Newton Method

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Outline

Newton method

- ❑ Finding a root
- ❑ Unconstrained minimization
  - Motivation with quadratic approximation
  - Rate of Newton's method

Newton method for finding a root

Newton method for finding a root

- Newton method: originally developed for finding a root of a function

- also known as the **Newton–Raphson method**

$$\phi : \mathbb{R} \to \mathbb{R}$$
$$\phi(x^*) = 0$$
$$x^* = ?$$

Newton Method for Finding a Root

Goal: $\phi : \mathbb{R} \to \mathbb{R}$

$$\phi(x^*) = 0$$

$$x^* = ?$$

Linear Approximation (1st order Taylor approx**):**

$$\underbrace{\phi(\underbrace{x + \Delta x}_{x^*})}_{\phi(x^*) = 0} = \phi(x) + \phi'(x)\Delta x + o(|\Delta x|)$$

Therefore,

$$0 \approx \phi(x) + \phi'(x)\Delta x$$

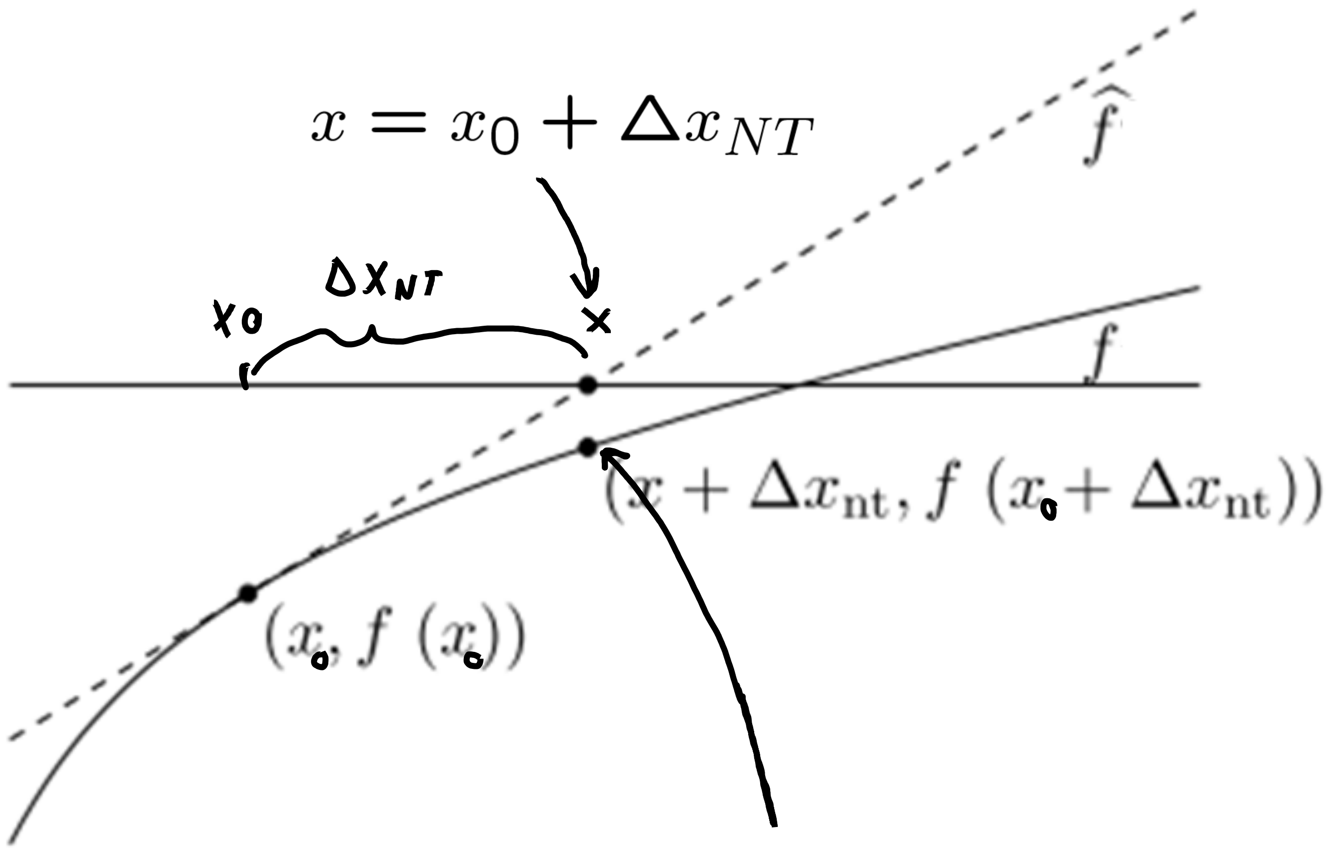
$$x^* - x = \Delta x = -\frac{\phi(x)}{\phi'(x)}$$

$$x_{k+1} = x_k - \frac{\phi(x)}{\phi'(x)}$$

Illustration of Newton’s method

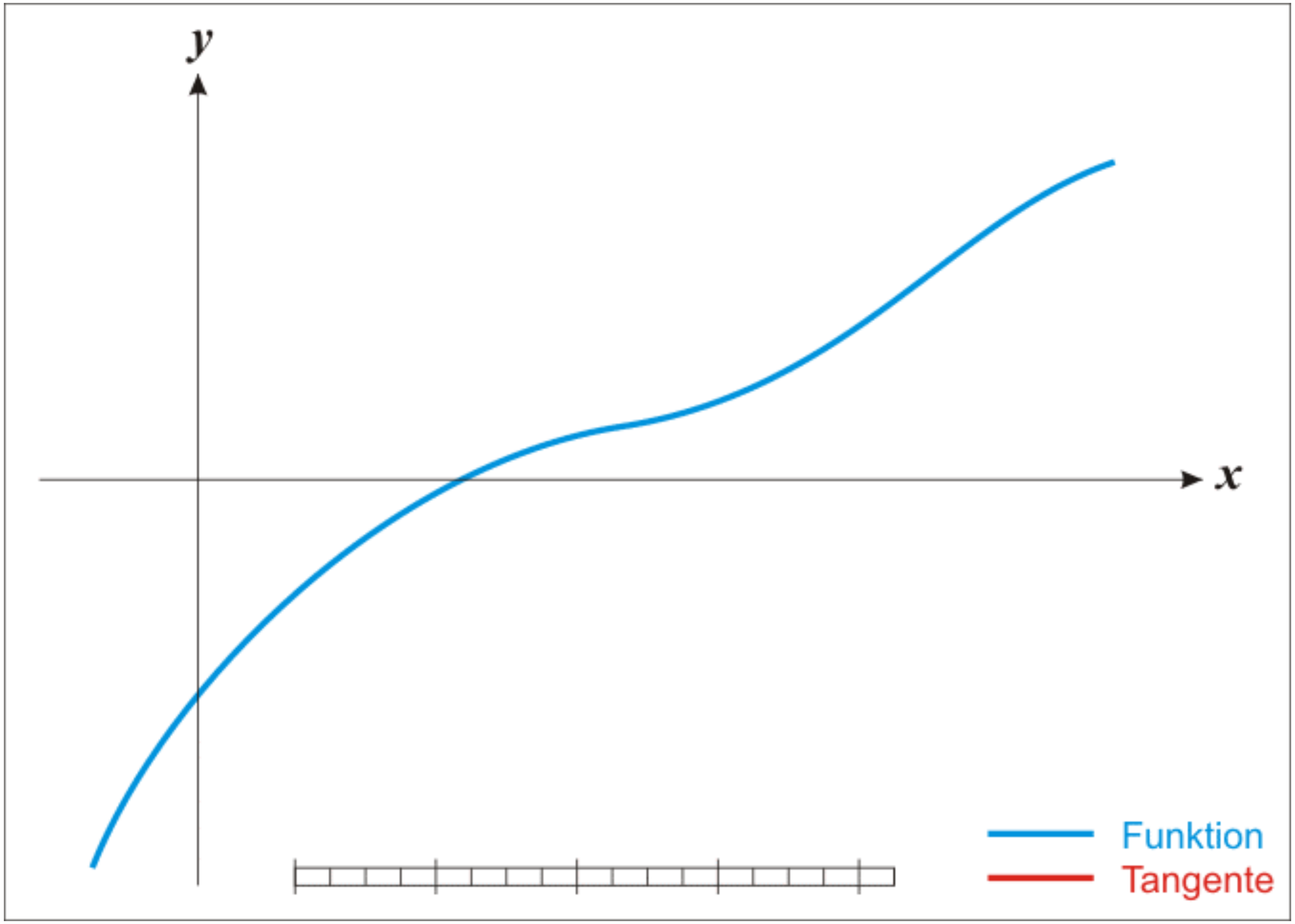
Goal: finding a root

$$\hat{f}(x) = f(x_0) + f'(x_0)(x - x_0)$$



In the next step we will linearize here in *x*

Example: Finding a Root



http://en.wikipedia.org/wiki/Newton%27s_method

Newton Method for Finding a Root

This can be generalized to multivariate functions

$F : \mathbb{R}^n \rightarrow \mathbb{R}^m$

$$0_m = F(x^*) = F(x + \Delta x) = F(x) + \underbrace{\nabla F(x)}_{\mathbb{R}^{m \times n}} \underbrace{\Delta x}_{\mathbb{R}^n} + \underbrace{o(|\Delta x|)}_{\text{NEGLECT}}$$

Therefore,

$$0_m = F(x) + \nabla F(x) \Delta x$$

$$\Delta x = -[\nabla F(x)]^{-1} F(x)$$

[Pseudo inverse if there is no inverse]

$\Delta x = x_{k+1} - x_k$, and thus

$$\underbrace{x_{k+1}}_{\mathbb{R}^n} = \underbrace{x_k}_{\mathbb{R}^n} - \underbrace{[\nabla F(x_k)]^{-1}}_{\mathbb{R}^{n \times m}} \underbrace{F(x_k)}_{\mathbb{R}^m}$$

Newton method: Start from x_0 and iterate.

Newton method for minimization

Newton method for minimization

Newton's method for the optimization problem

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

is the same as Newton's method for finding a root of

$$\nabla f(x) = 0.$$

History: The 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.

Newton method for minimization

$f : \mathbb{R}^n \to \mathbb{R}$, f is twice differentiable

$$\min_{x \in \mathbb{R}^n} f(x)$$

unconstrained

We need to find the roots of $\nabla f(x) = 0_n$

$$\nabla f : \mathbb{R}^n \to \mathbb{R}^n$$

Newton system: $\nabla f(x) + \nabla^2 f(x) \Delta x = 0_n$

Newton step: $\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x)]^{-1} \nabla f(x)$

Iterate until convergence, or max number of iterations exceeded

(divergence, loops, division by zero might happen...)

Motivation with Quadratic Approximation

Motivation with Quadratic Approximation

$f : \mathbb{R}^n \to \mathbb{R}$, f is twice differentiable

$\min_{x \in \mathbb{R}^n} f(x)$ unconstrained

Second order Taylor approximation:

Let $\phi(x) = f(x_k) + \nabla^T f(x_k)(x - x_k) + \frac{1}{2}(x - x_k)^T \nabla^2 f(x_k)(x - x_k)$

Assume that

$\nabla^2 f(x_k) \succ 0$ [i.e. ϕ has strict global minimum]

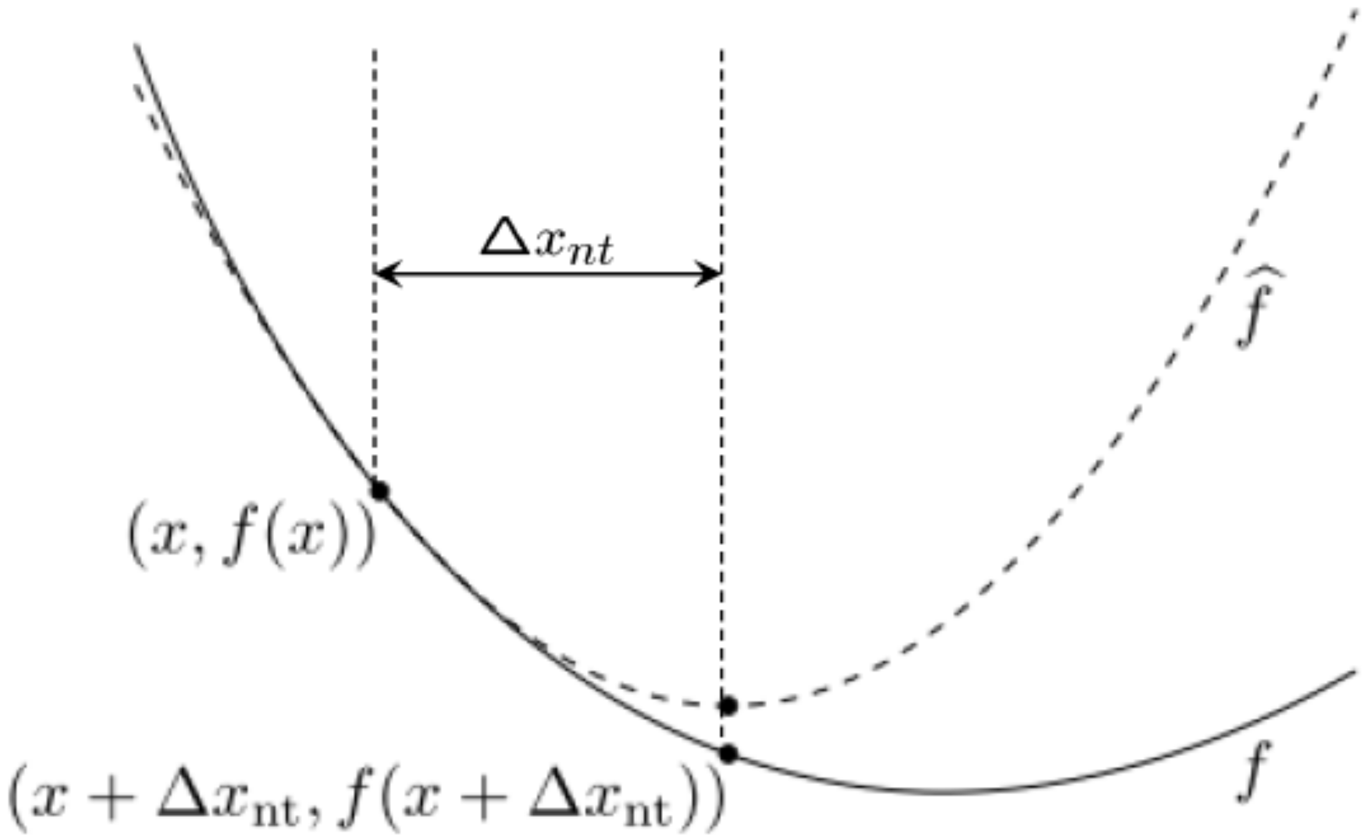
Now, if x_{k+1} is the global minimum of the quadratic function ϕ, then

$$0_n = \nabla \phi(x_{k+1}) = \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k)$$

Newton step:

$$\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x)]^{-1} \nabla f(x)$$

Motivation with Quadratic Approximation



Quadratic approaximation is good, when x is close to x^*

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

Comparison with Gradient Descent

Comparison with Gradient Descent

Newton's method: choose initial $x^{(0)} \in \mathbb{R}^n$, and

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

Compare to gradient descent: choose initial $x^{(0)} \in \mathbb{R}^n$, and

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

Newton method is obtained by minimizing over quadratic approximation:

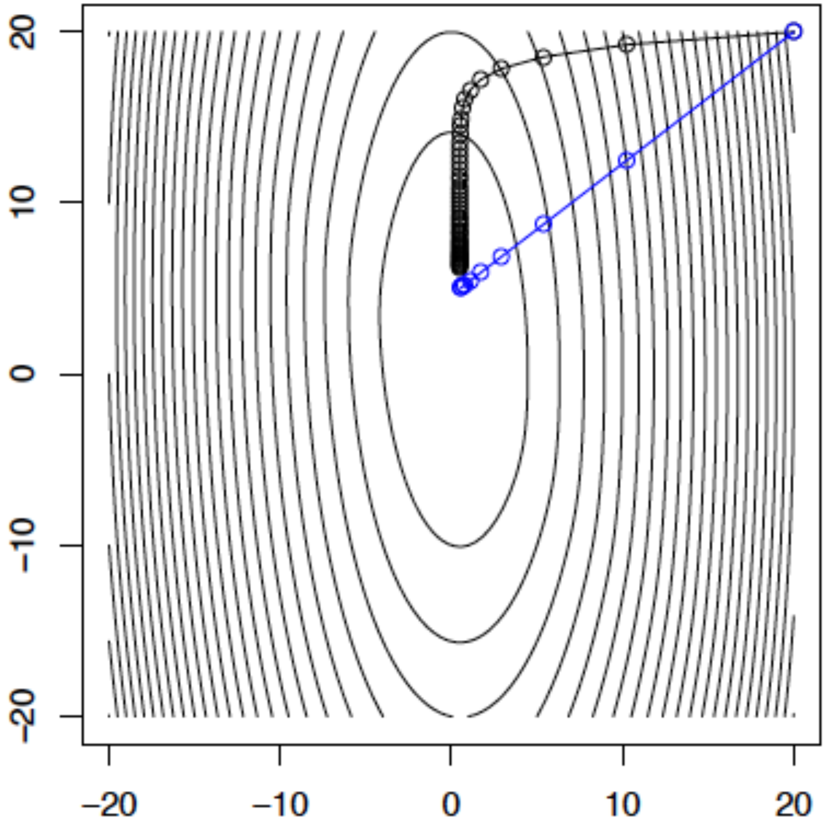
$$f(y) \approx f(x) + \nabla f(x)^T (y - x) + \frac{1}{2}(y - x)^T \nabla^2 f(x)(y - x)$$

Gradient descent uses a different quadratic approximation:

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

Comparison with Gradient Descent

For $f(x) = (10x_1^2 + x_2^2)/2 + 5\log(1 + e^{-x_1-x_2})$, compare gradient descent (black) to Newton's method (blue), where both take steps of roughly same length



How good is the Newton method?

Descent direction

Lemma [Descent direction]

If $\nabla^2 f \succ 0$, then Newton step is a descent direction.

Proof:

We know that if a vector has negative inner product with the gradient vector, then that direction is a descent direction

Newton step: $\Delta x = x_{k+1} - x_k = -[\nabla^2 f(x)]^{-1} \nabla f(x)$

$$\Rightarrow \nabla f(x)^T \Delta x = -\nabla f(x)^T [\nabla^2 f(x)]^{-1} \nabla f(x) < 0$$

Pre-Conditioning for Gradient descent

Recall convergence rate for gradient descent:

$$f(x^{(k)}) - f^\star \le c^k \frac{L}{2} \|x^{(0)} - x^\star\|_2^2$$

Constant c depends adversely on condition number L/m (higher condition number $\Rightarrow$ slower rate)

Can we convert it into well-conditioned problem by changing coordinates?

let $x = Ay$ and $g(y) = f(Ay)$

$$\nabla g(y) = A^T \nabla f(Ay), \nabla^2 g(y) = A^T \nabla^2 f(Ay) A$$

Can get $\nabla^2 g(y) = I$ if $A = [\nabla^2 f(x)]^{-1}$

Pre-Conditioning for Gradient descent

Can we convert it into well-conditioned problem by changing coordinates?

let $x = Ay$ and $g(y) = f(Ay)$

Can get $\nabla^2 g(y) = I$ if $A = [\nabla^2 f(x)]^{-1/2}$

Running gradient descent for g(y), gives best descent direction and convergence rate.

$$\begin{aligned} y_+ &= y - \eta \nabla g(y) \\ &= y - \eta A^T \nabla f(Ay), \\ Ay_+ &= Ay - \eta A A^T \nabla f(Ay) \\ x_+ &= x - \eta A A^T \nabla f(x). \end{aligned}$$

Equivalent to Newton step on f(x).

Affine Invariance

Important property Newton's method: affine invariance.

Assume $f : \mathbb{R}^n \to \mathbb{R}$ is twice differentiable and $A \in \mathbb{R}^{n \times n}$ is nonsingular. Let $g(y) := f(Ay)$.

Newton step for g starting from y is

$$y^+ = y - \left(\nabla^2 g(y)\right)^{-1} \nabla g(y).$$

It turns out that the Newton step for f starting from $x = Ay$ is $x^+ = Ay^+$.

Therefore progress is independent of problem scaling. By contrast, this is not true of gradient descent.

[Proof: HW3]

Affine Invariant stopping criterion

Stopping criterion for gradient descent:

$$\|\nabla f(x)\|_2 \leq \epsilon,$$

Not affine-invariant

Stopping criterion for Newton method:

$$\frac{\lambda^2(x)}{2} \leq \epsilon$$

where $\lambda(x) = \left(\nabla f(x)^T (\nabla^2 f(x))^{-1} \nabla f(x)\right)^{1/2}$ is the Newton decrement.

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 $x = Ay$

Affine Invariant stopping criterion

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

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

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

Another interpretation of Newton decrement: if Newton direction is $v = -(\nabla^2 f(x))^{-1} \nabla f(x)$, then

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

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

Newton method properties

- Quadratic convergence in the neighborhood of a strict local minimum [under some conditions].

- It can break down if $f''(x_k)$ is degenerate.
  [no inverse]

- It can diverge.

- It can be trapped in a loop.

- It can converge to a loop...

Damped Newton's Method

We have seen pure Newton's method, which need not converge. In practice, we instead 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 $t = 1$

Backtracking line search

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

Step sizes here typically are chosen by backtracking search, with parameters $0 < \alpha \le 1/2$, $0 < \beta < 1$. 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 $\nabla f(x)^T v = -\lambda^2(x)$

Convergence Rate

Local convergence for finding root

Theorem: Assume $F : \mathbb{R}^n \to \mathbb{R}^n$ is continuously differentiable and $x^\star \in \mathbb{R}^n$ is a root of F, that is, $F(x^\star) = 0$ such that $F'(x^\star)$ is non-singular. Then

(a) There exists $\delta > 0$ such that if $\|x^{(0)} - x^\star\| < \delta$ then Newton's method is well defined and

$$\lim_{k\to\infty} \frac{\|x^{(k+1)} - x^\star\|}{\|x^{(k)} - x^\star\|} = 0.$$

(b) If F' is Lipschitz continuous in a neighborhood of $x^\star$ then there exists $K > 0$ such that

$$\|x^{(k+1)} - x^\star\| \leq K\|x^{(k)} - x^\star\|^2.$$

Quadratic 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

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

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 $\|\nabla f(x^{(k_0+1)})\|_2 < \eta$

Convergence analysis

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

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

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

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

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

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

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

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

Convergence analysis

To reach $f(x^{(k)}) - f^\star \le \epsilon$, 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 $k_0 \le \frac{f(x^{(0)})-f^\star}{\gamma}$
- Somewhat bothersome may be the fact that the above bound depends on L, m, M, and yet the algorithm itself does not

Analysis can be improved e.g. for self-concordant functions

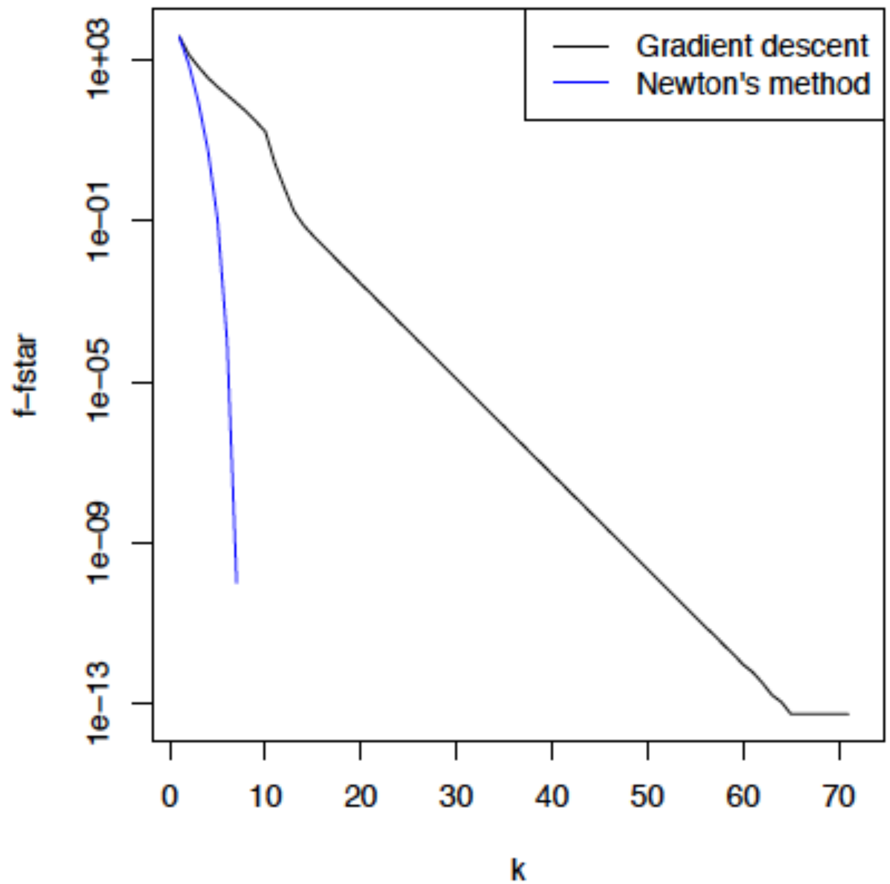
Comparison to first-order methods

Comparison to first-order methods

- 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

Example: Logistic regression

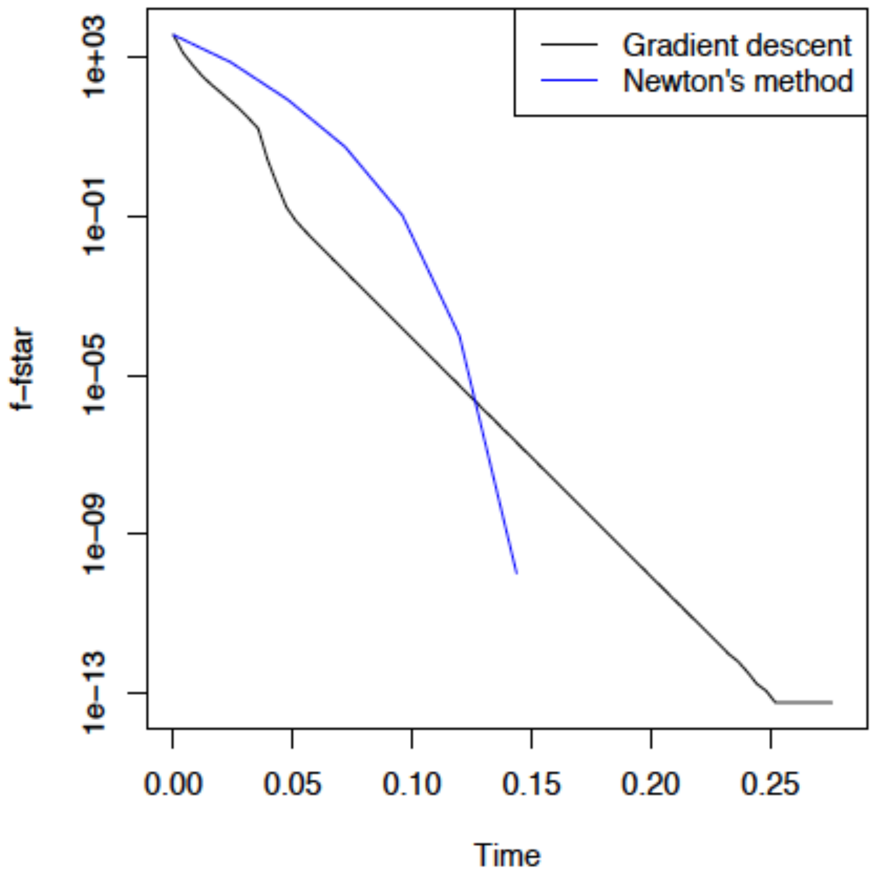
Logistic regression example, with $n = 500$, $p = 100$: we compare gradient descent and Newton's method, both with backtracking



Newton's method has a different regime of convergence.

Example: Logistic regression

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 $O(p^3)$