

Deep Learning

Summer Semester 2024

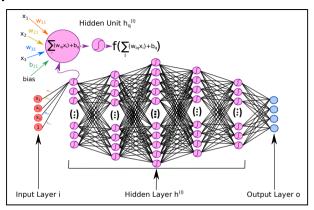
Monday, April 8, 2024

Prof. Dr.-Ing. Christian Bergler | OTH Amberg-Weider

Multi-Layer Perceptron

Ostbayerische Technische Hochschule Amberg-Weiden

Hidden Neuron



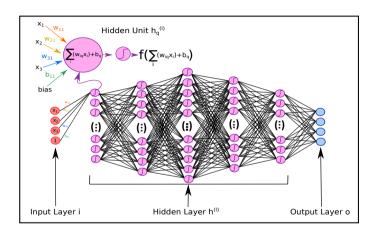
- Neural networks model a functional representation
- Input $x = [x_1, x_2, x_3, 1] \xrightarrow{f(x, \theta)} \text{Output } y = [y_1, y_2, y_3, y_4]$
- ullet Single layer-specific hidden neuron $\mathit{h}_q^{(\mathit{l})} = \mathtt{f}(\sum\limits_{\cdot} w_{iq} \mathsf{x}_i + b_q)$

Source: Christian Bergler, Dissertation "Deep Learning Applied To Animal Linguistics", Figure 10.2, 2023

Multi-Layer Perceptron

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Hidden Neuron





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Multi-Layer Perceptron

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Hidden Layer

Hidden Layer as Vector-Matrix-Product

$$h^{(I)} = \mathbf{f} \begin{pmatrix} \begin{bmatrix} w_{11} & \dots & w_{1M} \\ w_{21} & \dots & w_{2M} \\ \vdots & \vdots & \vdots \\ w_{N1} & \dots & w_{NM} \\ b_1 & \dots & b_M \end{bmatrix}^{T(I)} & \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_N \\ 1 \end{bmatrix}_{N+1 \times 1}^{(I-1)} = \begin{bmatrix} \mathbf{f}(w_{11}x_1 + \dots + w_{N1}x_N + b_1) \\ \mathbf{f}(w_{12}x_1 + \dots + w_{N2}x_N + b_2) \\ \vdots \\ \mathbf{f}(w_{1M}x_1 + \dots + w_{NM}x_N + b_M) \end{bmatrix}^{(I)}_{M \times 1}$$

- $h^{(l)} = f(z^{(l)}) = f(W^{T(l)}x + b^{(l)})$
- N = Number of inputs
- *M* = Number of hidden neurons
- / = Layer



Continuity of Functions

Continuity

Let $D \subseteq \mathbb{R}$ be an interval and $f: D \to \mathbb{R}$ a function. Then f is called continuous in $\bar{x} \in D$ if for all sequences (x_n) in D with $\lim_{n \to \infty} x_n = \bar{x}$ it holds that

$$\lim_{n\to\infty}f(x_n)=f(\bar x)$$

Furthermore, f is called continuous (in D) if f is continuous at all points $\bar{x} \in D$.

Alternative Specification:

f is called continuous in $\bar{x} \in D$ if $\lim_{x \to \bar{x}} = f(\bar{x})$ is valid.

Example Discontinuous Function:

The function $f: \mathbb{R} \to \mathbb{R}$ with

$$f(x) = \begin{cases} 1 & \text{if } x \ge 0 \\ 0 & \text{otherwise} \end{cases}$$

is discontinuous in $\bar{x} = 0$.



Differentiability

Derivation

Let $f : \mathbb{R} \to \mathbb{R}$ be a function and $x \in \mathbb{R}$. We say that f is differentiable at the point $x \in \mathbb{R}$ if the limit value

$$f'(x) := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

exists. The limit value is called the **derivative** of f at the point x, or f'(x) for short. The function f is called **differentiable** if it is differentiable at all points. The function $f': x \mapsto f'(x)$ is then called **derivative function** of f.

Exercise: Calculate the derivative of $f(x) = x^2$ at the point x



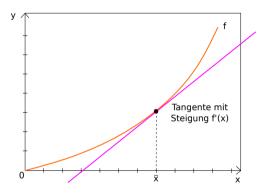
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(Geometric) Interpretation Derivative



• The derivative at a point \bar{x} indicates the gradient (slope) of a function at this point



Derivation Rules

Rule Set

Let $f,g:\mathbb{R}\to\mathbb{R}$, $x\in\mathbb{R}$ and f,g be differentiable at the point x Then

(i) f + g is differentiable at the point x with

$$(f+g)'(x) = f'(x) + g'(x)$$

(ii) $f \cdot g$ is differentiable at the point x with

$$(f \cdot g)'(x) = f'(x)g(x) + f(x)g'(x)$$

(iii) $\frac{f}{g}$ differentiable at the point x with

$$\left(\frac{f}{g}\right)'(x) = \frac{f'(x)g(x) - f(x)g'(x)}{g(x)^2}$$



Derivation Rules

 Of particular importance in the field of "Deep Learning" is the Chain Rule, which is used in a process called backpropagation

Rule Set

Let $f,g:\mathbb{R}\to\mathbb{R}$ be functions and let g be differentiable at the point $x\in\mathbb{R}$ and f at the point $y:=g(x)\in\mathbb{R}$. Then the concatenation $f\circ g$ is differentiable at the point x and the following applies

$$(f \circ g)'(x) = f'(y) \cdot g'(x) = f'(g(x)) \cdot g'(x)$$

Example: Calculate f'(x) for $f(x) = \sin(x)^2$



Local Optima of Functions

• The derivative can be used to specify an optimality criterion for differentiable functions

Criterion

If $f: \mathbb{R} \to \mathbb{R}$ is differentiable and $a \in \mathbb{R}$ is an extreme point of f (maximum or minimum), then

$$f'(a)=0$$

Remarks:

- This is a necessary optimality criterion
- Points where the derivative is zero are called critical points
- A critical point does not have to have a global maximum or minimum. There can also be a local maximum or minimum or a saddle point
- To decide whether there is a local optimum or a saddle point, the second derivative can be considered (see convexity)







Partial Derivative

- When training neural networks, functions $f: \mathbb{R}^n \to \mathbb{R}$ act as an error function, also known as loss function
- The input parameters are typically the weights of a neural network, the function value represents an error between the model prediction and the expected model output (ground truth) w.r.t. to the training data
- The aim is to determine the weights in such a way that the error is as small as possible

Partial derivative

Let $f : \mathbb{R}^n \to \mathbb{R}$ be a function of several variables and let $\mathbf{x} = (x_1, \dots, x_n)^T \in \mathbb{R}^n$ be given. If the limit value

$$\frac{\partial f}{\partial x_i}(\mathbf{x}) := \lim_{h \to 0} \frac{f(x_1, \dots, x_{i-1}, x_i + h, x_{i+1}, \dots, x_n) - f(x_1, \dots, x_n)}{h}$$

exists, it is called the partial derivative of f with respect to x_i at the point \mathbf{x} .



Gradient

• If you summarize all partial derivatives in a vector, you get the so-called gradient

Gradient

Let $f: \mathbb{R}^n \to \mathbb{R}$ be a real function whose partial derivatives exist at a point $\mathbf{x} \in \mathbb{R}^n$. Then

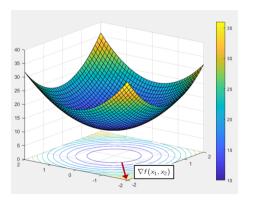
$$\nabla f(\mathbf{x}) := \left(\frac{\partial f}{\partial x_1}(\mathbf{x}), \dots, \frac{\partial f}{\partial x_n}(\mathbf{x})\right)^T$$

the **Gradient** of f at the point \mathbf{x} .



Interpretation Gradient

• The gradient at a point $\mathbf{x} = (x_1, x_2)$ always points in the direction of the steepest incline of the function f:





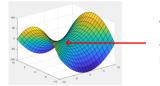
Optimality Condition

Criterion

If $f: \mathbb{R}^n \to \mathbb{R}$ is differentiable and $\mathbf{a} \in \mathbb{R}^n$ is an extreme point of f, then

$$\nabla f(\mathbf{a}) = \mathbf{0} = (0, \dots, 0)^T$$

- Points at which the gradient disappears are called critical points
- A critical point does not have to be a minimum or maximum, e.g. for the function $f(x_1, x_2) = x_1^2 x_2^2$ the point $\mathbf{x} = (0, 0)^T$ is a critical point, but it is neither a maximum nor a minimum \rightarrow Saddle point



The zero-point here is a critical point, but neither a local maximum nor a local minimum. It is rather a saddle point



Example

Exercise:

$$f: \mathbb{R}^3 \to \mathbb{R} , \quad f(x_1, x_2, x_3) = 2x_1^2 - 3x_2^2 + x_1x_3^2 .$$

- (a) Calculate the gradient of f
- (b) Determine all critical points of f
- (c) Investigate whether the critical points are local minima.



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Definiteness of Matrices

Semi-Positive-Definite (SPD) matrices

Let $A \in \mathbb{R}^{(n,n)}$ be a symmetric matrix. Then A is

positively definite, if $\mathbf{x}^T A \mathbf{x} > 0$ for all $\mathbf{x} \in \mathbb{R}^n$

positive semidefinite, if $\mathbf{x}^T A \mathbf{x} \ge 0$ for all $\mathbf{x} \in \mathbb{R}^n$

negative definite, if $\mathbf{x}^T A \mathbf{x} < 0$ for all $\mathbf{x} \in \mathbb{R}^n$

negative semidefinite, if $\mathbf{x}^T A \mathbf{x} \leq \mathbf{0}$ for all $\mathbf{x} \in \mathbb{R}^n$

If A is neither positive nor negative semidefinite, it is called **indefinite**.

Definiteness and Eigenvalues

A symmetric matrix $A \in \mathbb{R}^{(n,n)}$ is

positive (semi-)definite if all eigenvalues are positive (non-negative)

negative (semi-)definite if all eigenvalues are negative (non-positive)

indefinite if there are positive and negative eigenvalues



Optimality criterion

Criterion

Let the function $f: \mathbb{R}^n \to \mathbb{R}$ be twice continuously differentiable and let $\mathbf{a} \in \mathbb{R}^n$ be a critical point of f (i.e. $\nabla f(\mathbf{a}) = \mathbf{0}$) and let $H_f(\mathbf{a})$ be the Hessian matrix of f in \mathbf{a} . Is

 $H_f(\mathbf{a})$ positive definite, then \mathbf{a} is a strict local minimum of f,

 $H_f(\mathbf{a})$ negative definite, then \mathbf{a} is a strict local maximum of f,

 $H_f(\mathbf{a})$ indefinite, then \mathbf{a} is not a local extremum of f.



Convex and Concave Functions

 Convex and concave functions are particularly interesting from an optimization perspective. The lack of convexity makes the optimization problems in connection with neural networks challenging to solve.

Convex Function

A function $f: \mathbb{R}^n \to \mathbb{R}$ is called **convex** if for all $\mathbf{x_1}, \mathbf{x_2} \in \mathbb{R}^n$ and for all $\lambda \in [0, 1]$ it holds that

$$f(\lambda \mathbf{x_1} + (1 - \lambda)\mathbf{x_2}) \le \lambda f(\mathbf{x_1}) + (1 - \lambda)f(\mathbf{x_2})$$

It is called **strictly convex** if for all $\mathbf{x_1} \neq \mathbf{x_2}$ and $\lambda \in (0,1)$ it holds that

$$f(\lambda \mathbf{x_1} + (1 - \lambda)\mathbf{x_2}) < \lambda f(\mathbf{x_1}) + (1 - \lambda)f(\mathbf{x_2})$$

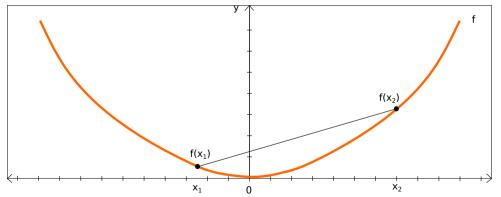
Concave Function

A function $f: \mathbb{R}^n \to \mathbb{R}$ is called (strictly) **concave** if -f is (strictly) convex



Visualization of Convexity der Konvexität

 In a one dimensional space, strictly convex functions have the property that the connecting line between any two points on the graph of the function always lies above the function:





Minimization

Local and global minimum of a real-valued function

Let $f: \mathbb{R}^n \to \mathbb{R}$. A point $\mathbf{x_1} \in \mathbb{R}^n$ is called

• local minimum of f if in a sufficiently small neighbourhood \mathcal{U} of $\mathbf{x_1}$ it holds that

$$f(\mathbf{x_1}) \le f(\mathbf{x_2})$$
 for all $\mathbf{x_2} \in \mathcal{U}$

• **global minimum** of f if for all $\mathbf{x}_2 \in \mathbb{R}^n$ it holds that

$$f(\mathbf{x_1}) \leq f(\mathbf{x_2})$$



Convexity and Minimization

Local minima for convex functions

Let $f: \mathbb{R}^n \to \mathbb{R}$ be a convex function. Then every local minimum is a global minimum

Local minima for strict convex functions

Let $f: \mathbb{R}^n \to \mathbb{R}$ be strictly convex. Then there is at most one local minimum $\bar{x} \in \mathbb{R}^n$ of f

Proof: Suppose there are two different local minima \tilde{x} and \bar{x} of f. Because of the above theorem, both are also global minima and $f(\tilde{x}) = f(\bar{x})$ must hold. From the strict convexity of f it follows for any $\lambda \in (0,1)$ that

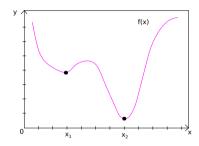
$$f(\lambda \tilde{x} + (1 - \lambda)\bar{x}) < \lambda f(\tilde{x}) + (1 - \lambda)f(\bar{x}) = f(\tilde{x})$$

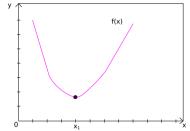
This is a contradiction to the actual assumption and thus every strict convex function possesses at most one local minimum!

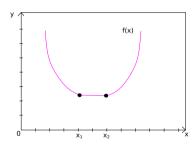


Convexity and Minimization

Examples







Type of convexity and minimum?



Convexity and Minimization

Second order convexity criteria

Let $f: \mathbb{R}^n \to \mathbb{R}$ be twice continuously differentiable. For $x \in \mathbb{R}^n$ let H(x) be the Hessian matrix at the point x. Then applies:

- If H(x) is positive semidefinite for all $x \in \mathbb{R}^n$, then f is convex
- If H(x) is even positive definite for all $x \in \mathbb{R}^n$, then f is strictly convex

Questions for Understanding:

- What does the above criterion mean for functions with a single variable?
- Does every strictly convex function have a global minimum? If not, give an example of a strictly convex function that does not have a global minimum.



Matrices

 The model function of neural networks can be written down compactly with the help of vectors and matrices.

Matrix

Let m and n be natural numbers. By an $m \times n$ -matrix over the body $\mathbb R$ we mean a scheme of numbers of the form

$$A=(a_{ij})_{i=1,\ldots,m\atop j=1,\ldots,n}=\left(egin{array}{cccc} a_{11}&a_{12}&\ldots&a_{1n}\ a_{21}&&&a_{2n}\ dots&&\ddots&dots\ a_{m1}&\ldots&\ldots&a_{mn} \end{array}
ight)$$

The set of all $m \times n$ matrices over the body \mathbb{R} is called $\mathbb{R}^{m \times n}$.



Addition and Scalar Multiplication for Matrices

$$A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & & & a_{2n} \\ \vdots & & \ddots & \vdots \\ a_{m1} & \dots & \dots & a_{mn} \end{pmatrix} \text{ und } B = \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ b_{21} & & & b_{2n} \\ \vdots & & \ddots & \vdots \\ b_{m1} & \dots & \dots & b_{mn} \end{pmatrix} \in \mathbb{R}^{m \times n}$$

Addition

$$A+B=\left(egin{array}{ccccc} a_{11}+b_{11} & a_{12}+b_{12} & \dots & a_{1n}+b_{1n} \ a_{21}+b_{21} & & a_{2n}+b_{2n} \ dots & & \ddots & dots \ a_{m1}+b_{m1} & \dots & \dots & a_{mn}+b_{mn} \end{array}
ight)$$

Scalar Multiplication

$$\lambda \cdot A = \begin{pmatrix} \lambda a_{11} & \lambda a_{12} & \dots & \lambda a_{1n} \\ \lambda a_{21} & & & \lambda a_{2n} \\ \vdots & & \ddots & \vdots \\ \lambda a_{m1} & \dots & \dots & \lambda a_{mn} \end{pmatrix}, \quad \lambda \in \mathbb{R}$$



Transposed Matrix

Definition

The transpose A^T of an $m \times n$ -matrix A is the $n \times m$ matrix whose columns are equal to the rows of A and whose rows are equal to the columns of A. The following therefore applies

$$(a_{ij})^T=(a_{ji}).$$

Rule Set

For any $m \times n$ -matrices A and B and $\lambda \in \mathbb{R}$ applies:

$$(A+B)^{T} = A^{T} + B^{T},$$

$$(\lambda A)^{T} = \lambda A^{T},$$

$$(A^{T})^{T} = A.$$



Transposed Matrix

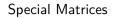
Exercise:

$$A = \begin{pmatrix} 2 & -1 \\ 1 & 4 \\ 3 & 5 \end{pmatrix} , \quad B = \begin{pmatrix} 1 & 2 \\ 1 & -1 \\ 1 & 1 \end{pmatrix} .$$

- Calculate A + B and $(A + B)^T$
- Determine the matrices A^T and B^T
- Calculate $A^T + B^T$



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Symmetric and adjoint matrix

• A square matrix $A \in \mathbb{R}^{n \times n}$ with real entries is called **symmetric** if

$$A = A^T$$

• A square matrix $A \in \mathbb{C}^{n \times n}$ with complex entries is called **adjoint** (refers to the conjugate transpose) if

$$A^* := \overline{A}^T = A$$



Multiplication of Matrices

 Besides the addition and scalar multiplication, matrices can also be multiplied under certain conditions

Matrix-matrix Multiplication

Let $A \in \mathbb{R}^{m \times n}$ and $B \in \mathbb{R}^{n \times k}$. The product $C := A \cdot B \in \mathbb{R}^{m \times k}$ is an $m \times k$ -matrix with the entries

$$c_{ij} = \sum_{k=1}^n \mathsf{a}_{ik} \cdot \mathsf{b}_{kj} \ .$$

Remarks:

- The prerequisite for multiplying two matrices is that the number of columns in the left-hand matrix is the same as the number of rows in the right-hand matrix.
- For square matrices $A, B \in \mathbb{R}^{n \times m}$, both the product $A \cdot B$ and the product $B \cdot A$ are well-defined.

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Example Matrix-Matrix Multiplication

• The following matrices are given:

$$A = \begin{pmatrix} 1 & 2 \\ -1 & 0 \\ 0 & 1 \end{pmatrix} , \quad B = \begin{pmatrix} 0 & 1 & 2 \\ 1 & 0 & 1 \end{pmatrix} ,$$

$$C = \begin{pmatrix} 1 & 1 \\ 2 & -1 \\ 1 & 0 \end{pmatrix} , \quad D = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Calculate all possible matrix products from these four matrices





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Matrix-Vector Multiplication

 A special case of matrix-matrix multiplication is the multiplication of a matrix with a vector (= matrix with single column)

Matrix-Vector Multiplication

For $A \in \mathbb{R}^{m \times n}$ and $\mathbf{x} = (x_1, \dots, x_n)^T \in \mathbb{R}^n$ applies

$$Ax = \mathbf{a}^{(1)} \cdot x_1 + \mathbf{a}^{(2)} \cdot x_2 + \ldots + \mathbf{a}^{(n)} \cdot x_n$$

where $\mathbf{a}^{(1)},\dots,\mathbf{a}^{(n)}\in\mathbb{R}^m$ denote the columns of the matrix A

 Note: When multiplying a matrix by a vector, linear combinations of the columns are formed



Rules for Matrix-Matrix Multiplication

• If A, B, C are matrices with suitable dimensions and $\lambda \in \mathbb{R}$ is a scalar, then:

$$(\lambda A)B = \lambda(AB) = A(\lambda B)$$

$$A(BC) = (AB)C$$

$$(A+B)C = AC + BC$$

$$A(B+C) = AB + AC$$

$$(AB)^{T} = B^{T}A^{T}$$

Remarks:

- The matrix-matrix multiplication is generally not commutative.
- Example: calculate the products $A \cdot B$ and $B \cdot A$ for the following matrices:

$$A = \left(\begin{array}{cc} 1 & 2 \\ -1 & 1 \end{array}\right) B = \left(\begin{array}{cc} 2 & 1 \\ 1 & 1 \end{array}\right)$$



Linear Illustrations

Linear Mapping

A mapping $f: \mathbb{R}^n \to \mathbb{R}^m$ is called **linear mapping** if the following applies to all $\mathbf{x}, \mathbf{y} \in \mathbb{R}^n$ and all $\lambda \in \mathbb{R}$:

- (i) $f(\mathbf{x} + \mathbf{y}) = f(\mathbf{x}) + f(\mathbf{y})$
- (ii) $f(\lambda \mathbf{x}) = \lambda f(\mathbf{x})$

Remarks:

- If $A \in \mathbb{R}^{m \times n}$ is a matrix, then the mapping $f : \mathbb{R}^n \to \mathbb{R}^m$ given by $f(\mathbf{x}) = A\mathbf{x}$ is a linear mapping.
- If you add a contant vector to a linear mapping, the resulting mapping is called affine-linear. For example, the mapping $g: \mathbb{R}^n \to \mathbb{R}^m$ given by $g(\mathbf{x}) = A\mathbf{x} + \mathbf{b}$ is an affine-linear mapping.



Norms

Norms are used to measure the lengths of vectors. These are functions that assign a non-negative number to a vector. The following properties must be fulfilled:

Norm on \mathbb{R}^n

A norm is a function $f: \mathbb{R}^n \to \mathbb{R}$ with the following properties:

- $f(\mathbf{x}) > 0$ for all $\mathbf{x} \in \mathbb{R}^n$ and $f(\mathbf{x}) = 0 \Leftrightarrow \mathbf{x} = \mathbf{0}$
- f(x + y) < f(x) + f(y)
- $f(\lambda \mathbf{x}) = |\lambda| f(\mathbf{x})$

- (positive definiteness)
 - (triangle inequality)
- (positive homogeneity)

- L_2 -Norm: $\|\mathbf{x}\|_2 = \sqrt{\mathbf{x}^T \cdot \mathbf{x}} = \sqrt{\sum_{i=1}^n x_i^2}$ L_1 -norm: $\|\mathbf{x}\|_1 = \sum_{i=1}^n |x_i|$
- L_p -norm: $\|\mathbf{x}\|_p = \left(\sum_{i=1}^n |x_i|^p\right)^{\frac{1}{p}}$ for p > 0.



Further Questions?





https://www.oth-aw.de/hochschule/ueber-uns/personen/bergler-christian/

 $Source: \ https://emekaboris.medium.com/the-intuition-behind-100-days-of-data-science-code-c98402cdc92c$