

The Newton Method

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Overview

- ▶ The Newton Method
- ▶ Newton Type Methods
- ▶ Convergence Theory
- ▶ Globalization
- ▶ Application to Unconstrained Optimization

Nonlinear Root Finding Problem

Regard nonlinear continuously differentiable function $F : \mathbb{R}^n \rightarrow \mathbb{R}^n$, $w \mapsto F(w)$. Aim is to solve **nonlinear root finding problem**

$$F(w) = 0.$$

Newton's idea: start with guess w_0 , and recursively generate sequence of iterates $\{w_k\}_{k=0}^{\infty}$ by linearizing the nonlinear equation at the current iterate:

$$F(w_k) + \frac{\partial F}{\partial w}(w_k)(w - w_k) = 0.$$

Can explicitly compute next iterate:

$$w_{k+1} = w_k - \left(\frac{\partial F}{\partial w}(w_k) \right)^{-1} F(w_k)$$

Note: we have to assume that Jacobian $\frac{\partial F}{\partial w}(w)$ is invertible.

Example: fifth root of two

Regard $F(w) = w^5 - 2$, where $\frac{\partial F}{\partial w}(w) = 5w^4$.

Newton iteration:

$$w_{k+1} = w_k - (5w_k^4)^{-1}(w_k^5 - 2)$$

Iterates quickly converge to solution w^* with $F(w^*) = 0$.

In fact, the convergence rate of Newton's method is *quadratic*.

Convergence Rates

Sequence w_k converges to limit point $w^* = \lim_{k \rightarrow \infty} w_k$. Rate of convergence is

- ▶ **q-linear** if there exists $\alpha < 1$ and k_0 such that for all $k \geq k_0$ holds

$$\|w_{k+1} - w^*\| \leq \alpha \|w_k - w^*\|$$

- ▶ **q-superlinear** if there exists a sequence α_k with $\lim_{k \rightarrow \infty} \alpha_k = 0$ such that

$$\|w_{k+1} - w^*\| \leq \alpha_k \|w_k - w^*\|$$

- ▶ **q-quadratic** if there exists a β and k_0 such that for all $k \geq k_0$ holds

$$\|w_{k+1} - w^*\| \leq \beta \|w_k - w^*\|^2$$

Correct digits double in each iteration. E.g.

$$\|w_k - w^*\| = 10^{-2^k} \text{ with } \beta = 1.$$

Newton Type Methods

More general, can use an approximation M_k of the Jacobian $J(w_k) := \frac{\partial F}{\partial w}(w_k)$. The Newton type iteration is

$$w_{k+1} = w_k - M_k^{-1}F(w_k)$$

Depending on how closely M_k approximates $J(w_k)$, the convergence rate can be faster or slower.

Local Contraction of Newton Type Methods

THEOREM: Sequence w_k converges to w^* with contraction rate

$$\|w_{k+1} - w^*\| \leq \left(\kappa + \frac{\omega}{2} \|w_k - w^*\| \right) \|w_k - w^*\|$$

if $\|w_0 - w^*\|$ is sufficiently small and there exist $\omega < \infty$ and $\kappa < 1$ such that for all w_k and w holds

$$\|M_k^{-1}(J(w_k) - J(w))\| \leq \omega \|w_k - w\| \quad (\text{Lipschitz condition})$$

$$\|M_k^{-1}(J(w_k) - M_k)\| \leq \kappa \quad (\text{compatibility condition})$$

Note: $\kappa = 0$ for exact Newton.

Proof (1):

$$\begin{aligned}w_{k+1} - w^* &= w_k - w^* - M_k^{-1}F(w_k) \\&= w_k - w^* - M_k^{-1}(F(w_k) - F(w^*)) \\&= M_k^{-1}(M_k(w_k - w^*)) \\&\quad - M_k^{-1} \int_0^1 J(w^* + t(w_k - w^*))(w_k - w^*)dt \\&= M_k^{-1}(M_k - J(w_k))(w_k - w^*) \\&\quad - M_k^{-1} \int_0^1 [J(w^* + t(w_k - w^*)) - F(w_k)](w_k - w^*)dt\end{aligned}$$

Proof (2):

Taking the norm of both sides:

$$\begin{aligned}\|w_{k+1} - w^*\| &\leq \kappa \|w_k - w^*\| \\ &\quad + \int_0^1 \omega \|w^* + t(w_k - w^*) - w_k\| dt \|w_k - w^*\| \\ &= \left(\kappa + \omega \underbrace{\int_0^1 (1-t) dt}_{=\frac{1}{2}} \|w_k - w^*\| \right) \|w_k - w^*\| \\ &= \left(\kappa + \frac{\omega}{2} \|w_k - w^*\| \right) \|w_k - w^*\|\end{aligned}$$

Globalization

The condition $\|w_0 - w^*\|$ is usually not satisfied, and the iteration needs to be *globalized* before it enters the area of local convergence. Different strategies:

- ▶ Homotopy: modify $F(w) = 0$ to an easier or solved problem (e.g. $F(w) - \lambda F(w_0) = 0$), slowly change homotopy parameter λ from 1 to 0, each time restarting Newton iteration at previous solution
- ▶ Line search: take smaller steps $\alpha_k \leq 1$

$$w_{k+1} = w_k - \alpha_k M_k^{-1} F(w_k)$$

(equivalent to an increase of M_k to $\alpha_k^{-1} M_k$)

- ▶ Trust region/Levenberg Marquard: modify iteration to ensure that steps $\|w_{k+1} - w_k\|$ remain sufficiently small, e.g.

$$w_{k+1} = w_k - (\beta_k I + M_k)^{-1} F(w_k)$$

Newton for unconstrained optimization

Optimization problem $\min_x f(x)$ is solved by $\nabla f(x^*) = 0$. Identify $w \equiv x$ and $F(w) \equiv \nabla f(x)$. Exact Newton method iterates

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

General Newton type methods iterate

$$x_{k+1} = x_k - B_k^{-1} \nabla f(x_k)$$

with some **Hessian approximation** B_k , for example:

- ▶ gradient method: $B_k = I$
- ▶ quasi Newton updates such as BFGS
- ▶ Gauss-Newton, for least squares problems $f(x) = \|R(x)\|_2^2$ use $B_k = 2 \frac{\partial R}{\partial x}(x_k)^\top \frac{\partial R}{\partial x}(x_k)$
- ▶ exact Hessian with Levenberg-Marquard modification: $B_k = \nabla^2 f(x_k) + \beta_k I$ to ensure positive definiteness and descent

Literature

- ▶ J. Nocedal and S. Wright: Numerical Optimization, Springer, 2006 (2nd edition)
- ▶ S. Boyd and L. Vandenberghe: Convex Optimization, Cambridge Univ. Press, 2004