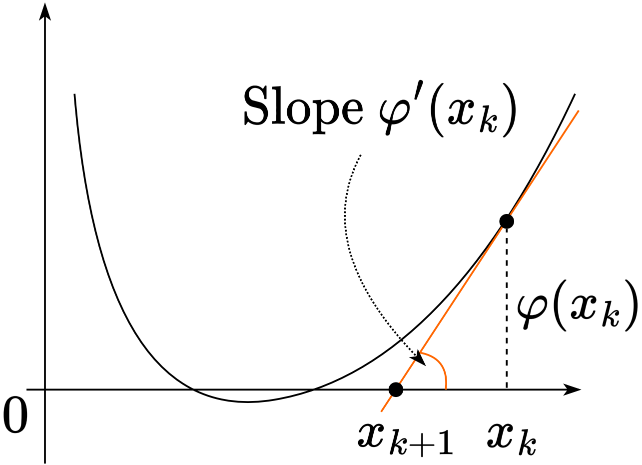
Newton method. Quasi-Newton methods

Seminar

Optimization for ML. Faculty of Computer Science. HSE University

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 $\nabla f(x) = 0$

Idea of Newton method of root findin

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$$\phi(t) = \frac{t}{\sqrt{1+t^2}}$$

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2. Then the iteration of the method takes the form:

$$x_{k+1} = x_k - \frac{\varphi(x_k)}{\varphi'(x_k)} = x_k - x_k(x_k^2+1) = -x_k^3$$

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It is easy to see that the method converges only if $|x_0| < 1$, emphasizing the **local** nature of the Newton method.

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:

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

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

$$\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) \\
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Pay attention to the restrictions related to the need for the Hessian to be non-degenerate (for the method to work), as well as for it to be positive definite (for convergence guarantee).

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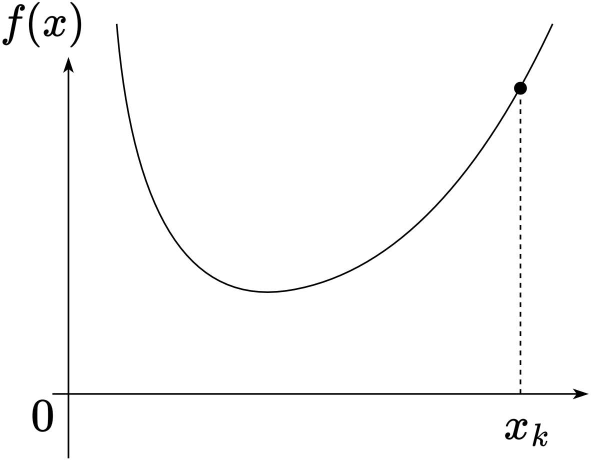

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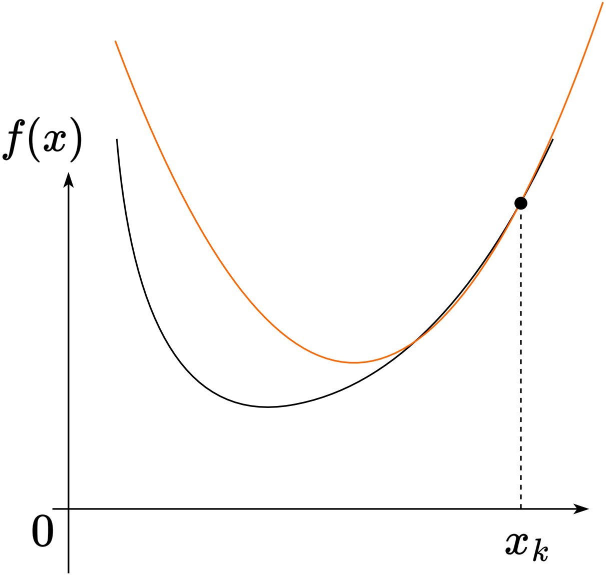

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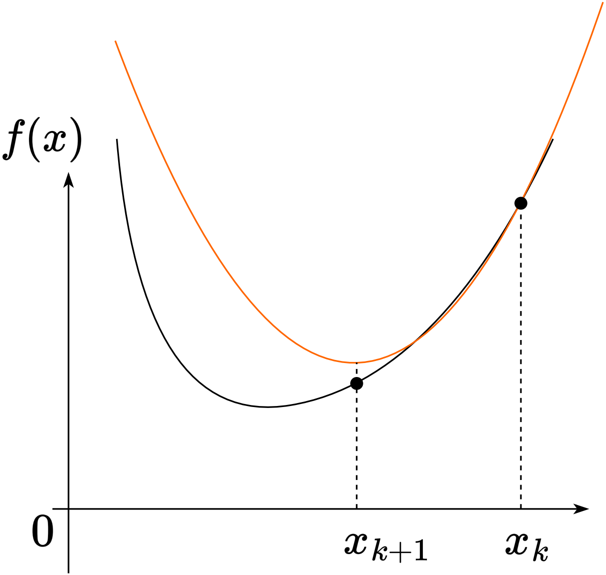

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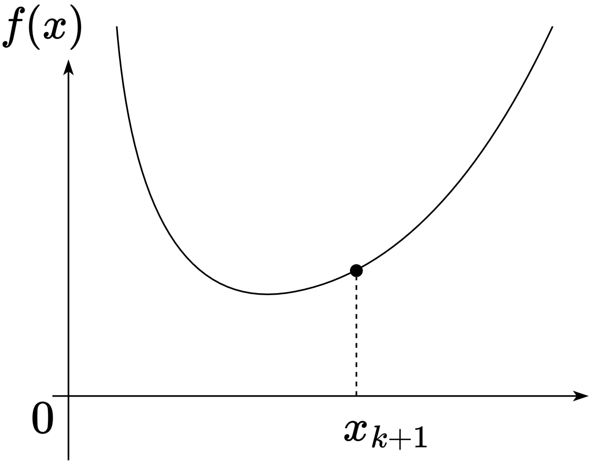

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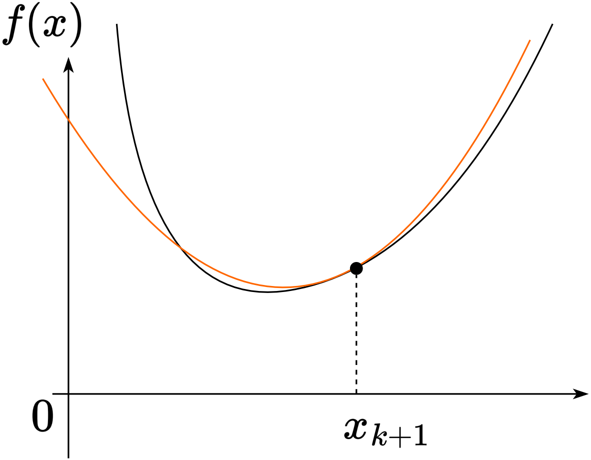

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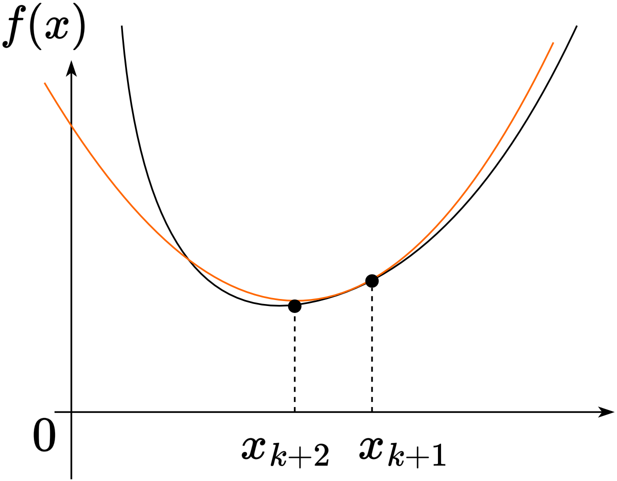

Newton method vs gradient descent

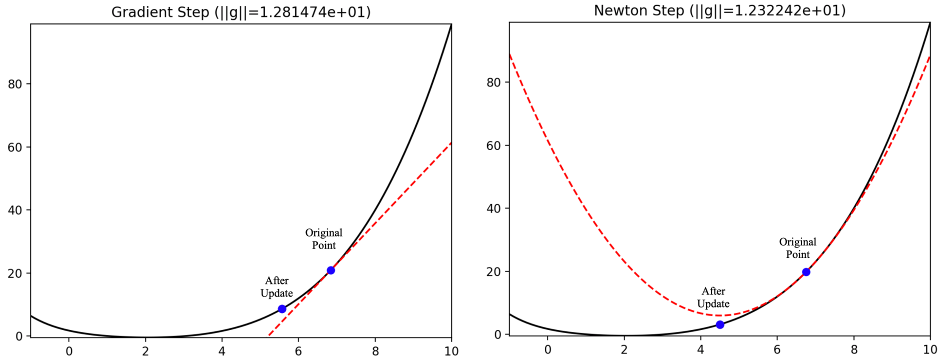

Figure 7: The loss function is depicted in black, the approximation as a dotted red line

The gradient descent $\equiv$ linear approximation

The Newton method $\equiv$ quadratic approximation

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

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

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:

$$\|x_{k+1} - x^*\|_2 \leq \frac{M \|x_k - x^*\|_2^2}{2\left(\mu - M \|x_k - x^*\|_2\right)}$$

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"**Converge locally**" means that the convergence rate described above is guaranteed to occur only if the starting point is quite close to the minimum point, in particular $\|x_0 - x^*\| < \frac{2\mu}{3M}$

Affine invariance

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2. Consider a quadratic approximation:

$$g(y+u) \approx g(y) + \langle g'(y), u \rangle + \frac{1}{2} u^\top g''(y) u \to \min_u$$

$$u^* = -\left(g''(y)\right)^{-1} g'(y) \quad y_{k+1} = y_k - \left(g''\left(y_k\right)\right)^{-1} g'\left(y_k\right)$$

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3. Substitute explicit expressions for $g''\left(y_k\right), g'\left(y_k\right)$:

$$y_{k+1} = y_k - \left(A^\top f''\left(Ay_k\right) A\right)^{-1} A^\top f'\left(Ay_k\right) = y_k - A^{-1}\left(f''\left(Ay_k\right)\right)^{-1} f'\left(Ay_k\right)$$

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4. Thus, the method's step is transformed by linear transformation in **the same way** as the coordinates:

$$Ay_{k+1} = Ay_k - \left(f''\left(Ay_k\right)\right)^{-1} f'\left(Ay_k\right) \quad x_{k+1} = x_k - \left(f''\left(x_k\right)\right)^{-1} f'\left(x_k\right)$$

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Pros

- quadratic convergence near the solution
- high accuracy of the obtained solution
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- it is necessary to store the 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
- the Hessian may not be positively determined $\to$ direction $-(f''(x))^{-1}f'(x)$ may not be a descending direction

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Quasi Newton methods partially solve these problems!

Quasi Newton methods

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:

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

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

$$s_k = -B_k \nabla f(x_k), \quad B_k = f_{xx}^{-1}(x_k)$$

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.

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> 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 true value of inverted Hessian in the local optimum $f_{xx}^{-1}(x_*)$.

Quasi Newton methods

Let's consider several schemes using iterative updating of B_k matrix in the following way:

$$B_{k+1} = B_k + \Delta B_k$$

Then if we use Taylor's approximation for the first order gradient, we get it:

$$\nabla f(x_k) - \nabla f(x_{k+1}) \approx f_{xx}(x_{k+1})(x_k - x_{k+1}).$$

Now let's formulate our method as:

$$\Delta x_k = B_{k+1} \Delta y_k, \text{ where } \quad \Delta y_k = \nabla f(x_{k+1}) - \nabla f(x_k)$$

in case you set the task of finding an update ΔB_k:

$$\Delta B_k \Delta y_k = \Delta x_k - B_k \Delta y_k$$

Broyden method

The simplest option is when the amendment ΔB_k has a rank equal to one. Then you can look for an amendment in the form

$$\Delta B_k = \mu_k q_k q_k^\top.$$

where μ_k is a scalar and q_k is a non-zero vector. Then mark the right side of the equation to find ΔB_k for Δz_k:

$$\Delta z_k = \Delta x_k - B_k \Delta y_k$$

We get it:

$$\mu_k q_k q_k^\top \Delta y_k = \Delta z_k$$

$$\left(\mu_k \cdot q_k^\top \Delta y_k\right) q_k = \Delta z_k$$

A possible solution is: $q_k = \Delta z_k$, $\mu_k = \left(q_k^\top \Delta y_k\right)^{-1}$. Then an iterative amendment to Hessian's evaluation at each iteration:

$$\Delta B_k = \frac{(\Delta x_k - B_k \Delta y_k)(\Delta x_k - B_k \Delta y_k)^\top}{\langle \Delta x_k - B_k \Delta y_k, \Delta y_k \rangle}.$$

Davidon–Fletcher–Powell method

$$\Delta B_k = \mu_1 \Delta x_k (\Delta x_k)^\top + \mu_2 B_k \Delta y_k (B_k \Delta y_k)^\top.$$

$$\Delta B_k = \frac{(\Delta x_k)(\Delta x_k)^\top}{\langle \Delta x_k, \Delta y_k \rangle} - \frac{(B_k \Delta y_k)(B_k \Delta y_k)^\top}{\langle B_k \Delta y_k, \Delta y_k \rangle}.$$

Broyden–Fletcher–Goldfarb–Shanno method

$$
\Delta B_k = QUQ^\top, \quad Q = [q_1, q_2], \quad q_1, q_2 \in \mathbb{R}^n, \quad U = \begin{pmatrix} a & c \\ c & b \end{pmatrix}.
$$

$$
\Delta B_k = \frac{(\Delta x_k)(\Delta x_k)^\top}{\langle \Delta x_k, \Delta y_k \rangle} - \frac{(B_k \Delta y_k)(B_k \Delta y_k)^\top}{\langle B_k \Delta y_k, \Delta y_k \rangle} + p_k p_k^\top.
$$

Computational experiments

Let's look at computational experiments for Newton and Quasi Newton methods .