Newton’s Method

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Newton's Method – Motivation

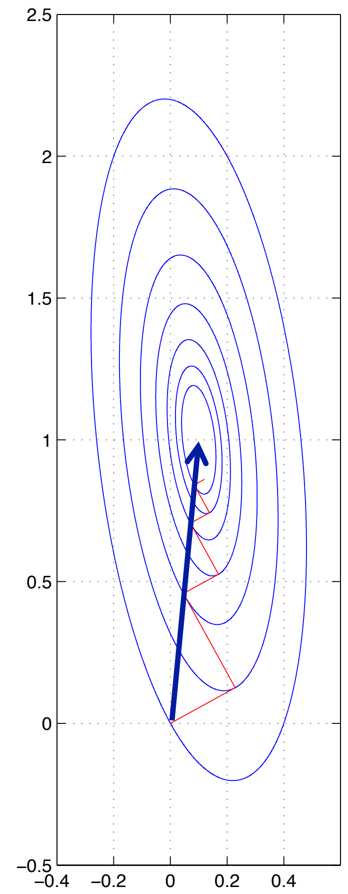
Quadratic Example:

$$\text{Min. } f(x) = \frac{1}{2}x^T Q x - b^T x$$

where $Q = Q^T$ is positive definite.

- At any current point x_k, the direction pointing to $x^* = Q^{-1}b$ is a perfect search direction, since exact line search along this direction will converge in just one step!

$$\begin{aligned} x^* &= x_k + \alpha p = Q^{-1}b \Longrightarrow \\ \alpha p &= Q^{-1}b - x_k = -Q^{-1}(Qx_k - b) \\ &= -\left[\nabla^2 f(x_k)\right]^{-1} \cdot \nabla f(x_k) \end{aligned}$$



Newton's Method – Motivation

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- Perfect search direction for quadratic and convex functions
- The step length is naturally $\alpha = 1$

Newton Iteration

Consider general nonlinear cost function f(x).

choose x_0 and tolerance $tol > 0$
$k \leftarrow 0$
evaluate $\nabla f(x_0)$ and $\nabla^2 f(x_0)$

while $\|\nabla f(x_k)\| > tol$
    Solve linear equation:
    $\nabla^2 f(x_k) p_k^N = -\nabla f(x_k)$ for p_k^N
    $x_{k+1} = x_k + p_k^N$
    $k = k + 1$
    evaluate gradient $\nabla f(x_k)$
    evaluate Hessian $\nabla^2 f(x_k)$
end

- Do not compute $[\nabla^2 f(x_k)]^{-1}$! Computing inverse of a matrix is very expensive!
- If the Hessian $\nabla^2 f(x_k)$ is positive definite, the Newton's direction p_k^N is a descent direction.
- If the Hessian $\nabla^2 f(x_k)$ is NOT positive definite, the Newton's direction p_k^N may not be a descent direction.
- Converge to minimum?

Newton Iteration – Example

Consider $\min_{x \in R} f(x) = \ln(1+x^2)$. $x^* = 0$ is the global minimizer.

$$f'(x) = \frac{2x}{1+x^2}, \qquad f''(x) = \frac{2(1-x^2)}{(1+x^2)^2}$$

$$\Longrightarrow \quad p_k^N = -\left[\nabla^2 f(x_k)\right]^{-1} \cdot \nabla f(x_k) = -\frac{x_k(1+x_k^2)}{1-x_k^2}$$

$$\Longrightarrow \quad x_{k+1} = x_k + p_k^N = \frac{2x_k^3}{x_k^2 - 1}$$

$\Longrightarrow$

- If $|x_0| > \frac{1}{\sqrt{3}}$, $\lim_{k\to\infty} |x_k| = \infty$;
- If $|x_0| < \frac{1}{\sqrt{3}}$, $\lim_{k\to\infty} x_k = 0$;
- If $|x_0| = \frac{1}{\sqrt{3}}$, $x_k = \{-\frac{1}{\sqrt{3}}, \frac{1}{\sqrt{3}}\}$.

- Unlike the steepest descent method, global convergence of Newton's method is NOT guaranteed.

Newton's Method – Convergence Results

Theorem 3.5.

Suppose that f is twice differentiable and that the Hessian $\nabla^2 f(x)$ is Lipschitz continuous (see (A.42)) in a neighborhood of a solution x^* at which the sufficient conditions (Theorem 2.4) are satisfied. Consider the iteration $x_{k+1} = x_k + p_k$, where p_k is given by (3.30). Then

(i) *if the starting point x_0 is sufficiently close to x^*, the sequence of iterates converges to x^*;*

(ii) *the rate of convergence of $\{x_k\}$ is quadratic; and*

(iii) *the sequence of gradient norms $\{\|\nabla f_k\|\}$ converges quadratically to zero.*

Let $\{x_k\}_{k=0}^{\infty}$ be a sequence in R^n that converges to x^*. The rate of convergence of $\{x_k\}$ is quadratic, if there is a constant $M > 0$ such that

$$\|x_{k+1} - x^*\| \leq M\|x_k - x^*\|^2$$

for all k sufficiently large.

Newton's Method – Convergence Analysis

Sketch of a proof:

1. Let $e_k = x_k - x^*$. Then

$$\begin{aligned} e_{k+1} &= x_k + p_k - x^* = x_k - x^* - \left[\nabla^2 f(x_k)\right]^{-1} \cdot \nabla f(x_k) \\ &= \left[\nabla^2 f(x_k)\right]^{-1} \left[\nabla^2 f(x_k)(x_k - x^*) - \nabla f(x_k)\right] \\ &= \left[\nabla^2 f(x_k)\right]^{-1} \left[\nabla^2 f(x_k)(x_k - x^*) - \boxed{(\nabla f(x_k) - \nabla f(x^*))}\right] \end{aligned}$$

Define $g(t) = \nabla f(x_k + t(x^* - x_k))$, $t \in [0,1]$. Then,

$$\begin{aligned} \nabla f(x_k) - \nabla f(x^*) &= g(0) - g(1) = -\int_0^1 g'(t)dt \\ &= \boxed{\int_0^1 \nabla^2 f(x_k + t(x^* - x_k))(x_k - x^*)dt} \end{aligned}$$

By Lipchitz continuity of $\nabla^2 f(x)$,

$$\|e_{k+1}\| \leq \frac{L}{2} \left\| \left[\nabla^2 f(x_k)\right]^{-1} \right\| \cdot \|e_k\|^2,$$

where L is the Lipchitz constant of $\nabla^2 f(x)$.

Newton's Method – Convergence Analysis

2. $\|e_{k+1}\| \;\leq\; \frac{L}{2}\boxed{\left\|\left[\nabla^2 f(x_k)\right]^{-1}\right\|}\cdot\|e_k\|^2$

Lemma. Let A and B be $n \times n$ matrices. Suppose A is invertible and $\|A - B\| \leq \frac{1}{\|A^{-1}\|}$. Then B is invertible. Moreover,

$$\|B^{-1}\| \leq \frac{\|A^{-1}\|}{1 - \|A^{-1}\| \cdot \|A - B\|}.$$

If B is sufficiently close to an invertible matrix A, B is invertible with a bounded inverse. In particular, if $\|A - B\| \leq \frac{1}{2\|A^{-1}\|}$, B is invertible, and $\|B^{-1}\| \leq 2\|A^{-1}\|$.

Since $\nabla^2 f(x)$ is continuous, there exist a sufficient small r, such that

$$\forall x \text{ with } \|x - x^*\| \leq r,\; \|\nabla^2 f(x) - \nabla^2 f(x^*)\| \leq \frac{1}{2\|\nabla^2 f(x^*)\|}.$$

By the Lemma, $\nabla^2 f(x)$ is invertible and

$$\left\|\left[\nabla^2 f(x)\right]^{-1}\right\| \leq \boxed{2\left\|\left[\nabla^2 f(x^*)\right]^{-1}\right\|}.$$

Newton's Method – Convergence Analysis

$\Longrightarrow$ There exist a sufficient small r, such that $\forall x_k$ with $\|x_k - x^*\| \leq r$,

$$\boxed{\|e_{k+1}\| \;\leq\; \tilde{L}\|e_k\|^2.} \qquad (\tilde{L} = L\left\|\left[\nabla^2 f(x^*)\right]^{-1}\right\|)$$

3. Define a set $\mathbb{B} = \{x \in R^n \mid \|x - x^*\| < \min(r, \frac{1}{2\tilde{L}})\}$. For all $x_0 \in \mathbb{B}$,

$\Longrightarrow$
$$\begin{aligned} \|x_1 - x^*\| \;&\leq\; \tilde{L}\|x_0 - x^*\|^2 \;=\; \tilde{L}\|x_0 - x^*\|\|x_0 - x^*\| \\ &\leq\; \tilde{L}\frac{1}{2\tilde{L}}\|x_0 - x^*\| \;=\; \frac{1}{2}\|x_0 - x^*\| \end{aligned}$$

$\Longrightarrow$ $x_1 \in \mathbb{B}$. By induction, the sequence $\{x_k\}_{k=0}^{\infty} \in \mathbb{B}$, and

$$\|x_{k+1} - x^*\| \;\leq\; \frac{1}{2}\|x_k - x^*\|$$

$\Longrightarrow$ For all $x_0 \in \mathbb{B}$, $\lim_{k\to\infty} x_k = x^*$, and the rate of convergence is quadratic.

Steepest Descent / Newton's Method

	Steepest Descent	Newton's Method
Robust?	Yes (global convergence)	No (local convergence)
Efficient?	No (linear rate of convergence)	Yes (quadratic rate of convergence)
Computational Cost	Cheap	Expensive

Needs $f(x_k)$ and $\nabla f(x_k)$

Needs gradient $\nabla f(x_k)$, Hessian $\nabla^2 f(x_k)$, and solving $\nabla^2 f(x_k) p_k^N = -\nabla f(x_k)$

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Tradeoffs among these goals are essential issues in numerical optimization! ⇒

- Conjugate gradient methods
- Trust region methods
- Quasi-Newton methods
- …