# Lecture 4: Second-order methods: Newton's method for unconstrained optimization

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C6.2/B2: Continuous Optimization

# Other search directions in Generic Linesearch Methods (GLMs)

Let $B^k$ symmetric, positive definite matrix [$B^k \succ 0$]. Let $s^k$ be defined by

$$B^k s^k = -\nabla f(x^k). \qquad (*)$$

- $\Longrightarrow \quad s^k$ descent direction:
  $\nabla f(x^k)^T s^k = -\nabla f(x^k)^T (B^k)^{-1} \nabla f(x^k) < 0$ whenever $\nabla f(x^k) \neq 0$ as $B^k$ pos. def. implies $(B^k)^{-1}$ pos. def.
- $\Longrightarrow \quad s^k$ uniquely solves

  $$\text{minimize}_{s \in \mathbb{R}^n} \; m_k(s) = f(x^k) + \nabla f(x^k)^T s + \tfrac{1}{2} s^T B^k s.$$

- $(*)$ is a scaled steepest descent direction;
- For some $B^k$, resulting GLMs can be made scale-invariant, and faster than steepest descent asymptotically

How to choose $B^k$ ?...[Newton, modified Newton, quasi-Newton; to follow.]

# Linesearch Newton's method

Let $f \in C^2(\mathbb{R}^n)$ and $B^k := \nabla^2 f(x^k)$ in GLM.

**Linesearch-Newton (also called Damped Newton's) method for minimization:**

Choose $\epsilon > 0$ and $x^0 \in \mathbb{R}^n$.

While $\|\nabla f(x^k)\| > \epsilon$, REPEAT:

- solve the linear system $\nabla^2 f(x^k) s^k = -\nabla f(x^k)$.
- set $x^{k+1} = x^k + \alpha^k s^k$, where $\alpha^k \in (0, 1]$; $k := k + 1$. END.

- Needs $\nabla^2 f(x^k)$ to be positive definite so that $s^k$ descent. Then $\alpha^k$ can be computed by exact linesearch, bArmijo, etc.

Some terminology:

Newton direction: $s^k = -(\nabla^2 f(x^k))^{-1} \nabla f(x^k)$.

(Pure) Newton's method: Newton's method without linesearch sets $x^{k+1} = x^k + s^k$ where $s^k$ is the Newton direction for all $k$.

- Whenever $\nabla^2 f(x^k)$ is positive definite, $s^k$ minimizes the second-order Taylor approximation of $f$ around $x^k$ (recall stp. descent minimizes first-order Taylor).

# Connection to Newton's method for root-finding

$x^*$ stationary point of $f \iff \nabla f(x^*) = 0$.

Let $r(x) := \nabla f(x) = 0 \quad n \times n$ system of nonlinear equations

$\longrightarrow$ apply Newton's method for root-finding to $\nabla f(x) = 0$:

Let $x^{k+1}$ s. t. $r(x^k) + J(x^k)(x^{k+1} - x^k) = 0$, where $J(x^k)$ is the Jacobian (matrix) of $r(x)$ at $x = x^k$, i.e., $J(x^k)_{ij} = \left(\frac{\partial r_i}{\partial x_j}\right)(x^k)$.

$$\overset{J(x^k)\ \text{nonsingular}}{\Longrightarrow} \qquad x^{k+1} = x^k - (J(x^k))^{-1} r(x^k).$$

- The Jacobian of $\nabla f$ at $x$ is the Hessian matrix $\nabla^2 f(x)$

$$\Downarrow \ \nabla^2 f(x^k) \ \text{nonsingular}$$

$$\text{(Pure) Newton iterate}: \ x^{k+1} = x^k - (\nabla^2 f(x^k))^{-1} \nabla f(x^k).$$

# Advantages of Newton's method for optimization

- Fast (i.e., quadratic) local rate of convergence.

Theorem 7 (local convergence of (pure) Newton's method):

- let $f \in \mathcal{C}^2(\mathbb{R}^n)$, $\nabla f(x^*) = 0$ with $\nabla^2 f(x^*)$ nonsingular;
- $\nabla^2 f$ locally Lipschitz continuous at $x^*$.

If $x^{k_0}$ is sufficiently close to $x^*$, for some $k_0 \geq 0$,

$\Longrightarrow$ $x^k$ is well-defined for all $k \geq k_0$;

$x^k \to x^*$ as $k \to \infty$, at quadratic rate. $\square$

- In the conditions of Th 7: $\nabla f(x^k) \to 0$ quadratically as well.

- "$x^{k_0}$ sufficiently close to $x^*$"= there exists $\mathcal{N}(x^*, \delta)$ such that $x^{k_0} \in \mathcal{N}$. In general, $\mathcal{N}$ not known beforehand (depends on unknown $x^*$ and problem-dependent constants).

# Advantages of Newton's method for optimization

<u>Sketch of Proof for Theorem 7:</u>

Taylor expansion of $\nabla f$ around x [vector form]:

$$\nabla f(x^*) = \nabla f(x) + \nabla^2 f(x)(x^* - x) + \mathcal{O}(\|x^* - x\|^2),$$

where $x$ is sufficiently close to $x^*$ and $\mathcal{O}(\cdot)$ depends on the Lipschitz constant of $\nabla^2 f(x^*)$. Using $\nabla f(x^*) = 0$ and $x := x^k$, whenever $x^k$ suff. close to $x^*$, we have

$$0 = \nabla f(x^k) + \nabla^2 f(x^k)(x^* - x^k) + \mathcal{O}(\|x^* - x^k\|^2). \;(**)$$

$\nabla^2 f(x^*)$ nonsingular $\Longrightarrow$ $\nabla^2 f(x^k)$ nonsingular whenever $x^k$ suff. close to $x^*$. Now (**) implies $x^k - x^* = [\nabla^2 f(x^k)]^{-1} \nabla f(x^k) + \mathcal{O}(\|x^* - x^k\|^2)$. Letting $s^k$ be the Newton direction, and $x^{k+1} = x^k + s^k$, we deduce that, whenever $x^k$ suff. close to $x^*$, $x^{k+1} - x^* = \mathcal{O}(\|x^k - x^*\|^2)$. $\Box$

# Local convergence for linesearch-Newton's method

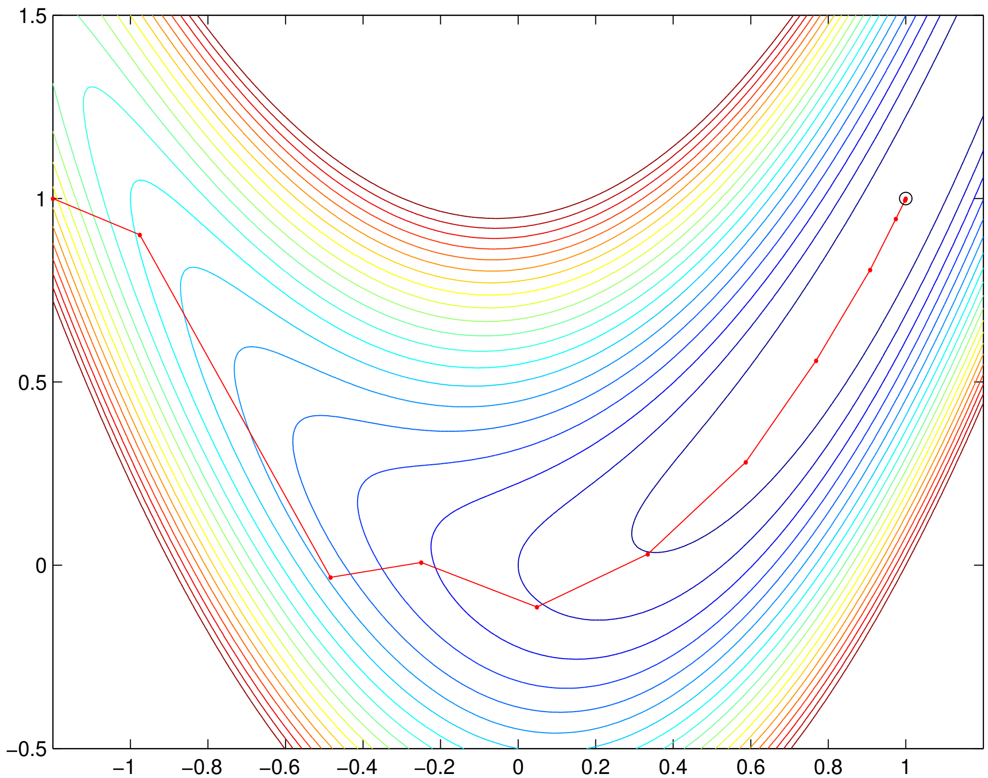
Theorem 8  Let $f \in \mathcal{C}^2(\mathbb{R}^n)$ and $\nabla^2 f$ be Lipschitz continuous and positive definite at the iterates.

Apply Newton's method with bArmijo linesearch and the choices $\beta \leq 0.5$ and $\alpha_{(0)} = 1$. Assume the iterates $x^k \to x^*$ as $k \to \infty$, where $\nabla^2 f(x^*) \succ 0$.

Then $\alpha^k = 1$ for all $k$ sufficiently large, and the rate of convergence of $x^k$ to $x^*$ is quadratic (asymptotically).

# Local convergence for Newton with bArmijo linesearch

$$f(x_1, x_2) = 10(x_2 - x_1^2)^2 + (x_1 - 1)^2; \quad x^* = (1, 1).$$




Newton with bArmijo linesearch applied to the Rosenbrock function $f$.

- $\beta < 0.5$ and $\alpha_{(0)} = 1$ in bArmijo; $\alpha^k = 1$ for suff. large $k$.

# Advantages of Newton's method for optimization

- Newton's method (with or without linesearch) is scale invariant with respect to linear transformations of variables.

Let $A \in \mathbb{R}^{n\times n}$ nonsingular matrix and $y = Ax$
($A$ is constant, independent of $x$ and $y$); let $B = A^{-1}$.

Let $\overline{f}(y) := f(x(y)) = f(By)$; minimize $\overline{f}$ wrt $y$.

$\Longrightarrow \nabla \overline{f}(y) = B^T \nabla f(x)$ and $\nabla^2 \overline{f}(y) = B^T \nabla^2 f(x) B$.

Newton direction at $y$:
$$\begin{aligned} s_y &= -[B^T \nabla^2 f(x) B]^{-1} B^T \nabla f(x) \\ &= -B^{-1}[\nabla^2 f(x)]^{-1} B^{-T} B^T \nabla f(x) \\ &= -B^{-1}[\nabla^2 f(x)]^{-1} \nabla f(x) \\ &= A s_x. \end{aligned}$$

$\Longrightarrow \quad y + \alpha s_y = A(x + \alpha s_x)$.

Thus $y + \alpha s_y \approx y^* \quad \Longrightarrow \quad x + \alpha s_x \approx x^*$, where $y^* = Ax^*$.

# Disadvantages of Newton's method for optimization

- Newton's method with/without linesearch: the Newton direction $s^k$ is not well-defined if $\nabla^2 f(x^k)$ singular; $s^k$ may not be descent if $\nabla^2 f(x^k)$ is not positive definite.
- Newton's method ('pure', without linesearch): iterates can get attracted to local maxima or saddle points of $f$ if sufficiently close to them (in the conditions of local convergence Theorem 7, $\nabla^2 f(x^*)$ only required to be nonsingular).
- Newton's method ('pure', without linesearch): iterates may fail to converge at all if $x^0$ 'too far' from solution (outside neighbourhood of local convergence, failure may occur). Thus linesearch is needed to make Newton's method globally convergent.

# Disadvantages of Newton's method for optimization

Example of failure of (pure) Newton's method to converge globally.

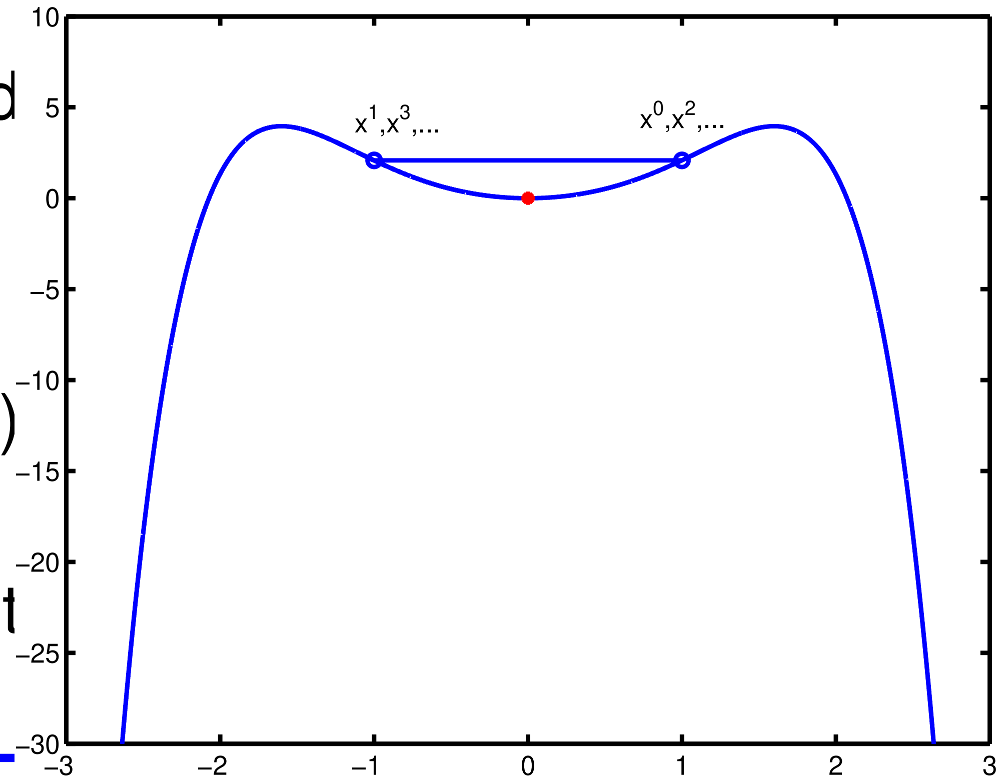
$$f : \mathbb{R} \to \mathbb{R}, \qquad f(x) = -\frac{x^6}{6} + \frac{x^4}{4} + 2x^2.$$

$x^* = 0$ local minimizer; $x = \pm\sqrt{(1+\sqrt{17})/2} \approx \pm 1.6$ global max.

Newton's method applied to $f$, with $x^0 = 1$;
$\Rightarrow$ $x^{2k} = 1$ and $x^{2k+1} = -1$, for all $k$.

$-1$ and $1$ are not (even) stationary points of $f$.

Note that $s^k$ descent but we have gone 'too far'.




Newton's method applied to $f$.