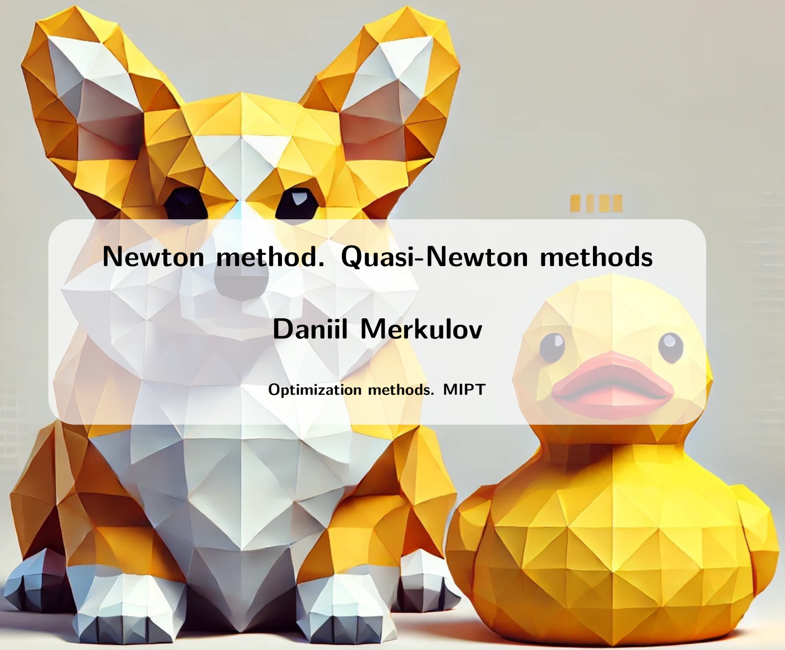


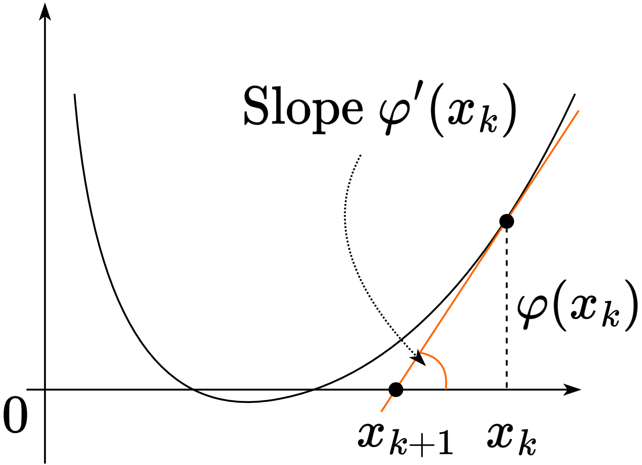
Newton method. Quasi-Newton methods

Daniil Merkulov

Optimization methods. MIPT

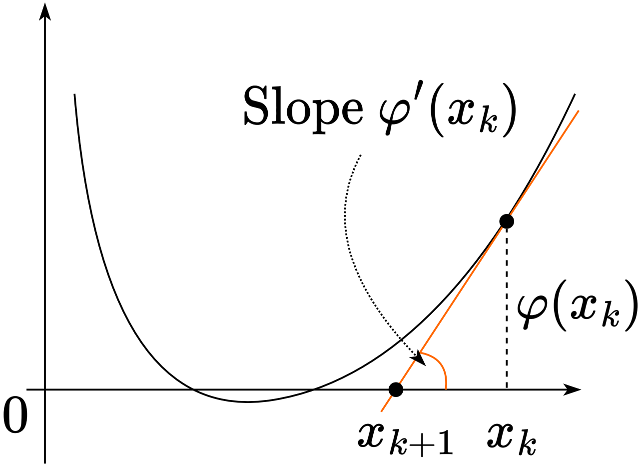
Newton method

Idea of Newton method of root finding



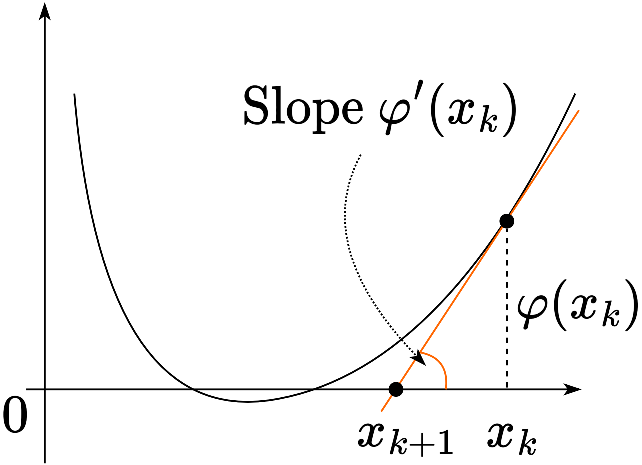
Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.

Idea of Newton method of root finding



Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

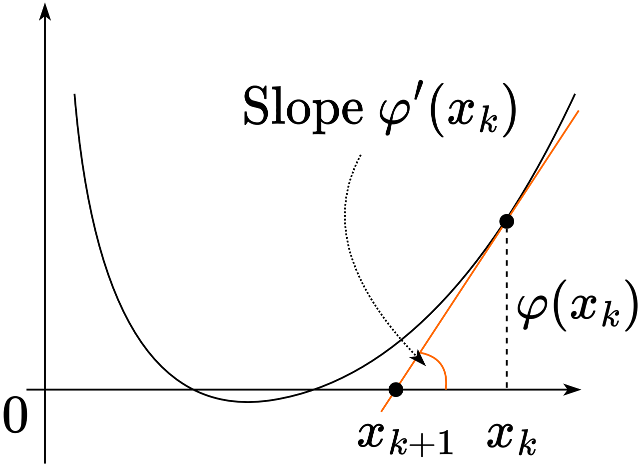
Idea of Newton method of root finding



Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

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

Idea of Newton method of root finding

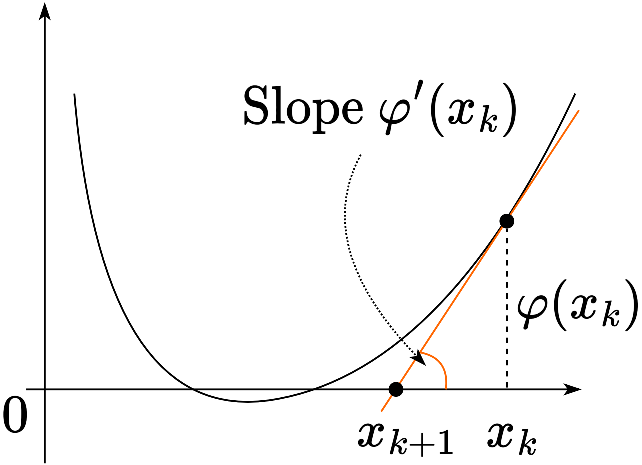


Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

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

We get an iterative scheme:

Idea of Newton method of root finding



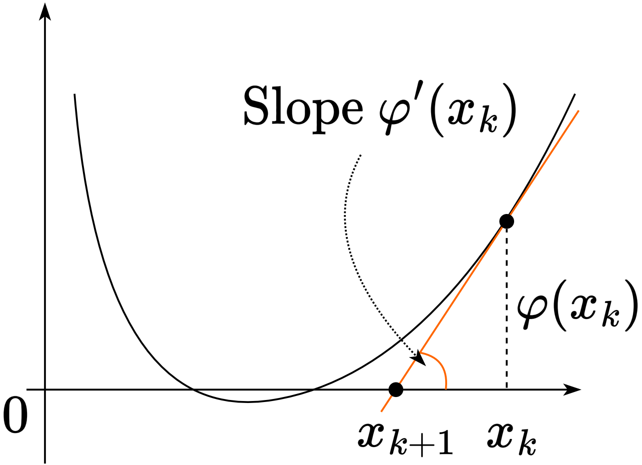
Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

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

We get an iterative scheme:

$$x_{k+1} = x_k - \frac{\varphi(x_k)}{\varphi'(x_k)}.$$

Idea of Newton method of root finding



Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

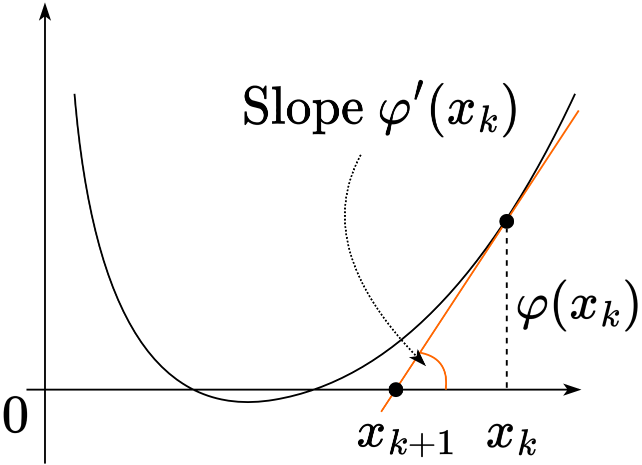
$$\varphi'(x_k) = \frac{\varphi(x_k)}{x_{k+1} - x_k}$$

We get an iterative scheme:

$$x_{k+1} = x_k - \frac{\varphi(x_k)}{\varphi'(x_k)}.$$

Which will become a Newton optimization method in case $f'(x) = \varphi(x)$[a]:

Idea of Newton method of root finding



Consider the function $\varphi(x) : \mathbb{R} \to \mathbb{R}$.
The whole idea came from building a linear approximation at the point x_k and find its root, which will be the new iteration point:

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

We get an iterative scheme:

$$x_{k+1} = x_k - \frac{\varphi(x_k)}{\varphi'(x_k)}.$$

Which will become a Newton optimization method in case $f'(x) = \varphi(x)$[a]:

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

[a] Literally we aim to solve the problem of finding stationary points $\nabla f(x) = 0$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x - x_k), x - x_k\rangle.$$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k \rangle.$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k \rangle.$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

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

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k\rangle.$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

$$\begin{aligned}
\nabla f^{II}_{x_k}(x_{k+1}) &= \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k) = 0 \\
\nabla^2 f(x_k)(x_{k+1} - x_k) &= -\nabla f(x_k)
\end{aligned}$$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$
f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k \rangle.
$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

$$
\begin{aligned}
\nabla f^{II}_{x_k}(x_{k+1}) &= \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k) = 0 \\
\nabla^2 f(x_k)(x_{k+1} - x_k) &= -\nabla f(x_k) \\
\left[\nabla^2 f(x_k)\right]^{-1} \nabla^2 f(x_k)(x_{k+1} - x_k) &= -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k)
\end{aligned}
$$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$
f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k \rangle.
$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

$$
\begin{aligned}
\nabla f^{II}_{x_k}(x_{k+1}) &= \nabla f(x_{k}) + \nabla^2 f(x_k)(x_{k+1} - x_k) = 0 \\
\nabla^2 f(x_k)(x_{k+1} - x_k) &= -\nabla f(x_{k}) \\
\left[\nabla^2 f(x_k)\right]^{-1} \nabla^2 f(x_k)(x_{k+1} - x_k) &= -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_{k}) \\
x_{k+1} &= x_k -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_{k}).
\end{aligned}
$$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k\rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x-x_k), x-x_k \rangle.$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

$$\begin{aligned}
\nabla f^{II}_{x_k}(x_{k+1}) &= \nabla f(x_{k}) + \nabla^2 f(x_k)(x_{k+1} - x_k) = 0 \\
\nabla^2 f(x_k)(x_{k+1} - x_k) &= -\nabla f(x_{k}) \\
\left[\nabla^2 f(x_k)\right]^{-1} \nabla^2 f(x_k)(x_{k+1} - x_k) &= -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_{k}) \\
x_{k+1} &= x_k -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_{k}).
\end{aligned}$$

Newton method as a local quadratic Taylor approximation minimizer

Let us now have the function $f(x)$ and a certain point x_k. Let us consider the quadratic approximation of this function near x_k:

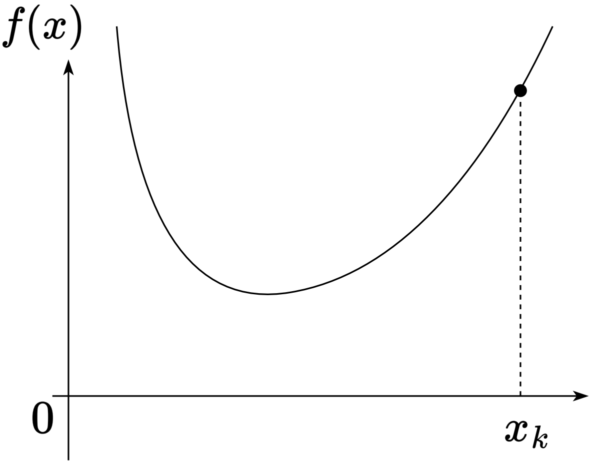
$$f^{II}_{x_k}(x) = f(x_k) + \langle \nabla f(x_k), x - x_k \rangle + \frac{1}{2} \langle \nabla^2 f(x_k)(x - x_k), x - x_k \rangle.$$

The idea of the method is to find the point x_{k+1}, that minimizes the function $f^{II}_{x_k}(x)$, i.e. $\nabla f^{II}_{x_k}(x_{k+1}) = 0$.

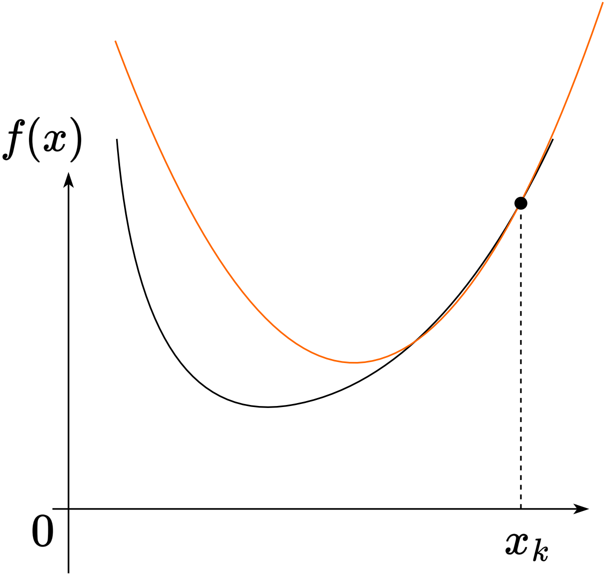
$$\begin{aligned}
\nabla f^{II}_{x_k}(x_{k+1}) &= \nabla f(x_k) + \nabla^2 f(x_k)(x_{k+1} - x_k) = 0 \\
\nabla^2 f(x_k)(x_{k+1} - x_k) &= -\nabla f(x_k) \\
\left[\nabla^2 f(x_k)\right]^{-1} \nabla^2 f(x_k)(x_{k+1} - x_k) &= -\left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k) \\
x_{k+1} &= x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k).
\end{aligned}$$

Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

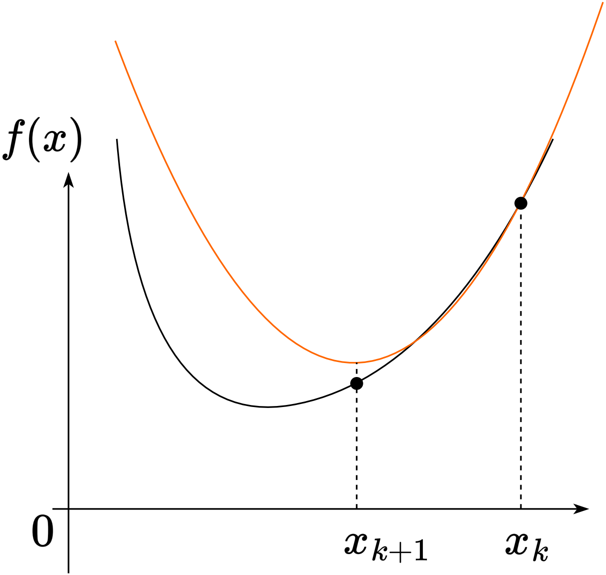
Newton method as a local quadratic Taylor approximation minimizer



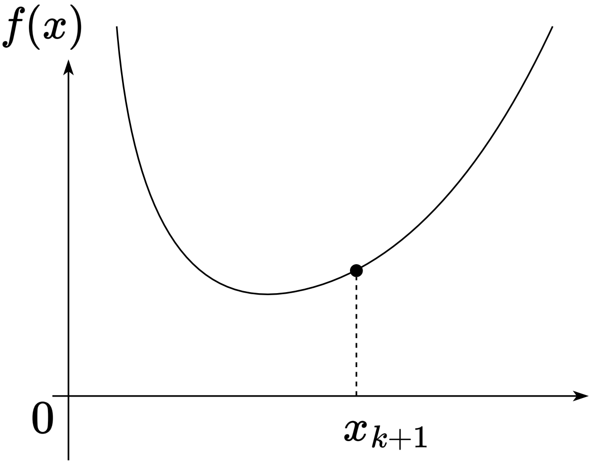
Newton method as a local quadratic Taylor approximation minimizer



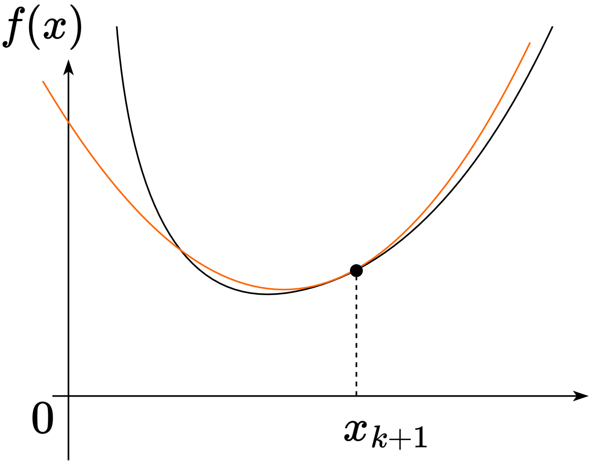
Newton method as a local quadratic Taylor approximation minimizer



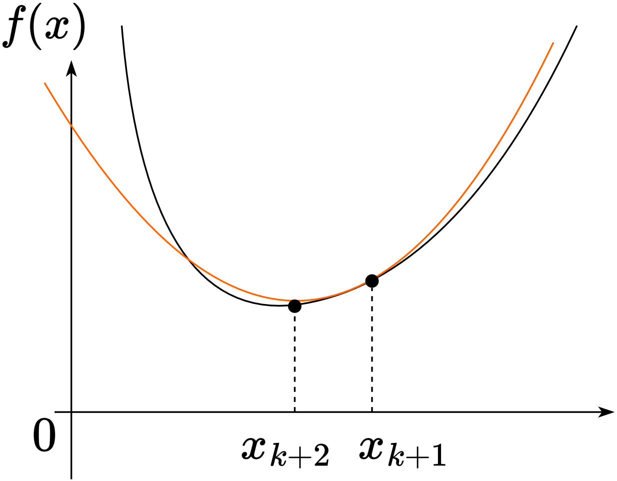
Newton method as a local quadratic Taylor approximation minimizer



Newton method as a local quadratic Taylor approximation minimizer



Newton method as a local quadratic Taylor approximation minimizer



Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Proof

Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Proof

1. We will use Newton-Leibniz formula

$$\nabla f(x_k) - \nabla f(x^*) = \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau$$

Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Proof

1. We will use Newton-Leibniz formula

$$\nabla f(x_k) - \nabla f(x^*) = \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau$$

2. Then we track the distance to the solution

Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Proof

1. We will use Newton-Leibniz formula

$$
\nabla f(x_k) - \nabla f(x^*) = \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*)d\tau
$$

2. Then we track the distance to the solution

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

Convergence

Theorem

Let $f(x)$ be a strongly convex twice continuously differentiable function at $\mathbb{R}^n$, for the second derivative of which inequalities are executed: $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$. Then Newton's method with a constant step locally converges to solving the problem with superlinear speed. If, in addition, Hessian is M-Lipschitz continuous, then this method converges locally to x^* at a quadratic rate.

Proof

1. We will use Newton-Leibniz formula

$$
\nabla f(x_k) - \nabla f(x^*) = \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau
$$

2. Then we track the distance to the solution

$$
\begin{aligned}
x_{k+1} - x^* = x_k - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k) - x^* = x_k - x^* - \left[\nabla^2 f(x_k)\right]^{-1} \nabla f(x_k) = \\
= x_k - x^* - \left[\nabla^2 f(x_k)\right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))(x_k - x^*) d\tau
\end{aligned}
$$

Convergence

3.

$$
= \left(I - \left[\nabla^2 f(x_k) \right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau \right) (x_k - x^*) =
$$

Convergence

3.

$$
= \left(I - \left[\nabla^2 f(x_k)\right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau \right) (x_k - x^*) =
$$

$$
= \left[\nabla^2 f(x_k)\right]^{-1} \left(\nabla^2 f(x_k) - \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau \right) (x_k - x^*) =
$$

Convergence

3.

$$
\begin{aligned}
&= \left(I - \left[\nabla^2 f(x_k)\right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\nabla^2 f(x_k) - \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)\right)(x_k - x^*) =
\end{aligned}
$$

Convergence

3.

$$
\begin{aligned}
&= \left(I - \left[\nabla^2 f(x_k)\right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\nabla^2 f(x_k) - \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} G_k (x_k - x^*)
\end{aligned}
$$

Convergence

3.

$$
\begin{aligned}
&= \left(I - \left[\nabla^2 f(x_k)\right]^{-1} \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\nabla^2 f(x_k) - \int_0^1 \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} \left(\int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right)\right)(x_k - x^*) = \\
&= \left[\nabla^2 f(x_k)\right]^{-1} G_k (x_k - x^*)
\end{aligned}
$$

4. We have introduced:

$$
G_k = \int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right).
$$

Convergence

5. Let's try to estimate the size of G_k:

   where $r_k = \|x_k - x^*\|$.

Convergence

5. Let's try to estimate the size of G_k:

$$\|G_k\| = \left\| \int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*))d\tau\right) \right\| \leq$$

where $r_k = \|x_k - x^*\|$.

Convergence

5. Let's try to estimate the size of G_k:

$$\|G_k\| = \left\| \int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau \right) \right\| \leq$$

$$\leq \int_0^1 \left\| \nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) \right\| d\tau \leq \qquad \text{(Hessian's Lipschitz continuity)}$$

where $r_k = \|x_k - x^*\|$.

Convergence

5. Let's try to estimate the size of G_k:

$$
\begin{aligned}
\|G_k\| = \left\| \int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau\right) \right\| \leq \\
\leq \int_0^1 \left\| \nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) \right\| d\tau \leq \qquad \text{(Hessian's Lipschitz continuity)} \\
\leq \int_0^1 M\|x_k - x^* - \tau(x_k - x^*)\| d\tau = \int_0^1 M\|x_k - x^*\|(1-\tau) d\tau = \frac{r_k}{2} M,
\end{aligned}
$$

where $r_k = \|x_k - x^*\|$.

Convergence

5. Let's try to estimate the size of G_k:

$$
\begin{aligned}
\|G_k\| = \left\| \int_0^1 \left(\nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) d\tau \right) \right\| \leq \\
\leq \int_0^1 \left\| \nabla^2 f(x_k) - \nabla^2 f(x^* + \tau(x_k - x^*)) \right\| d\tau \leq \qquad \text{(Hessian's Lipschitz continuity)} \\
\leq \int_0^1 M \|x_k - x^* - \tau(x_k - x^*)\| d\tau = \int_0^1 M \|x_k - x^*\| (1 - \tau) d\tau = \frac{r_k}{2} M,
\end{aligned}
$$

where $r_k = \|x_k - x^*\|$.

6. So, we have:

$$
r_{k+1} \leq \left\| \left[\nabla^2 f(x_k) \right]^{-1} \right\| \cdot \frac{r_k}{2} M \cdot r_k
$$

and we need to bound the norm of the inverse hessian

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$\nabla^2 f(x_k) - \nabla^2 f(x^*) \succeq -Mr_k I_n$$

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$
\begin{aligned}
\nabla^2 f(x_k) - \nabla^2 f(x^*) &\succeq -M r_k I_n \\
\nabla^2 f(x_k) &\succeq \nabla^2 f(x^*) - M r_k I_n
\end{aligned}
$$

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$
\begin{aligned}
\nabla^2 f(x_k) - \nabla^2 f(x^*) &\succeq -Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \nabla^2 f(x^*) - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \mu I_n - Mr_k I_n
\end{aligned}
$$

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$
\begin{aligned}
\nabla^2 f(x_k) - \nabla^2 f(x^*) &\succeq -Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \nabla^2 f(x^*) - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \mu I_n - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq (\mu - Mr_k) I_n
\end{aligned}
$$

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$
\begin{aligned}
\nabla^2 f(x_k) - \nabla^2 f(x^*) &\succeq -Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \nabla^2 f(x^*) - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \mu I_n - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq (\mu - Mr_k) I_n
\end{aligned}
$$

Convexity implies $\nabla^2 f(x_k) \succ 0$, i.e. $r_k < \frac{\mu}{M}$.

$$
\begin{aligned}
\left\| \left[\nabla^2 f(x_k) \right]^{-1} \right\| &\leq (\mu - Mr_k)^{-1} \\
r_{k+1} &\leq \frac{r_k^2 M}{2(\mu - Mr_k)}
\end{aligned}
$$

Convergence

7. Because of Hessian's Lipschitz continuity and symmetry:

$$
\begin{aligned}
\nabla^2 f(x_k) - \nabla^2 f(x^*) &\succeq -Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \nabla^2 f(x^*) - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq \mu I_n - Mr_k I_n \\
\nabla^2 f(x_k) &\succeq (\mu - Mr_k) I_n
\end{aligned}
$$

Convexity implies $\nabla^2 f(x_k) \succ 0$, i.e. $r_k < \frac{\mu}{M}$.

$$
\begin{aligned}
\left\| \left[\nabla^2 f(x_k) \right]^{-1} \right\| &\leq (\mu - Mr_k)^{-1} \\
r_{k+1} &\leq \frac{r_k^2 M}{2(\mu - Mr_k)}
\end{aligned}
$$

8. The convergence condition $r_{k+1} < r_k$ imposes additional conditions on r_k : $\quad r_k < \frac{2\mu}{3M}$

   Thus, we have an important result: Newton's method for the function with Lipschitz positive-definite Hessian converges **quadratically** near ($\| x_0 - x^* \| < \frac{2\mu}{3M}$) to the solution.

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n\times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

$$y_{k+1} = y_k - \left(\nabla^2 g(y_k)\right)^{-1} \nabla g(y_k)$$

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

$$y_{k+1} = y_k - \left(\nabla^2 g(y_k)\right)^{-1} \nabla g(y_k)$$

Expanding this, we get:

$$y_{k+1} = y_k - \left(A^T \nabla^2 f(Ay_k) A\right)^{-1} A^T \nabla f(Ay_k)$$

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

$$
y_{k+1} = y_k - \left(\nabla^2 g(y_k)\right)^{-1} \nabla g(y_k)
$$

Expanding this, we get:

$$
y_{k+1} = y_k - \left(A^T \nabla^2 f(Ay_k) A\right)^{-1} A^T \nabla f(Ay_k)
$$

Using the property of matrix inverse $(AB)^{-1} = B^{-1}A^{-1}$, this simplifies to:

$$
\begin{aligned}
y_{k+1} &= y_k - A^{-1} \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k) \\
Ay_{k+1} &= Ay_k - \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k)
\end{aligned}
$$

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

$$y_{k+1} = y_k - \left(\nabla^2 g(y_k)\right)^{-1} \nabla g(y_k)$$

Expanding this, we get:

$$y_{k+1} = y_k - \left(A^T \nabla^2 f(Ay_k) A\right)^{-1} A^T \nabla f(Ay_k)$$

Using the property of matrix inverse $(AB)^{-1} = B^{-1} A^{-1}$, this simplifies to:

$$\begin{aligned} y_{k+1} &= y_k - A^{-1} \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k) \\ Ay_{k+1} &= Ay_k - \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k) \end{aligned}$$

Thus, the update rule for x is:

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

Affine Invariance of Newton's Method

An important property of Newton's method is **affine invariance**. Given a function f and a nonsingular matrix $A \in \mathbb{R}^{n \times n}$, let $x = Ay$, and define $g(y) = f(Ay)$. Note, that $\nabla g(y) = A^T \nabla f(x)$ and $\nabla^2 g(y) = A^T \nabla^2 f(x) A$. The Newton steps on g are expressed as:

$$y_{k+1} = y_k - \left(\nabla^2 g(y_k)\right)^{-1} \nabla g(y_k)$$

Expanding this, we get:

$$y_{k+1} = y_k - \left(A^T \nabla^2 f(Ay_k) A\right)^{-1} A^T \nabla f(Ay_k)$$

Using the property of matrix inverse $(AB)^{-1} = B^{-1} A^{-1}$, this simplifies to:

$$y_{k+1} = y_k - A^{-1} \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k)$$
$$Ay_{k+1} = Ay_k - \left(\nabla^2 f(Ay_k)\right)^{-1} \nabla f(Ay_k)$$

Thus, the update rule for x is:

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

This shows that the progress made by Newton's method is independent of problem scaling. This property is not shared by the gradient descent method!

Summary

What's nice:

- quadratic convergence near the solution x^*

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

What's not nice:

- it is necessary to store the (inverse) hessian on each iteration: $\mathcal{O}(n^2)$ memory

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

What's not nice:

- it is necessary to store the (inverse) hessian on each iteration: $\mathcal{O}(n^2)$ memory
- it is necessary to solve linear systems: $\mathcal{O}(n^3)$ operations

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

What's not nice:

- it is necessary to store the (inverse) hessian on each iteration: $\mathcal{O}(n^2)$ memory
- it is necessary to solve linear systems: $\mathcal{O}(n^3)$ operations
- the Hessian can be degenerate at x^*

Summary

What's nice:

- quadratic convergence near the solution x^*
- affine invariance
- the parameters have little effect on the convergence rate

What's not nice:

- it is necessary to store the (inverse) hessian on each iteration: $\mathcal{O}(n^2)$ memory
- it is necessary to solve linear systems: $\mathcal{O}(n^3)$ operations
- the Hessian can be degenerate at x^*
- the hessian may not be positively determined $\to$ direction $-(f''(x))^{-1}f'(x)$ may not be a descending direction

Newton method problems

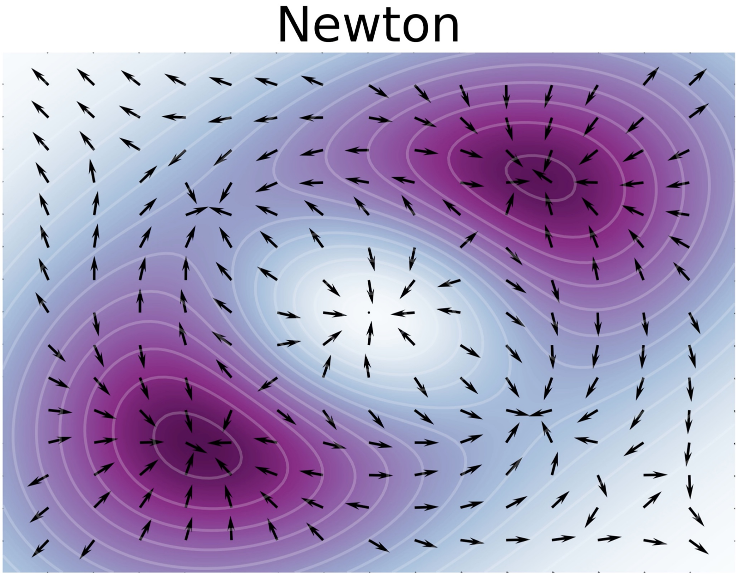


Figure 7: Animation

Newton method problems

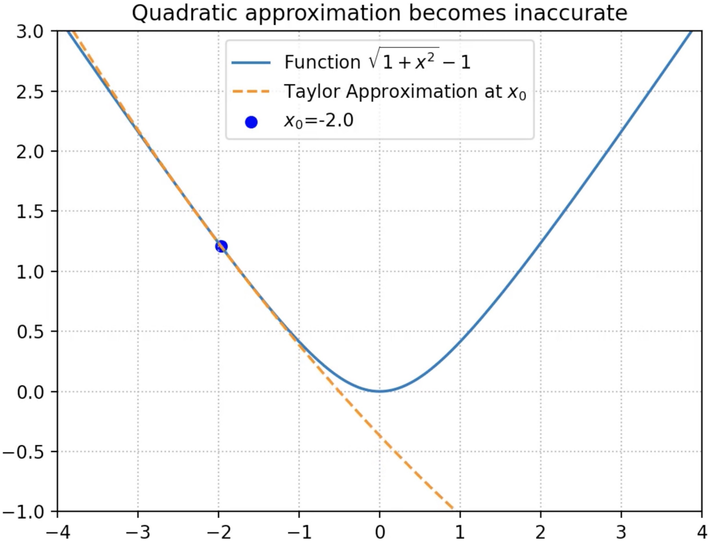


Figure 8: Animation

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$
s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$
s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

Let us assume that the distance is defined locally by some metric A:

$$
d(x, x_0) = (x - x_0)^\top A(x - x_0)
$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$
s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

Let us assume that the distance is defined locally by some metric A:

$$
d(x, x_0) = (x - x_0)^\top A (x - x_0)
$$

Let us also consider first order Taylor approximation of a function $f(x)$ near the point x_0:

$$
f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \tag{1}
$$

Now we can explicitly pose a problem of finding s, as it was stated above.

$$
\begin{aligned}
&\min_{\delta x \in \mathbb{R}^{\ltimes}} f(x_0 + \delta x) \\
&\text{s.t. } \delta x^\top A \delta x = \varepsilon^2
\end{aligned}
$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$
s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

Let us assume that the distance is defined locally by some metric A:

$$
d(x, x_0) = (x - x_0)^\top A (x - x_0)
$$

Let us also consider first order Taylor approximation of a function $f(x)$ near the point x_0:

$$
f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \tag{1}
$$

Now we can explicitly pose a problem of finding s, as it was stated above.

$$
\begin{aligned}
&\min_{\delta x \in \mathbb{R}^{\ltimes}} f(x_0 + \delta x) \\
&\text{s.t. } \delta x^\top A \delta x = \varepsilon^2
\end{aligned}
$$

Using equation (1 it can be written as:

$$
\begin{aligned}
&\min_{\delta x \in \mathbb{R}^{\ltimes}} \nabla f(x_0)^\top \delta x \\
&\text{s.t. } \delta x^\top A \delta x = \varepsilon^2
\end{aligned}
$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$
x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)
$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$
s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

Let us assume that the distance is defined locally by some metric A:

$$
d(x, x_0) = (x - x_0)^\top A(x - x_0)
$$

Let us also consider first order Taylor approximation of a function $f(x)$ near the point x_0:

$$
f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \tag{1}
$$

Now we can explicitly pose a problem of finding s, as it was stated above.

$$
\begin{aligned}
&\min_{\delta x \in \mathbb{R}^{\ltimes}} f(x_0 + \delta x) \\
&\text{s.t. } \delta x^\top A \delta x = \varepsilon^2
\end{aligned}
$$

Using equation (1 it can be written as:

$$
\begin{aligned}
&\min_{\delta x \in \mathbb{R}^{\ltimes}} \nabla f(x_0)^\top \delta x \\
&\text{s.t. } \delta x^\top A \delta x = \varepsilon^2
\end{aligned}
$$

Using Lagrange multipliers method, we can easily conclude, that the answer is:

$$
\delta x = - \frac{2\varepsilon^2}{\nabla f(x_0)^\top A^{-1} \nabla f(x_0)} A^{-1} \nabla f
$$

The idea of adapive metrics

Given $f(x)$ and a point x_0. Define $B_\varepsilon(x_0) = \{x \in \mathbb{R}^n : d(x, x_0) = \varepsilon^2\}$ as the set of points with distance ε to x_0. Here we presume the existence of a distance function $d(x, x_0)$.

$$x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)$$

Then, we can define another *steepest descent* direction in terms of minimizer of function on a sphere:

$$s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}$$

Let us assume that the distance is defined locally by some metric A:

$$d(x, x_0) = (x - x_0)^\top A(x - x_0)$$

Let us also consider first order Taylor approximation of a function $f(x)$ near the point x_0:

$$f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \tag{1}$$

Now we can explicitly pose a problem of finding s, as it was stated above.

$$\min_{\delta x \in \mathbb{R}^\ltimes} f(x_0 + \delta x)$$
$$\text{s.t. } \delta x^\top A \delta x = \varepsilon^2$$

Using equation (1 it can be written as:

$$\min_{\delta x \in \mathbb{R}^\ltimes} \nabla f(x_0)^\top \delta x$$
$$\text{s.t. } \delta x^\top A \delta x = \varepsilon^2$$

Using Lagrange multipliers method, we can easily conclude, that the answer is:

$$\delta x = -\frac{2\varepsilon^2}{\nabla f(x_0)^\top A^{-1} \nabla f(x_0)} A^{-1} \nabla f$$

Which means, that new direction of steepest descent is nothing else, but $A^{-1} \nabla f(x_0)$.

. . . Indeed, if the space is isotropic and $A = I$, we immediately have gradient descent formula, while Newton method uses local Hessian as a metric matrix.

Quasi-Newton methods

Quasi-Newton methods intuition

For the classic task of unconditional optimization $f(x) \to \min\limits_{x \in \mathbb{R}^n}$ the general scheme of iteration method is written as:

$$x_{k+1} = x_k + \alpha_k d_k$$

Quasi-Newton methods intuition

For the classic task of unconditional optimization $f(x) \to \min\limits_{x \in \mathbb{R}^n}$ the general scheme of iteration method is written as:

$$
x_{k+1} = x_k + \alpha_k d_k
$$

In the Newton method, the d_k direction (Newton's direction) is set by the linear system solution at each step:

$$
B_k d_k = -\nabla f(x_k), \quad B_k = \nabla^2 f(x_k)
$$

Quasi-Newton methods intuition

For the classic task of unconditional optimization $f(x) \to \min\limits_{x \in \mathbb{R}^n}$ the general scheme of iteration method is written as:

$$x_{k+1} = x_k + \alpha_k d_k$$

In the Newton method, the d_k direction (Newton's direction) is set by the linear system solution at each step:

$$B_k d_k = -\nabla f(x_k), \quad B_k = \nabla^2 f(x_k)$$

i.e. at each iteration it is necessary to **compute** hessian and gradient and **solve** linear system.

Quasi-Newton methods intuition

For the classic task of unconditional optimization $f(x) \to \min\limits_{x \in \mathbb{R}^n}$ the general scheme of iteration method is written as:

$$x_{k+1} = x_k + \alpha_k d_k$$

In the Newton method, the d_k direction (Newton's direction) is set by the linear system solution at each step:

$$B_k d_k = -\nabla f(x_k), \quad B_k = \nabla^2 f(x_k)$$

i.e. at each iteration it is necessary to **compute** hessian and gradient and **solve** linear system.

Note here that if we take a single matrix of $B_k = I_n$ as B_k at each step, we will exactly get the gradient descent method.

The general scheme of quasi-Newton methods is based on the selection of the B_k matrix so that it tends in some sense at $k \to \infty$ to the truth value of the Hessian $\nabla^2 f(x_k)$.

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \dots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Basic Idea: As B_k already contains information about the Hessian, use a suitable matrix update to form B_{k+1}.

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Basic Idea: As B_k already contains information about the Hessian, use a suitable matrix update to form B_{k+1}.

Reasonable Requirement for B_{k+1} (motivated by the secant method):

$$\nabla f(x_{k+1}) - \nabla f(x_k) = B_{k+1}(x_{k+1} - x_k) = B_{k+1} d_k$$

$$\Delta y_k = B_{k+1} \Delta x_k$$

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \dots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Basic Idea: As B_k already contains information about the Hessian, use a suitable matrix update to form B_{k+1}.

Reasonable Requirement for B_{k+1} (motivated by the secant method):

$$\nabla f(x_{k+1}) - \nabla f(x_k) = B_{k+1}(x_{k+1} - x_k) = B_{k+1} d_k$$
$$\Delta y_k = B_{k+1} \Delta x_k$$

In addition to the secant equation, we want:

- B_{k+1} to be symmetric

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Basic Idea: As B_k already contains information about the Hessian, use a suitable matrix update to form B_{k+1}.

Reasonable Requirement for B_{k+1} (motivated by the secant method):

$$\nabla f(x_{k+1}) - \nabla f(x_k) = B_{k+1}(x_{k+1} - x_k) = B_{k+1} d_k$$
$$\Delta y_k = B_{k+1} \Delta x_k$$

In addition to the secant equation, we want:

- B_{k+1} to be symmetric
- B_{k+1} to be "close" to B_k

Quasi-Newton Method Template

Let $x_0 \in \mathbb{R}^n$, $B_0 \succ 0$. For $k = 1, 2, 3, \ldots$, repeat:

1. Solve $B_k d_k = -\nabla f(x_k)$
2. Update $x_{k+1} = x_k + \alpha_k d_k$
3. Compute B_{k+1} from B_k

Different quasi-Newton methods implement Step 3 differently. As we will see, commonly we can compute $(B_{k+1})^{-1}$ from $(B_k)^{-1}$.

Basic Idea: As B_k already contains information about the Hessian, use a suitable matrix update to form B_{k+1}.

Reasonable Requirement for B_{k+1} (motivated by the secant method):

$$\nabla f(x_{k+1}) - \nabla f(x_k) = B_{k+1}(x_{k+1} - x_k) = B_{k+1} d_k$$
$$\Delta y_k = B_{k+1} \Delta x_k$$

In addition to the secant equation, we want:

- B_{k+1} to be symmetric
- B_{k+1} to be "close" to B_k
- $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$

Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + auu^T$$

Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + auu^T$$

The secant equation $B_{k+1}d_k = \Delta y_k$ yields:

$$(au^T d_k)u = \Delta y_k - B_k d_k$$

Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + auu^T$$

The secant equation $B_{k+1}d_k = \Delta y_k$ yields:

$$(au^T d_k)u = \Delta y_k - B_k d_k$$

This only holds if u is a multiple of $\Delta y_k - B_k d_k$. Putting $u = \Delta y_k - B_k d_k$, we solve the above,

$$a = \frac{1}{(\Delta y_k - B_k d_k)^T d_k},$$

Symmetric Rank-One Update

Let's try an update of the form:

$$B_{k+1} = B_k + auu^T$$

The secant equation $B_{k+1}d_k = \Delta y_k$ yields:

$$(au^Td_k)u = \Delta y_k - B_kd_k$$

This only holds if u is a multiple of $\Delta y_k - B_kd_k$. Putting $u = \Delta y_k - B_kd_k$, we solve the above,

$$a = \frac{1}{(\Delta y_k - B_kd_k)^T d_k},$$

which leads to

$$B_{k+1} = B_k + \frac{(\Delta y_k - B_kd_k)(\Delta y_k - B_kd_k)^T}{(\Delta y_k - B_kd_k)^T d_k}$$

called the symmetric rank-one (SR1) update or Broyden method.

Symmetric Rank-One Update with inverse

How can we solve

$$B_{k+1}d_{k+1} = -\nabla f(x_{k+1}),$$

in order to take the next step? In addition to propagating B_k to B_{k+1}, let's propagate inverses, i.e., $C_k = B_k^{-1}$ to $C_{k+1} = (B_{k+1})^{-1}$.

Sherman-Morrison Formula:

The Sherman-Morrison formula states:

$$(A + uv^T)^{-1} = A^{-1} - \frac{A^{-1}uv^TA^{-1}}{1 + v^TA^{-1}u}$$

Thus, for the SR1 update, the inverse is also easily updated:

$$C_{k+1} = C_k + \frac{(d_k - C_k\Delta y_k)(d_k - C_k\Delta y_k)^T}{(d_k - C_k\Delta y_k)^T\Delta y_k}$$

In general, SR1 is simple and cheap, but it has a key shortcoming: it does not preserve positive definiteness.

Davidon-Fletcher-Powell Update

We could have pursued the same idea to update the inverse C:

$$C_{k+1} = C_k + auu^T + bvv^T.$$

Davidon-Fletcher-Powell Update

We could have pursued the same idea to update the inverse C:

$$C_{k+1} = C_k + auu^T + bvv^T.$$

Multiplying by Δy_k, using the secant equation $d_k = C_k \Delta y_k$, and solving for a, b, yields:

$$C_{k+1} = C_k - \frac{C_k \Delta y_k \Delta y_k^T C_k}{\Delta y_k^T C_k \Delta y_k} + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

Woodbury Formula Application

Woodbury then shows:

$$B_{k+1} = \left(I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k}\right) B_k \left(I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k}\right) + \frac{\Delta y_k \Delta y_k^T}{\Delta y_k^T d_k}$$

This is the Davidon-Fletcher-Powell (DFP) update. Also cheap: $O(n^2)$, preserves positive definiteness. Not as popular as BFGS.

Broyden-Fletcher-Goldfarb-Shanno update

Let's now try a rank-two update:

$$B_{k+1} = B_k + auu^T + bvv^T.$$

Broyden-Fletcher-Goldfarb-Shanno update

Let's now try a rank-two update:

$$B_{k+1} = B_k + auu^T + bvv^T.$$

The secant equation $\Delta y_k = B_{k+1}d_k$ yields:

$$\Delta y_k - B_k d_k = (au^T d_k)u + (bv^T d_k)v$$

Broyden-Fletcher-Goldfarb-Shanno update

Let's now try a rank-two update:

$$B_{k+1} = B_k + auu^T + bvv^T.$$

The secant equation $\Delta y_k = B_{k+1} d_k$ yields:

$$\Delta y_k - B_k d_k = (au^T d_k)u + (bv^T d_k)v$$

Putting $u = \Delta y_k$, $v = B_k d_k$, and solving for a, b we get:

$$B_{k+1} = B_k - \frac{B_k d_k d_k^T B_k}{d_k^T B_k d_k} + \frac{\Delta y_k \Delta y_k^T}{d_k^T \Delta y_k}$$

called the Broyden-Fletcher-Goldfarb-Shanno (BFGS) update.

Broyden-Fletcher-Goldfarb-Shanno update with inverse

Woodbury Formula

The Woodbury formula, a generalization of the Sherman-Morrison formula, is given by:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Broyden-Fletcher-Goldfarb-Shanno update with inverse

Woodbury Formula

The Woodbury formula, a generalization of the Sherman-Morrison formula, is given by:

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Applied to our case, we get a rank-two update on the inverse C:

$$C_{k+1} = C_k + \frac{(d_k - C_k \Delta y_k)d_k^T}{\Delta y_k^T d_k} + \frac{d_k(d_k - C_k \Delta y_k)^T}{\Delta y_k^T d_k} - \frac{(d_k - C_k \Delta y_k)^T \Delta y_k}{(\Delta y_k^T d_k)^2} d_k d_k^T$$

$$C_{k+1} = \left(I - \frac{d_k \Delta y_k^T}{\Delta y_k^T d_k}\right) C_k \left(I - \frac{\Delta y_k d_k^T}{\Delta y_k^T d_k}\right) + \frac{d_k d_k^T}{\Delta y_k^T d_k}$$

This formulation ensures that the BFGS update, while comprehensive, remains computationally efficient, requiring $O(n^2)$ operations. Importantly, BFGS update preserves positive definiteness. Recall this means $B_k \succ 0 \Rightarrow B_{k+1} \succ 0$. Equivalently, $C_k \succ 0 \Rightarrow C_{k+1} \succ 0$

Code

- Open In Colab

Code

- Open In Colab
- Comparison of quasi Newton methods

Code

- Open In Colab
- Comparison of quasi Newton methods
- Some practical notes about Newton method