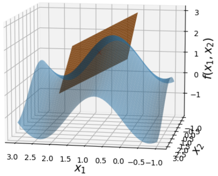
Optimization in Machine Learning

Mathematical Concepts
´ Taylor Approximation

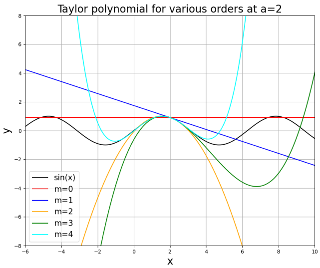


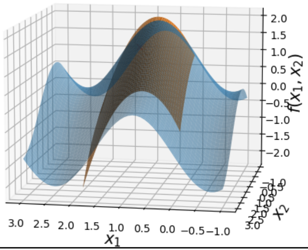
Learning goals

- Taylor’s theorem (univariate)
- Taylor series (univariate)
- Taylor’s theorem (multivariate)
- Taylor series (multivariate)

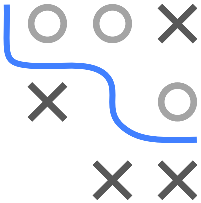
TAYLOR APPROXIMATIONS: OVERVIEW

- To optimize (find minima and maxima) it can be extremely helpful to approximate nonlinear functions locally
- We can use **Taylor polynomials** to approximate functions and
- **Taylor's theorem** provides us with the tools to estimate the error of this approximation $\implies$ helpful for analyzing optimization algorithms
- Some functions can locally or even globally equal their **Taylor series**, i.e. the limit of Taylor polynomials





TAYLOR APPROXIMATIONS: MOTIVATION



- Since the geometry of linear and quadratic functions is very well understood we will often want to use those for approximations
- For example, for a function $f : \mathcal{S} \subseteq \mathbb{R}^d \to \mathbb{R}$

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

- You might also often see an approximation via the gradient and Hessian of a function:

$$f(\mathbf{x} + \mathbf{h}) \approx f(\mathbf{x}) + \nabla_{\mathbf{x}} f(\mathbf{x})\mathbf{h} + \frac{1}{2}\mathbf{h}^\top \nabla^2_{\mathbf{x}} f(\mathbf{x})\mathbf{h}$$

- In fact, $f(\mathbf{x}) + \nabla_{\mathbf{x}} f(\mathbf{x})\mathbf{h}$ and $f(\mathbf{x}) + \nabla_{\mathbf{x}} f(\mathbf{x})\mathbf{h} + \frac{1}{2}\mathbf{h}^\top \nabla^2_{\mathbf{x}} f(\mathbf{x})\mathbf{h}$ are, respectively, the first and second **Taylor polynomial of f at $\mathbf{x}$**, evaluated at $\mathbf{x} + \mathbf{h}$

TAYLOR POLYNOMIALS

- Idea: Find a polynomial that locally behaves like a function f at point $\boldsymbol{a}$, i.e. matches f's value (f), slope (f'), curvature (f''), etc.

$\Leftrightarrow$ Find polynomial so that

$$f(x) \approx T_k(x, \boldsymbol{a}) \quad \text{for all } x \text{ near } \boldsymbol{a}$$

where k denotes the highest order of derivative of f used in T_k

- Wording: We "*expand f (via Taylor) around $\boldsymbol{a}$*"

Definition of Taylor polynomial (univariate): Let $I \subseteq \mathbb{R}$ be an open interval and $f \in \mathcal{C}^k(I, \mathbb{R})$. For each $a, x \in I$, the kth order Taylor polynomial for f at a is defined as

$$T_k(x, a) := \sum_{j=0}^{k} \frac{f^{(j)}(a)}{j!}(x-a)^j$$

MULTIVARIATE TAYLOR POLYNOMIALS

For the multivariate version, we need a concise way to express derivatives and powers involving several variables

- A **multi-index** is a vector $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_d) \in \mathbb{N}^d$.
- Its **order** is the sum of its components: $|\boldsymbol{\alpha}| = \alpha_1 + \alpha_2 + \cdots + \alpha_d$.
- Partial derivative is written as $D^{\boldsymbol{\alpha}} f = \dfrac{\partial^{|\boldsymbol{\alpha}|} f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}}$
- Factorials generalize componentwise: $\boldsymbol{\alpha}! = \alpha_1!\,\alpha_2! \cdots \alpha_d!$.
- For $\mathbf{x},\ \boldsymbol{a} \in \mathbb{R}^d$: $(\mathbf{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} = (x_1 - a_1)^{\alpha_1} \cdots (x_d - a_d)^{\alpha_d}$.

Definition of Taylor polynomial (multivariate): Let I be an open subset of $\mathbb{R}^n$ and $f \in \mathcal{C}^k(I, \mathbb{R})$. For each $\boldsymbol{a}, \mathbf{x} \in I$, the kth order Taylor polynomial for f at $\boldsymbol{a}$ is defined as

$$T_k(\mathbf{x}, \boldsymbol{a}) := \sum_{|\boldsymbol{\alpha}| \le k} \frac{D^{\boldsymbol{\alpha}} f(\boldsymbol{a})}{\boldsymbol{\alpha}!} (\mathbf{x} - \boldsymbol{a})^{\boldsymbol{\alpha}}$$

MULTIVARIATE TAYLOR POLYNOMIAL IDENTITIES

For $f \in \mathcal{C}^k(I, \mathbb{R})$ as before, we will often use the following identities:

- $T_1(\mathbf{x}, \boldsymbol{a}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})$
- $T_2(\mathbf{x}, \boldsymbol{a}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{a})^T \boldsymbol{H}(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})$

(Which squares with the notation of the motivation slide by setting $\boldsymbol{a} \hat{=} \mathbf{x}$ and $\mathbf{x} \hat{=} \mathbf{x} + \boldsymbol{h}$)

Example: Specifically deriving T_1 for bivariate f ($d = 2$)

α_1	α_2	$\lvert\boldsymbol{\alpha}\rvert$	$D^{\boldsymbol{\alpha}} f$	$\boldsymbol{\alpha}!$	$(\mathbf{x} - \boldsymbol{a})^{\boldsymbol{\alpha}}$
0	0	0	f	1	1
1	0	1	$\partial f / \partial x_1$	1	$x_1 - a_1$
0	1	1	$\partial f / \partial x_2$	1	$x_2 - a_2$

and, therefore

$$
\begin{aligned}
T_1(\mathbf{x}, \boldsymbol{a}) &= \frac{f(\boldsymbol{a})}{1} \cdot 1 + \frac{\partial f(\boldsymbol{a})}{\partial x_1}(x_1 - a_1) + \frac{\partial f(\boldsymbol{a})}{\partial x_2}(x_2 - a_2) \\
&= f(\boldsymbol{a}) + \begin{pmatrix} \frac{\partial f(\boldsymbol{a})}{\partial x_1} \\ \frac{\partial f(\boldsymbol{a})}{\partial x_2} \end{pmatrix}^T \begin{pmatrix} x_1 - a_1 \\ x_2 - a_2 \end{pmatrix} = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})
\end{aligned}
$$

TAYLOR'S THEOREM

General version for both univariate and multivariate functions:
Let I be an open subset of $\mathbb{R}^n$, $n \in \mathbb{N}_{>0}$, and $f \in \mathcal{C}^k(I, \mathbb{R})$. There exists a function $R_k : I \times I \to \mathbb{R}$ so that for each $\boldsymbol{a}, \mathbf{x} \in I$

$$R_k(\mathbf{x}, \boldsymbol{a}) = o(\|\mathbf{x} - \boldsymbol{a}\|^k) \text{ as } \mathbf{x} \to \boldsymbol{a}$$

and

$$f(\mathbf{x}) = T_k(\mathbf{x}, \boldsymbol{a}) + R_k(\mathbf{x}, \boldsymbol{a})$$

- $R_k(\mathbf{x}, \boldsymbol{a})$ is called **remainder term** and different specific forms have been established
- However, we will usually focus on the property $R_k(\mathbf{x}, \boldsymbol{a}) = o(\|\mathbf{x} - \boldsymbol{a}\|^k)$ as $\mathbf{x} \to \boldsymbol{a}$ or upper bounds derived for specific function classes when analyzing optimization algorithms

TAYLOR SERIES

- For $f \in \mathcal{C}^\infty$, there might exist an open ball $B_r(\boldsymbol{a})$ with radius $r > 0$ around $\boldsymbol{a}$ such that the **Taylor series**

$$T_\infty(\mathbf{x}, \boldsymbol{a}) = \begin{cases} \sum_{k=0}^{\infty} \frac{f^{(k)}(a)}{k!}(x - a)^k & \text{if } f \text{ is univariate} \\ \sum_{|\boldsymbol{\alpha}| \geq 0} \frac{D^{\boldsymbol{\alpha}} f(\boldsymbol{a})}{\boldsymbol{\alpha}!}(\mathbf{x} - \boldsymbol{a})^{\boldsymbol{\alpha}} & \text{if } f \text{ is multivariate} \end{cases}$$

  converges to f on $B_r(\boldsymbol{a})$
- If such an open Ball exists for all $\boldsymbol{a}$ in the domain of f, f is called an **analytic function**
- Even if Taylor series converges, it might not converge to f
- Upper bound $R = \sup \{r \mid \text{Taylor series converges on } B_r(\boldsymbol{a})\}$ is called the radius of convergence of Taylor series around $\boldsymbol{a}$
- If $R > 0$ and f analytic, Taylor series converges absolutely and uniformly to f on compact sets inside $B_R(\boldsymbol{a})$
- No general convergence behaviour on boundary of $B_R(\boldsymbol{a})$

EXAMPLES OF ANALYTIC FUNCTIONS

For analytic functions the remainder term eventually vanishes, i.e.
$R_k(\mathbf{x}, \boldsymbol{a}) \to 0$ as $k \to \infty$ for all $\mathbf{x} \in B_r(\boldsymbol{a})$.

Important examples are

- Polynomials
- Exponential function $(\exp)$
- Trigonometric functions $(\sin, \cos)$

And important rules are

- Any analytic function of a polynomial is again an analytic function
- Analytic functions are closed under sum and product
  (due to the properties of series)
- The derivative of an analytic function is again an analytic function

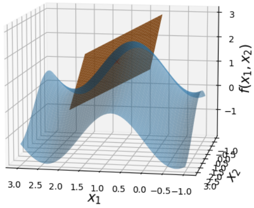
One specific example: $f : \mathbb{R}^2 \longrightarrow \mathbb{R}\ \mathbf{x} \mapsto \sin(2x_1) + \cos(x_2)$

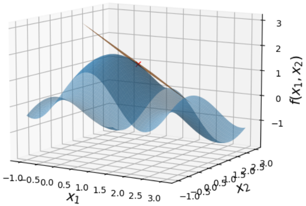
EXAMPLE: TAYLOR APPROXIMATION OF $f(\mathbf{x}) = \sin(2x_1) + \cos(x_2)$ AT $\boldsymbol{a} = (1, 1)^T$

1st order: we know that $f(\mathbf{x}) = \underbrace{f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})}_{T_1(\mathbf{x},\boldsymbol{a})} + R_1(\mathbf{x}, \boldsymbol{a})$ and since

$\nabla f(\mathbf{x}) = (2\cos(2x_1), -\sin(x_2))$,

$$\begin{aligned} f(\mathbf{x}) &= T_1(\mathbf{x}) + R_1(\mathbf{x}, \boldsymbol{a}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a}) + R_1(\mathbf{x}, \boldsymbol{a}) \\ &= \sin(2) + \cos(1) + (2\cos(2), -\sin(1)) \begin{pmatrix} x_1 - 1 \\ x_2 - 1 \end{pmatrix} + R_1(\mathbf{x}, \boldsymbol{a}) \end{aligned}$$





EXAMPLE: TAYLOR APPROXIMATION OF $f(\mathbf{x}) = \sin(2x_1) + \cos(x_2)$ AT $\boldsymbol{a} = (1, 1)^T$

2nd order: we know that

$$f(\mathbf{x}) = \underbrace{f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{a})^T \boldsymbol{H}(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})}_{T_2(\mathbf{x}, \boldsymbol{a})} + R_2(\mathbf{x}, \boldsymbol{a})$$

and since $H(\mathbf{x}) = \begin{pmatrix} -4\sin(2x_1) & 0 \\ 0 & -\cos(x_2) \end{pmatrix}$,

$$f(\mathbf{x}) = T_1(\mathbf{x}, \boldsymbol{a}) + \frac{1}{2}\begin{pmatrix} x_1 - 1 \\ x_2 - 1 \end{pmatrix}^T \begin{pmatrix} -4\sin(2) & 0 \\ 0 & -\cos(1) \end{pmatrix} \begin{pmatrix} x_1 - 1 \\ x_2 - 1 \end{pmatrix} + R_2(\mathbf{x}, \boldsymbol{a})$$