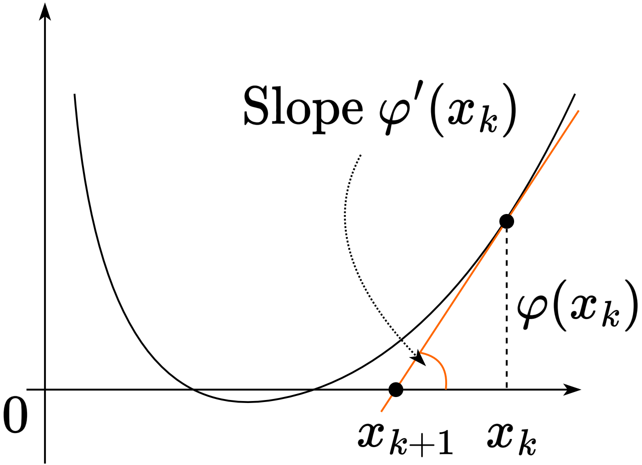
Newton method. Quasi-Newton methods

Daniil Merkulov

Optimization methods. MIPT

Newton method

Idea of Newton method of root finding



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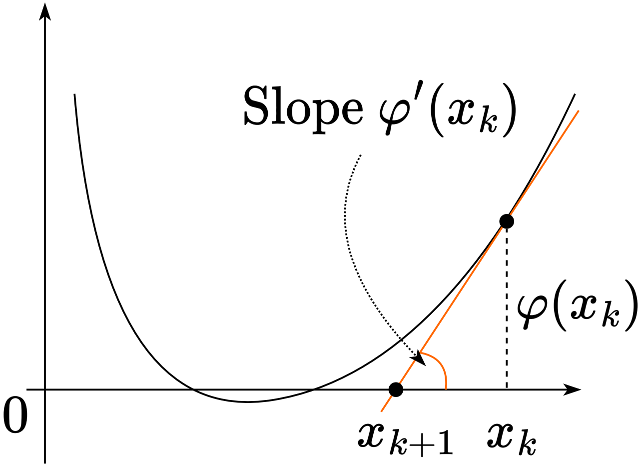

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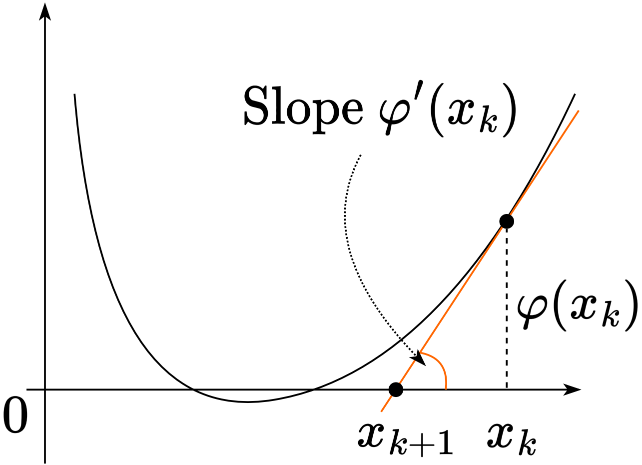

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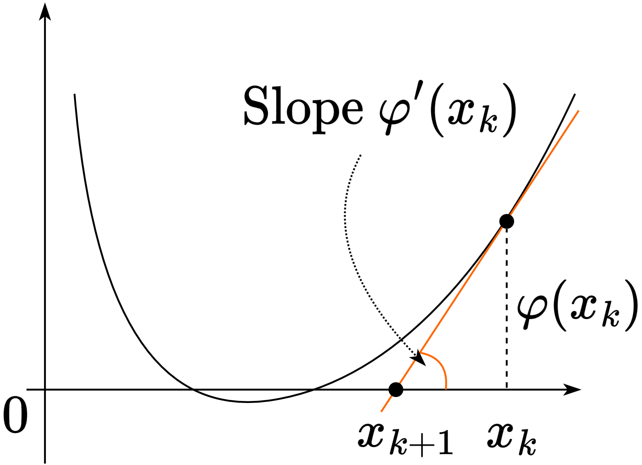

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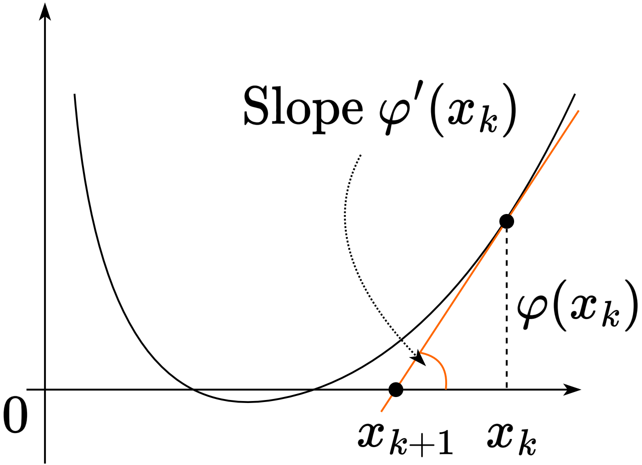

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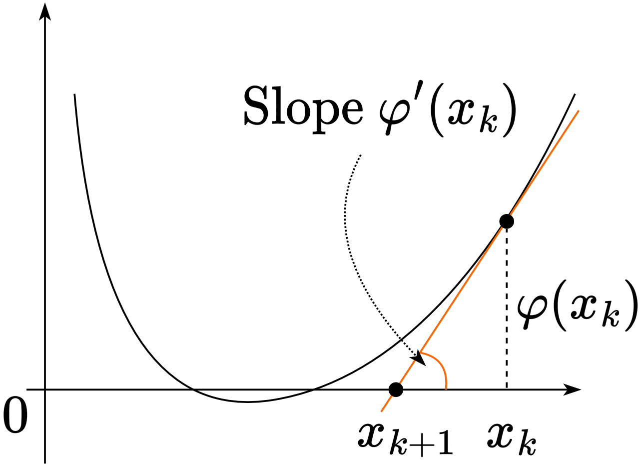

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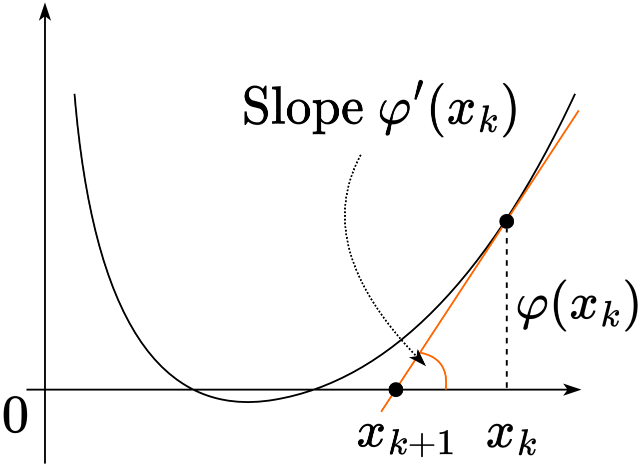

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Which will become a Newton optimization method in case $f'(x) = \varphi(x)$[a]:

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

[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:

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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).

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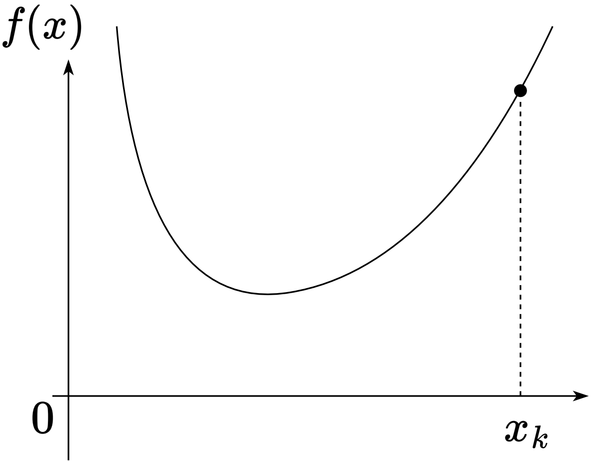

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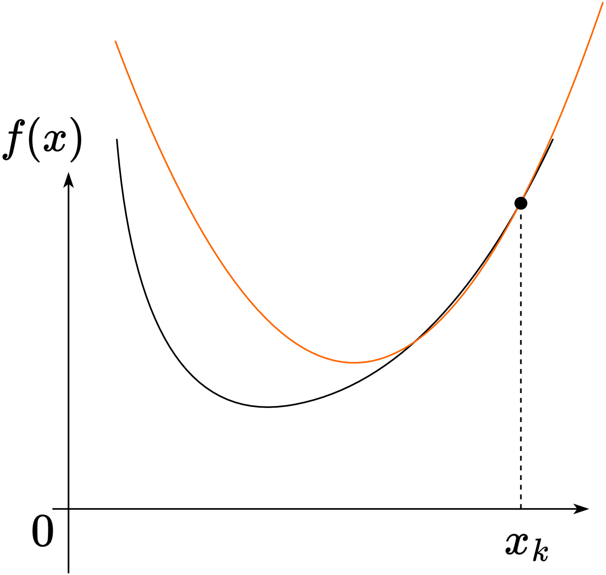

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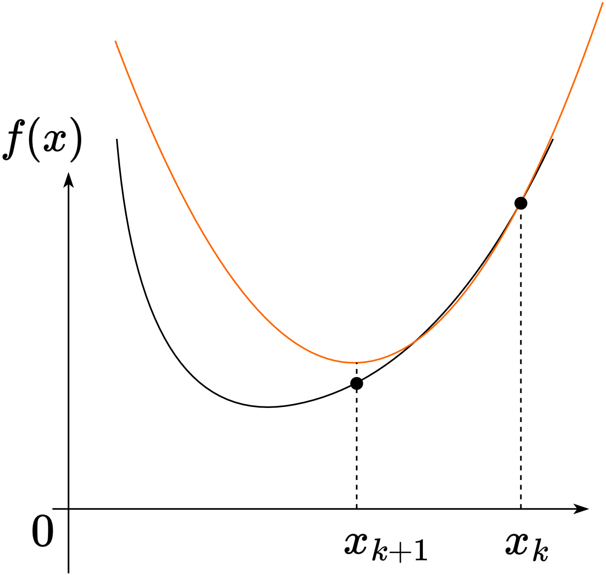

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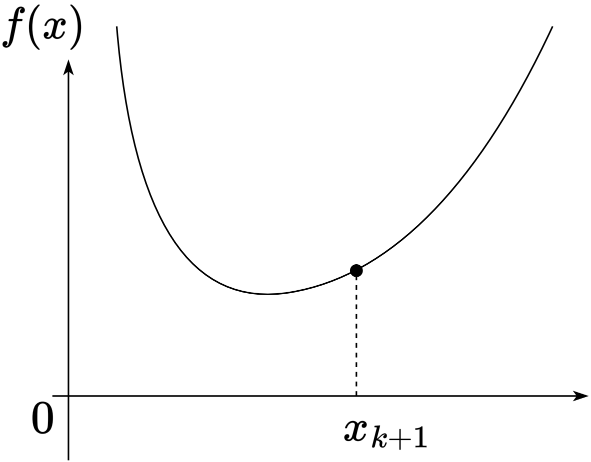

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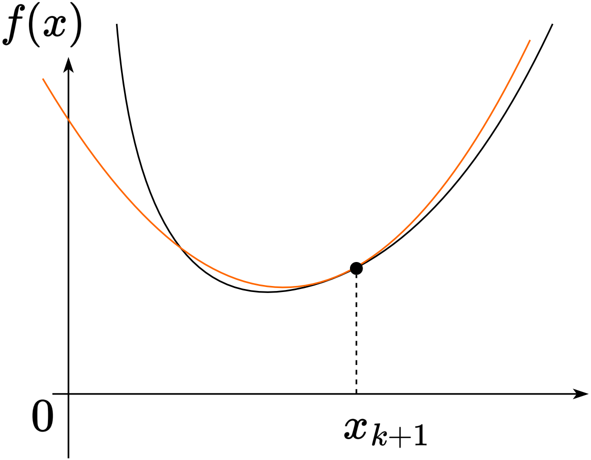

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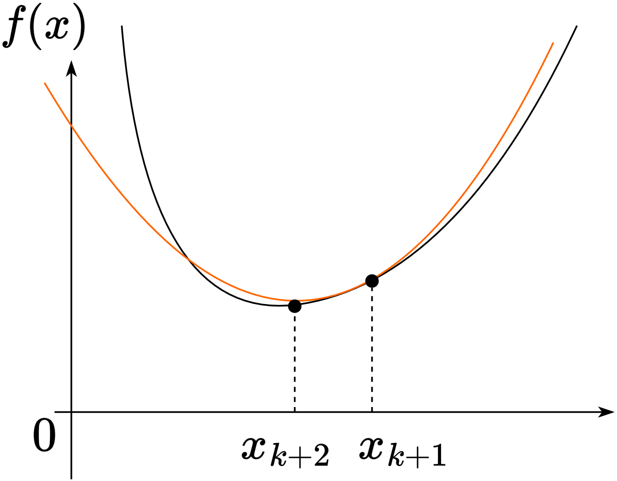

Convergence

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.

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

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

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&= \left[\nabla^2 f(x_k) \right]^{-1} G_k (x_k - x^*)
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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).
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\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 = \frac{r_k}{2} M,
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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

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

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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:

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

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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^*

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- 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

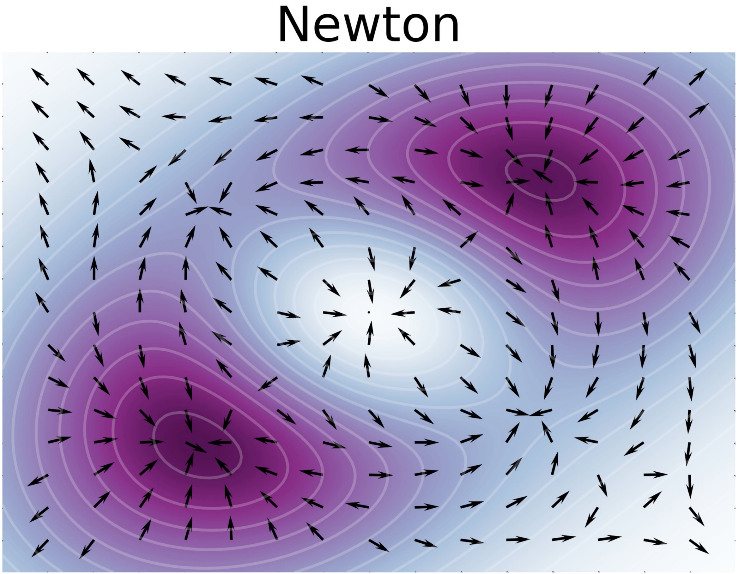

Figure 7: Animation

Newton method problems

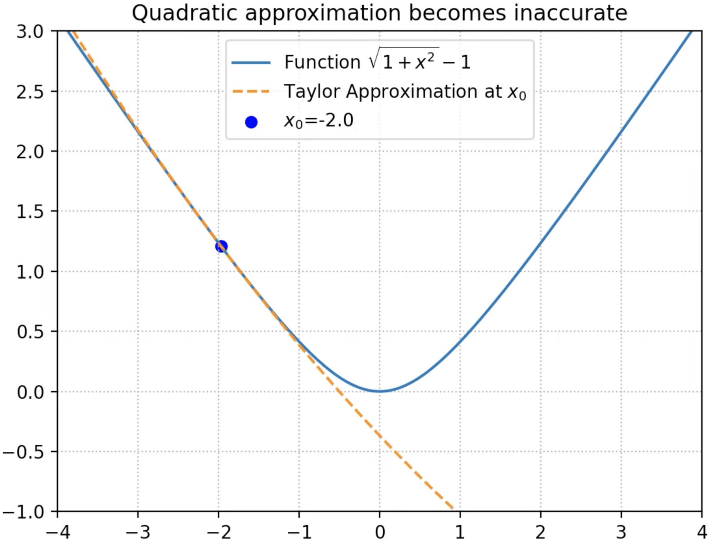

Figure 8: Animation

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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f(x_0 + \delta x) \approx f(x_0) + \nabla f(x_0)^\top \delta x \tag{1}
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Now we can explicitly pose a problem of finding s, as it was stated above.

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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:

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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 $\nabla^2 f(x_k)$.

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

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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):

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

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:

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

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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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which leads to

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

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:

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

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:

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

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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:

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

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:

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

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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:

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

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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