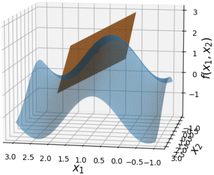
Optimization

Hessian Matrix & Taylor Series



Learning goals

- Taylor series (Univariate)
- Hessian Matrix
- Taylor series (Multivariate)

TAYLOR SERIES (UNIVARIATE)

Definition (Taylor's Theorem): Let $I \subseteq \mathbb{R}$ an open interval and $a, x \in I$. Further, let $f \in \mathcal{C}^{m+1}(I, \mathbb{R})$ for $m \in \mathbb{N}$. Then

$$f(x) = T_m(x, a) + R_m(x, a).$$

We call

$$T_m(x, a) = \sum_{k=}^{m} \frac{f^k(a)}{k!}(x - a)^k =$$

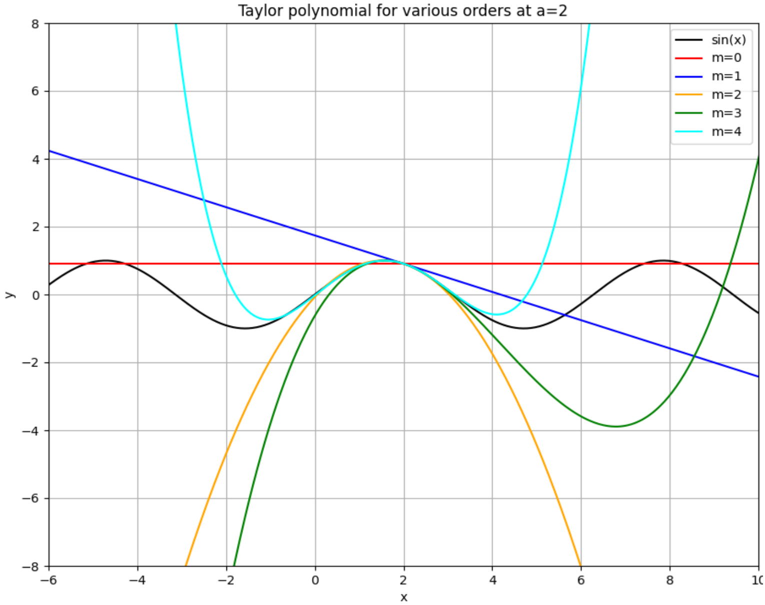
$$f(a) + f'(a)(x - a) + \frac{f''(a)}{2!}(x - a)^2 + ... + \frac{f^{(m)}(a)}{m!}(x - a)^m$$

the m-th Taylor polynomial.

$$R_m(x, a)$$

is called **remainder term**. We will cover this term later.

TAYLOR SERIES (UNIVARIATE)



DIFFERENTIATION (MULTIVARIATE)

The second derivative of a multivariate function is defined by its Hessian (if it exists).

Definition (Hessian): Let $f \in \mathcal{C}^2(\mathcal{S}, \mathbb{R})$, $\mathcal{S} \subseteq \mathbb{R}^d$. The **Hessian matrix** is defined as

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

Example: Let $f(x_1, x_2) = sin(x_1) \cdot cos(x_2)$. Then:

$$H(\mathbf{x}) = \begin{pmatrix} \text{-}\cos(x_2) \cdot \sin(x_1) & \text{-}\cos(x_1) \cdot \cos(x_2) \\ \text{-}\cos(x_1) \cdot \sin(x_2) & \text{-}\cos(x_2) \cdot \sin(x_1) \end{pmatrix}$$

HESSIAN DESCRIBES LOCAL CURVATURE

Local curvature can be analyzed via Eigenspecturm of $H(\mathbf{x})$:

- The Eigenvector $\boldsymbol{v}_{\text{max}}$ belonging to the largest Eigenvalue λ_{max} (in absolute terms) points into the the direction of largest curvature.
- Respectively: $\boldsymbol{v}_{\text{min}}$ points into direction of smallest curvature.
- Eigenvalues tell us about the definiteness and therefore the curvature of the matrix at a given point.

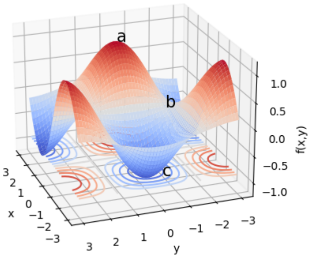
  positive-definite: all eigenvalues positive -> concave up
  positive-definite: all eigenvalues positive -> concave down
  saddle point: if eigenvalues are positive & negative.
  no statement possible: if either eigenvalue is $= 0$.

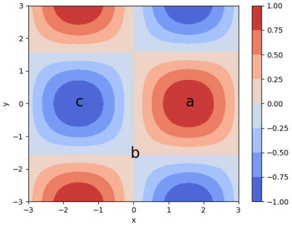
HESSIAN DESCRIBES LOCAL CURVATURE

Example (continued): $f(x_1, x_2) = sin(x_1) \cdot cos(x_2)$ and

$$H(\mathbf{x}) = \begin{pmatrix} \text{-}\cos(x_2) \cdot \sin(x_1) & \text{-}\cos(x_1) \cdot \cos(x_2) \\ \text{-}\cos(x_1) \cdot \sin(x_2) & \text{-}\cos(x_2) \cdot \sin(x_1) \end{pmatrix}$$

The Eigenvalues at $a = (\frac{-\pi}{2}, 0)$, $b = (0, \frac{-\pi}{2})$ and $c = (\frac{-\pi}{2}, 0)$ are -1 & -1, 1 & -1 and 1 & 1, respectively. The signs can each be retraced in the following plots:





Therefore, the hessian at a is negative-definite, has a saddle point at b and is positive-definite at c.

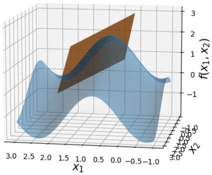
MULTIVARIATE TAYLOR SERIES

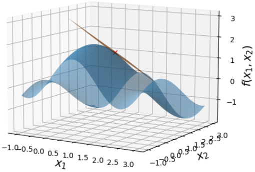
Taylor's theorem (1st order):

$$f(\mathbf{x}) = \underbrace{f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})^\top (\mathbf{x} - \boldsymbol{a})}_{T_1(\mathbf{x}, \boldsymbol{a})} + R_1(\mathbf{x}, a)$$

Example: $f(\mathbf{x}) = \sin(2x_1) + \cos(x_2)$, $\boldsymbol{a} = (1, 1)^\top$. Since $\nabla f(\mathbf{x}) = \begin{pmatrix} 2 \cdot \cos(2x_1) \\ -\sin(x_2) \end{pmatrix}$

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





MULTIVARIATE TAYLOR SERIES

Taylor's theorem (2nd order):

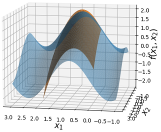
$$f(\mathbf{x}) = \underbrace{f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})^\top (\mathbf{x} - \boldsymbol{a}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{a})^\top \boldsymbol{H}(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})}_{T_2(\mathbf{x}, \boldsymbol{a})} + R_2(\mathbf{x}, a)$$

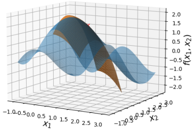
Example (continued): $f(\mathbf{x}) = \sin(2x_1) + \cos(x_2)$, $\boldsymbol{a} = (1, 1)^\top$. Since

$$\nabla f(\mathbf{x}) = \begin{pmatrix} 2 \cdot \cos(2x_1) \\ -\sin(x_2) \end{pmatrix} \text{ and } H(\mathbf{x}) = \begin{pmatrix} -4\sin(2x_1) & 0 \\ 0 & -\cos(x_2) \end{pmatrix}$$

we get

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





MULTIVARIATE TAYLOR SERIES

@Julia: Update notation

Formally, Taylor's theorem states:

Definition (Taylor's Theorem): Let $G \subseteq \mathbb{R}^n$ open, $f \in \mathcal{C}^{m+1}(G, \mathbb{R})$ for $m \in \mathbb{N}_0$. If $a \in G$, $h \in \mathbb{R}^n$ so that the line segment $S_{a,a+h}$ between a and $a + h \in G$, then

$$f(\boldsymbol{a}+\boldsymbol{h}) = \sum_{k=0}^{m} \frac{(\boldsymbol{h}\nabla^k(f)(\boldsymbol{a})}{k!} + R_m(\boldsymbol{a}) =$$

$$f(\boldsymbol{a}) + \frac{(\boldsymbol{h}\nabla)(f)(\boldsymbol{a})}{1!} + \frac{(\boldsymbol{h}\nabla)^2(f)(\boldsymbol{a})}{2!} + \ldots + \frac{(\boldsymbol{h}\nabla)^m(f)(\boldsymbol{a})}{m!} + R_m(\boldsymbol{a})$$

MULTIVARIATE TAYLOR SERIES

@Julia: Update notation

Definition (Mutlivariate Directional derivative): $\boldsymbol{h} = (h_1, ..., h_n) \in \mathbb{R}^n$, $G \subseteq \mathbb{R}^n$ open, $f : G \to \mathbb{R}^n$ differentiable, $a \in G$.

$$(\boldsymbol{h}\nabla(f)(\boldsymbol{a}) := \frac{\partial f}{\partial h}(\boldsymbol{a}) = \sum_{j=1}^{n} h_j \partial_j f((a)) = h_1 \partial_j f((a)) + ... + h_n \partial_n f((a))$$

with $(\boldsymbol{h}\nabla)$ called **Differential operator**.

If $f \in \mathcal{C}^2(G, \mathbb{R})$, we can apply $(\boldsymbol{h}\nabla)$ again:

$$(\boldsymbol{h}\nabla)(f)^2(\boldsymbol{a}) := (\boldsymbol{h}\nabla)(\boldsymbol{h}\nabla)(f)(\boldsymbol{a}) =$$

$$= \sum_{j=1}^{n} (\boldsymbol{h}\nabla)(\boldsymbol{h}_j \partial_j (f)(\boldsymbol{a}) = \sum_{k,j=1}^{n} h_k h_j \partial_k \partial_j f(\boldsymbol{a})$$

TAYLOR APPROXIMATION

@Julia: Update notation

The remainder term $R_m(\boldsymbol{a})$ can be written down quantitatively

$$R_m(\boldsymbol{a}) := \int_0^1 \frac{(1-t)^m}{m!} (\boldsymbol{h}\nabla^{m+1})(f)(\boldsymbol{a} + t\boldsymbol{h})\mathrm{d}t$$

(this is called the integral form; alternative formulas for the remainder term exist as well, but are not covered here.)

or qualitatively

$$R_m(\boldsymbol{a}) \in \mathcal{O}(\|\mathbf{x} - \boldsymbol{a}\|^m) \text{ for } \mathbf{x} \to \boldsymbol{a}$$

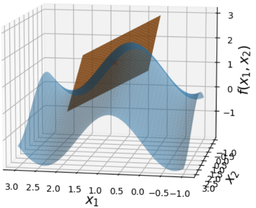
If we don't care too much about the approximation error, we just write:

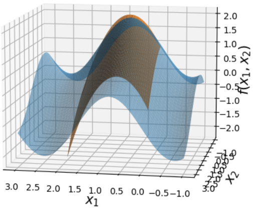
$$f(\mathbf{x}) \approx T_m(\mathbf{x}, \boldsymbol{a}).$$

TAYLOR APPROXIMATION

Note:

- Higher m gives a better approximation
- The m^{th} order taylor series is the best m^{th} order approximation to $f(\mathbf{x})$ near $\boldsymbol{a}$





Consider $T_2(\mathbf{x}, \boldsymbol{a}) = f(\boldsymbol{a}) + \nabla f(\boldsymbol{a})^\top (\mathbf{x} - \boldsymbol{a}) + \frac{1}{2}(\mathbf{x} - \boldsymbol{a})^\top \boldsymbol{H}(\boldsymbol{a})(\mathbf{x} - \boldsymbol{a})$. The first term ensures the **value** of T_2 and f match at $\boldsymbol{a}$. The second term ensures the **slopes** of T_2 and f match at $\boldsymbol{a}$. The third term ensures the **curvature** of T_2 and f match at $\boldsymbol{a}$.