CSE 840: Computational Foundations of Artificial Intelligence Nov 06, 2023

Higher Order Derivatives, Minima/Maxima, Matrix/Vector Calculus

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Higher Order Derivatives

Definition 1 (Higher - order derivatives) *refer to the derivatives of derivatives, taking higher-order derivatives involves repeatedly finding the derivative of a function. Example: the second derivative is the derivative of the first derivative, the third derivative is the derivative of the second derivative, and so on.*

Consider $f:\mathbb{R}^n \to \mathbb{R}$, assume it is differentiable, so all partial derivatives $\frac{\partial f}{\partial x_i}:\mathbb{R}^n \to \mathbb{R}$ exist. If this function is differentiable, we can take its derivative: $\frac{\partial}{\partial x_i}(\frac{\partial f}{\partial x_j}) = \frac{\partial^2 f}{\partial x_i \partial x_j}$ These are called second order partial derivatives.

⚠ In general, we cannot change the order of derivatives: $\frac{\partial^2 f}{\partial x_i \partial x_j} \neq \frac{\partial^2 f}{\partial x_j \partial x_i}$

Example:

$$
\begin{aligned}
f(x,y) &= \frac{x.y^3}{x^2+y^2} \\
\nabla f(x,y) &= (\frac{y^3(y^2-x^2)}{(x^2+y^2)^2}, \frac{xy^2(3x^2+y^2)}{(x^2+y^2)^2})
\end{aligned}
$$

Have:

$$
\begin{aligned}
&\frac{\partial f}{\partial x}(0,y) = y \quad \forall y, \quad \frac{\partial}{\partial y}(\frac{\partial f}{\partial x}) = 1 \\
&\frac{\partial f}{\partial y}(x,0) = 0 \quad \forall x, \quad \frac{\partial}{\partial x}(\frac{\partial f}{\partial y}) = 0
\end{aligned}
$$

we can see that $1 \neq 0$.

Definition 2 (Continuously Differentiable:) *We say that $f:\mathbb{R}^n \to \mathbb{R}$ is continuously differentiable if all partial derivatives exist and are continuous.*
We say that f is twice continuously differentiable if f is continuously differentiable and all its partial derivatives $\frac{\partial f}{\partial x_i}$ are again continuously differentiable.

Analogously: k times continuously differentiable

Notation:
$\mathscr{C}^k(\mathbb{R}^n, \mathbb{R}^m) = \{f : \mathbb{R}^n \to \mathbb{R}^m | k$ times continuously differentiable$\}$
$\mathscr{C}^\infty(\mathbb{R}^n, \mathbb{R}^m) = \{f : \mathbb{R}^n \to \mathbb{R}^m | \infty$ often continuously differentiable$\}$

Theorem 3 (Schwartz) *Assume that f is twice continuously differentiable. Then we can exchange the order in which we take partial derivatives:* $\frac{\partial^2 f}{\partial x_i \partial x_j} = \frac{\partial^2 f}{\partial x_j \partial x_j}$

Analogously: k times continuously differentiable $\implies$ can exchange order of first k partial derivatives.

⚠ Caution about derivatives:

$f : \mathbb{R}^n \to \mathbb{R}$ $\leftarrow$ function

$\nabla f : \mathbb{R}^n \to \mathbb{R}^n$ $\leftarrow$ first derivatives($\dfrac{\partial f}{\partial x_i}$): n partial derivatives

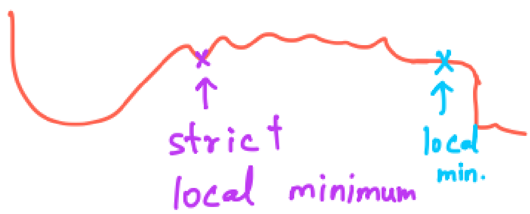
$Hf : \mathbb{R}^n \to \mathbb{R}^{n \times n}$ $\leftarrow$ second derivatives($\dfrac{\partial^2 f}{\partial x_i \partial x_j}$): n^2 partial derivatives

Definition 4 (Hessian Matrix) $f : \mathbb{R}^n \to \mathbb{R}$, *then we define the Hessian of* f *at point* x *by,*
$(Hf)_{ij}(x) := \frac{\partial^2 f(x)}{\partial x_i \partial x_j} \quad i, j = 1, 2, 3, ..., n$

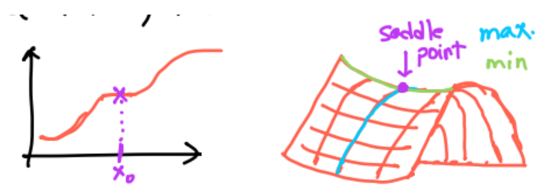
Minima/Maxima

Definition 5 (Critical Point) *$f : \mathbb{R}^n \to \mathbb{R}$ differentiable. If $\nabla f(x) = 0$ then we call x a critical point.*

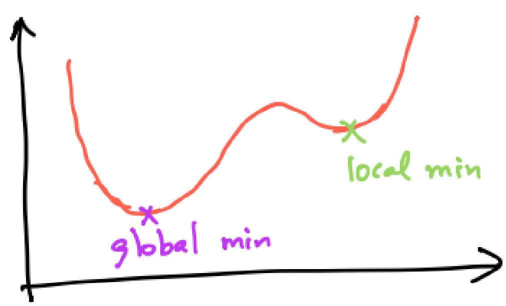
- f has a local minimum at x_0 if there exists $\epsilon > 0$, such that $\forall x \in B_\epsilon(x_0) : f(x) \geq f(x_0)$
- f has a strict local minimum at x_0 if there exists $\epsilon > 0$, such that $\forall x \in B_\epsilon(x_0) : f(x) > f(x_0)$



- f has a local maximum at x_0 if there exists $\epsilon > 0$, such that $\forall x \in B_\epsilon(x_0) : f(x) \leq f(x_0)$
- f has a strict local maximum at x_0 if there exists $\epsilon > 0$, such that $\forall x \in B_\epsilon(x_0) : f(x) < f(x_0)$
- If f is differentiable and x_0 is a critical point that is neither a local minima nor a local maximum. We call it a saddle point.



- f has a global minimum at x_0 if $\forall x : f(x) \geq f(x_0)$



- f has a global maximum at x_0 if $\forall x : f(x) \leq f(x_0)$

How can we identitywhich type of point we have?

Intuition in $\mathbb{R}$:

local min. $f'(x)=0$, $f''(x)>0$

local max. $f'(x)=0$, $f''(x)<0$

saddle point $f'(x)=0$, $f''(x)=0$

Theorem 6 $f:\mathbb{R}^n \to \mathbb{R}$, $f \in \mathscr{C}^2(\mathbb{R}^n)$. *Assume that x_0 is a critical point, i.e $\nabla f(x_0)=0$. Then:*

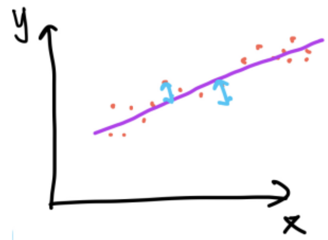
(i) If x_0 is a local minimum(maximum), then the Hessian $Hf(x_0)$ is positive semi definite (negative semi definite).

(ii) If $Hf(x_0)$ is positive definite (negative definite), then x_0 is a strict local minimum(maximum). If $Hf(x_0)$ is indefinite then (x_0) is a saddle point.

Matrix/Vector Calculus

Example: Linear Least Squares

$f : \mathbb{R}^n \to \mathbb{R}$
pred $\hat{y}(w) = Aw$ where,
$\hat{y}$ is prediction, A - input data
w - weight vector (parameters we want to find).



$f(w) = \|y - \hat{y}(w)\|_2^2 = \|y - Aw\|_2^2$
$f(w)$ - how good pred. is with parameter w.

We want to minimize $f(w)$. Thus, we need to look at $\nabla f : \mathbb{R}^n \to \mathbb{R}^n$.

Compute Gradient:

$$f\begin{pmatrix} w_1 \\ \vdots \\ w_n \end{pmatrix} = \sum_{j=1}^{n} (y_j - \sum_{k=1}^{n} a_{jk} w_k)^2 \qquad \text{where } \sum_{k=1}^{n} a_{jk} w_r = (Aw)_j$$

$$\frac{\partial f}{\partial w_i} = \sum_{j=1}^{n} 2(-a_{ji})(y_j - \sum_{k=1}^{n} a_{jk} w_k) \qquad \text{where } \sum_{k=1}^{n} a_{jk} w_r = (Aw)_j,$$

$$(y_j - \sum_{k=1}^{n} a_{jk} w_k) = y - (Aw)_j, \quad \text{and}$$

$$-2 \sum_{j=i}^{n} 2(-a_{ji})(y_j - \sum_{k=1}^{n} a_{jk} w_k) = (A^T(y - Aw))_i$$

$$\nabla f(w) = -2A^T(y - Aw)$$

Intuition: "syntax" close to 1-dim case:
$f(w) = (y - aw)^2$
$f'(w) = -a(y - aw) \cdot 2 = -2a(y - aw)$

Matrix-Vector Calculus: Lookup table ("matrix cookbook") for gradients of many important functions:

$f : \mathbb{R}^n \to \mathbb{R}$.

- $f(x) = a^T x \quad (a \in \mathbb{R}^n)$
  $f(x) = \langle a, x \rangle$
  $\frac{\partial f}{\partial x} = a \in \mathbb{R}^n$
- $f(x) = x^T A x \implies \frac{\partial f}{\partial x} = (A + A^T)x \in \mathbb{R}^n$

$f: \mathbb{R}^{n\times m} \to \mathbb{R}.$

- $f(x) = a^T X b \implies \frac{\partial f}{\partial x} = ab^T \in \mathbb{R}^{n\times m}$
  where X is $\mathbb{R}^{n\times m}$, a^T is $1\times n$ and b is $m\times 1$ dimensions.

- $f(x) = a^T X^T C X b \implies \frac{\partial f}{\partial x} = C^T X ab + CXba^T$
  where a^T is $a\times m$, X^T is $m\times n$, C is $n\times n$, X $n\times m$, and b is $m\times 1$ dimensions.

- $f(X) = tr(X) \implies \frac{\partial x}{\partial x} = I$
  where $tr(X)$ is the trace and I is the identity matrix.

- $f(X) = tr(AX) \implies \frac{\partial x}{\partial x} = A$
  $f(X) = tr(X^T AX) \implies \frac{\partial x}{\partial x} = (A + A^T)X$

- $f(X) = det(X) \to$ Determinant

  $\frac{\partial x}{\partial x} = det(X)(X^T)^{-1}$

  $\frac{\partial det}{\partial x_{sr}} = det(X)(X^{-1})_{rs}$

$f: \mathbb{R}^{n\times m} \to \mathbb{R}^{n\times m}$ Inverse.

- $f(A) = A^{-1}, \quad f_{ij} := (A^{-1})_{ij}$

  $\frac{\partial f_{ij}}{\partial a_{uv}} = -(a_{iu})^{-1}(a_{vj})^{-1}$