

# Matrix calculus. Line search.

## Seminar

Optimization for ML. Faculty of Computer Science. HSE University

# Theory recap. Differential

- Differential  $df(x)[\cdot] : U \rightarrow V$  in point  $x \in U$  for  $f(\cdot) : U \rightarrow V$ :

$$f(x+h) - f(x) = \underbrace{df(x)[h]}_{\text{differential}} + o(||h||)$$

$U \rightarrow V$	$\mathbb{R}$	$\mathbb{R}^n$	$\mathbb{R}^{n \times m}$
$\mathbb{R}$	$f'(x)dx$	$\nabla f(x)dx$	$\nabla f(x)dx$
$\mathbb{R}^n$	$\nabla f(x)^T dx$	$J(x)dx$	—
$\mathbb{R}^{n \times m}$	$tr(\nabla f(X)^T dX)$	—	—

# Theory recap. Differential

- Differential  $df(x)[\cdot] : U \rightarrow V$  in point  $x \in U$  for  $f(\cdot) : U \rightarrow V$ :

$$f(x+h) - f(x) = \underbrace{df(x)[h]}_{\text{differential}} + \bar{o}(\|h\|)$$

- Canonical form of the differential:

$U \rightarrow V$	$\mathbb{R}$	$\mathbb{R}^n$	$\mathbb{R}^{n \times m}$
$\mathbb{R}$	$f'(x)dx$	$\nabla f(x)dx$	$\nabla f(x)dx$
$\mathbb{R}^n$	$\nabla f(x)^T dx$	$J(x)dx$	—
$\mathbb{R}^{n \times m}$	$tr(\nabla f(X)^T dX)$	—	—

# Theory recap. Differentiation Rules

- Useful differentiation rules and standard derivatives:

---

## Differentiation Rules

$$dA = 0$$

$$d(\alpha X) = \alpha(dX)$$

$$d(AXB) = A(dX)B$$

$$d(X + Y) = dX + dY$$

$$d(X^T) = (dX)^T$$

$$d(XY) = (dX)Y + X(dY)$$

$$d(\langle X, Y \rangle) = \langle dX, Y \rangle + \langle X, dY \rangle$$

$$d\left(\frac{X}{\phi}\right) = \frac{\phi dX - (d\phi)X}{\phi^2}$$

---

## Standard Derivatives

$$d(\langle A, X \rangle) = \langle A, dX \rangle$$

$$d(\langle Ax, x \rangle) = \langle (A + A^T)x, dx \rangle$$

$$d(\text{Det}(X)) = \text{Det}(X) \langle X^{-T}, dX \rangle$$

$$d(X^{-1}) = -X^{-1}(dX)X^{-1}$$

# Theory recap. Differential and Gradient / Hessian

We can retrieve the gradient using the following formula:

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

# Theory recap. Differential and Gradient / Hessian

We can retrieve the gradient using the following formula:

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

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  $d(df) = d^2f(x)$

# Theory recap. Differential and Gradient / Hessian

We can retrieve the gradient using the following formula:

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

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  $d(df) = d^2f(x)$

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

# Theory recap. Line Search

- Solution localization methods:



# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method
- Inexact line search:

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method
- Inexact line search:
  - Sufficient decrease

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method
- Inexact line search:
  - Sufficient decrease
  - Goldstein conditions

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method
- Inexact line search:
  - Sufficient decrease
  - Goldstein conditions
  - Curvature conditions

# Theory recap. Line Search

- Solution localization methods:
  - Dichotomy search method
  - Golden selection search method
- Inexact line search:
  - Sufficient decrease
  - Goldstein conditions
  - Curvature conditions
  - The idea behind backtracking line search

# Matrix Calculus. Problem 1

## Example

Find  $\nabla f(x)$ , if  $f(x) = \frac{1}{2}x^T Ax + b^T x + c$ .



## Matrix Calculus. Problem 2

### Example

Find  $\nabla f(X)$ , if  $f(X) = \text{tr}(AX^{-1}B)$

## Matrix Calculus. Problem 3

### Example

Find the gradient  $\nabla f(x)$  and hessian  $\nabla^2 f(x)$ , if  $f(x) = \frac{1}{3}\|x\|_2^3$

## Line Search. Example 1: Comparison of Methods (Colab ♣)

$$f_1(x) = x(x-2)(x+2)^2$$

$$[a, b] = [-3, 2]$$

Random search: 72 function calls. 36 iterations.  $f_1^* = 0.09$

Binary search: 23 function calls. 13 iterations.  $f_1^* = 10.00$

Golden search: 19 function calls. 18 iterations.  $f_1^* = 10.00$

Parabolic search: 20 function calls. 17 iterations.  $f_1^* = 10.00$



Figure 1: Comparison of different line search algorithms with  $f_1$

## Line Search. Example 1: Comparison of Methods (Colab ♣)

$$f_2(x) = -\sqrt{\frac{2}{\pi}} \frac{x^2 e^{-\frac{x^2}{8}}}{8}$$

$$[a, b] = [0, 6]$$

Random search: 68 function calls. 34 iterations.  $f_2^* = 0.71$

Binary search: 23 function calls. 13 iterations.  $f_2^* = 0.71$

Golden search: 20 function calls. 19 iterations.  $f_2^* = 0.71$

Parabolic search: 17 function calls. 14 iterations.  $f_2^* = 0.71$



Figure 2: Comparison of different line search algorithms with  $f_2$

## Line Search. Example 1: Comparison of Methods (Colab ♣)

$$f_3(x) = \sin \left( \sin \left( \sin \left( \sqrt{\frac{x}{2}} \right) \right) \right)$$
$$[a, b] = [5, 70]$$

Random search: 66 function calls. 33 iterations.  $f_3^* = 0.25$

Binary search: 32 function calls. 17 iterations.  $f_3^* = 0.25$

Golden search: 25 function calls. 24 iterations.  $f_3^* = 0.25$

Parabolic search: 103 function calls. 100 iterations.  $f_3^* = 0.25$

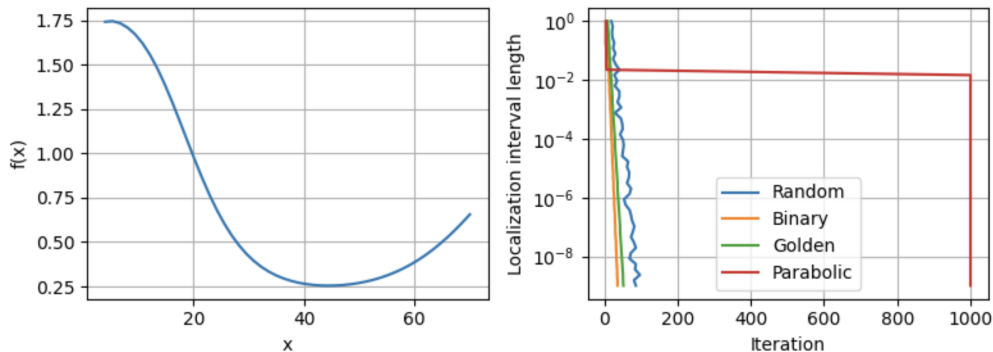


Figure 3: Comparison of different line search algorithms with  $f_3$

## Line Search. Example 2: The Brent Method

- Parabolic Interpolation + Golden Search = Brent Method



Figure 4: Idea of Brent Method

## Line Search. Example 2: The Brent Method

- Parabolic Interpolation + Golden Search = Brent Method
- The key idea of the method is to track the value of the optimized scalar function at six points  $a, b, x, w, v, u$



Figure 4: Idea of Brent Method

## Line Search. Example 2: The Brent Method

- Parabolic Interpolation + Golden Search = Brent Method
- The key idea of the method is to track the value of the optimized scalar function at six points  $a, b, x, w, v, u$
- $[a, b]$  – localization interval in the current iteration

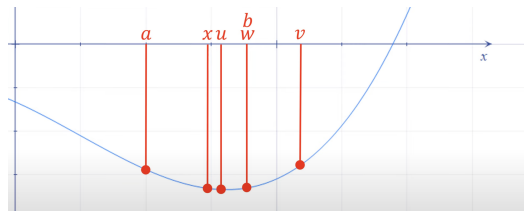


Figure 4: Idea of Brent Method



## Line Search. Example 2: The Brent Method

- Parabolic Interpolation + Golden Search = Brent Method
- The key idea of the method is to track the value of the optimized scalar function at six points  $a, b, x, w, v, u$
- $[a, b]$  – localization interval in the current iteration
- The points  $x, w$  and  $v$  such that the inequality  $f(x) \leq f(w) \leq f(v)$  is valid



Figure 4: Idea of Brent Method

## Line Search. Example 2: The Brent Method

- Parabolic Interpolation + Golden Search = Brent Method
- The key idea of the method is to track the value of the optimized scalar function at six points  $a, b, x, w, v, u$
- $[a, b]$  – localization interval in the current iteration
- The points  $x, w$  and  $v$  such that the inequality  $f(x) \leq f(w) \leq f(v)$  is valid
- $u$  – minimum of a parabola built on points  $x, w$  and  $v$  or the point of the golden section of the largest of the intervals  $[a, x]$   $[x, b]$ .

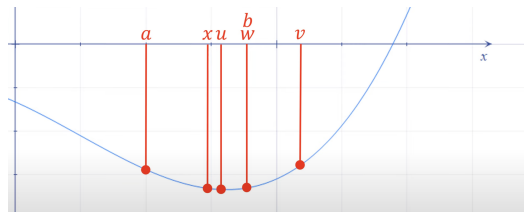


Figure 4: Idea of Brent Method

## Line Search. Example 2: The Brent Method

A parabola is constructed only if the points  $x$ ,  $w$  and  $v$  are different, and its vertex  $u^*$  is taken as the point  $u$  only if

- $u^* \in [a, b]$



Figure 5: An example of how the Brent Method works

## Line Search. Example 2: The Brent Method

A parabola is constructed only if the points  $x$ ,  $w$  and  $v$  are different, and its vertex  $u^*$  is taken as the point  $u$  only if

- $u^* \in [a, b]$
- $u^*$  is no more than half the length of the step that was before the previous one, from the point  $x$



Figure 5: An example of how the Brent Method works

## Line Search. Example 2: The Brent Method

A parabola is constructed only if the points  $x$ ,  $w$  and  $v$  are different, and its vertex  $u^*$  is taken as the point  $u$  only if

- $u^* \in [a, b]$
- $u^*$  is no more than half the length of the step that was before the previous one, from the point  $x$
- If the conditions above are not met, then point  $u$  is located from the golden search



Figure 5: An example of how the Brent Method works

## Line Search. Example 2: The Brent Method

A parabola is constructed only if the points  $x$ ,  $w$  and  $v$  are different, and its vertex  $u^*$  is taken as the point  $u$  only if

- $u^* \in [a, b]$
- $u^*$  is no more than half the length of the step that was before the previous one, from the point  $x$
- If the conditions above are not met, then point  $u$  is located from the golden search
- Example In Colab ♣

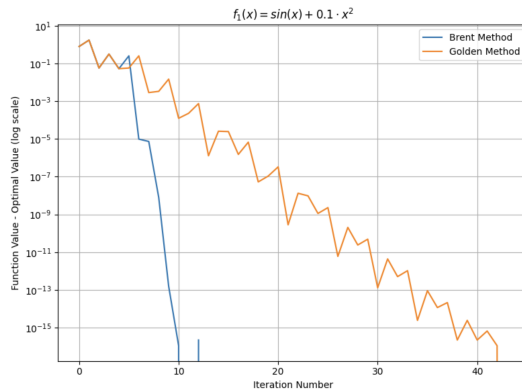


Figure 5: An example of how the Brent Method works