LECTURE 17: SECOND-ORDER DERIVATIVES

1. Second-Order Derivatives

Notice: If $f : \mathbb{R}^n \to \mathbb{R}$ is real-valued, then so are its partial derivatives $f_{x_1}, f_{x_2}, \dots, f_{x_n}$

If the partial derivatives f_{x_i} happen themselves to be differentiable, then we can define the **second-order partial derivatives** as

Definition: $(f_{x_i})_{x_j} = \frac{\partial}{\partial x_j}(f_{x_i})$ (Rudin uses D_{ji} for this)

In general, we do **not** have $(f_{x_i})_{x_j} \neq \left(f_{x_j}\right)_{x_i}$

Example: If $f(0,0) = 0$ and

$$f(x,y) = \frac{xy(x^2 - y^2)}{x^2 + y^2}$$

Then $(f_{x_1})_{x_2}(0,0) = -1$ but $(f_{x_2})_{x_1}(0,0) = 1$ (see homework)

(The problem is once again interchange of limits in the derivatives)

That said, *if* the second-order partial derivatives are continuous, then the above is true.

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Rectangle Lemma: Suppose f_{x_1} and $(f_{x_1})_{x_2}$ are exist in $\mathbb{R}^2$. Let Q be the rectangle with opposite vertices (a, b) and $(a+h, b+k)$ where $h, k \neq 0$ (see picture in lecture) and let

$$\Delta(f, Q) = f(a+h, b+k) - f(a+h, b) - f(a, b+k) + f(a, b)$$

Then there is a point (x, y) inside Q such that

$$\frac{\Delta(f, Q)}{hk} = (f_{x_1})_{x_2}(x, y)$$

Compare this with the Mean Value Theorem $\frac{f(b)-f(a)}{b-a} = f'(c)$. Here we're saying that a difference quotient can be estimated with second derivatives. It should remind you a little bit of the formula

$$\lim_{h \to 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x)$$

Proof:

STEP 1: Let $u(t) = f(t, b+k) - f(t, b)$, then

$$\Delta(f, Q) = u(a+h) - u(a)$$

By the Mean-Value Theorem applied to u, there is x between a and $a+h$ such that $u(a+h) - u(a) = hu'(x)$

But $u'(t) = f_{x_1}(t, b+k) - f_{x_1}(t, b)$ and so

$$u'(x) = f_{x_1}(x, b+k) - f_{x_1}(x, b)$$

Let $v(t) = f_{x_1}(x, t)$ then

$$u'(x) = v(b+k) - v(b)$$

By the mean-value theorem applied to v, there is y between b and $b+k$ such that $v(b+k)-v(b)=kv'(y)$

But $v'(t)=\left(f_{x_1}\right)_{x_2}(x,t)$ and so $v'(y)=\left(f_{x_1}\right)_{x_2}(x,y)$.

STEP 2: Combining everything we get

$$\begin{aligned}\Delta(f,Q)=&u(a+h)-u(a)\\=&hu'(x)\\=&h(v(b+k)-v(b))\\=&hkv'(y)\\=&hk\left(f_{x_1}\right)_{x_2}(x,y)\quad\square\end{aligned}$$

Theorem: [Clairaut/Schwarz Theorem]

If moreover $\left(f_{x_1}\right)_{x_2}$ is continuous at (a,b) then $\left(f_{x_2}\right)_{x_1}(a,b)$ exists and

$$\left(f_{x_2}\right)_{x_1}(a,b)=\left(f_{x_1}\right)_{x_2}(a,b)$$

Fun Fact: Clairaut had 19 siblings, and published his first math paper at 12 years old!

Proof: Let $\epsilon>0$ be given and $A=:\left(f_{x_1}\right)_{x_2}(a,b)$. By continuity, if h and k are small enough, then for all $(x,y)\in Q$ (rectangle) we have

$$\left|\left(f_{x_1}\right)_{x_2}(x,y)-A\right|<\epsilon$$

Therefore by the Rectangle Lemma above, we have

$$\left|\frac{\Delta(f,Q)}{hk}-A\right|<\epsilon$$

Now if we let $k\to 0$ first, then we get

$$\left|\left(\lim_{k\to 0}\frac{\Delta(f,Q)}{hk}\right)-A\right|\leq\epsilon$$

But $\dfrac{\Delta(f,Q)}{hk}=\dfrac{1}{h}\left[\left(\dfrac{f(a+h,b+k)-f(a+h,b)}{k}\right)-\left(\dfrac{f(a,b+k)-f(a,b)}{k}\right)\right]$

So as $k\to 0$ this just tends to $\frac{f_{x_2}(a+h,b)-f_{x_2}(a,b)}{h}$ and hence

$$\left|\frac{f_{x_2}(a+h,b)-f_{x_2}(a,b)}{h}-A\right|\leq\epsilon$$

Finally, if you let $h\to 0$, since this is true for all $\epsilon>0$ we get

$$\left(f_{x_2}\right)_{x_1}(a,b)=A=:\left(f_{x_1}\right)_{x_2}(a,b)\quad\square$$

Definition: In that case (unambiguous by Clairaut)

$$\frac{\partial^2 f}{\partial x_1\partial x_2}=f_{x_1x_2}=\left(f_{x_1}\right)_{x_2}=\left(f_{x_2}\right)_{x_1}$$

Definition: f is C^2 if f is C^1 and all the second-order partial derivatives are continuous.

2. The True Second-Derivative Test

Video: The True Second-Derivative Test

Definition: The **Hessian** of f is

$$D^2 f=\left[\frac{\partial^2 f}{\partial x_i\partial x_j}\right]$$

Note: If f is C^2 then this matrix is symmetric

As an application of this, let's state the **true** second derivative test for max/min (not the fake version you learned in multivariable calculus)

The True Second-Derivative Test: Suppose $f'(a) = 0$ for some a

(1) If all the eigenvalues of $D^2 f(a)$ are > 0, f has a local min at a

(2) If all the eigenvalues of $D^2 f(a)$ are < 0, f has a local max at a

(3) If the eigenvalues of $D^2 f(a)$ are mixed (positive/neg) then f has a saddle point at a

(4) Else the test is inconclusive

Example: $f(x, y) = x^3 - 3x + 3xy^2$

Can show that f has a critical point at $(1, 0)$ and

$$D^2 f = \begin{bmatrix} f_{xx} & f_{xy} \\ f_{yx} & f_{yy} \end{bmatrix} = \begin{bmatrix} 6x & 6y \\ 6y & 6x \end{bmatrix} \Rightarrow D^2 f(1, 0) = \begin{bmatrix} 6 & 0 \\ 0 & 6 \end{bmatrix}$$

The eigenvalues are $\lambda = 6$ and $\lambda = 6$, which are positive, hence f has a local min at $(1, 0)$

3. Differentiation of Integrals

Finally, let's discuss the **very** delicate question of differentiation of integrals.

Question: When do we have

$$\frac{d}{dt} \int_a^b \phi(x, t) dx = \int_a^b \frac{\partial \phi}{\partial t}(x, t) dx$$

In general, this is not true (see homework), but we can show that this does hold provided $\frac{\partial \phi}{\partial t}$ is continuous

Fact: Suppose $\phi : [a, b] \times [c, d] \to \mathbb{R}$ and $\frac{\partial \phi}{\partial t}$ are continuous, and if

$$f(t) = \int_a^b \phi(x, t) dx \text{ then } f'(t) = \int_a^b \frac{\partial \phi}{\partial t}(x, t) dx$$

Proof:

STEP 1: Fix t and consider the difference quotient

$$\psi(x, s) = \frac{\phi(x, s) - \phi(x, t)}{s - t}$$

Claim:

$$\lim_{s \to t} \psi(x, s) = \frac{\partial \phi}{\partial t}(x, t)$$

This convergence is uniform in x (independent of x)

Why? Let $\epsilon > 0$ be given. By uniform continuity of $\frac{\partial \phi}{\partial t}$ there is $\delta > 0$ such that if $|s - t| < \delta$ and all x, we have

$$\left| \frac{\partial \phi}{\partial t}(x, s) - \frac{\partial \phi}{\partial t}(x, t) \right| < \epsilon$$

With that $\delta > 0$, if $|s - t| < \delta$, then by the Mean-Value Theorem applied to $\phi(x, \cdot)$, there is a u between s and t such that

$$\psi(x, s) = \frac{\partial \phi}{\partial t}(x, u)$$

But in particular $|u - t| < \delta$ (u is closer to t than s is) and so

$$\left| \frac{\partial \phi}{\partial t}(x, u) - \frac{\partial \phi}{\partial t}(x, t) \right| < \epsilon \Rightarrow \left| \psi(x, s) - \frac{\partial \phi}{\partial t}(x, t) \right| < \epsilon \checkmark$$

STEP 2: By definition of f, we have

$$\frac{f(s)-f(t)}{s-t} = \int_a^b \psi(x,s)dx$$

But since $\psi(x,s) \to \frac{\partial \phi}{\partial t}(x,t)$ as $s \to t$, uniformly in x, we get

$$\lim_{s\to t} \frac{f(s)-f(t)}{s-t} = \lim_{s\to t} \int_a^b \psi(x,s)dx = \int_a^b \frac{\partial \phi}{\partial t}(x,t)dx$$

(We can put the limit inside the integral by uniform convergence)

This implies that $f'(t)$ exists as a limit and $f'(t) = \int_a^b \frac{\partial \phi}{\partial t}(x,t)dx$ □

Note: There's a related identity called the **Leibniz rule for integrals** that is often used in practice

$$\frac{d}{dt}\int_a^t \phi(x,t)dx = \phi(t,t) + \int_a^t \frac{\partial \phi}{\partial t}(x,t)dx$$

4. An Interesting Example

$$\text{Let } f(t) = \int_{-\infty}^{\infty} e^{-x^2}\cos(xt)dx$$

In this section we will find an explicit formula for f

Claim # 1:

$$f'(t) = g(t) \text{ where } g(t) = \int_{-\infty}^{\infty} -xe^{-x^2}\sin(xt)dx$$

(This is what you expect if you naively differentiate under the integral)

Proof: First of all, notice that for all α and β we have

$$\begin{aligned}\cos(\alpha+\beta)-\cos(\alpha) &= \int_{\alpha}^{\alpha+\beta} -\sin(t)dt\\ \frac{\cos(\alpha+\beta)-\cos(\alpha)}{\beta} &= \frac{1}{\beta}\int_{\alpha}^{\alpha+\beta} -\sin(t)dt\\ \frac{\cos(\alpha+\beta)-\cos(\alpha)}{\beta}+\sin(\alpha) &= \frac{1}{\beta}\int_{\alpha}^{\alpha+\beta} \sin(\alpha)-\sin(t)dt\end{aligned}$$

(Here we used that $\sin(\alpha)$ is constant)

If $\beta > 0$ and using $|\sin(x)-\sin(y)| \leq |x-y|$ and $\alpha - t \leq 0$ we get

$$\begin{aligned}\left|\frac{\cos(\alpha+\beta)-\cos(\alpha)}{\beta}+\sin(\alpha)\right| &= \left|\frac{1}{\beta}\int_{\alpha}^{\alpha+\beta} \sin(\alpha)-\sin(t)dt\right|\\ &\leq \frac{1}{|\beta|}\int_{\alpha}^{\alpha+\beta} \left|\sin(\alpha)-\sin(t)\right| dt\\ &\leq \frac{1}{\beta}\int_{\alpha}^{\alpha+\beta} |\alpha - t|\, dt\\ &= \frac{1}{\beta}\left[\frac{(t-\alpha)^2}{2}\right]_{\alpha}^{\alpha+\beta} = \frac{1}{\beta}\left(\frac{\beta^2}{2}\right) = \frac{\beta}{2}\end{aligned}$$

A similar formula holds if $\beta < 0$ and so

$$\left|\frac{\cos(\alpha+\beta)-\cos(\alpha)}{\beta}+\sin(\alpha)\right| \leq |\beta|$$

Now apply the above with $\alpha = xt$ and $\beta = xh$ and use the definitions of f and g to get

$$\left|\frac{f(t+h)-f(t)}{h} - g(t)\right| \leq |h| \left(\int_{-\infty}^{\infty} x^2 e^{-x^2} dx\right)$$

Therefore, letting $h \to 0$ we obtain that $f'(t) = g(t)$ ✓

Claim # 2: $f(t) = \sqrt{\pi} e^{-\frac{t^2}{4}}$

Proof: Integrate $f(t) = \int_{-\infty}^{\infty} e^{-x^2} \cos(xt) dx$ by parts with $du = \cos(xt)$ and $v = e^{-x^2}$ to get

$$f(t) = -\int_{-\infty}^{\infty} -2xe^{-x^2} \left(\frac{\sin(xt)}{t} \right) dx = -2 \left(\frac{g(t)}{t} \right)$$

$$\begin{aligned} tf(t) &= -2g(t) \\ tf(t) &= -2f'(t) \qquad \text{(Since } f' = g\text{)} \\ \frac{f'(t)}{f(t)} &= -\frac{t}{2} \\ (\ln |f(t)|)' &= -\frac{t}{2} \\ \ln |f(t)| &= -\frac{t^2}{4} + C \\ |f(t)| &= e^C \, e^{-\frac{t^2}{4}} \\ f(t) &= \underbrace{\pm e^C}_{C} e^{-\frac{t^2}{4}} \Rightarrow f(t) = Ce^{-\frac{t^2}{4}} \end{aligned}$$

$$C = f(0) = \int_{-\infty}^{\infty} e^{-x^2} \cos(x0) dx = \int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi}$$

$$\text{Therefore } f(t) = \sqrt{\pi} e^{-\frac{t^2}{4}}$$