Line Search. Matrix Calculus

Daniil Merkulov

Optimization for ML. Faculty of Computer Science. HSE University

Line search

Problem

Suppose, we have a problem of minimization of a function $f(x) : \mathbb{R} \to \mathbb{R}$ of scalar variable:

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f(x) \to \min_{x \in \mathbb{R}}
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Typical example of line search problem is selecting appropriate stepsize for gradient descent algorithm:

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The line search is a fundamental optimization problem that plays a crucial role in solving complex tasks. To simplify the problem, let's assume that the function, $f(x)$, is *unimodal*, meaning it has a single peak or valley.

Unimodal function

Definition

Function $f(x)$ is called **unimodal** on $[a, b]$, if there is $x_* \in [a, b]$, that $f(x_1) > f(x_2) \quad \forall a \leq x_1 < x_2 < x_*$ and $f(x_1) < f(x_2) \quad \forall x_* < x_1 < x_2 \leq b$

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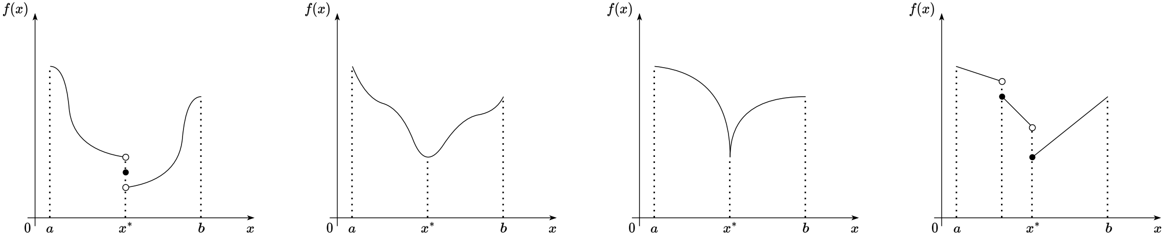

Рис. 1: Examples of unimodal functions

Key property of unimodal functions

Let $f(x)$ be unimodal function on $[a, b]$. Than if $x_1 < x_2 \in [a, b]$, then:

- if $f(x_1) \leq f(x_2) \to x_* \in [a, x_2]$

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Proof Let's prove the first statement. On the contrary, suppose that $f(x_1) \leq f(x_2)$, but $x^* > x_2$. Then necessarily $x_1 < x_2 < x^*$ and by the unimodality of the function $f(x)$ the inequality: $f(x_1) > f(x_2)$ must be satisfied. We have obtained a contradiction.

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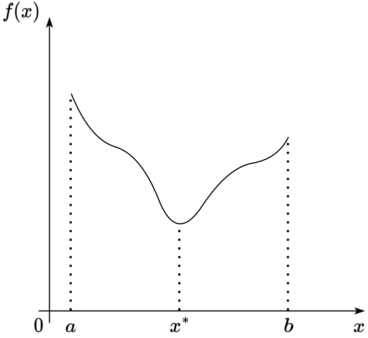

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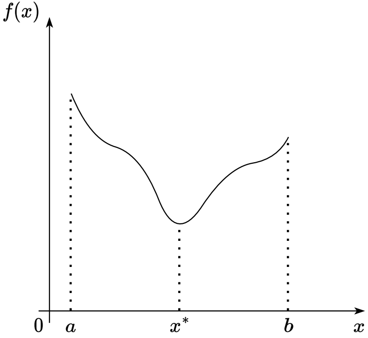

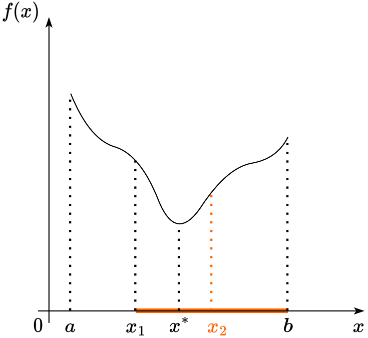

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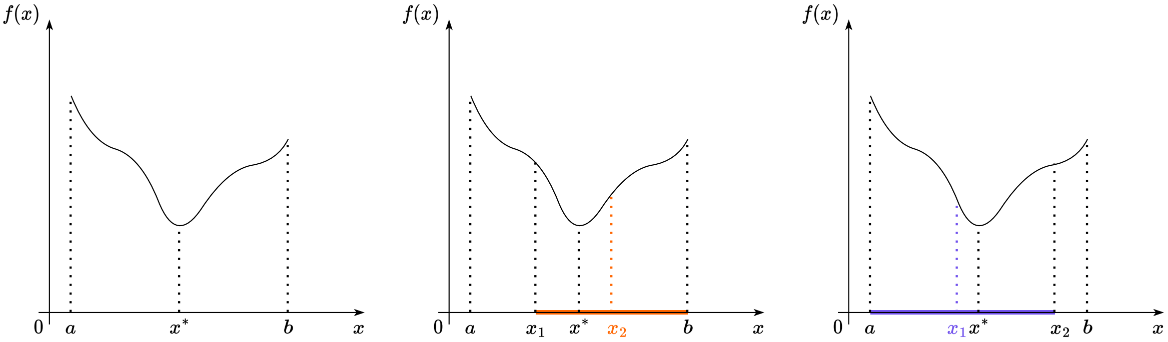

Dichotomy method

We aim to solve the following problem:

$$f(x) \to \min_{x \in [a,b]}$$

We divide a segment into two equal parts and choose the one that contains the solution of the problem using the values of functions, based on the key property described above. Our goal after one iteration of the method is to halve the solution region.

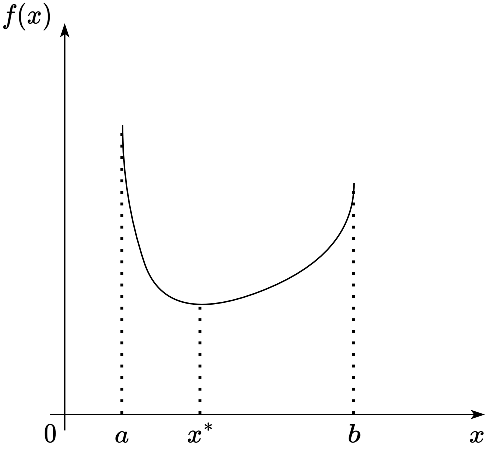

Рис. 2: Dichotomy method for unimodal function

Dichotomy method

We measure the function value at the middle of the line segment

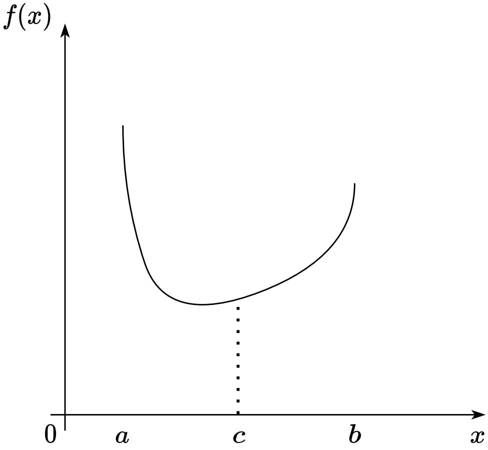

Рис. 3: Dichotomy method for unimodal function

Dichotomy method

In order to apply the key property we perform another measurement.

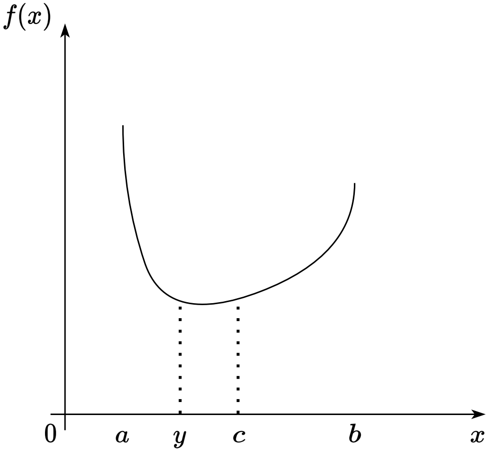

Рис. 4: Dichotomy method for unimodal function

Dichotomy method

We select the target line segment. And in this case we are lucky since we already halved the solution region. But that is not always the case.

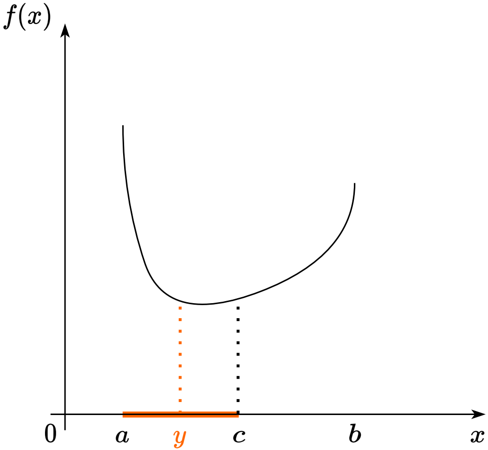

Рис. 5: Dichotomy method for unimodal function

Dichotomy method

Let's consider another unimodal function.

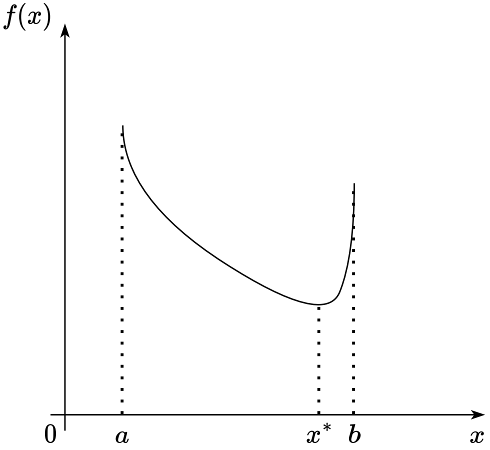

Рис. 6: Dichotomy method for unimodal function

Dichotomy method

Measure the middle of the line segment.

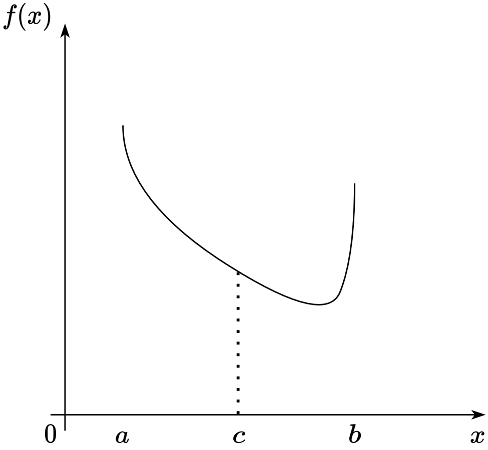

Рис. 7: Dichotomy method for unimodal function

Dichotomy method

Get another measurement.

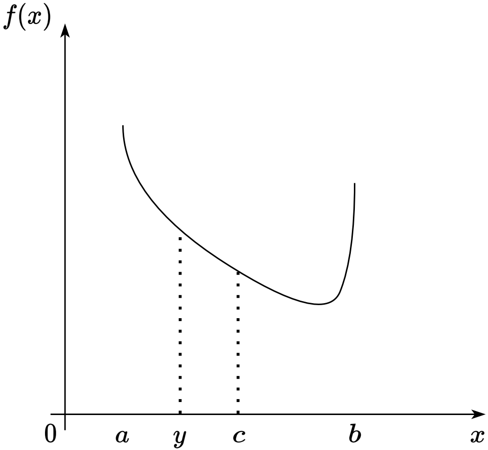

Рис. 8: Dichotomy method for unimodal function

Dichotomy method

Select the target line segment. You can clearly see, that the obtained line segment is not the half of the initial one. It is $\frac{3}{4}(b-a)$. So to fix it we need another step of the algorithm.

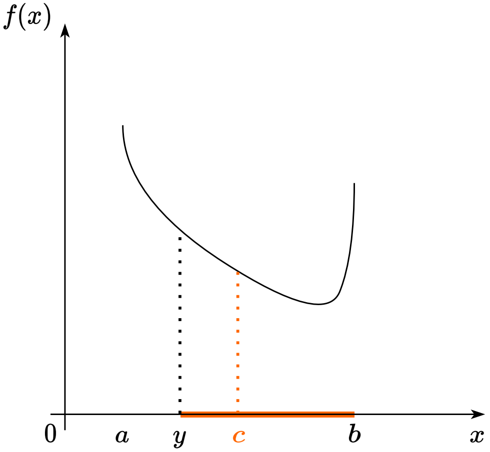

Рис. 9: Dichotomy method for unimodal function

Dichotomy method

After another additional measurement, we will surely get

$\frac{2}{3}\frac{3}{4}(b-a) = \frac{1}{2}(b-a)$

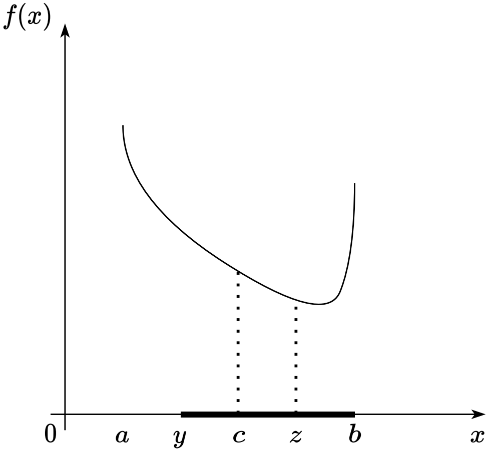

Рис. 10: Dichotomy method for unimodal function

Dichotomy method

To sum it up, each subsequent iteration will require at most two function value measurements.

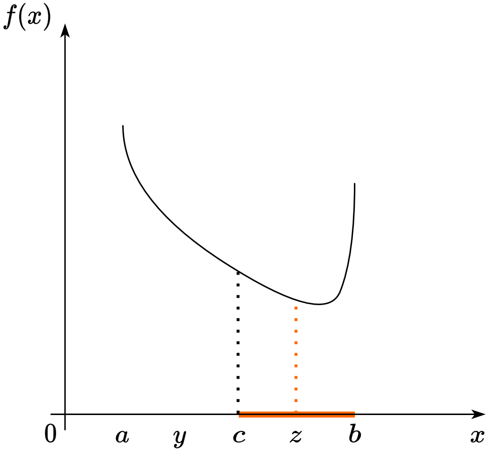

Рис. 11: Dichotomy method for unimodal function

Dichotomy method. Algorithm

```python
def binary_search(f, a, b, epsilon):
    c = (a + b) / 2
    while abs(b - a) > epsilon:
        y = (a + c) / 2.0
        if f(y) <= f(c):
            b = c
            c = y
        else:
            z = (b + c) / 2.0
            if f(c) <= f(z):
                a = y
                b = z
            else:
                a = c
                c = z
    return c
```

Dichotomy method. Bounds

The length of the line segment on $k+1$-th iteration:

$$\Delta_{k+1} = b_{k+1} - a_{k+1} = \frac{1}{2^k}(b-a)$$

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For unimodal functions, this holds if we select the middle of a segment as an output of the iteration x_{k+1}:

$$|x_{k+1} - x_*| \leq \frac{\Delta_{k+1}}{2} \leq \frac{1}{2^{k+1}}(b-a) \leq (0.5)^{k+1} \cdot (b-a)$$

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Note, that at each iteration we ask oracle no more, than 2 times, so the number of function evaluations is $N = 2 \cdot k$, which implies:

$$|x_{k+1} - x_*| \leq (0.5)^{\frac{N}{2}+1} \cdot (b-a) \leq (0.707)^N \frac{b-a}{2}$$

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By marking the right side of the last inequality for ε, we get the number of method iterations needed to achieve ε accuracy:

$$K = \left\lceil \log_2 \frac{b-a}{\varepsilon} - 1 \right\rceil$$

Golden-section search

The idea is quite similar to the dichotomy method. There are two golden points on the line segment (left and right) and the insightful idea is, that on the next iteration one of the points will remain the golden point.

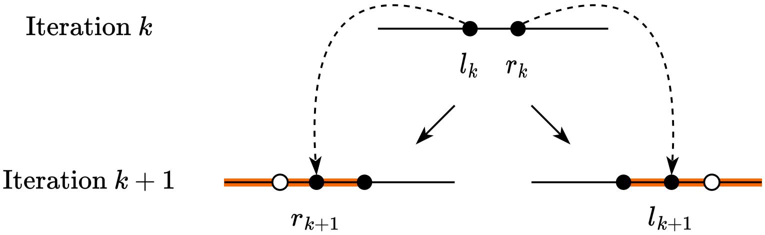

Рис. 12: Key idea, that allows us to decrease function evaluations

Golden-section search. Algorithm

```python
def golden_search(f, a, b, epsilon):
    tau = (sqrt(5) + 1) / 2
    y = a + (b - a) / tau**2
    z = a + (b - a) / tau
    while b - a > epsilon:
        if f(y) <= f(z):
            b = z
            z = y
            y = a + (b - a) / tau**2
        else:
            a = y
            y = z
            z = a + (b - a) / tau
    return (a + b) / 2
```

Golden-section search. Bounds

$$
|x_{k+1} - x_*| \leq b_{k+1} - a_{k+1} = \left(\frac{1}{\tau} \right)^{N-1} (b-a) \approx 0.618^k (b-a),
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where $\tau = \frac{\sqrt{5}+1}{2}$.

- The geometric progression constant **more** than the dichotomy method - 0.618 worse than 0.5

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where $\tau = \frac{\sqrt{5}+1}{2}$.

- The geometric progression constant **more** than the dichotomy method - 0.618 worse than 0.5
- The number of function calls **is less** than for the dichotomy method - 0.707 worse than 0.618 - (for each iteration of the dichotomy method, except for the first one, the function is calculated no more than 2 times, and for the gold method - no more than one)

Successive parabolic interpolation

Sampling 3 points of a function determines unique parabola. Using this information we will go directly to its minimum. Suppose, we have 3 points $x_1 < x_2 < x_3$ such that line segment $[x_1, x_3]$ contains minimum of a function $f(x)$. Then, we need to solve the following system of equations:

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$$ax_i^2 + bx_i + c = f_i = f(x_i), i = 1, 2, 3$$

Note, that this system is linear, since we need to solve it on a, b, c. Minimum of this parabola will be calculated as:

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$$
u = -\frac{b}{2a} = x_2 - \frac{(x_2 - x_1)^2(f_2 - f_3) - (x_2 - x_3)^2(f_2 - f_1)}{2\left[(x_2 - x_1)(f_2 - f_3) - (x_2 - x_3)(f_2 - f_1)\right]}
$$

Note, that if $f_2 < f_1, f_2 < f_3$, than u will lie in $[x_1, x_3]$

Successive parabolic interpolation. Algorithm [1]

```
def parabola_search(f, x1, x2, x3, epsilon):
    f1, f2, f3 = f(x1), f(x2), f(x3)
    while x3 - x1 > epsilon:
        u = x2 - ((x2 - x1)**2*(f2 - f3) - (x2 - x3)**2*(f2 - f1))/(2*((x2 - x1)*(f2 - f3) - (x2 - x3)*(f2 - f1)))
        fu = f(u)

        if x2 <= u:
            if f2 <= fu:
                x1, x2, x3 = x1, x2, u
                f1, f2, f3 = f1, f2, fu
            else:
                x1, x2, x3 = x2, u, x3
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        else:
            if fu <= f2:
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                f1, f2, f3 = f1, fu, f2
            else:
                x1, x2, x3 = u, x2, x3
                f1, f2, f3 = fu, f2, f3
    return (x1 + x3) / 2
```
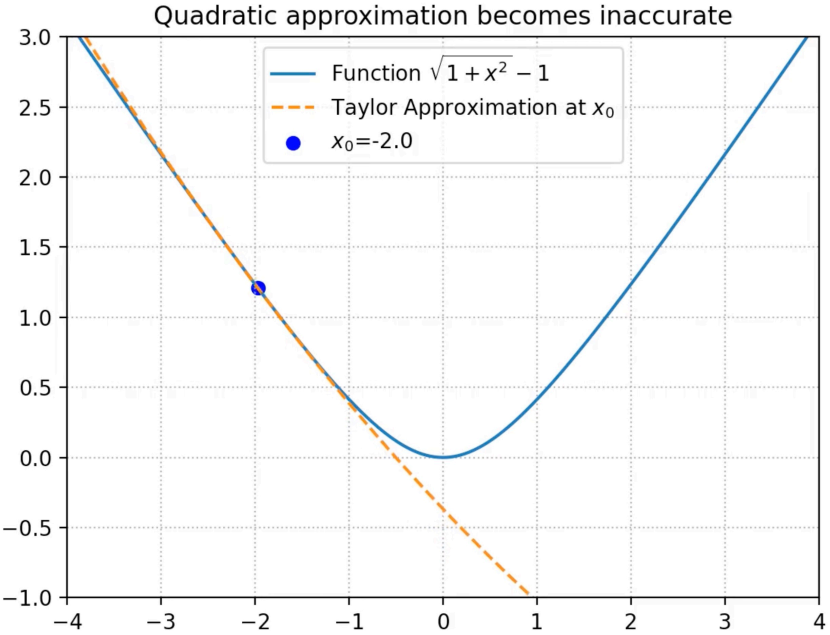

[1] The convergence of this method is superlinear, but local, which means, that you can take profit from using this method only near some neighbour of optimum. *Here* is the proof of superlinear convergence of order 1.32.


Quadratic approximation becomes inaccurate
Function $\sqrt{1+x^2}-1$
Taylor Approximation at x_0
x_0=-2.0
3.0
2.5
2.0
1.5
1.0
0.5
0.0
−0.5
−1.0
−4
−3
−2
−1
0
1
2
3
4

Inexact line search

Sometimes it is enough to find a solution, which will approximately solve out problem. This is very typical scenario for mentioned stepsize selection problem

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\begin{aligned}
x_{k+1} &= x_k - \alpha \nabla f(x_k) \\
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\phi(\alpha) = f(x_k - \alpha \nabla f(x_k)), \alpha \geq 0
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The first-order approximation of $\phi(\alpha)$ near $\alpha = 0$ is:

$$
\phi(\alpha) \approx f(x_k) - \alpha \nabla f(x_k)^T \nabla f(x_k)
$$

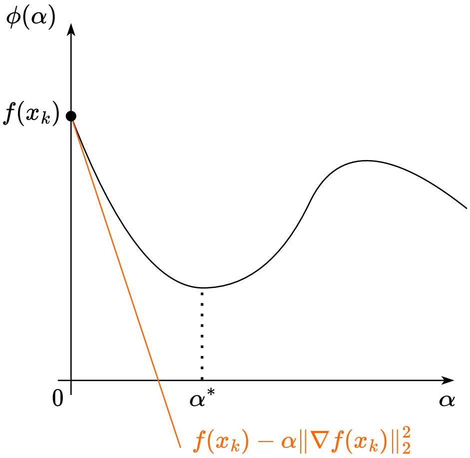

Рис. 13: Illustration of Taylor approximation of $\phi_0^I(\alpha)$

Inexact line search. Sufficient Decrease

The inexact line search condition, known as the Armijo condition, states that α should provide sufficient decrease in the function f, satisfying:

$$f(x_k - \alpha \nabla f(x_k)) \leq f(x_k) - c_1 \cdot \alpha \nabla f(x_k)^T \nabla f(x_k)$$

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for some constant $c_1 \in (0, 1)$. Note that setting $c_1 = 1$ corresponds to the first-order Taylor approximation of $\phi(\alpha)$. However, this condition can accept very small values of α, potentially slowing down the solution process. Typically, $c_1 \approx 10^{-4}$ is used in practice.

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Example

If $f(x)$ represents a cost function in an optimization problem, choosing an appropriate c_1 value is crucial. For instance, in a machine learning model training scenario, an improper c_1 might lead to either very slow convergence or missing the minimum.

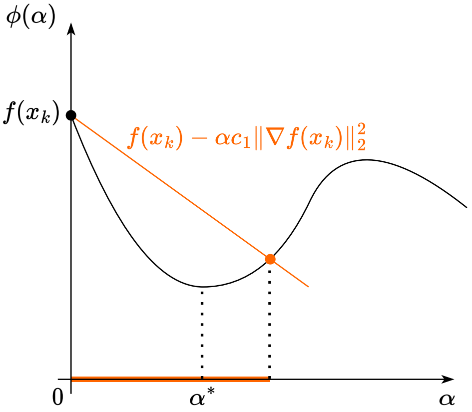

Рис. 14: Illustration of sufficient decrease condition with coefficient c_1

Inexact line search. Goldstein Conditions

Consider two linear scalar functions $\phi_1(\alpha)$ and $\phi_2(\alpha)$:

$$\phi_1(\alpha) = f(x_k) - c_1\alpha\|\nabla f(x_k)\|^2$$

$$\phi_2(\alpha) = f(x_k) - c_2\alpha\|\nabla f(x_k)\|^2$$

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$$\phi_1(\alpha) = f(x_k) - c_1 \alpha \|\nabla f(x_k)\|^2$$

$$\phi_2(\alpha) = f(x_k) - c_2 \alpha \|\nabla f(x_k)\|^2$$

The Goldstein-Armijo conditions locate the function $\phi(\alpha)$ between $\phi_1(\alpha)$ and $\phi_2(\alpha)$. Typically, $c_1 = \rho$ and $c_2 = 1 - \rho$, with $\rho \in (0, 0.5)$.

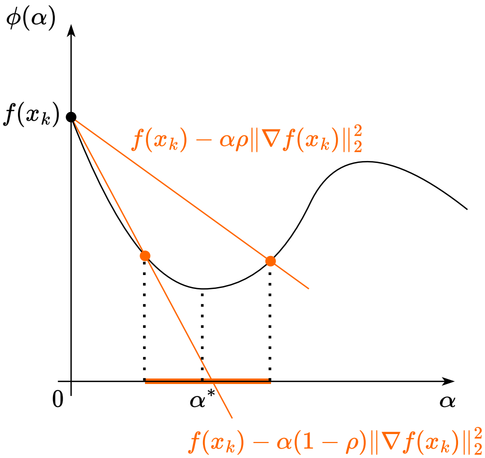

Рис. 15: Illustration of Goldstein conditions

Inexact line search. Curvature Condition

To avoid excessively short steps, we introduce a second criterion:

$$-\nabla f(x_k - \alpha \nabla f(x_k))^T \nabla f(x_k) \geq c_2 \nabla f(x_k)^T(-\nabla f(x_k))$$

Inexact line search. Curvature Condition

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for some $c_2 \in (c_1, 1)$. Here, c_1 is from the Armijo condition.

The left-hand side is the derivative $\nabla_\alpha \phi(\alpha)$, ensuring that the slope of $\phi(\alpha)$ at the target point is at least c_2 times the initial slope $\nabla_\alpha \phi(\alpha)(0)$.

Commonly, $c_2 \approx 0.9$ is used for Newton or quasi-Newton methods. Together, the sufficient decrease and curvature conditions form the Wolfe conditions.

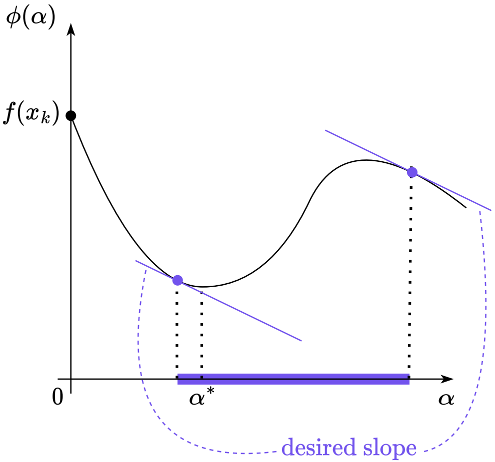

Рис. 16: Illustration of curvature condition

Inexact line search. Wolfe Condition

$$-\nabla f(x_k - \alpha \nabla f(x_k))^T \nabla f(x_k) \geq c_2 \nabla f(x_k)^T(-\nabla f(x_k))$$

Together, the sufficient decrease and curvature conditions form the Wolfe conditions.

Theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be continuously differentiable, and let $\phi(\alpha) = f(x_k - \alpha \nabla f(x_k))$. Assume $\nabla f(x_k)^T p_k < 0$, where $p_k = -\nabla f(x_k)$, making p_k a descent direction. Also, assume f is bounded below along the ray $\{x_k + \alpha p_k \mid \alpha > 0\}$. We aim to show that for $0 < c_1 < c_2 < 1$, there exist intervals of step lengths satisfying the Wolfe conditions.

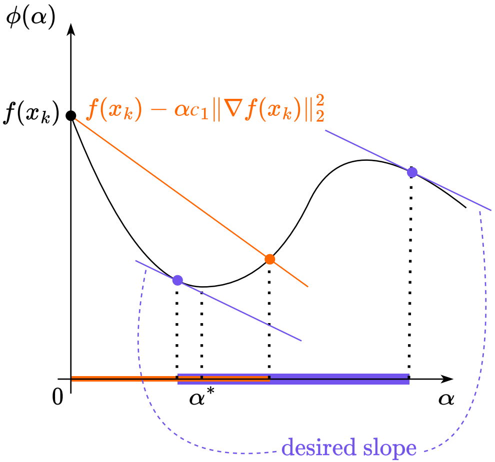

Рис. 17: Illustration of Wolfe condition

Inexact line search. Wolfe Condition. Proof

1. Since $\phi(\alpha) = f(x_k + \alpha p_k)$ is bounded below and $l(\alpha) = f(x_k) + \alpha c_1 \nabla f(x_k)^T p_k$ is unbounded below (as $\nabla f(x_k)^T p_k < 0$), the graph of $l(\alpha)$ must intersect the graph of $\phi(\alpha)$ at least once. Let $\alpha' > 0$ be the smallest such value satisfying:

$$f(x_k + \alpha' p_k) \leq f(x_k) + \alpha' c_1 \nabla f(x_k)^T p_k. \tag{1}$$

   This ensures the **sufficient decrease condition** is satisfied.

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   This ensures the **sufficient decrease condition** is satisfied.

2. By the Mean Value Theorem, there exists $\alpha'' \in (0, \alpha')$ such that:

$$f(x_k + \alpha' p_k) - f(x_k) = \alpha' \nabla f(x_k + \alpha'' p_k)^T p_k. \tag{2}$$

   Substituting $f(x_k + \alpha' p_k)$ from (1) into (2), we have:

$$\alpha' \nabla f(x_k + \alpha'' p_k)^T p_k \leq \alpha' c_1 \nabla f(x_k)^T p_k.$$

   Dividing through by $\alpha' > 0$, this simplifies to:

$$\nabla f(x_k + \alpha'' p_k)^T p_k \leq c_1 \nabla f(x_k)^T p_k. \tag{3}$$

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3. Since $c_1 < c_2$ and $\nabla f(x_k)^T p_k < 0$, the inequality $c_1 \nabla f(x_k)^T p_k < c_2 \nabla f(x_k)^T p_k$ holds. This implies there exists α'' such that:

$$\nabla f(x_k + \alpha'' p_k)^T p_k \leq c_2 \nabla f(x_k)^T p_k. \tag{4}$$

   Inequalities (3) and (4) together ensure the Wolfe conditions are satisfied.

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4. For the strong Wolfe conditions, the curvature condition:

$$\left|\nabla f(x_k + \alpha p_k)^T p_k\right| \leq c_2 \left|\nabla f(x_k)^T p_k\right| \tag{5}$$

   is met because $\nabla f(x_k + \alpha p_k)^T p_k$ is negative and bounded below by $c_2 \nabla f(x_k)^T p_k$.

Inexact line search. Wolfe Condition. Proof

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5. Due to the smoothness of f, there exists an interval around α'' where the Wolfe conditions (and thus the strong Wolfe conditions) hold. Hence, the proof is complete.

Backtracking Line Search

Backtracking line search is a technique to find a step size that satisfies the Armijo condition, Goldstein conditions, or other criteria of inexact line search. It begins with a relatively large step size and iteratively scales it down until a condition is met.

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1. Choose an initial step size, α_0, and parameters $\beta \in (0, 1)$ and $c_1 \in (0, 1)$.

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2. Check if the chosen step size satisfies the chosen condition (e.g., Armijo condition).
3. If the condition is satisfied, stop; else, set $\alpha := \beta\alpha$ and repeat step 2.

The step size α is updated as

$$\alpha_{k+1} := \beta\alpha_k$$

in each iteration until the chosen condition is satisfied.

Example

In machine learning model training, the backtracking line search can be used to adjust the learning rate. If the loss doesn't decrease sufficiently, the learning rate is reduced multiplicatively until the Armijo condition is met.

Numerical illustration

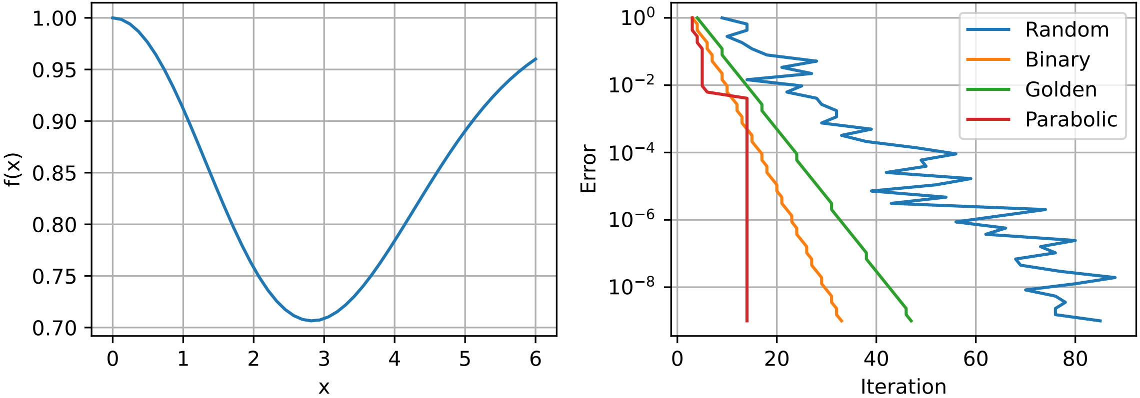

Рис. 18: Comparison of different line search algorithms

Open In Colab ♣

Matrix calculus

Gradient

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$, then vector, which contains all first-order partial derivatives:

$$\nabla f(x) = \dfrac{df}{dx} = \begin{pmatrix} \frac{\partial f}{\partial x_1} \\ \frac{\partial f}{\partial x_2} \\ \vdots \\ \frac{\partial f}{\partial x_n} \end{pmatrix}$$

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named gradient of $f(x)$. This vector indicates the direction of the steepest ascent. Thus, vector $-\nabla f(x)$ means the direction of the steepest descent of the function in the point. Moreover, the gradient vector is always orthogonal to the contour line in the point.

Example

For the function $f(x, y) = x^2 + y^2$, the gradient is:

$$\nabla f(x, y) = \begin{bmatrix} 2x \\ 2y \end{bmatrix}$$

This gradient points in the direction of the steepest ascent of the function.

Question

How does the magnitude of the gradient relate to the steepness of the function?

Hessian

Let $f(x) : \mathbb{R}^n \to \mathbb{R}$, then matrix, containing all the second order partial derivatives:

$$f''(x) = \nabla^2 f(x) = \frac{\partial^2 f}{\partial x_i \partial x_j} = \begin{pmatrix} \frac{\partial^2 f}{\partial x_1 \partial x_1} & \frac{\partial^2 f}{\partial x_1 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_1 \partial x_n} \\ \frac{\partial^2 f}{\partial x_2 \partial x_1} & \frac{\partial^2 f}{\partial x_2 \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_2 \partial x_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 f}{\partial x_n \partial x_1} & \frac{\partial^2 f}{\partial x_n \partial x_2} & \cdots & \frac{\partial^2 f}{\partial x_n \partial x_n} \end{pmatrix}$$

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In fact, Hessian could be a tensor in such a way: $(f(x) : \mathbb{R}^n \to \mathbb{R}^m)$ is just 3d tensor, every slice is just hessian of corresponding scalar function $(\nabla^2 f_1(x), \dots, \nabla^2 f_m(x))$.

Example

For the function $f(x, y) = x^2 + y^2$, the Hessian is:

$$H_f(x, y) = \begin{bmatrix} 2 & 0 \\ 0 & 2 \end{bmatrix}$$

This matrix provides information about the curvature of the function in different directions.

Question

How can the Hessian matrix be used to determine the concavity or convexity of a function?

Schwartz theorem

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function. If the mixed partial derivatives $\frac{\partial^2 f}{\partial x_i \partial x_j}$ and $\frac{\partial^2 f}{\partial x_j \partial x_i}$ are both continuous on an open set containing a point a, then they are equal at the point a. That is,

$$\frac{\partial^2 f}{\partial x_i \partial x_j}(a) = \frac{\partial^2 f}{\partial x_j \partial x_i}(a)$$

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$$\frac{\partial^2 f}{\partial x_i \partial x_j}(a) = \frac{\partial^2 f}{\partial x_j \partial x_i}(a)$$

Given the Schwartz theorem, if the mixed partials are continuous on an open set, the Hessian matrix is symmetric. That means the entries above the main diagonal mirror those below the main diagonal:

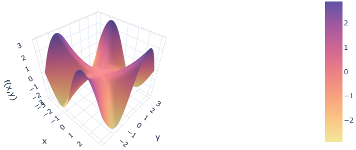
$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i} \quad \nabla^2 f(x) = (\nabla^2 f(x))^T$$

This symmetry simplifies computations and analysis involving the Hessian matrix in various applications, particularly in optimization.

Schwartz counterexample

$$f(x,y) = \begin{cases} \frac{xy(x^2-y^2)}{x^2+y^2} & \text{for } (x,\, y) \neq (0,\, 0), \\ 0 & \text{for } (x, y) = (0, 0). \end{cases}$$

Counterexample ♣



One can verify, that $\frac{\partial^2 f}{\partial x \partial y}(0,0) \neq \frac{\partial^2 f}{\partial y \partial x}(0,0)$, although the mixed partial derivatives do exist, and at every other point the symmetry does hold.

Jacobian

The extension of the gradient of multidimensional $f(x) : \mathbb{R}^n \to \mathbb{R}^m$ is the following matrix:

$$
J_f = f'(x) = \dfrac{df}{dx^T} = \begin{pmatrix}
\frac{\partial f_1}{\partial x_1} & \frac{\partial f_2}{\partial x_1} & \dots & \frac{\partial f_m}{\partial x_1} \\
\frac{\partial f_1}{\partial x_2} & \frac{\partial f_2}{\partial x_2} & \dots & \frac{\partial f_m}{\partial x_2} \\
\vdots & \vdots & \ddots & \vdots \\
\frac{\partial f_1}{\partial x_n} & \frac{\partial f_2}{\partial x_n} & \dots & \frac{\partial f_m}{\partial x_n}
\end{pmatrix}
$$

This matrix provides information about the rate of change of the function with respect to its inputs.

Question

Can we somehow connect those three definitions above (gradient, jacobian, and hessian) using a single correct statement?

Example

For the function

$$
f(x, y) = \begin{bmatrix} x + y \\ x - y \end{bmatrix},
$$

the Jacobian is:

$$
J_f(x, y) = \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}
$$

Question

How does the Jacobian matrix relate to the gradient for scalar-valued functions?

Summary

$$f(x) : X \to Y; \qquad \frac{\partial f(x)}{\partial x} \in G$$

X	Y	G	Name
$\mathbb{R}$	$\mathbb{R}$	$\mathbb{R}$	$f'(x)$ (derivative)
$\mathbb{R}^n$	$\mathbb{R}$	$\mathbb{R}^n$	$\dfrac{\partial f}{\partial x_i}$ (gradient)
$\mathbb{R}^n$	$\mathbb{R}^m$	$\mathbb{R}^{n \times m}$	$\dfrac{\partial f_i}{\partial x_j}$ (jacobian)
$\mathbb{R}^{m \times n}$	$\mathbb{R}$	$\mathbb{R}^{m \times n}$	$\dfrac{\partial f}{\partial x_{ij}}$

Differentials

Theorem

Let $x \in S$ be an interior point of the set S, and let $D : U \to V$ be a linear operator. We say that the function f is differentiable at the point x with derivative D if for all sufficiently small $h \in U$ the following decomposition holds:

$$f(x + h) = f(x) + D[h] + o(\|h\|)$$

If for any linear operator $D : U \to V$ the function f is not differentiable at the point x with derivative D, then we say that f is not differentiable at the point x.

Differentials

After obtaining the differential notation of df we can retrieve the gradient using the following formula:

$$df(x) = \langle \nabla f(x), dx \rangle$$

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Then, if we have a differential of the above form and we need to calculate the second derivative of the matrix/vector function, we treat ``old'' dx as the constant dx_1, then calculate $d(df) = d^2 f(x)$

$$d^2 f(x) = \langle \nabla^2 f(x) dx_1, dx \rangle = \langle H_f(x) dx_1, dx \rangle$$

Differential properties

Let A and B be the constant matrices, while X and Y are the variables (or matrix functions).

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- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$
- $d\left(\dfrac{X}{\phi}\right) = \dfrac{\phi dX - (d\phi)X}{\phi^2}$
- $d\left(\det X\right) = \det X \langle X^{-T}, dX\rangle$

Differential properties

Let A and B be the constant matrices, while X and Y are the variables (or matrix functions).

- $dA = 0$
- $d(\alpha X) = \alpha(dX)$
- $d(AXB) = A(dX)B$
- $d(X+Y) = dX + dY$
- $d(X^T) = (dX)^T$
- $d(XY) = (dX)Y + X(dY)$
- $d\langle X, Y\rangle = \langle dX, Y\rangle + \langle X, dY\rangle$
- $d\left(\frac{X}{\phi}\right) = \frac{\phi dX - (d\phi)X}{\phi^2}$
- $d\left(\det X\right) = \det X \langle X^{-T}, dX\rangle$
- $d\left(\text{tr } X\right) = \langle I, dX\rangle$

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- $H = (J(\nabla f))^T$
- $d(X^{-1}) = -X^{-1}(dX)X^{-1}$

Matrix calculus. Example 1

Example

Find $df, \nabla f(x)$, if $f(x) = \langle x, Ax\rangle - b^T x + c$.

Matrix calculus. Example 2

Example

Find $df, \nabla f(x)$, if $f(x) = \ln \langle x, Ax\rangle$.

1. It is essential for A to be positive definite, because it is a logarithm argument. So, $A \in \mathbb{S}^n_{++}$Let's find the differential first:

$$
\begin{split}
df = d\left(\ln \langle x, Ax\rangle\right) = \dfrac{d\left(\langle x, Ax\rangle\right)}{\langle x, Ax\rangle} = \dfrac{\langle dx, Ax\rangle + \langle x, d(Ax)\rangle}{\langle x, Ax\rangle} = \\
= \dfrac{\langle Ax, dx\rangle + \langle x, Adx\rangle}{\langle x, Ax\rangle} = \dfrac{\langle Ax, dx\rangle + \langle A^T x, dx\rangle}{\langle x, Ax\rangle} = \dfrac{\langle (A + A^T) x, dx\rangle}{\langle x, Ax\rangle}
\end{split}
$$

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$$

2. Note, that our main goal is to derive the form $df = \langle \cdot, dx\rangle$

$$
df = \left\langle \frac{2Ax}{\langle x, Ax\rangle}, dx\right\rangle
$$

Hence, the gradient is $\nabla f(x) = \dfrac{2Ax}{\langle x, Ax\rangle}$

Matrix calculus. Example 3

Example

Find $df, \nabla f(X)$, if $f(X) = \langle S, X \rangle - \log \det X$.

Summary

Summary

Определения

1. Унимодальная функция.
2. Метод дихотомии.
3. Метод золотого сечения.
4. Метод параболической интерполяции.
5. Условие достаточного убывания для неточного линейного поиска.
6. Условия Гольдштейна для неточного линейного поиска.
7. Условие ограничения на кривизну для неточного линейного поиска.
8. Градиент функции $f(x) : \mathbb{R}^n \to \mathbb{R}$.
9. Гессиан функции $f(x) : \mathbb{R}^n \to \mathbb{R}$.
10. Якобиан функции $f(x) : \mathbb{R}^n \to \mathbb{R}^m$.
11. Формула для аппроксимации Тейлора первого порядка $f^I_{x_0}(x)$ функции $f(x) : \mathbb{R}^n \to \mathbb{R}$ в точке x_0.
12. Формула для аппроксимации Тейлора второго порядка $f^{II}_{x_0}(x)$ функции $f(x) : \mathbb{R}^n \to \mathbb{R}$ в точке x_0.
13. Связь дифференциала функции df и градиента ∇f для функции $f(x) : \mathbb{R}^n \to \mathbb{R}$.
14. Связь второго дифференциала функции $d^2 f$ и гессиана $\nabla^2 f$ для функции $f(x) : \mathbb{R}^n \to \mathbb{R}$.

Теоремы

1. Метод дихотомии и золотого сечения для унимодальных функций. Скорость сходимости.