabla f(x)^T w$$

we get $\tilde{v} = -u^{-1}(\nabla^2 f(x))^{-1}\nabla f(x) = \frac{1}{\|v\|_{\nabla^2 f(x)}} v$.
Note that $\|\tilde{v}\|_{\nabla^2 f(x)} = 1$ and

$$\max_{w:\|w\|_{\nabla^2 f(x)} \leq 1} \nabla f(x)^T w = \|\nabla f(x)\|_{[\nabla^2 f(x)]^{-1}} = \|v\|_{\nabla^2 f(x)} = \lambda(x)$$

i.e., $\lambda(x)$ is the length of the Newton step in the norm defined by the Hessian $\nabla^2 f(x)$— a local adaptive choice of the norm.

Note that the Newton decrement, like the Newton steps, are affine invariant; i.e., if we defined $g(y) = f(Ay)$ for nonsingular A, then $\lambda_g(y)$ would match $\lambda_f(x)$ at $x = Ay$.

Pure Newton's method may not converge

The original use of Newton's method was to solve the roots of nonlinear equation $g(x) = 0$. This is more general than solving $\nabla f(x) = 0$. (Why?)

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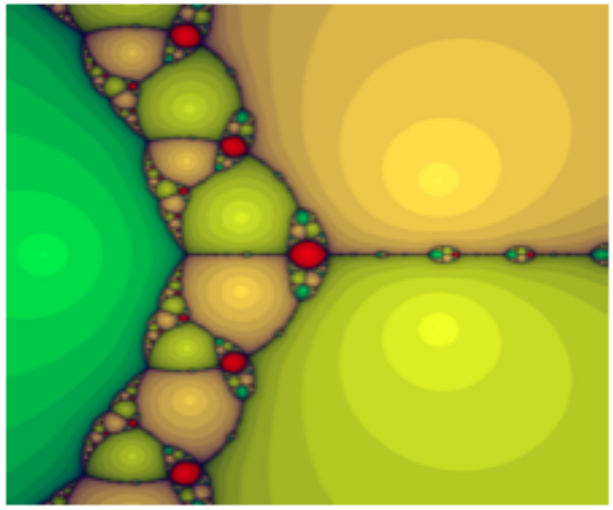
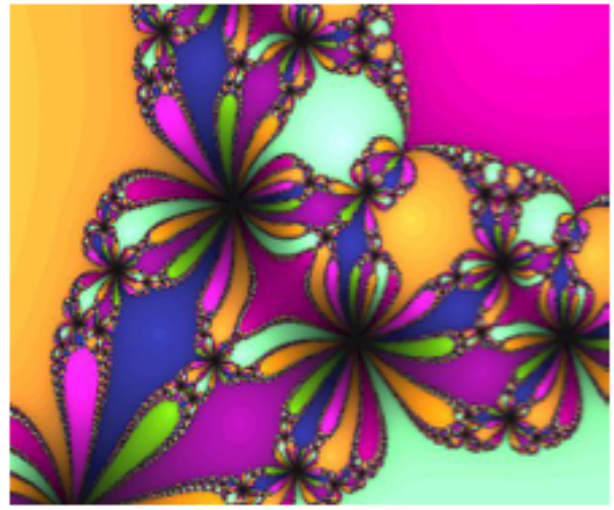
When Newton's method converges and when not is rather complex.



$z^3 - 2z + 2$



$x^8 + 15x^4 - 16$

(Examples from Suvrit Sra)

See more Newton fractals here:

`https://www.chiark.greenend.org.uk/~sgtatham/newton/`

Backtracking line search

In practice, we use damped Newton's method (i.e., Newton's method), which repeats

$$x^+ = x - t\big(\nabla^2 f(x)\big)^{-1}\nabla f(x)$$

Note that the pure method uses $t = 1$

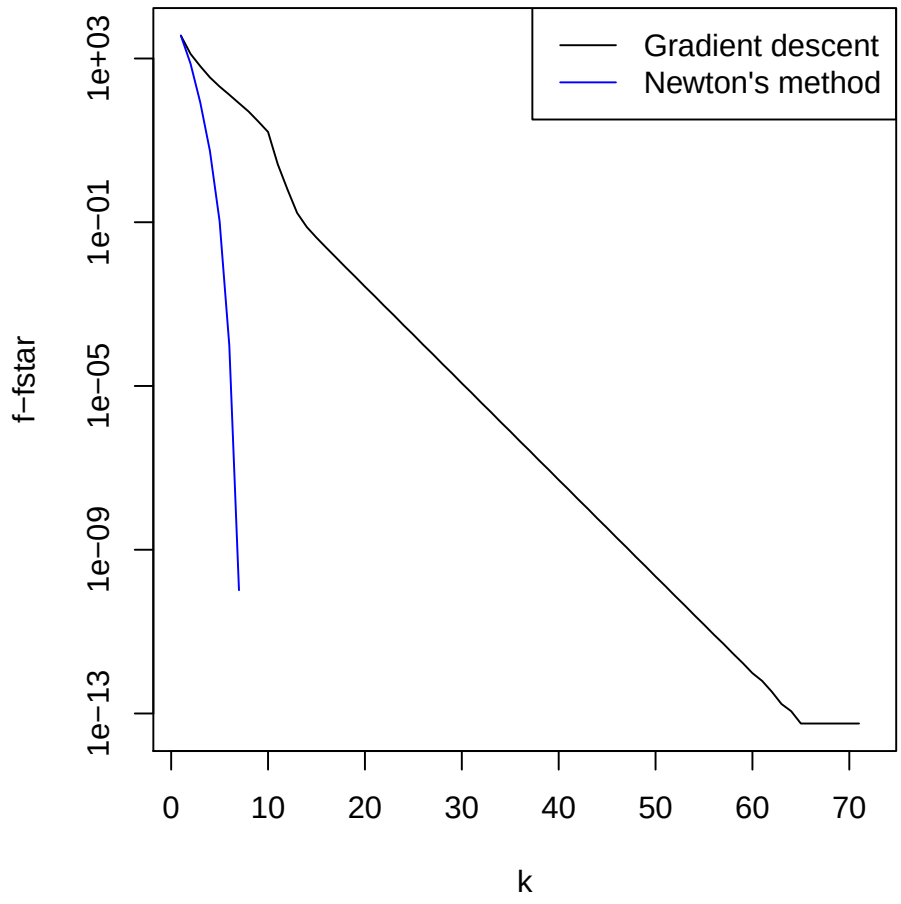
Step sizes here typically are chosen by backtracking search, with parameters $0 < \alpha \leq 1/2$, $0 < \beta < 1$. At each iteration, we start with $t = 1$ and while

$$f(x + tv) > f(x) + \alpha t \nabla f(x)^T v$$

we shrink $t = \beta t$, else we perform the Newton update. Note that here $v = -(\nabla^2 f(x))^{-1}\nabla f(x)$, so $\nabla f(x)^T v = -\lambda^2(x)$

Example: logistic regression

Logistic regression example, with $n = 500$, $p = 100$: we compare gradient descent and Newton's method, both with backtracking



Newton's method: in a totally different regime of convergence...!

Convergence analysis

Assume that f convex, twice differentiable, having $\mathrm{dom}(f) = \mathbb{R}^n$, and additionally

- ∇f is Lipschitz with parameter L
- f is strongly convex with parameter m
- $\nabla^2 f$ is Lipschitz with parameter M

Theorem: Newton's method with backtracking line search satisfies the following two-stage convergence bounds

$$f(x^{(k)}) - f^\star \leq \begin{cases} (f(x^{(0)}) - f^\star) - \gamma k & \text{if } k \leq k_0 \\ \dfrac{2m^3}{M^2}\left(\dfrac{1}{2}\right)^{2^{k-k_0+1}} & \text{if } k > k_0 \end{cases}$$

Here $\gamma = \alpha\beta^2\eta^2 m/L^2$, $\eta = \min\{1, 3(1-2\alpha)\}m^2/M$, and k_0 is the number of steps until $\|\nabla f(x^{(k_0+1)})\|_2 < \eta$

In more detail, convergence analysis reveals $\gamma > 0$, $0 < \eta \leq m^2/M$ such that convergence follows two stages

- Damped phase: $\|\nabla f(x^{(k)})\|_2 \geq \eta$, and

$$f(x^{(k+1)}) - f(x^{(k)}) \leq -\gamma$$

- Pure phase: $\|\nabla f(x^{(k)})\|_2 < \eta$, backtracking selects $t = 1$, and

$$\frac{M}{2m^2}\|\nabla f(x^{(k+1)})\|_2 \leq \left(\frac{M}{2m^2}\|\nabla f(x^{(k)})\|_2\right)^2$$

Note that once we enter pure phase, we won't leave, because

$$\frac{2m^2}{M}\left(\frac{M}{2m^2}\eta\right)^2 \leq \eta$$

when $\eta \leq m^2/M$

Unraveling this result, what does it say? To get $f(x^{(k)}) - f^\star \leq \epsilon$, we need at most

$$\frac{f(x^{(0)}) - f^\star}{\gamma} + \log\log(\epsilon_0/\epsilon)$$

iterations, where $\epsilon_0 = 2m^3/M^2$

- This is called quadratic convergence. Compare this to linear convergence (which, recall, is what gradient descent achieves under strong convexity)
- The above result is a local convergence rate, i.e., we are only guaranteed quadratic convergence after some number of steps k_0, where $k_0 \leq \frac{f(x^{(0)}) - f^\star}{\gamma}$
- Somewhat bothersome may be the fact that the above bound depends on L, m, M, and yet the algorithm itself does not ...

Self-concordance

A scale-free analysis is possible for self-concordant functions: on $\mathbb{R}$, a convex function f is called self-concordant if

$$|f'''(x)| \leq 2f''(x)^{3/2} \quad \text{for all } x$$

and on $\mathbb{R}^n$ is called self-concordant if its projection onto every line segment is so

Theorem (Nesterov and Nemirovskii): Newton's method with backtracking line search requires at most

$$C(\alpha, \beta)\big(f(x^{(0)}) - f^\star\big) + \log\log(1/\epsilon)$$

iterations to reach $f(x^{(k)}) - f^\star \leq \epsilon$, where $C(\alpha, \beta)$ is a constant that only depends on α, β

Implications of self-concordance

We say that three-times differentiable function $f : \mathbb{R}^d \to \mathbb{R}$ is R-self-concordant at x if for all $v \in \mathbb{R}^d$

$$\nabla^3 f(x)[v, v, v] \leq 2R(\nabla^2 f(x)[v, v])^{3/2}.$$

Let $H_x := \nabla^2 f(x)$. If f is R-self-concordant at x. Then for any v such that $R\|v\|_{H_x} < 1$, we have that

$$(1 - R\|v\|_{H_x})^2 \nabla^2 f(x) \prec \nabla^2 f(x + v) \prec \frac{1}{(1 - R\|v\|_{H_x})^2} \nabla^2 f(x).$$

This semidefinite ordering informally allows us to approximately cancel out $\nabla^2 f(x + v)$ with $\nabla^2 f(x)^{-1}$ hence leading to a convergence bound that is independent to the condition number!

What kind of functions are self-concordant?

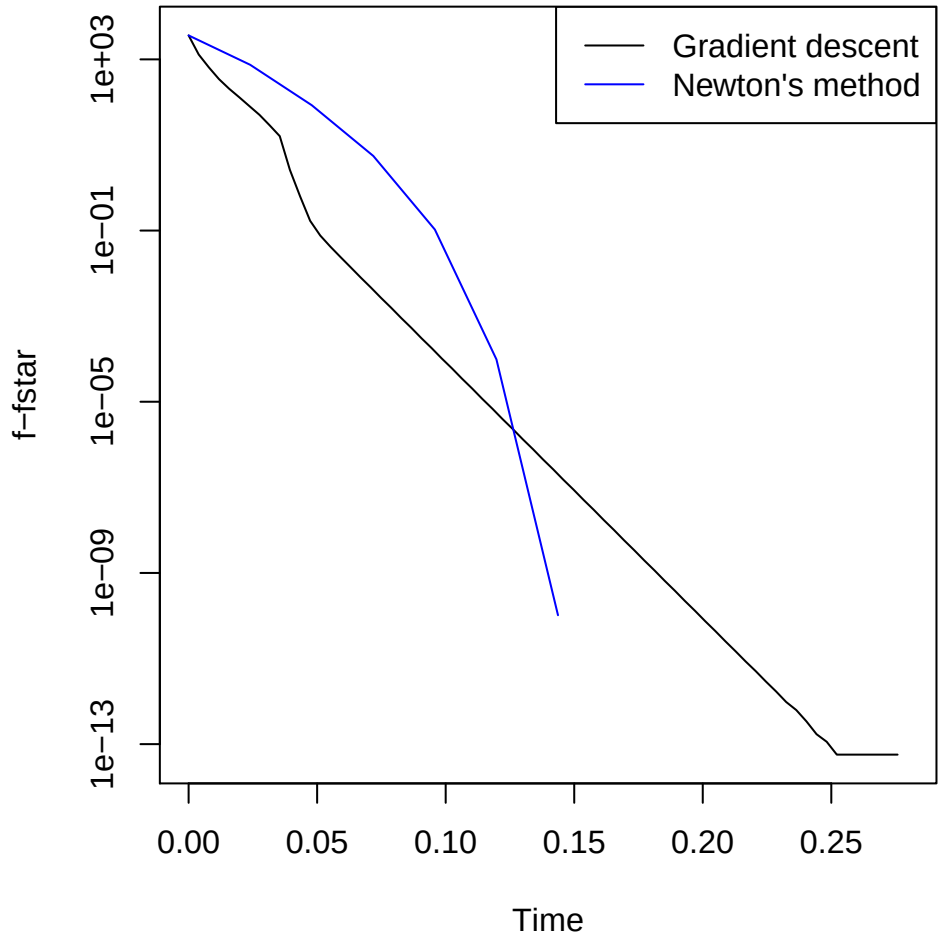
- $f(x) = -\sum_{i=1}^{n} \log(x_i)$ on $\mathbb{R}^n_{++}$
- $f(X) = -\log(\det(X))$ on $\mathbb{S}^n_{++}$
- If g is self-concordant, then so is $f(x) = g(Ax + b)$
- In the definition of self-concordance, we can replace factor of 2 by a general $\kappa > 0$
- If g is κ-self-concordant, then we can rescale: $f(x) = \frac{\kappa^2}{4} g(x)$ is self-concordant (2-self-concordant)

Comparison to first-order methods

At a high-level:

- Memory: each iteration of Newton's method requires $O(n^2)$ storage ($n \times n$ Hessian); each gradient iteration requires $O(n)$ storage (n-dimensional gradient)
- Computation: each Newton iteration requires $O(n^3)$ flops (solving a dense $n \times n$ linear system); each gradient iteration requires $O(n)$ flops (scaling/adding n-dimensional vectors)
- Backtracking: backtracking line search has roughly the same cost, both use $O(n)$ flops per inner backtracking step
- Conditioning: Newton's method is not affected by a problem's conditioning, but gradient descent can seriously degrade
- Fragility: Newton's method may be empirically more sensitive to bugs/numerical errors, gradient descent is more robust

Back to logistic regression example: now x-axis is parametrized in terms of time taken per iteration



Each gradient descent step is $O(p)$, but each Newton step is $O(p^3)$

Sparse, structured problems

When the inner linear systems (in Hessian) can be solved efficiently and reliably, Newton's method can strive

E.g., if $\nabla^2 f(x)$ is sparse and structured for all x, say banded, then both memory and computation are $O(n)$ with Newton iterations

What functions admit a structured Hessian? Two examples:

- If $g(\beta) = f(X\beta)$, then $\nabla^2 g(\beta) = X^T \nabla^2 f(X\beta) X$. Hence if X is a structured predictor matrix and $\nabla^2 f$ is diagonal, then $\nabla^2 g$ is structured
- If we seek to minimize $f(\beta) + g(D\beta)$, where $\nabla^2 f$ is diagonal, g is not smooth, and D is a structured penalty matrix, then the Lagrange dual function is $-f^*(-D^T u) - g^*(-u)$. Often $-D\nabla^2 f^*(-D^T u)D^T$ can be structured

Equality-constrained Newton's method

Consider now a problem with equality constraints, as in

$$\min_x \ f(x) \ \text{ subject to } \ Ax = b$$

Several options:

- Eliminating equality constraints: write $x = Fy + x_0$, where F spans null space of A, and $Ax_0 = b$. Solve in terms of y
- Deriving the dual: can check that the Lagrange dual function is $-f^*(-A^T v) - b^T v$, and strong duality holds. With luck, we can express $x^\star$ in terms of $v^\star$
- Equality-constrained Newton: in many cases, this is the most straightforward option

In equality-constrained Newton's method, we start with $x^{(0)}$ such that $Ax^{(0)} = b$. Then we repeat the updates

$$x^+ = x + tv, \quad \text{where}$$

$$v = \underset{Az=0}{\operatorname{argmin}} \ \nabla f(x)^T (z - x) + \frac{1}{2}(z - x)^T \nabla^2 f(x)(z - x)$$

This keeps x^+ in feasible set, since $Ax^+ = Ax + tAv = b + 0 = b$

Furthermore, v is the solution to minimizing a quadratic subject to equality constraints. We know from KKT conditions that v satisfies

$$\begin{bmatrix} \nabla^2 f(x) & A^T \\ A & 0 \end{bmatrix} \begin{bmatrix} v \\ w \end{bmatrix} = \begin{bmatrix} -\nabla f(x) \\ 0 \end{bmatrix}$$

for some w. Hence Newton direction v is again given by solving a linear system in the Hessian (albeit a bigger one)

Quasi-Newton methods

If the Hessian is too expensive (or singular), then a quasi-Newton method can be used to approximate $\nabla^2 f(x)$ with $H \succ 0$, and we update according to

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

- Approximate Hessian H is recomputed at each step. Goal is to make H^{-1} cheap to apply (possibly, cheap storage too)
- Convergence is fast: superlinear, but not the same as Newton. Roughly n steps of quasi-Newton make same progress as one Newton step
- Very wide variety of quasi-Newton methods; common theme is to "propogate" computation of H across iterations

Davidon-Fletcher-Powell or DFP:

- Update H, H^{-1} via rank 2 updates from previous iterations; cost is $O(n^2)$ for these updates
- Since it is being stored, applying H^{-1} is simply $O(n^2)$ flops
- Can be motivated by Taylor series expansion

Broyden-Fletcher-Goldfarb-Shanno or BFGS:

- Came after DFP, but BFGS is now much more widely used
- Again, updates H, H^{-1} via rank 2 updates, but does so in a "dual" fashion to DFP; cost is still $O(n^2)$
- Also has a limited-memory version, L-BFGS: instead of letting updates propogate over all iterations, only keeps updates from last m iterations; storage is now $O(mn)$ instead of $O(n^2)$

References and further reading

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- L. Vandenberghe, Lecture notes for EE 236C, UCLA, Spring 2011-2012
- Fractals derived from Newton-Raphson iteration: `https://www.chiark.greenend.org.uk/~sgtatham/newton/`