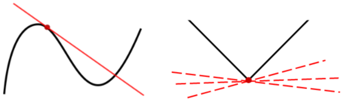
Optimization in Machine Learning

Mathematical Concepts
Differentiation and Derivatives



Learning goals

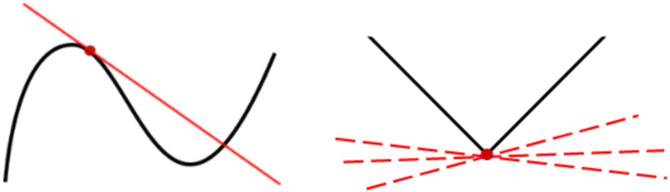
- Definition of smoothness
- Uni- & multivariate differentiation
- Gradient, partial derivatives
- Jacobian matrix
- Hessian matrix
- Lipschitz continuity

UNIVARIATE DIFFERENTIABILITY

Definition: A function $f : \mathcal{S} \subseteq \mathbb{R} \to \mathbb{R}$ is said to be **differentiable** for each inner point $x \in \mathcal{S}$ if the following limit exists:

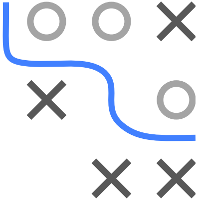
$$f'(x) := \lim_{h \to 0} \frac{f(x+h) - f(x)}{h}$$

Intuitively: f can be approximated locally by a lin. fun. with slope $m = f'(x)$.

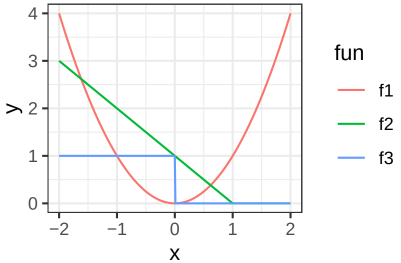


Left: Function is differentiable everywhere. **Right:** Not differentiable at the red point.

SMOOTH VS. NON-SMOOTH



- **Smoothness** of a function $f : \mathcal{S} \to \mathbb{R}$ is measured by the number of its continuous derivatives
- $\mathcal{C}^k$ is class of k-times continuously differentiable functions ($f \in \mathcal{C}^k$ means $f^{(k)}$ exists and is continuous)
- In this lecture, we call f "smooth", if at least $f \in \mathcal{C}^1$



f_1 is smooth, f_2 is continuous but not differentiable, and f_3 is non-continuous.

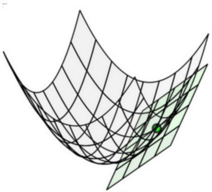
MULTIVARIATE DIFFERENTIABILITY

Definition: For a function $f : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}$ of d variables $x_1, \dots, x_d$, **partial derivatives** are defined as

$$\frac{\partial f}{\partial x_1} = \lim_{h \to 0} \frac{f\left(x_1 + h, x_2, \dots, x_d\right) - f(\boldsymbol{x})}{h}$$

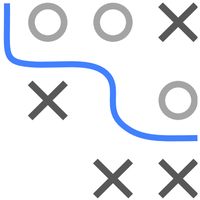
$$\vdots$$

$$\frac{\partial f}{\partial x_d} = \lim_{h \to 0} \frac{f\left(x_1, \dots, x_{d-1}, x_d + h\right) - f(\boldsymbol{x})}{h}$$



Geometrically: Similarly to the 1D case, the vector of partial derivatives can be used to determine a tangent hyperplane. Source: jermwatt/machine_learning_refined.

GRADIENT



- Specifically, the vector of partial derivatives is called the **gradient**:

$$\nabla_{\boldsymbol{x}} f \text{ or } \nabla f := \left(\frac{\partial f}{\partial x_1}, \frac{\partial f}{\partial x_2}, \ldots, \frac{\partial f}{\partial x_d} \right) \qquad \text{(note that this is a row vector!)}$$

- This gradient of f can be used to linearly approximate f:

$$f(\boldsymbol{x} + \mathbf{h}) = f(\boldsymbol{x}) + \nabla_{\boldsymbol{x}} f(\boldsymbol{x})\mathbf{h} + o(\mathbf{h})$$

Example: $f(\boldsymbol{x}) = x_1^2/2 + x_1 x_2 + x_2^2 \Rightarrow \nabla f(\boldsymbol{x}) = (x_1 + x_2, x_1 + 2x_2)$

DIRECTIONAL DERIVATIVE

The **directional derivative** tells how fast $f : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}$ is changing w.r.t. an arbitrary direction $\boldsymbol{v}$:

$$D_{\boldsymbol{v}} f(\boldsymbol{x}) := \lim_{h \to 0} \frac{f(\boldsymbol{x} + h\boldsymbol{v}) - f(\boldsymbol{x})}{h} = \nabla f(\boldsymbol{x}) \boldsymbol{v}$$

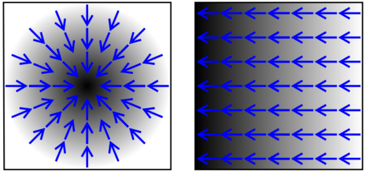
Example: The directional derivative for $\boldsymbol{v} = (1, 1)$ is:

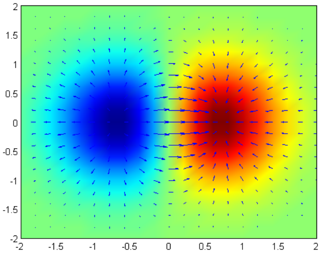
$$D_{\boldsymbol{v}} f(\boldsymbol{x}) = \nabla f(\boldsymbol{x}) \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \frac{\partial f}{\partial x_1} + \frac{\partial f}{\partial x_2}$$

NB: Some people require that $||\boldsymbol{v}|| = 1$. Then, we can identify $D_{\boldsymbol{v}} f(\boldsymbol{x})$ with the instantaneous rate of change in direction $\boldsymbol{v}$, i.e. $\lim_{h \to 0} \frac{f(\boldsymbol{x}+h\boldsymbol{v}) - f(\boldsymbol{x})}{h}$ – and in our example we would have to divide by $\sqrt{2}$.

IMPORTANT PROPERTIES OF THE GRADIENT

1. **Orthogonal** to level curves/surfaces of a function
2. Points in direction of **greatest increase** of f





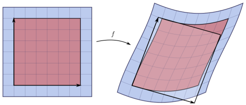
JACOBIAN MATRIX

For vector-valued function $f :\subseteq \mathbb{R}^d \longrightarrow \mathbb{R}^m,\ \boldsymbol{x} \mapsto (f_1(\boldsymbol{x}), \dots, f_m(\boldsymbol{x}))^\top$, $f_j : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}$, the **Jacobian** matrix $J_f : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}^{m\times d}$ generalizes gradient by placing all ∇f_j in its rows:

$$J_f(\boldsymbol{x}) \text{ or } \nabla f(\boldsymbol{x}) = \begin{pmatrix} \nabla f_1(\boldsymbol{x}) \\ \vdots \\ \nabla f_m(\boldsymbol{x}) \end{pmatrix} = \begin{pmatrix} \frac{\partial f_1(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_1(\boldsymbol{x})}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m(\boldsymbol{x})}{\partial x_1} & \cdots & \frac{\partial f_m(\boldsymbol{x})}{\partial x_d} \end{pmatrix}$$

We will mainly use the ∇f notation.

- Jacobian gives best linear approximation of distorted volumes



Source: Wikipedia

JACOBIAN DETERMINANT

Let $f \in \mathcal{C}^1$ and $\mathbf{x}_0 \in \mathcal{S} \subseteq \mathbb{R}^d$.

Inverse function theorem: Let $\mathbf{y}_0 = f(\mathbf{x}_0)$. If $\det(J_f(\mathbf{x}_0)) \neq 0$, then

1. f is invertible in a neighborhood of $\mathbf{x}_0$,
2. $f^{-1} \in \mathcal{C}^1$ with $J_{f^{-1}}(\mathbf{y}_0) = J_f(\mathbf{x}_0)^{-1}$.

- $|\det(J_f(\mathbf{x}_0))|$: factor by which f expands/shrinks volumes near $\mathbf{x}_0$
- If $\det(J_f(\mathbf{x}_0)) > 0$, f preserves orientation near $\mathbf{x}_0$
- If $\det(J_f(\mathbf{x}_0)) < 0$, f reverses orientation near $\mathbf{x}_0$

HESSIAN MATRIX

For real-valued function $f : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}$, the **Hessian** matrix $\nabla^2 : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}^{d \times d}$ contains all their second derivatives (if they exist):

$$\nabla^2 f(\boldsymbol{x}) = \left(\frac{\partial^2 f(\boldsymbol{x})}{\partial x_i \partial x_j} \right)_{i,j=1,\ldots,d}$$

Note: Hessian of f is Jacobian of ∇f. Also, the Hessian is often denoted by $H(\boldsymbol{x}) \hat{=} \nabla^2 f(\boldsymbol{x})$

Example: Let $f(\boldsymbol{x}) = \sin(x_1) \cdot \cos(2x_2)$. Then:

$$\nabla^2 f(\boldsymbol{x}) = \begin{pmatrix} -\cos(2x_2) \cdot \sin(x_1) & -2\cos(x_1) \cdot \sin(2x_2) \\ -2\cos(x_1) \cdot \sin(2x_2) & -4\cos(2x_2) \cdot \sin(x_1) \end{pmatrix}$$

- If $f \in \mathcal{C}^2$, then $\nabla^2 f$ is symmetric
- Many local properties (geometry, convexity, critical points) are encoded by the Hessian and its spectrum ($\rightarrow$ later)

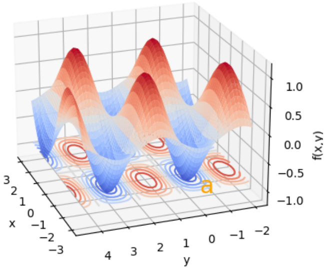
LOCAL CURVATURE BY HESSIAN

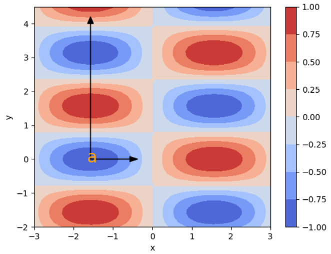
Eigenvector corresponding to largest (resp. smallest) **eigenvalue** of Hessian points in direction of largest (resp. smallest) **curvature**

Example (previous slide)**:** For $\boldsymbol{a} = (-\pi/2, 0)^T$, we have

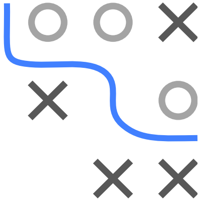
$$\nabla^2 f(\boldsymbol{a}) = \begin{pmatrix} 1 & 0 \\ 0 & 4 \end{pmatrix}$$

and thus $\lambda_1 = 4$, $\lambda_2 = 1$, $\boldsymbol{v}_1 = (0, 1)^T$, and $\boldsymbol{v}_2 = (1, 0)^T$.





LIPSCHITZ CONTINUITY



Function $h : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}^m$ is **Lipschitz continuous** if slopes are bounded:

$$\|h(\mathbf{x}) - h(\mathbf{y})\| \leq L\|\mathbf{x} - \mathbf{y}\| \quad \text{for each } \mathbf{x}, \mathbf{y} \in \mathcal{S} \subseteq \mathbb{R}^d \text{ and some } L > 0$$

- **Examples** ($d = m = 1$)**:** $\sin(x)$, $|x|$
- **Not** examples: $1/x$ (but *locally* Lipschitz continuous), $\sqrt{x}$
- If $m = d$ and h **differentiable**:

$$h \text{ Lipschitz continuous with constant } L \iff J_h \preccurlyeq L \cdot \mathbf{I}_d$$

Note: $\mathbf{A} \preccurlyeq \mathbf{B} :\iff \mathbf{B} - \mathbf{A}$ is positive semidefinite, i.e., $\mathbf{v}^T(\mathbf{B} - \mathbf{A})\mathbf{v} \geq 0 \;\; \forall \mathbf{v} \neq 0$

Proof of "$\Rightarrow$" for $d = m = 1$**:**

$$h'(x) = \lim_{\epsilon \to 0} \frac{h(x+\epsilon) - h(x)}{\epsilon} \leq \lim_{\epsilon \to 0} \underbrace{\left| \frac{h(x+\epsilon) - h(x)}{\epsilon} \right|}_{\leq L} \leq \lim_{\epsilon \to 0} L = L$$

[**Proof** of "$\Leftarrow$" by mean value theorem: Show that $\lambda_{\max}(J_h) \leq L$.]

LIPSCHITZ GRADIENTS

- Let $f \in \mathcal{C}^2$. Since $\nabla^2 f$ is Jacobian of $h = \nabla f$ ($m = d$):

$$\nabla f \text{ Lipschitz continuous with constant } L \iff \nabla^2 f \preccurlyeq L \cdot \mathbf{I}_d$$

- Equivalently, eigenvalues of $\nabla^2 f$ are bounded by L
- **Interpretation:** Curvature in any direction is bounded by L
- Lipschitz gradients occur frequently in machine learning
  $\Longrightarrow$ Fairly **weak assumption**
- Important for analysis of **gradient descent** optimization
  $\Longrightarrow$ Descent lemma (later)