

# Newton method. Quasi-Newton methods.

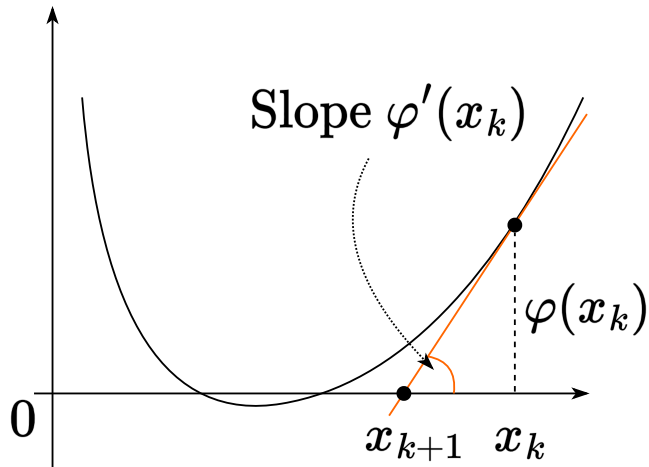
Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

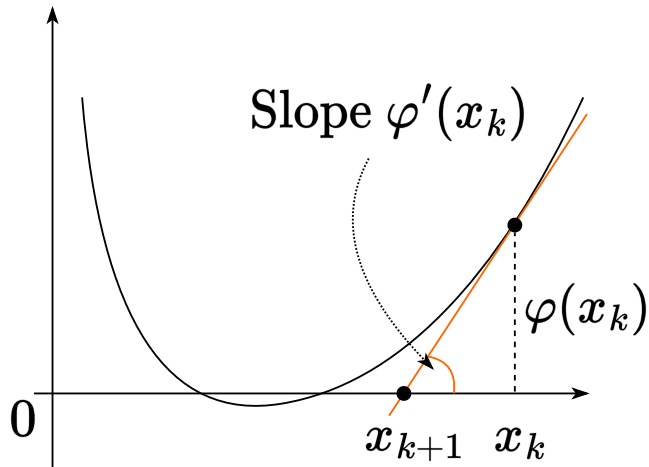


## Idea of Newton method of root finding

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

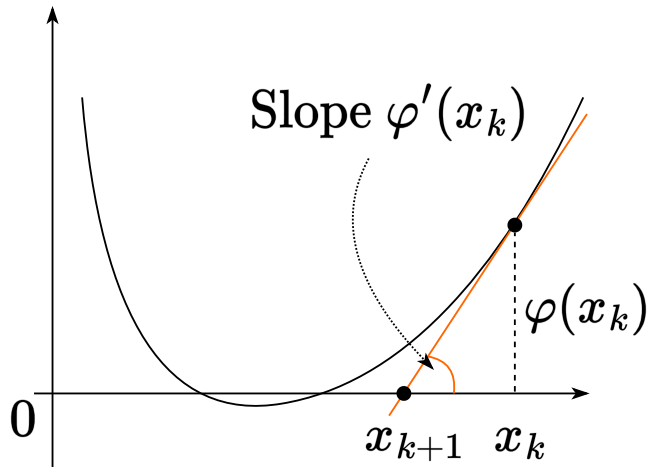


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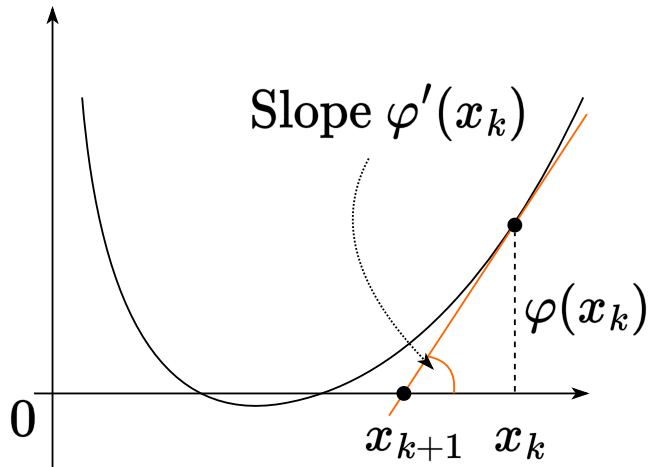
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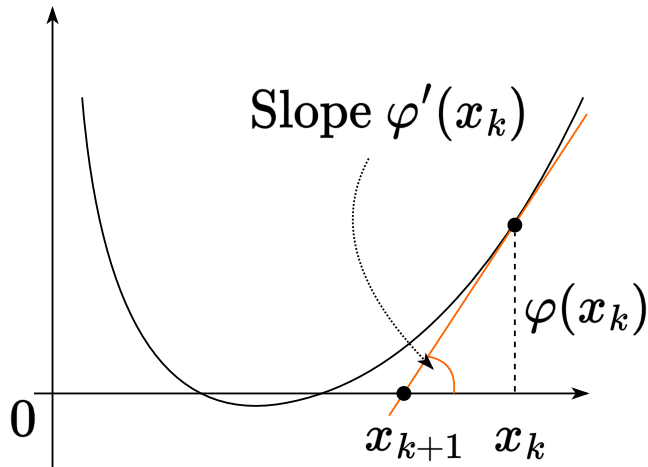
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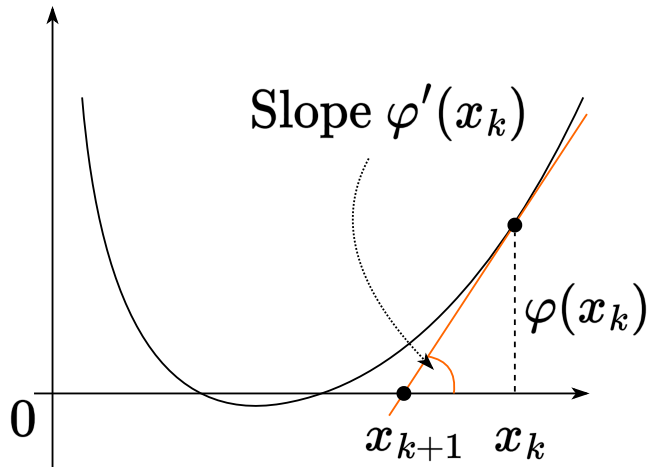
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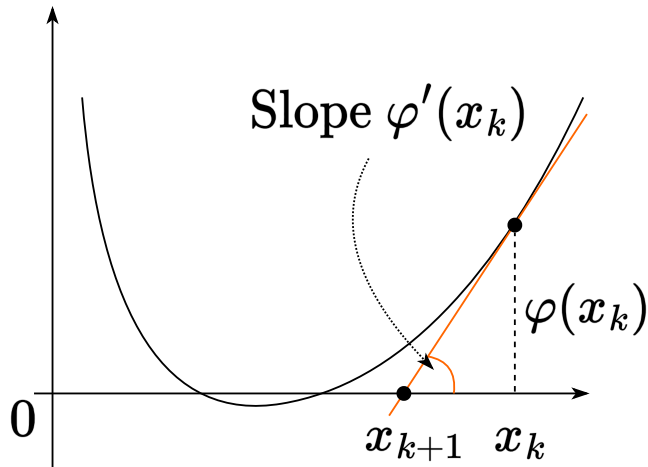
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$$x_{k+1} = x_k - [\nabla^2 f(x_k)]^{-1} \nabla f(x_k)$$

<sup>a</sup>Literally we aim to solve the problem of finding stationary points  $\nabla f(x) = 0$



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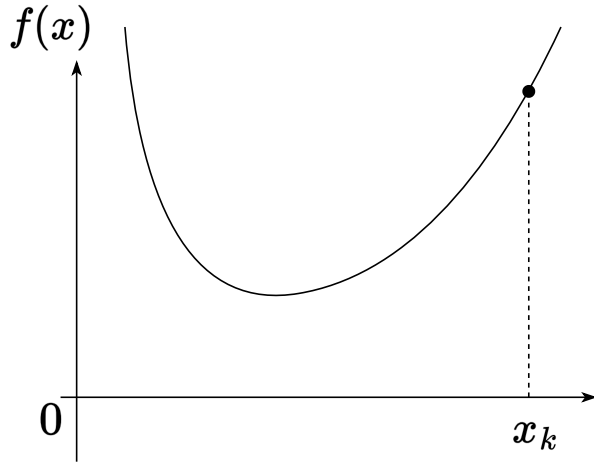
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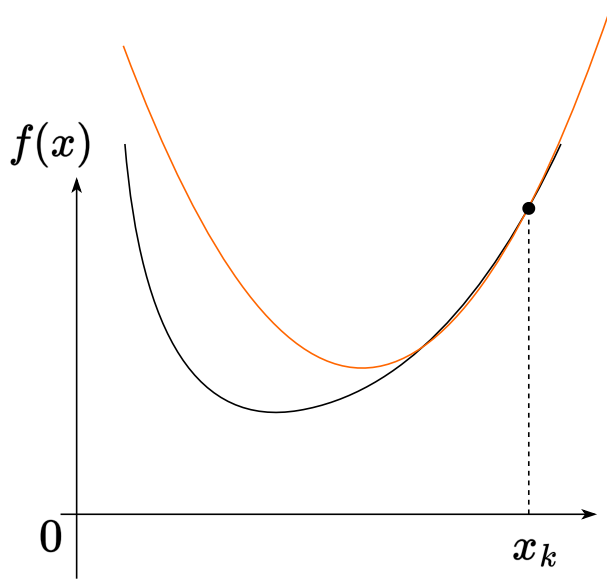
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Let us immediately note the limitations related to the necessity of the Hessian's non-degeneracy (for the method to exist), as well as its positive definiteness (for the convergence guarantee).

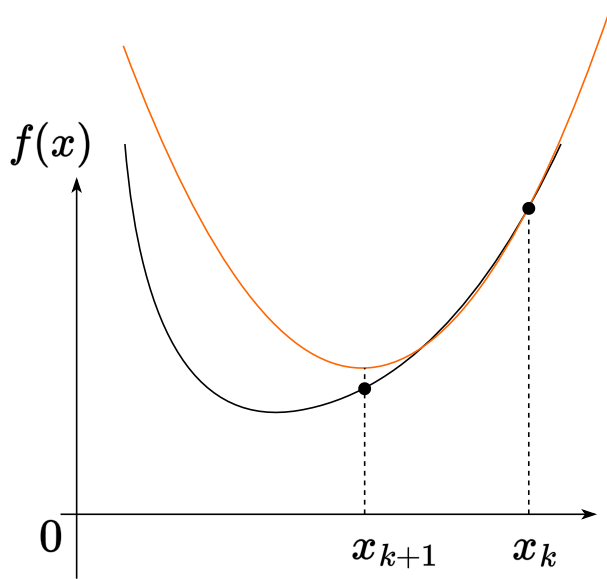
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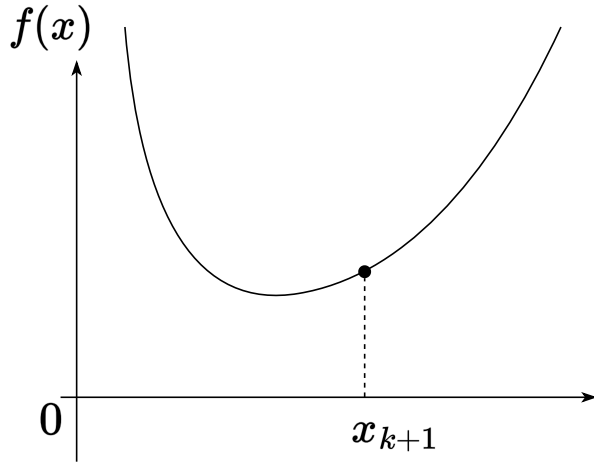
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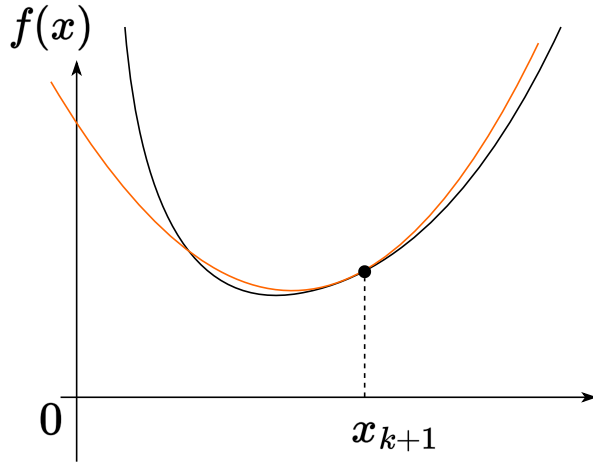
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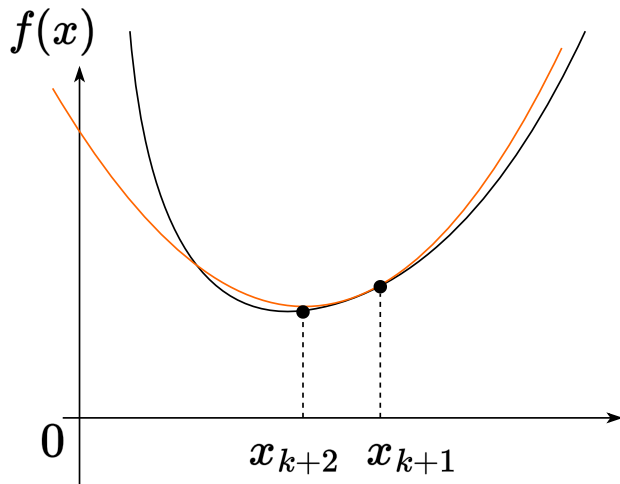
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Let  $f(x)$  be a strongly convex twice continuously differentiable function at  $\mathbb{R}^n$ , for the second derivative of which inequalities are executed:  $\mu I_n \preceq \nabla^2 f(x) \preceq L I_n$ . Then Newton's method with a constant step 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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4. We have introduced:

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

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6. So, we have:

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

and we need to bound the norm of the inverse hessian

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

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

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

## Convergence

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

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

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

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

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

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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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!

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- the Hessian can be degenerate at  $x^*$
- the hessian may not be positively determined  $\rightarrow$  direction  $-(f''(x))^{-1}f'(x)$  may not be a descending direction

# Newton

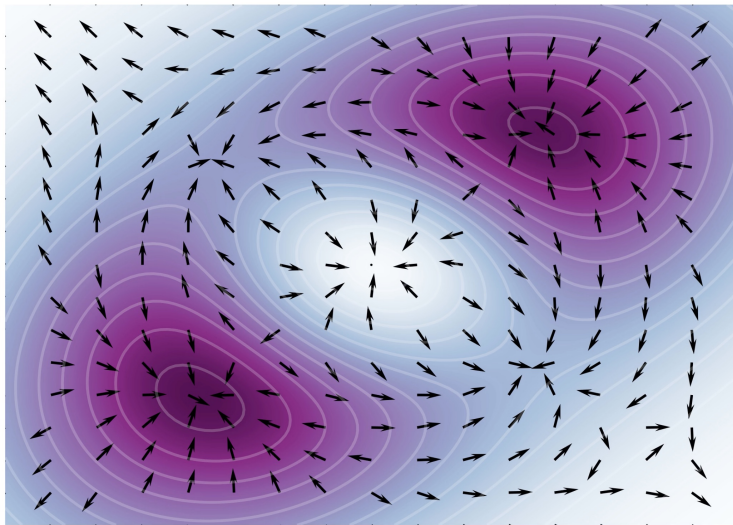


Figure 7: Animation 

# Newton method problems

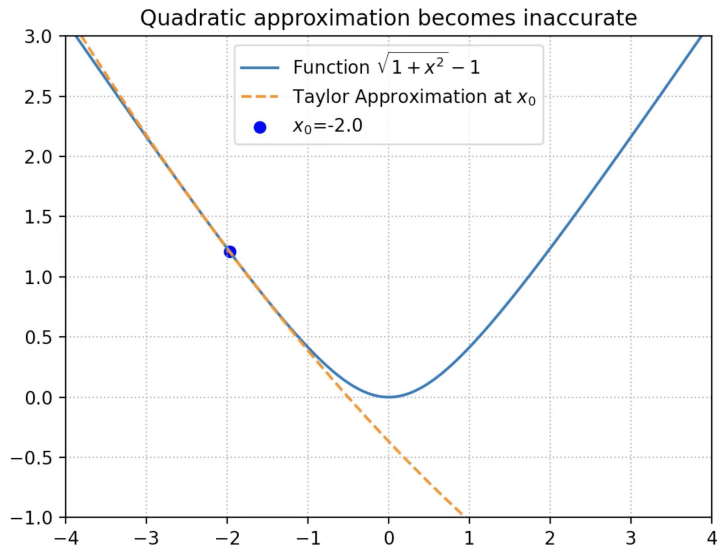


Figure 8: Animation

## The idea of adaptive metrics

Given  $f(x)$  and a point  $x_0$ . Define

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

(1) . . . 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  $f(x) \rightarrow \min_{x \in \mathbb{R}^n}$  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  $k \rightarrow \infty$  to the truth value of the Hessian  $\nabla^2 f(x_k)$ .

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**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):

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

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:

$$B_{k+1} = B_k + \alpha uu^T$$

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

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,

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

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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:

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

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  $C$ :

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

# Davidon-Fletcher-Powell Update

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

$$C_{k+1} = C_k + a u u^T + b v v^T.$$

Multiplying by  $\Delta y_k$ , 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:

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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:

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

# 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

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