Newton method. Quasi-Newton methods.

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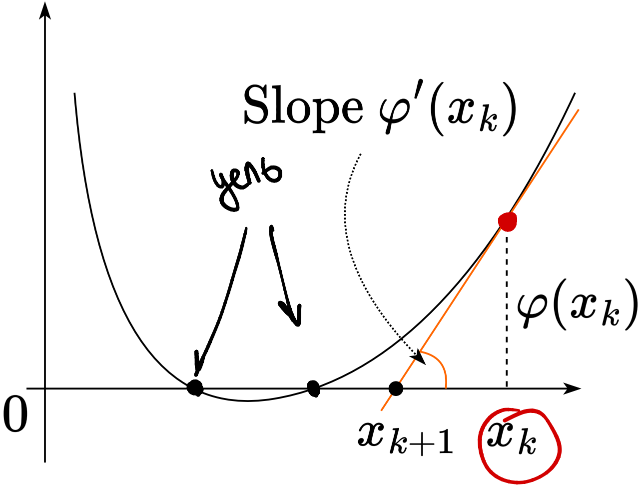
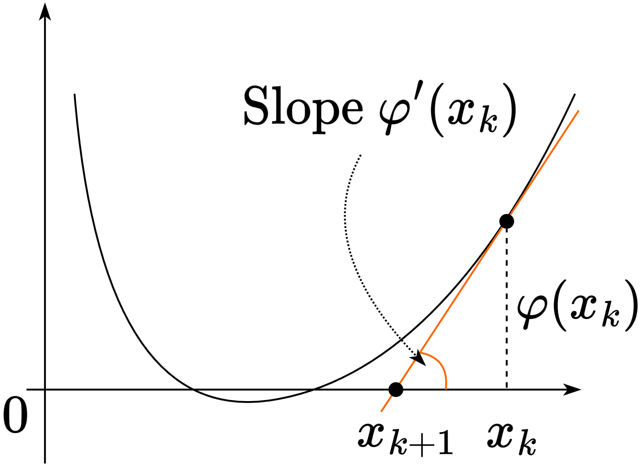
Idea of Newton method of root finding



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

Idea of Newton method of root finding



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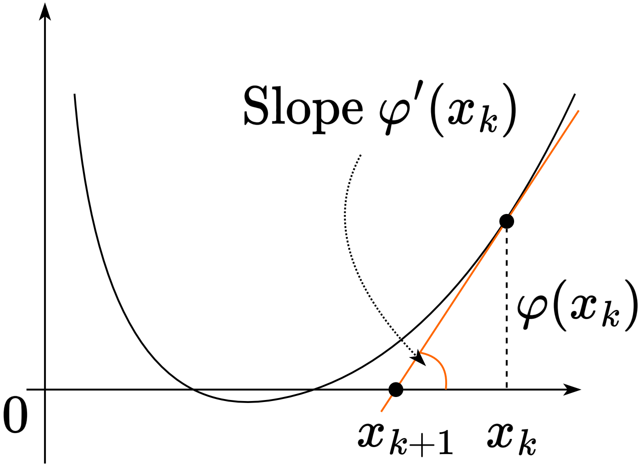

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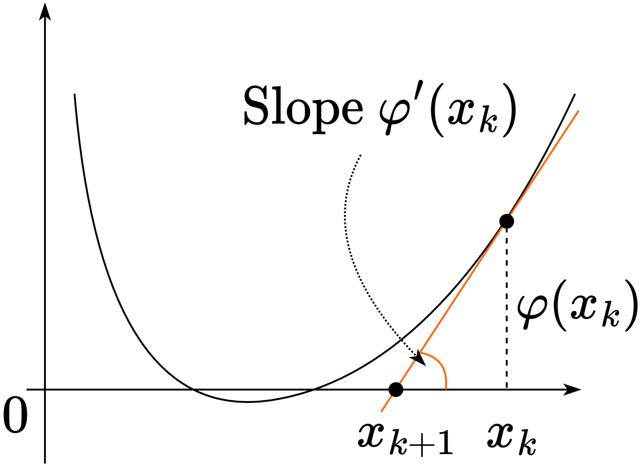

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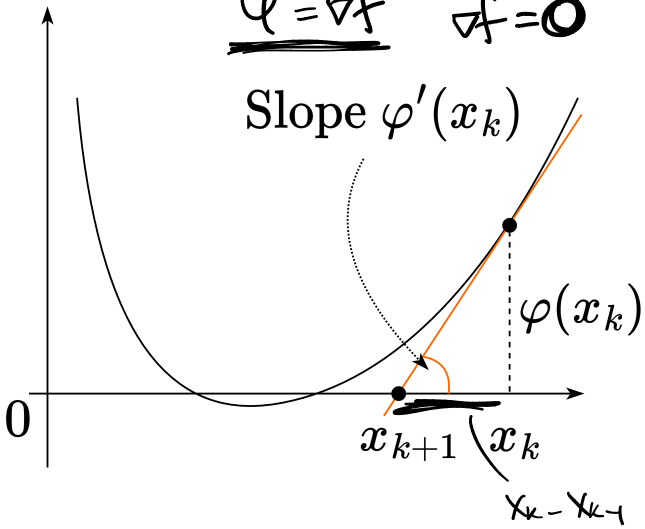
We get an iterative scheme:

Idea of Newton method of root finding

$\varphi = \nabla f \qquad \nabla f = 0$



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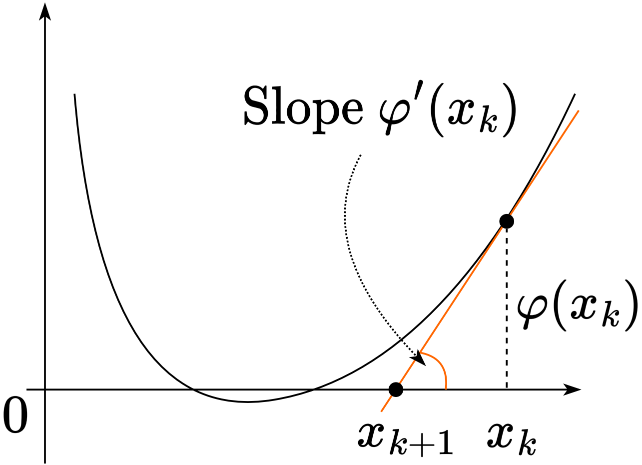
Idea of Newton method of root finding



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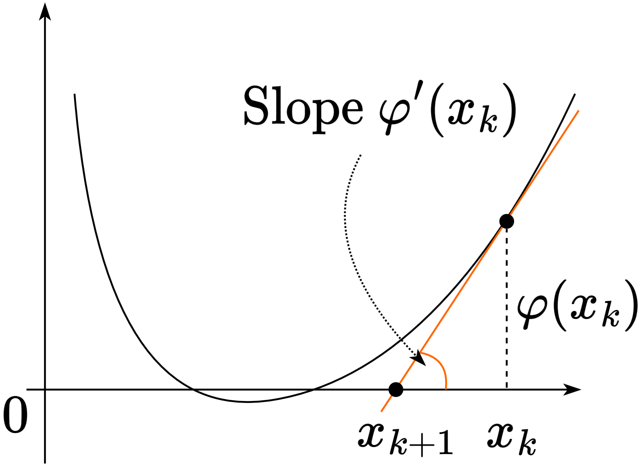
We get an iterative scheme:

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

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

Idea of Newton method of root finding



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We get an iterative scheme: ✓ f'

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

f''

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

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

[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:

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

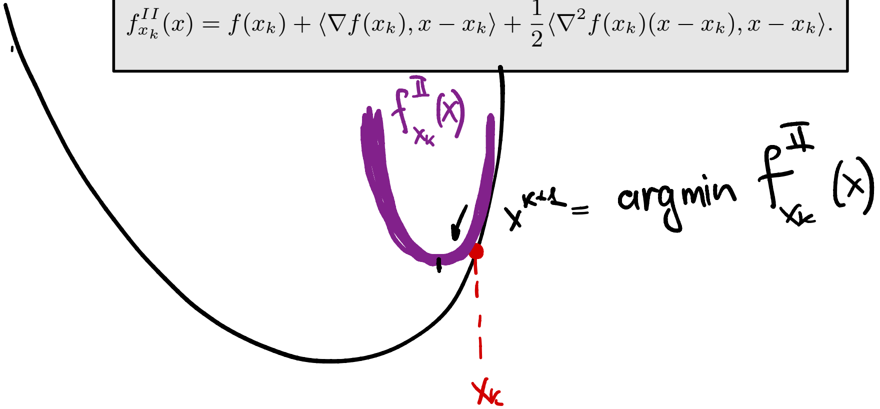
x_k

давайте построим $f^{II}_{x_k}(x)$

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:

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



Newton method as a local quadratic Taylor approximation minimizer

хотим

$\nabla^2 f(x) \succ 0$

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:

0 $\quad \nabla f(x_k) \quad\quad x^T A x \to 2\frac{A+A^T}{2}x \to 2Ax$

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

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

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

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$x_{k+1} = \dots\dots$

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$$

метод Ньютона

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

для кв. Ньютон сх-ся за 1 итерацию

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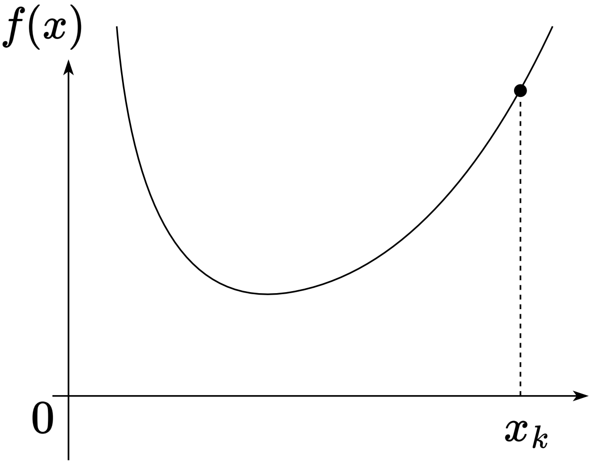
Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

Newton method as a local quadratic Taylor approximation minimizer



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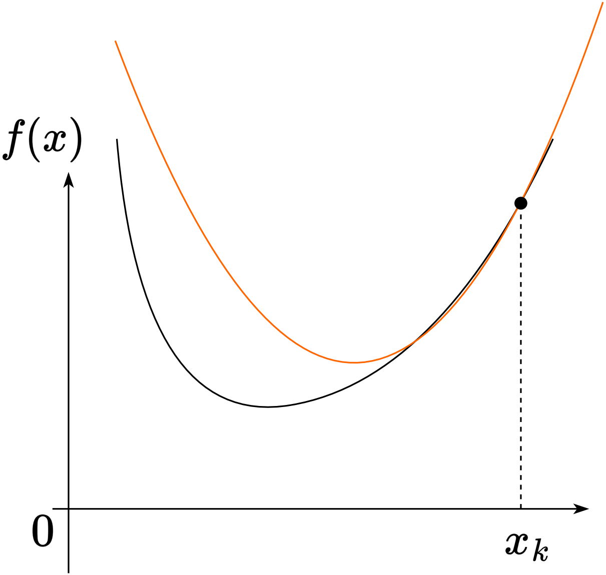

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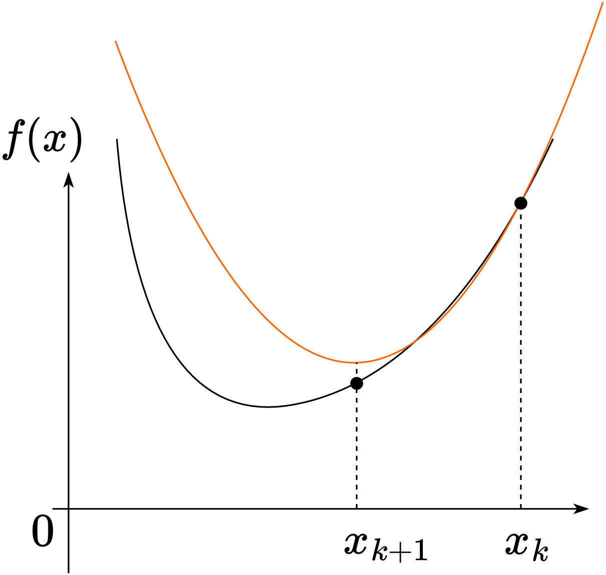

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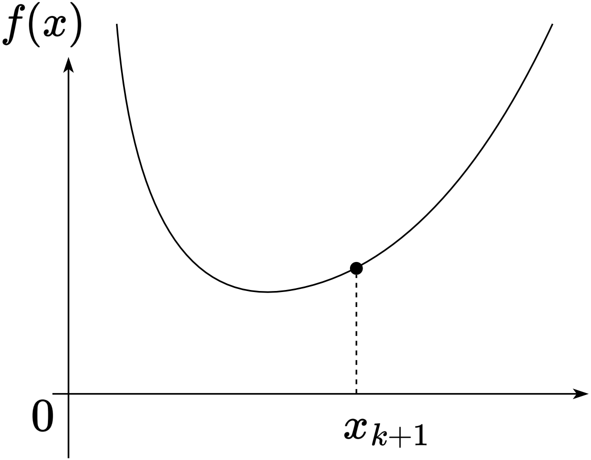

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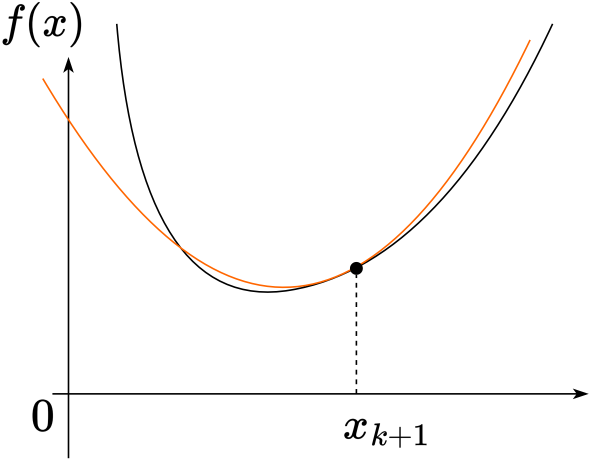

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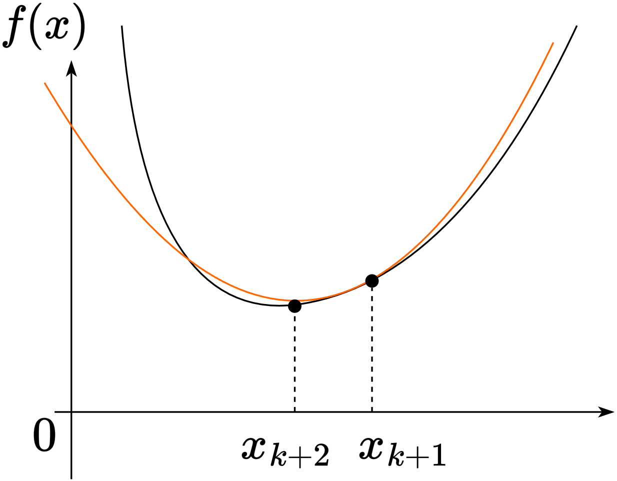

Convergence

μ-сильно выпуклая

L-гладкая (липшицевость градиента)

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.

липшицевость гессиана

$$\|\nabla^2 f(x) - \nabla^2 f(y)\| \leq M\|x-y\|$$

локальная сх-ть: если x_0 вблизи некоторой окр-ти x^*

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Proof

1. We will use Newton-Leibniz formula

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

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2. Then we track the distance to the solution

Convergence

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

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

$\nabla f(x^*) = 0$

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

Convergence

вынос
↓
за
скобку
$(x_k - x^*)$

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.

$$
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$$

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

вынос за скобки $\nabla^2 f^{-1}$

Convergence

$\nabla^2 f(x_k) \qquad y = \int_0^1 y \, dt$

3.

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

Convergence

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

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

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

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Convergence

$$\left\| \int \right\| \leq \int \| \cdot \|$$

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

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

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$$\leq \int_0^1 M\|x_k - x^* - \tau(x_k - x^*)\|d\tau = \int_0^1 M\|x_k - x^*\|(1-\tau)d\tau = \boxed{\frac{r_k}{2}M,}$$

$$\int_0^1 (1-\tau)d\tau = \tau - \frac{\tau^2}{2}\Big|_0^1 = \frac{1}{2}$$

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

Convergence

$\mu \leq \lambda(\nabla^2 f(x_k)) \leq L$

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

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

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

$$\leq \int_0^1 M\|x_k - x^* - \tau(x_k - x^*)\| d\tau = \int_0^1 M\|x_k - x^*\|(1-\tau)d\tau = \frac{r_k}{2}M,$$

where $r_k = \|x_k - x^*\|$. $\|x_{k+1} - x^*\| = r_{k+1}$

6. So, we have:

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

$\|\nabla^2 f(x_k)^{-1}\| \leq \frac{1}{\mu}$

$\frac{M}{2\mu} r_k^2.$

and we need to bound the norm of the inverse hessian

Convergence

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

Convergence

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

$$\|\nabla^2 f(x_k) - \nabla^2 f(x^*)\| \leq M \|x_k - x^*\| \leq Mr_k$$

r_k

$$-Mr_k I \preceq \nabla^2 f(x_k) - \nabla^2 f(x^*) \preceq Mr_k I$$

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:

$$\nabla^2 f(x^*) \succeq \mu I$$

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

Convergence

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\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

$\| \cdot \|_2$

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$$

μI

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

$$
\left\| \left[\nabla^2 f(x_k) \right]^{-1} \right\| \leq (\mu - Mr_k)^{-1}
$$

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

$$
r_{k+1} \leq \frac{r_k^2 M}{2(\mu - Mr_k)}
$$

Convergence

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

Потребуем

$r_{k+1} < r_k$

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

$\dfrac{r_k^2 M - 2(\mu - Mr_k) r_k}{2(\mu - Mr_k)} < 0$

$3r_k^2 M - 2\mu r_k$

$r_k < \frac{2\mu}{3M}$

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

$$
\left\| \left[\nabla^2 f(x_k) \right]^{-1} \right\| \leq (\mu - Mr_k)^{-1}
$$

$$
r_{k+1} \leq \boxed{\frac{r_k^2 M}{2(\mu - Mr_k)} < r_k}
$$

Точка r_0

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

Thus, we have an important result: Newton's method for the function with Lipschitz positive-definite Hessian converges **quadratically** near $\left(\|x_0 - x^*\| < \frac{2\mu}{3M}\right)$ 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 $\boxed{x = Ay,}$ and define $\boxed{g(y) = f(Ay)}$. Note, that $\boxed{\nabla g(y) = A^T \nabla f(x)}$ and $\boxed{\nabla^2 g(y) = A^T \nabla^2 f(x) A}$. The Newton steps on g are expressed as:

Ньютон в y переменных →

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

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$$

Expanding this, we get:

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

$$
A^{-1} \cdot \left(A^T \nabla^2 f\right)^{-1}
$$

$$
A^{-1} \left(\nabla^2 f\right)^{-1} A^{T^{-1}}
$$

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

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

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

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Thus, the update rule for x is:

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

Affine Invariance of Newton's Method

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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

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

Summary

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

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- the parameters have little effect on the convergence rate

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Summary

$10^{22} \cdot$ 16 бит

$2 \cdot 10^{22}$ байта $2 \cdot 10^{13} \cdot 10^{9}$ байт

$2 \cdot 10^{13}$ ГБ

16 ГБ

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

Метод Ньютона для GPT-3

$n = 175B =$

$\approx 100 \cdot 10^{9} = 10^{11}$

$n^2 \approx 10^{22}$

Summary

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

What's nice:

- quadratic convergence near the solution x^*
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- 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

$$\boxed{\underbrace{\nabla^2 f(x_k)}_{A} \cdot \underbrace{(x_{k+1} - x_k)}_{x} = \underbrace{-\nabla f(x_k)}_{b}}$$

x = реш. лин. системы

Summary

What's nice:

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

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- the parameters have little effect on the convergence rate

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- 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

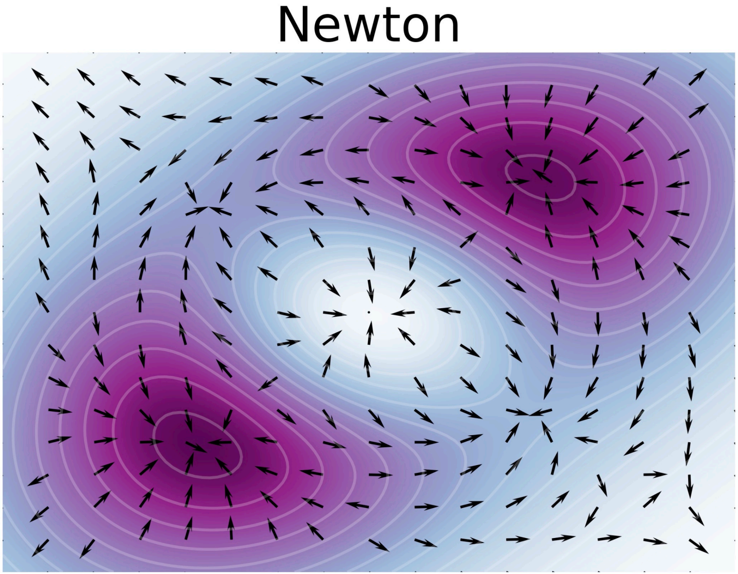

Figure 7: Animation

Newton method problems

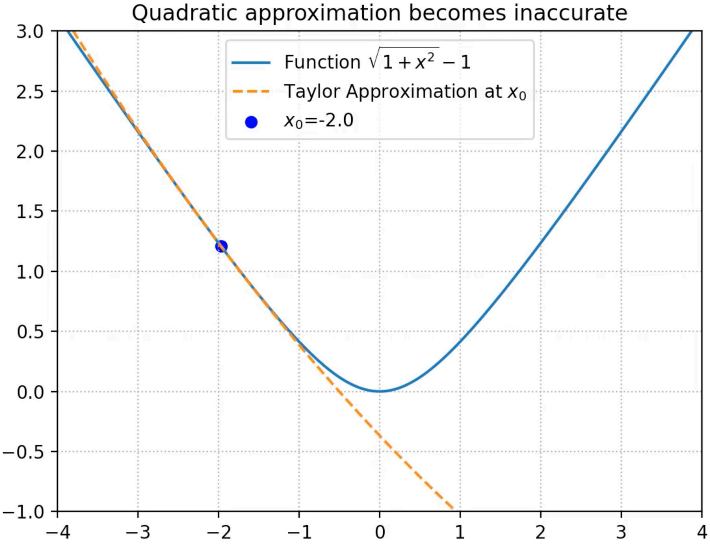

Figure 8: Animation

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 $d(x, x_0)$.

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\boxed{x^* = \text{arg} \min_{x \in B_\varepsilon(x_0)} f(x)}
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s = \lim_{\varepsilon \to 0} \frac{x^* - x_0}{\varepsilon}
$$

GD $\quad d(x, x_0) = \langle x - x_0, x - x_0 \rangle$

Newton $\quad d(x, x_0) = \langle \nabla^2 f(x_0)(x - x_0), x - x_0 \rangle$

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

$$f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \qquad (1)$$

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

$$\min_{\delta x \in \mathbb{R}^{\ltimes}} f(x_0 + \delta x)$$

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

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

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\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 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:

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

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

$$
B_k d_k = -\nabla f(x_k), \quad \boxed{B_k = \nabla^2 f(x_k)} \leftarrow \text{Newton}
$$

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

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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 $B_k d_k = -\nabla f(x_k)$

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3. Compute B_{k+1} from B_k

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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 $(B_k)^{-1}$.

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

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

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

SECANT
Equation

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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:

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

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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,

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

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$B_k > 0$

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SR-1
не гарантирует
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which leads to

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

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:

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

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:

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

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

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

BFGS

Let's now try a rank-two update:

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

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

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

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

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

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:

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

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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

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