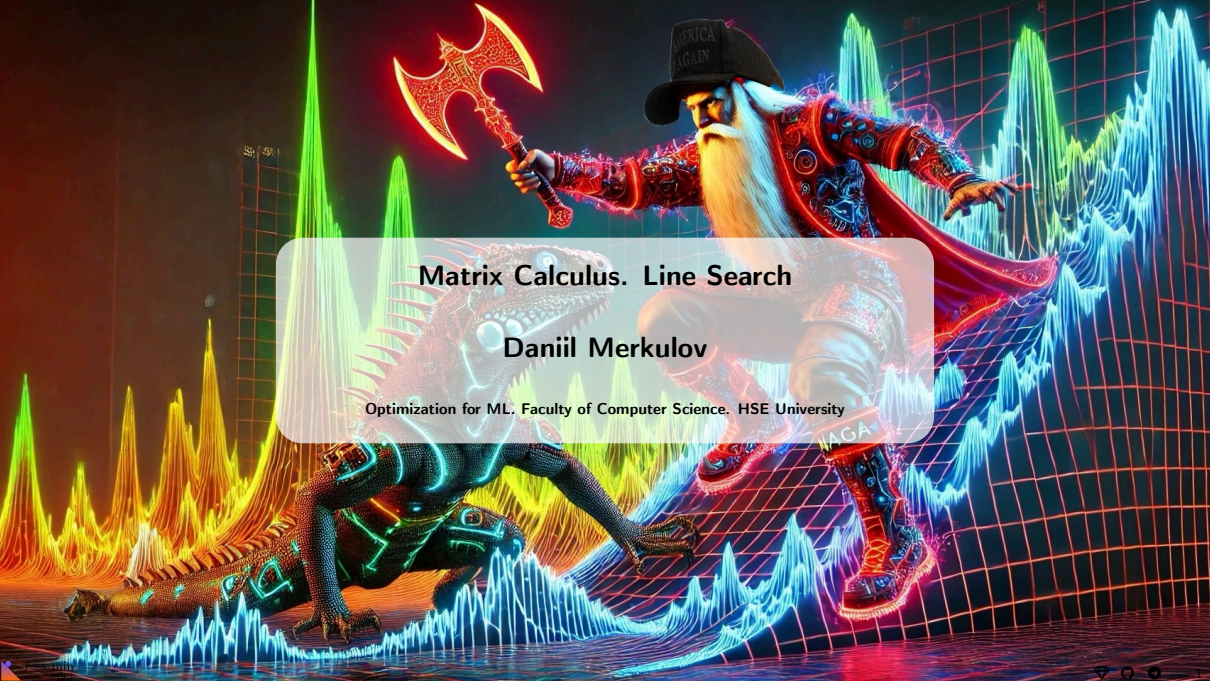

Matrix Calculus. Line Search

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Matrix calculus

Gradient

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

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

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

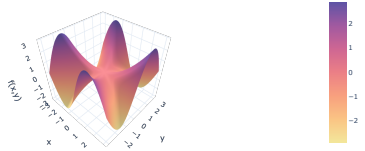
$$\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_i} \quad \nabla^2 f(x) = (\nabla^2 f(x))^T$$

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:

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

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

Question

Can we 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)
$\mathbb{R}^n$	$\mathbb{R}$	$\mathbb{R}^n$	$\frac{\partial f}{\partial x_i}$ (gradient)
$\mathbb{R}^n$	$\mathbb{R}^m$	$\mathbb{R}^{n \times m}$	$\frac{\partial f_i}{\partial x_j}$ (jacobian)
$\mathbb{R}^{m \times n}$	$\mathbb{R}$	$\mathbb{R}^{m \times n}$	$\frac{\partial f}{\partial x_{ij}}$

First-order Taylor approximation

The first-order Taylor approximation, also known as the linear approximation, is centered around some point x_0. If $f : \mathbb{R}^n \to \mathbb{R}$ is a differentiable function, then its first-order Taylor approximation is given by:

$$f^I_{x_0}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0)$$

Where:

- $f(x_0)$ is the value of the function at the point x_0.

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It is very usual to replace the $f(x)$ with $f^I_{x_0}(x)$ near the point x_0 for simple analysis of some approaches.

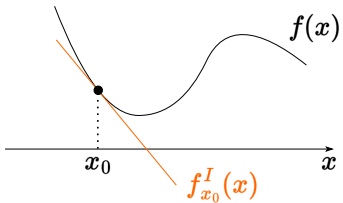

Figure 1: First order Taylor approximation near the point x_0

Second-order Taylor approximation

The second-order Taylor approximation, also known as the quadratic approximation, includes the curvature of the function. For a twice-differentiable function $f : \mathbb{R}^n \to \mathbb{R}$, its second-order Taylor approximation centered at some point x_0 is:

$$f_{x_0}^{II}(x) = f(x_0) + \nabla f(x_0)^T (x - x_0) + \frac{1}{2}(x - x_0)^T \nabla^2 f(x_0)(x - x_0)$$

Where $\nabla^2 f(x_0)$ is the Hessian matrix of f at the point x_0.

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Where $\nabla^2 f(x_0)$ is the Hessian matrix of f at the point x_0.
When using the linear approximation of the function is not sufficient one can consider replacing the $f(x)$ with $f_{x_0}^{II}(x)$ near the point x_0. In general, Taylor approximations give us a way to locally approximate functions. The first-order approximation is a plane tangent to the function at the point x_0, while the second-order approximation includes the curvature and is represented by a parabola. These approximations are especially useful in optimization and numerical methods because they provide a tractable way to work with complex functions.

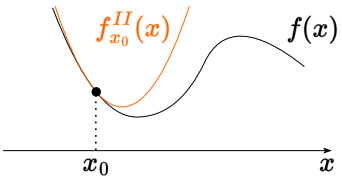

Figure 2: Second order Taylor approximation near the point x_0

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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- $df(g(x)) = \frac{df}{dg} \cdot dg(x)$
- $H = (J(\nabla f))^T$
- $d(X^{-1}) = -X^{-1}(dX)X^{-1}$

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

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

Matrix calculus. Example 2

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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 the argument of a logarithm. So, $A \in \mathbb{S}^n_{++}$Let's find the differential first:

$$df = d\left(\ln\langle x, Ax\rangle\right) = \frac{d\left(\langle x, Ax\rangle\right)}{\langle x, Ax\rangle} = \frac{\langle dx, Ax\rangle + \langle x, d(Ax)\rangle}{\langle x, Ax\rangle} =$$

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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 $f(X) = \langle S, X \rangle - \log\det X$.

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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Example

A typical example of a line search problem is selecting the appropriate stepsize for the gradient descent algorithm:

$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$
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Line search is a fundamental optimization problem that is crucial to 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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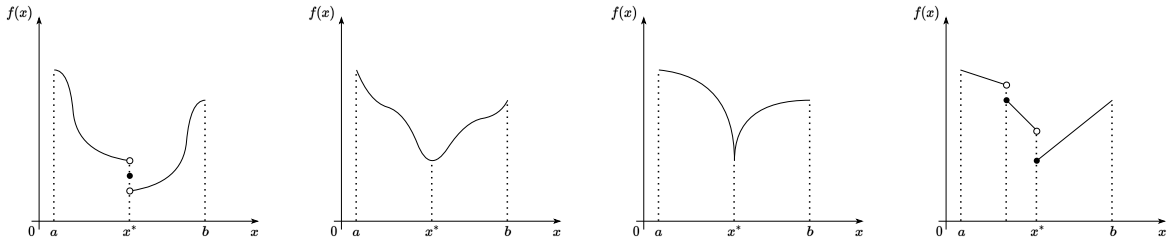

Figure 3: Examples of unimodal functions

Key property of unimodal functions

Let $f(x)$ be an unimodal function on $[a, b]$. Then 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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- if $f(x_1) \geq f(x_2) \to x_* \in [x_1, b]$

Key property of unimodal functions

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

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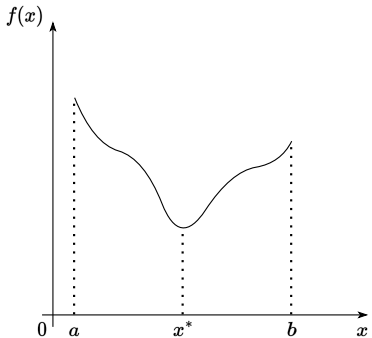

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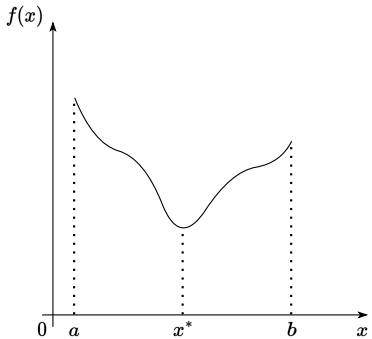

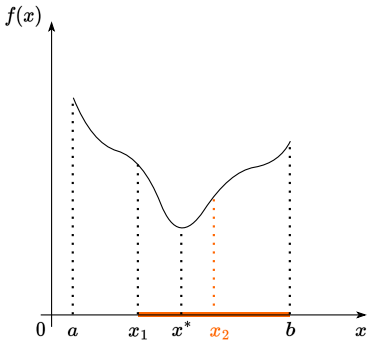

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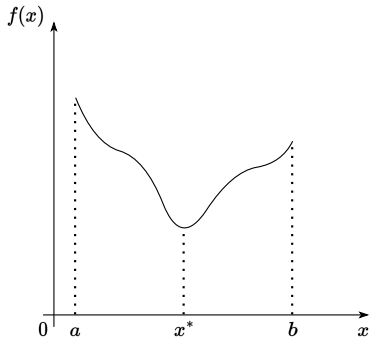

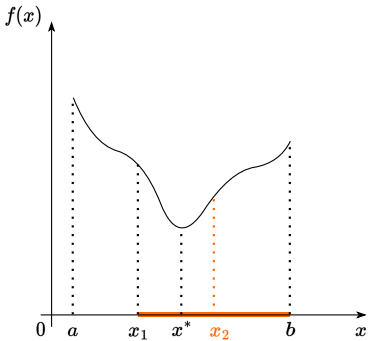

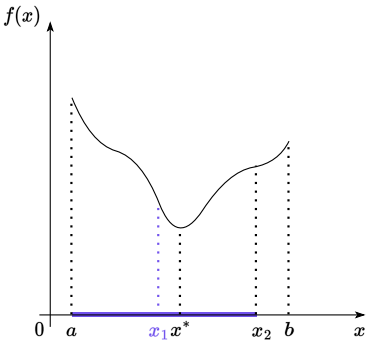

Dichotomy method

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.

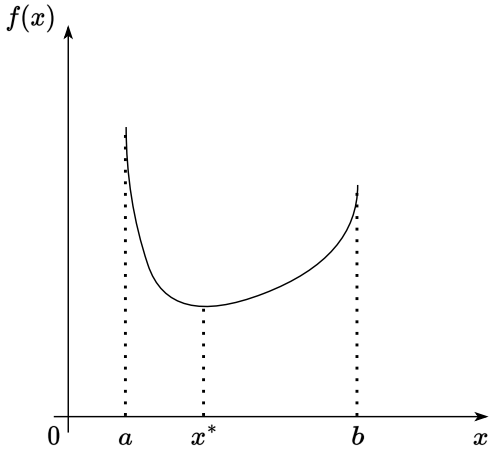

Figure 4: Dichotomy method for unimodal function

Dichotomy method

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

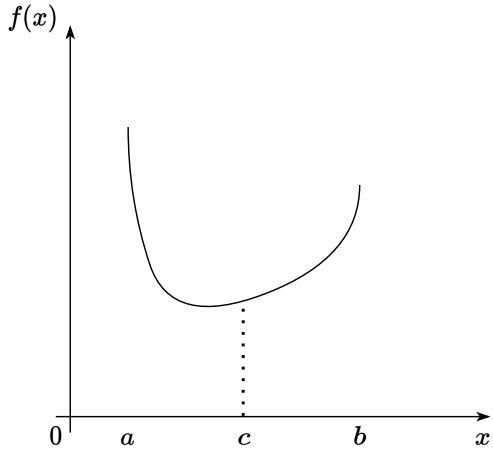

Figure 5: Dichotomy method for unimodal function

Dichotomy method

To apply the key property we perform another measurement.

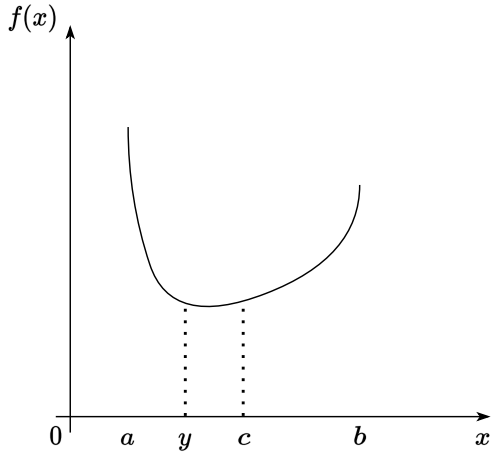

Figure 6: Dichotomy method for unimodal function

Dichotomy method

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

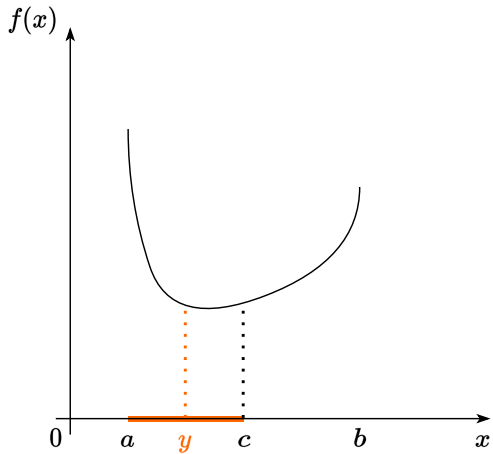

Figure 7: Dichotomy method for unimodal function

Dichotomy method

Let's consider another unimodal function.

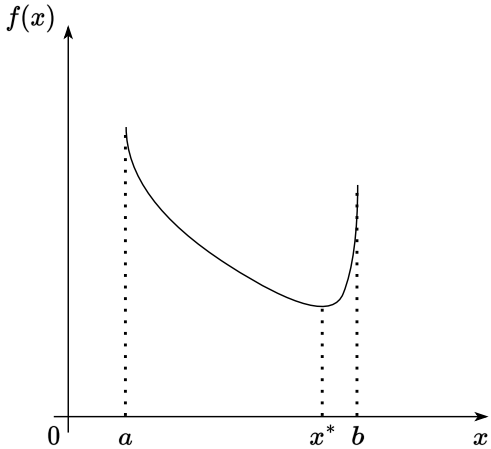

Figure 8: Dichotomy method for unimodal function

Dichotomy method

Measure the middle of the line segment.

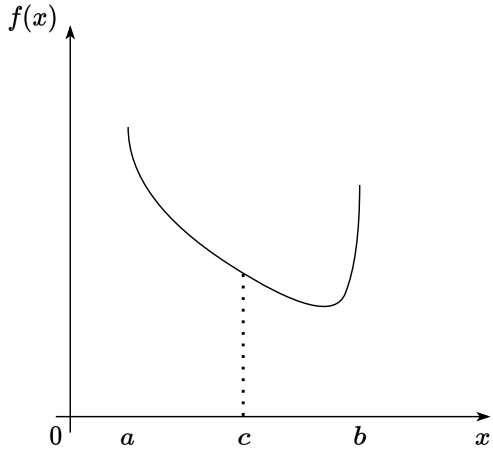

Figure 9: Dichotomy method for unimodal function

Dichotomy method

Get another measurement.

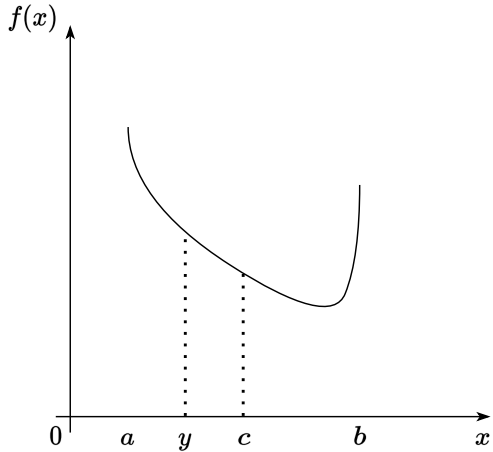

Figure 10: Dichotomy method for unimodal function

Dichotomy method

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

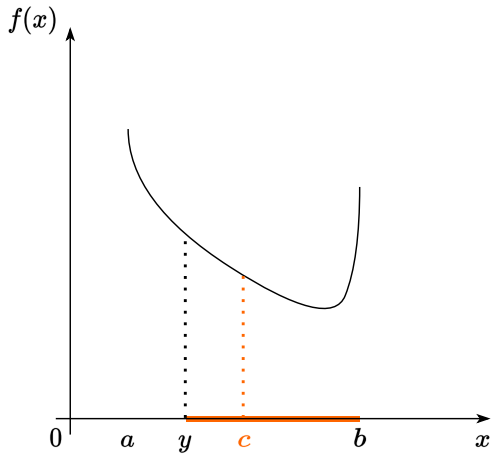

Figure 11: Dichotomy method for unimodal function

Dichotomy method

After another additional measurement, we will surely get $\frac{2}{3}\frac{3}{4}(b-a) = \frac{1}{2}(b-a)$

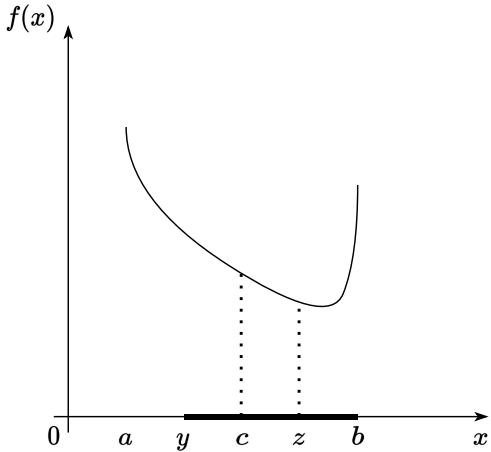

Figure 12: Dichotomy method for unimodal function

Dichotomy method

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

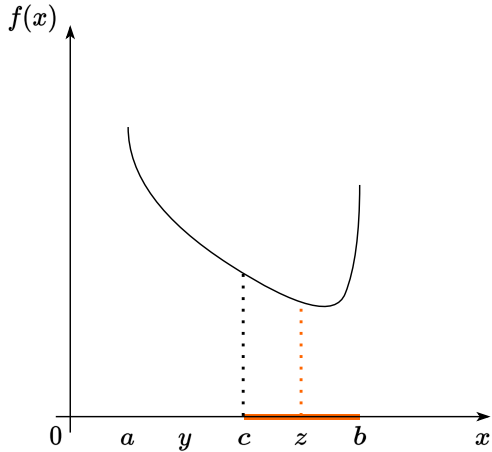

Figure 13: Dichotomy method for unimodal function

Dichotomy method. Algorithm

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

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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.

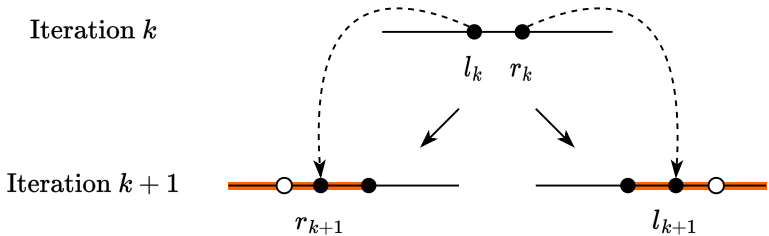

Figure 14: Key idea, that allows us to decrease function evaluations

Golden-section search. Algorithm

```
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

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

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

- The geometric progression constant **is larger** for the golden-section method compared to the dichotomy method: 0.618 is worse than 0.5.

Golden-section search. Bounds

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

- The geometric progression constant **is larger** for the golden-section method compared to the dichotomy method: 0.618 is worse than 0.5.
- The number of function calls **is fewer** for the golden-section method compared to the dichotomy method: 0.707 is worse than 0.618. For each iteration of the dichotomy method (except the first one), the function is evaluated no more than twice, whereas for the golden-section method, it is evaluated no more than once per iteration.

Successive parabolic interpolation

Sampling 3 points of a function determines a 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. The minimum of this parabola will be calculated as:

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

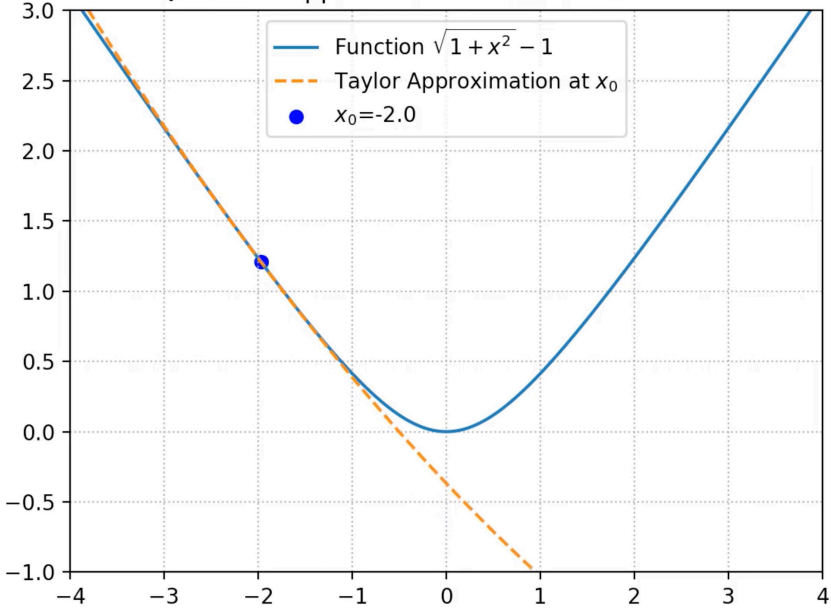
Note, that if $f_2 < f_1, f_2 < f_3$, then u will lie in $[x_1, x_3]$

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
 f1, f2, f3 = f2, fu, f3
        else:
            if fu <= f2:
 x1, x2, x3 = x1, u, x2
 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 neighbor 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 sufficient to find a solution that approximately solves our problem. This is a very typical scenario for the mentioned stepsize selection problem.

$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$
$$\alpha = \text{argmin } f(x_{k+1})$$

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$$x_{k+1} = x_k - \alpha \nabla f(x_k)$$
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Consider a scalar function $\phi(\alpha)$ at a point x_k:

$$\phi(\alpha) = f(x_k - \alpha \nabla f(x_k)), \alpha \geq 0$$

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Consider a scalar function $\phi(\alpha)$ at a point x_k:

$$\phi(\alpha) = f(x_k - \alpha \nabla f(x_k)), \alpha \geq 0$$

The first-order approximation of $\phi(\alpha)$ near $\alpha = 0$ is:

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

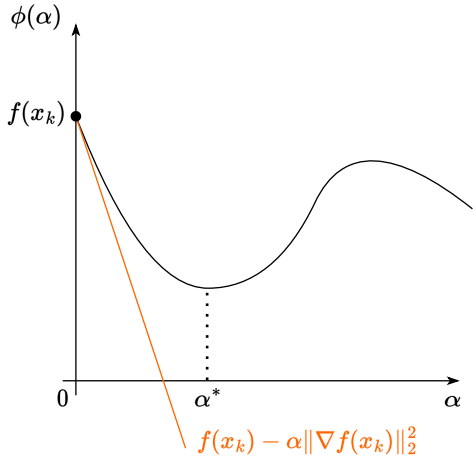

Figure 15: Illustration of Taylor approximation of $\phi_0^I(\alpha)$

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.

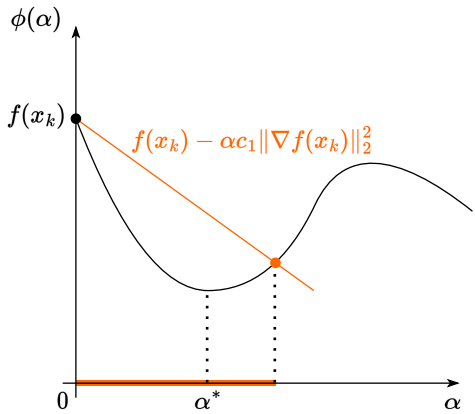

Figure 16: Illustration of sufficient decrease condition with coefficient c_1

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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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 $\rho \in (0, 0.5)$.

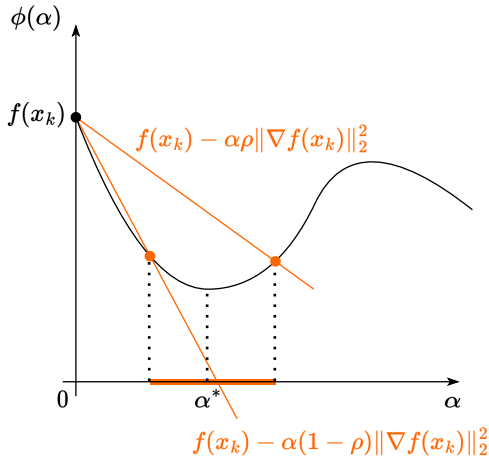

Figure 17: Illustration of Goldstein conditions

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

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

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

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.

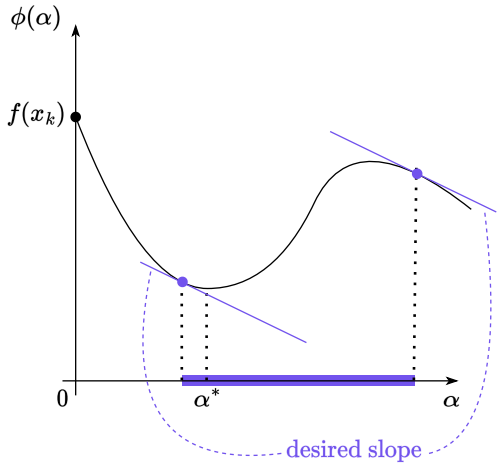

Figure 18: Illustration of curvature condition

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.

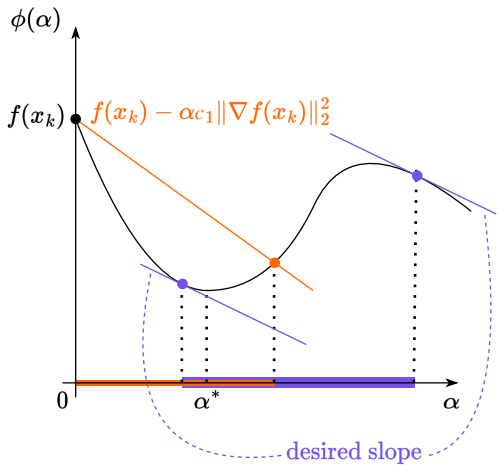

Figure 19: Illustration of Wolfe condition

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:

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

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

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:

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

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

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

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

   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:

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

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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:

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

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

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

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

   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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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

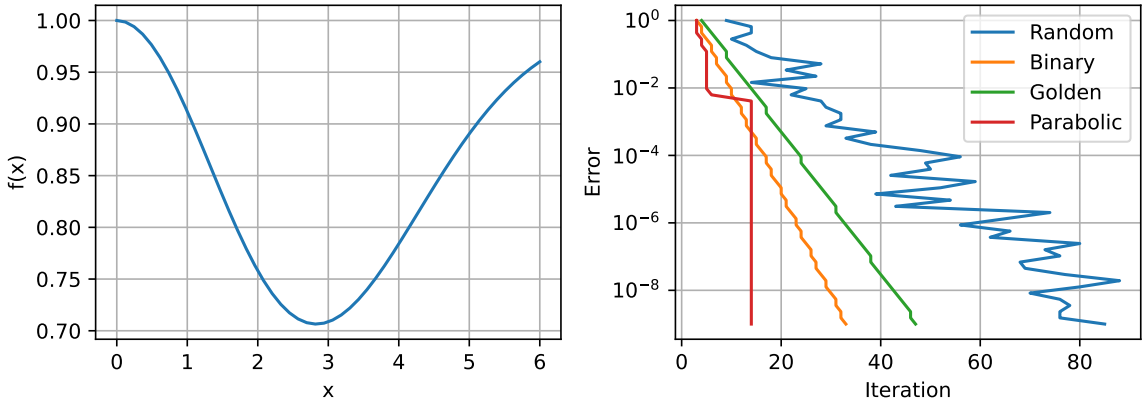
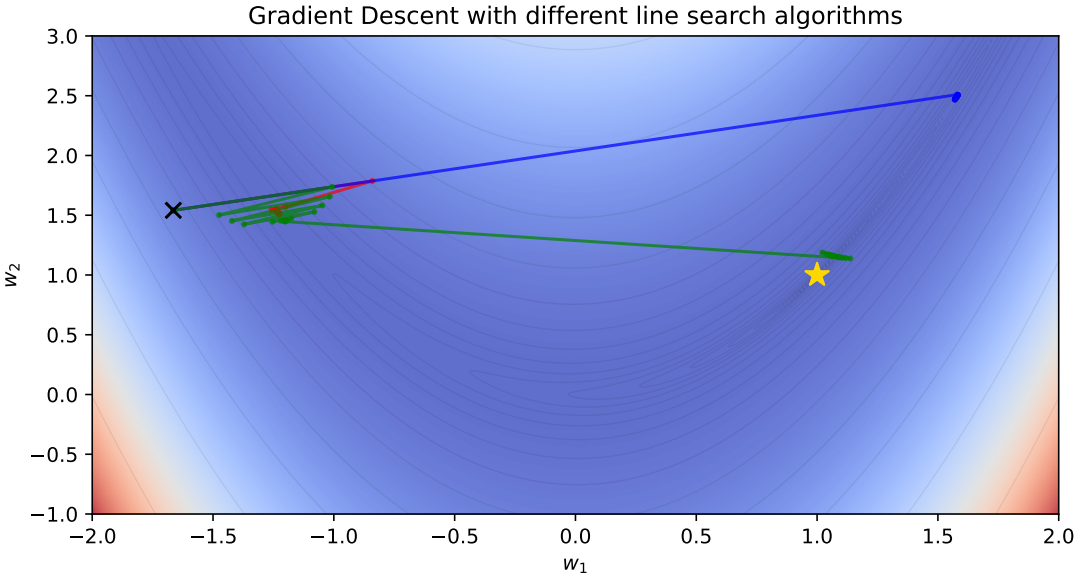


Figure 20: Comparison of different line search algorithms

Open In Colab ♣

Gradient Descent with Line Search



Summary

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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.