Lecture 8

Math Foundations Team

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Introduction

- Till now we have discussed about Taylor/Maclaurian series, Partial Derivatives and Gradients.
- Now we are interested in Higher order Derivatives.
- Multivariate Taylor Series and its uses in the expansion of a function with multivariables.

Higher-Order Derivatives

Consider a function $f : \mathbb{R}^2 \to \mathbb{R}$

Notations for Higher-Order Partial Derivatives:

$\frac{\partial^2 f}{\partial x^2}$: Second Partial Derivative of x w.r.t. x

$\frac{\partial^n f}{\partial x^n}$: n^{th} Partial Derivative of x w.r.t. x

$\frac{\partial^2 f}{\partial y \partial x} = \frac{\partial}{\partial y}(\frac{\partial f}{\partial x})$: is the partial derivative obtained by first partial differentiating with respect to x and then with respect to y.

$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial}{\partial x}(\frac{\partial f}{\partial y})$: is the partial derivative obtained by first partial differentiating by y and then x.

Hessian Matrix

The Hessian is the collection of all second-order partial derivatives. If f(x, y) is a twice (continuously) differentiable function, then $\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial^2 f}{\partial y \partial x}$ i.e., the order of differentiation does not matter, and the corresponding Hessian matrix

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial x \partial y} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix}$$

is symmetric. The Hessian is denoted as $\nabla^2_{x,y} f(x, y)$
In general, if $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable, multivariable function, the Hessian matrix $\boldsymbol{H} = \nabla^2_{\boldsymbol{x}} f(\boldsymbol{x})$ is of order $n \times n$.

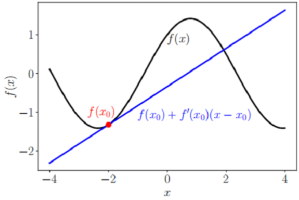
Linearization and Multivariate Taylor Series

The gradient ∇f of a function f is often used for a locally linear approximation of f around x_0 :

$$f(x) \approx f(x_0) + (\nabla_x f)(x_0)(x - x_0) \tag{1}$$

Here $(\nabla_x f)(x_0)$ is the gradient of f with respect to x, evaluated atx_0. Figure illustrates the linear approximation of a function f at an input x_0. The original function is approximated by a straight line.

This approximation is locally accurate, but the farther we move away from x_0 the worse the approximation gets. Equation (1) is a special case of a multivariate Taylor series expansion of f at x_0, where we consider only the first two terms. We discuss the more general case in the following, which will allow for better approximations.



Linear approximation of a function. The original function f is linearized at $x_0 = -2$ using a first-order Taylor series expansion.

Multivariate Taylor Series

Consider a function $f : \mathbb{R}^D \to \mathbb{R}$, $x \to f(x)$,

$$x \in \mathbb{R}^D$$

that is smooth at x_0. When we define the difference vector $\delta := x - x_0$ the multivariate Taylor series of f at (x_0) is defined as multivariate Taylor series

$$f(x) = \sum_{k=0}^{\infty} \frac{D_x^k f(x_0)}{k!} \delta^k \tag{2}$$

where $D_x^k f(x_0)$ is the k^{th} (total) derivative of f with respect to x, evaluated at x_0.

Taylor Polynomial

The Taylor polynomial of degree n of Taylor polynomial f at x_0 contains the first n + 1 components of the series in (2) and is defined as

$$T_n(x) = \sum_{k=0}^{n} \frac{D_x^k f(x_0)}{k!} \delta^k \tag{3}$$

In (2) and (3), we used the slightly sloppy notation of δ^k, which is not defined for vectors

$$x \in \mathbb{R}^D,$$

$D > 1$, and $k > 1$. Note that both $D_x^k f$ and δ^k are k^{th} order tensors, i.e., k-dimensional arrays.

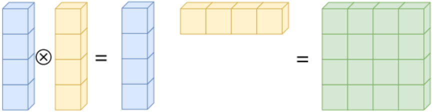
Taylor Polynomial...

kth-order tensor $\boldsymbol{\delta}^k \in \mathbb{R}^{\overbrace{D\times D\times\ldots\times D}^{k \text{ times}}}$ is obtained as a k-fold outer product, denoted by $\otimes$, of the vector $\boldsymbol{\delta} \in \mathbb{R}^D$. For example,

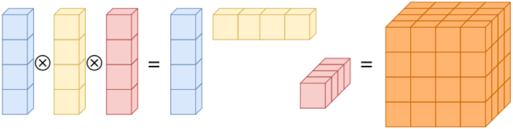
$$\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top, \quad \boldsymbol{\delta}^2[i,j] = \delta[i]\delta[j]$$

$$\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta}, \quad \boldsymbol{\delta}^3[i,j,k] = \delta[i]\delta[j]\delta[k]\,.$$

Taylor Polynomial...



(a) Given a vector $\boldsymbol{\delta} \in \mathbb{R}^4$, we obtain the outer product $\boldsymbol{\delta}^2 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} = \boldsymbol{\delta}\boldsymbol{\delta}^\top \in \mathbb{R}^{4\times4}$ as a matrix.



(b) An outer product $\boldsymbol{\delta}^3 := \boldsymbol{\delta} \otimes \boldsymbol{\delta} \otimes \boldsymbol{\delta} \in \mathbb{R}^{4\times4\times4}$ results in a third-order tensor ("three-dimensional matrix"), i.e., an array with three indexes.

$$D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)\boldsymbol{\delta}^k = \sum_{i_1=1}^{D} \cdots \sum_{i_k=1}^{D} D_{\boldsymbol{x}}^k f(\boldsymbol{x}_0)[i_1, \ldots, i_k]\delta[i_1] \cdots \delta[i_k]$$

Taylor Polynomial...

In general, we obtain the terms in the Taylor series, where $D_x^k f(x_0)\delta^k$ contains k^{th} order polynomials.Now that we defined the Taylor series for vector fields, let us explicitly write down the first terms $D_x^k f(x_0)\delta^k$ of the Taylor series expansion for

$k = 0, \ldots, 3$ and $\boldsymbol{\delta} := \boldsymbol{x} - \boldsymbol{x}_0$:

$$k = 0 : D_{\boldsymbol{x}}^0 f(\boldsymbol{x}_0)\boldsymbol{\delta}^0 = f(\boldsymbol{x}_0) \in \mathbb{R}$$

$$k = 1 : D_{\boldsymbol{x}}^1 f(\boldsymbol{x}_0)\boldsymbol{\delta}^1 = \underbrace{\nabla_{\boldsymbol{x}} f(\boldsymbol{x}_0)}_{1\times D} \underbrace{\boldsymbol{\delta}}_{D\times 1} = \sum_{i=1}^{D} \nabla_{\boldsymbol{x}} f(\boldsymbol{x}_0)[i]\delta[i] \in \mathbb{R}$$

$$k = 2 : D_{\boldsymbol{x}}^2 f(\boldsymbol{x}_0)\boldsymbol{\delta}^2 = \mathrm{tr}\big(\underbrace{\boldsymbol{H}(\boldsymbol{x}_0)}_{D\times D} \underbrace{\boldsymbol{\delta}}_{D\times 1} \underbrace{\boldsymbol{\delta}^\top}_{1\times D}\big) = \boldsymbol{\delta}^\top \boldsymbol{H}(\boldsymbol{x}_0)\boldsymbol{\delta}$$

$$= \sum_{i=1}^{D}\sum_{j=1}^{D} H[i,j]\delta[i]\delta[j] \in \mathbb{R}$$

$$k = 3 : D_{\boldsymbol{x}}^3 f(\boldsymbol{x}_0)\boldsymbol{\delta}^3 = \sum_{i=1}^{D}\sum_{j=1}^{D}\sum_{k=1}^{D} D_{\boldsymbol{x}}^3 f(\boldsymbol{x}_0)[i,j,k]\delta[i]\delta[j]\delta[k] \in \mathbb{R}$$

Here, $\boldsymbol{H}(\boldsymbol{x}_0)$ is the Hessian of f evaluated at $\boldsymbol{x}_0$.

Taylor Series Expansion of a Function with Two Variables

Consider the function $f(x, y) = x^2 + 2xy + y^3$.
We want to compute the Taylor series expansion of f at $(x_0, y_0) = (1, 2)$.
Before we start, let us discuss what to expect: The function in $f(x, y)$ is a polynomial of degree 3. We are looking for a Taylor series expansion,which itself is a linear combination of polynomials. Therefore, we do not expect the Taylor series expansion to contain terms of fourth or higher order to express a third-order polynomial. This means that it should be sufficient to determine the first four terms of $f(x) = \sum_{k=0}^{\infty} \frac{D_x^k f(x_0)}{k!} \delta^k$ for an exact alternative representation of $f(x, y)$. To determine the Taylor series expansion, we start with the constant term and the first-order derivatives, which are given by $f(1, 2) = 13$

$$\frac{\partial f}{\partial x} = 2x + 2y \implies \frac{\partial f}{\partial x}(1,2) = 6$$
$$\frac{\partial f}{\partial y} = 2x + 3y^2 \implies \frac{\partial f}{\partial y}(1,2) = 14\,.$$

Therefore, we obtain

$$D^1_{x,y} f(1,2) = \nabla_{x,y} f(1,2) = \begin{bmatrix} \frac{\partial f}{\partial x}(1,2) & \frac{\partial f}{\partial y}(1,2) \end{bmatrix} = \begin{bmatrix} 6 & 14 \end{bmatrix} \in \mathbb{R}^{1\times 2}$$

such that

$$\frac{D^1_{x,y} f(1,2)}{1!} \boldsymbol{\delta} = \begin{bmatrix} 6 & 14 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} = 6(x-1) + 14(y-2)\,.$$

When we collect the second-order partial derivatives, we obtain the Hessian

$$\boldsymbol{H} = \begin{bmatrix} \frac{\partial^2 f}{\partial x^2} & \frac{\partial^2 f}{\partial x \partial y} \\ \frac{\partial^2 f}{\partial y \partial x} & \frac{\partial^2 f}{\partial y^2} \end{bmatrix} = \begin{bmatrix} 2 & 2 \\ 2 & 6y \end{bmatrix},$$

such that

$$\boldsymbol{H}(1,2) = \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \in \mathbb{R}^{2\times 2}.$$

Therefore, the next term of the Taylor-series expansion is given

$$\begin{aligned} \frac{D^2_{x,y} f(1,2)}{2!} \boldsymbol{\delta}^2 &= \frac{1}{2} \boldsymbol{\delta}^\top \boldsymbol{H}(1,2) \boldsymbol{\delta} \\ &= \frac{1}{2} \begin{bmatrix} x-1 & y-2 \end{bmatrix} \begin{bmatrix} 2 & 2 \\ 2 & 12 \end{bmatrix} \begin{bmatrix} x-1 \\ y-2 \end{bmatrix} \\ &= (x-1)^2 + 2(x-1)(y-2) + 6(y-2)^2. \end{aligned}$$

The third-order derivatives are obtained as

$$D^3_{x,y}f = \begin{bmatrix} \frac{\partial \boldsymbol{H}}{\partial x} & \frac{\partial \boldsymbol{H}}{\partial y} \end{bmatrix} \in \mathbb{R}^{2\times 2\times 2},$$

$$D^3_{x,y}f[:,:,1] = \frac{\partial \boldsymbol{H}}{\partial x} = \begin{bmatrix} \frac{\partial^3 f}{\partial x^3} & \frac{\partial^3 f}{\partial x^2 \partial y} \\ \frac{\partial^3 f}{\partial x \partial y \partial x} & \frac{\partial^3 f}{\partial x \partial y^2} \end{bmatrix},$$

$$D^3_{x,y}f[:,:,2] = \frac{\partial \boldsymbol{H}}{\partial y} = \begin{bmatrix} \frac{\partial^3 f}{\partial y \partial x^2} & \frac{\partial^3 f}{\partial y \partial x \partial y} \\ \frac{\partial^3 f}{\partial y^2 \partial x} & \frac{\partial^3 f}{\partial y^3} \end{bmatrix}.$$

Since most second-order partial derivatives in the Hessian, are constant, the only nonzero third-order partial derivative is $\frac{\partial^3 f}{\partial y^3} = 6 \implies \frac{\partial^3 f}{\partial y^3}(1,2) = 6$ Higher-order derivatives and the mixed derivatives of degree 3 (e.g., $\frac{\partial^3 f}{\partial x^2 \partial y}$) vanish, such that

$$D^3_{x,y} f[:,:,1] = \begin{bmatrix} 0 & 0 \\ 0 & 0 \end{bmatrix}, \quad D^3_{x,y} f[:,:,2] = \begin{bmatrix} 0 & 0 \\ 0 & 6 \end{bmatrix}$$

and

$$\frac{D^3_{x,y} f(1,2)}{3!} \boldsymbol{\delta}^3 = (y-2)^3,$$

which collects all cubic terms of the Taylor series. Overall, the (exact) Taylor series expansion of f at $(x_0, y_0) = (1, 2)$ is

$$
\begin{aligned}
f(x) &= f(1,2) + D^1_{x,y} f(1,2)\boldsymbol{\delta} + \frac{D^2_{x,y} f(1,2)}{2!}\boldsymbol{\delta}^2 + \frac{D^3_{x,y} f(1,2)}{3!}\boldsymbol{\delta}^3 \\
&= f(1,2) + \frac{\partial f(1,2)}{\partial x}(x-1) + \frac{\partial f(1,2)}{\partial y}(y-2) \\
&\quad + \frac{1}{2!}\left(\frac{\partial^2 f(1,2)}{\partial x^2}(x-1)^2 + \frac{\partial^2 f(1,2)}{\partial y^2}(y-2)^2 \right. \\
&\quad \left. + 2\frac{\partial^2 f(1,2)}{\partial x \partial y}(x-1)(y-2)\right) + \frac{1}{6}\frac{\partial^3 f(1,2)}{\partial y^3}(y-2)^3 \\
&= 13 + 6(x-1) + 14(y-2) \\
&\quad + (x-1)^2 + 6(y-2)^2 + 2(x-1)(y-2) + (y-2)^3 .
\end{aligned}
$$

- A set $A \subset \mathbb{R}^n$ is called as an open set if $\forall \boldsymbol{a} \in A$ there exists $\delta > 0$ such that $\boldsymbol{x} \in A$ whenever $\|\boldsymbol{x} - \boldsymbol{a}\| < \delta$.
- Let $f : \mathbb{R}^n \to \mathbb{R}$ is twice continuously differentiable, multivariable function on an open set containing $\boldsymbol{x_0}$. Then the point $\boldsymbol{x_0}$ is said to be a critical point of f if $\nabla_{\boldsymbol{x}} f(\boldsymbol{x_0}) = \mathbf{0}$.
- Using Taylor's polynomial approximation, we get $f(\boldsymbol{x}) \approx f(\boldsymbol{x_0}) + \nabla_{\boldsymbol{x}} f(\boldsymbol{x_0})\delta + \delta^T \boldsymbol{H}(\boldsymbol{x_0})\delta$, where $\delta = \boldsymbol{x} - \boldsymbol{x_0}$.
- So at critical point, we get $f(\boldsymbol{x}) \approx f(\boldsymbol{x_0}) + \delta^T \boldsymbol{H}(\boldsymbol{x_0})\delta$

Second Derivative Test

Let $\boldsymbol{x_0}$ be a critical point of f.

i) If the Hessian matrix $\boldsymbol{H}$ is positive definite (i.e. all eigenvalues are strictly positive) then $\delta^T \boldsymbol{H}(\boldsymbol{x_0})\delta > 0$. So $f(\boldsymbol{x}) > f(\boldsymbol{x_0})$ and hence $\boldsymbol{x_0}$ is a point of local minima.

ii) If the Hessian matrix $\boldsymbol{H}$ is negative definite (i.e. all eigenvalues are strictly negative) then $\delta^T \boldsymbol{H}(\boldsymbol{x_0})\delta < 0$. So $f(\boldsymbol{x}) < f(\boldsymbol{x_0})$ and hence $\boldsymbol{x_0}$ is a point of local maxima.

iii) If the Hessian matrix $\boldsymbol{H}$ has both positive and negative eigenvalues then $\boldsymbol{x_0}$ is a saddle point.

iv) If the determinant of Hessian matrix $\boldsymbol{H}$ is zero then the test is inconclusive.

An Example

Let $f(x,y) = 3x^2y + y^3 - 3x^2 - 3y^2 + 2$, then

$$\begin{aligned}
\nabla_{x,y} f(x,y) &= [6xy - 6x, 3x^2 + 3y^2 - 6y] \\
\nabla_{x,y} f(x,y) = 0 &\Rightarrow (0,0), (0,2), (1,1), (-1,1) \text{ are critical points} \\
\boldsymbol{H}(x,y) &= \begin{bmatrix} 6y-6 & -6x \\ -6x & 6y-6 \end{bmatrix}
\end{aligned}$$

The eigenvalues of $\boldsymbol{H}(0,0)$ are $-6,-6$ and hence $[0,0]^T$ is a maxima
The eigenvalues of $\boldsymbol{H}(0,2)$ are $6,6$ and hence $[0,2]^T$ is a minima.
The eigenvalues of $\boldsymbol{H}(1,1)$ are $-6,6$ and hence $[1,1]^T$ is a saddle point.
The eigenvalues of $\boldsymbol{H}(-1,1)$ are $-6,6$ and hence $[1,1]^T$ is a saddle point.