MAT235 Tutorial 7: Solutions to Additional Problems

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5. Let $g : \mathbb{R}^2 \times [0, \infty)^2 \to \mathbb{R}$ be a function defined by

$$g(x, y, z, w) = \int_w^z \frac{\arctan(x^2)}{1 + u^u} du$$

where $x, y \in \mathbb{R}$ but $z, w \geq 0$. Compute the following partial derivatives of g:

$$\frac{\partial g}{\partial x}, \quad \frac{\partial g}{\partial y}$$

$$\frac{\partial^2 g}{\partial w^2}, \quad \frac{\partial^2 g}{\partial z^2}, \quad \frac{\partial^2 g}{\partial w \partial z}, \quad \frac{\partial^2 g}{\partial z \partial w}$$

Solution: Let $f : [0, \infty) \to \mathbb{R}$ be defined by $f(u) = \dfrac{1}{1 + u^u}$. Then

$$g(x, y, z, w) = \int_w^z \arctan(x^2) f(u)\, du = \arctan(x^2) \int_w^z f(u)\, du \tag{5.1}$$

where the last equality follows because $\arctan(x^2)$ is independent of u, z and w so the term can be brought outside the integrand. Let us begin by determining the first-order partials. The derivative of $\arctan(x)$ is $\dfrac{1}{1 + x^2}$. Thus, treating the integral as a constant with respect to x and applying the chain rule,

$$\begin{aligned} \frac{\partial g}{\partial x} &= \left[\frac{\partial}{\partial x} \arctan(x^2)\right] \int_w^z f(u)\, du &(5.2)\\ &= \left[\frac{1}{1 + x^4} \cdot 2x\right] \int_w^z f(u)\, du &(5.3)\\ &= \frac{2x}{1 + x^4} \int_w^z f(u)\, du. &(5.4) \end{aligned}$$

The derivative in y is zero: there are no y terms. Hence

$$\boxed{\frac{\partial g}{\partial x} = \frac{2x}{1 + x^4} \int_w^z f(u)\, du, \qquad \frac{\partial g}{\partial y} = 0} \tag{5.5}$$

The second-order derivatives are slightly different, since the z and w terms are the bounds of the integral. Let us recall some single-variable integral identities. Let $g(x)$ be an integrable function over some domain $[a, b]$. Let $c \in [a, b]$ be a point in the domain. Then:

$$\begin{aligned} \int_a^b g(x)\, dx &= -\int_b^a g(x)\, dx &(5.6)\\ \int_a^b g(x)\, dx &= \int_a^c g(x)\, dx + \int_c^b g(x)\, dx. &(5.7) \end{aligned}$$

Furthermore, the Fundamental Theorem of Calculus. Let $G(x) = \int_a^x g(t)\,dt$. Then, for all $x \in [a, b]$,

$$\frac{dG}{dx} = \frac{d}{dx}\int_a^x g(t)\,dt = g(x). \tag{5.8}$$

Consider (5.7) first. If our lower and upper bounds $z, w \geq 0$, then we can expand the integral term as

$$\begin{aligned}\int_w^z f(u)\,du &= \int_w^0 f(u)\,du + \int_0^z f(u)\,du && (5.9)\\ &= \int_0^z f(u)\,du - \int_0^w f(u)\,du && (5.10)\end{aligned}$$

where (5.10) follows from (5.6). Intuitively, this is just the area under f up to z, minus that of the area up to w. If $w > z$, this integral will be negative. If $w = z$, zero. We can now write (5.1) as a sum of integrals via variable separation:

$$g(x, y, z, w) = \arctan(x^2)\left[\int_0^z f(u)\,du - \int_0^w f(u)\,du\right] \tag{5.11}$$

Next, I note that the Fundamental Theorem of Calculus applies along isolated axes, which includes partial derivatives. By (5.8), we can easily calculate the first-order derivatives in z and w:

$$\begin{aligned}\frac{\partial g}{\partial z} &= \arctan(x^2)\frac{\partial}{\partial z}\left[\int_0^z f(u)\,du - \int_0^w f(u)\,du\right] && (5.12)\\ &= \arctan(x^2)\,[f(z) + 0] && (5.13)\\ &= \frac{\arctan(x^2)}{1 + z^z}. && (5.14)\end{aligned}$$

Similarly,

$$\frac{\partial g}{\partial w} = -\frac{\arctan(x^2)}{1 + w^w}. \tag{5.15}$$

The mixed partials are the easiest to find, since each function is only a function of (x, z) or (x, w). Thus any mixed derivative will give zero. Since g is continuous differentiable on $[0, \infty)$, Clairaut's theorem applies and therefore

$$\boxed{\frac{\partial^2 g}{\partial z \partial w} = \frac{\partial^2 g}{\partial w \partial z} = 0} \tag{5.16}$$

The second-order zz/ww derivatives arise by finding the derivative of $f(u)$. We have

$$\begin{aligned}\frac{df}{du} &= \frac{d}{du}\left[\frac{1}{1 + u^u}\right] && (5.17)\\ &= \left(-\frac{1}{(1 + u^u)^2}\right)\frac{d}{du}[1 + u^u] && (5.18)\\ &= \left(-\frac{1}{(1 + u^u)^2}\right)\frac{d}{du}[e^{u\ln u}] && (5.19)\\ &= \left(-\frac{1}{(1 + u^u)^2}\right)e^{u\ln u}\frac{d}{du}[u\ln u] && (5.20)\end{aligned}$$

$$= \left(-\frac{1}{(1+u^u)^2}\right) e^{u\ln u}(\ln u + 1) \tag{5.21}$$

$$= -\frac{(\ln u + 1)u^u}{(1+u^u)^2} \tag{5.22}$$

We note that this function is defined for $u > 0$, and undefined at $u = 0$ although the limit $u \to 0$ exists (but diverges). Therefore

$$\boxed{\frac{\partial^2 g}{\partial z^2} = -\arctan(x^2)\frac{(\ln z + 1)z^z}{(1+z^z)^2}, \qquad \frac{\partial^2 g}{\partial w^2} = \arctan(x^2)\frac{(\ln w + 1)w^w}{(1+w^w)^2}}$$

valid on the domain $z, w \in (0, \infty)$.

6. Determine the Quadratic Taylor polynomial $P_2(x, y)$ of the function $j : \mathbb{R}^2 \to \mathbb{R}$ given by $j(x, y) = \arctan(x + 2y)$ centered about the point (1,0).

Solution: A second-order quadratic Taylor polynomial about a point $\mathbf{p} = (a, b)$ is given by

$$P_2(\mathbf{x}) = f(\mathbf{p}) + \nabla f(\mathbf{p})(\mathbf{x} - \mathbf{p}) + \frac{1}{2}(\mathbf{x} - \mathbf{p})^T Hf(\mathbf{p})(\mathbf{x} - \mathbf{p}) \tag{6.1}$$

where $\mathbf{x} \equiv (x, y)$ and $Hf(\mathbf{p}) = \begin{pmatrix} f_{xx}(\mathbf{p}) & f_{xy}(\mathbf{p}) \\ f_{yx}(\mathbf{p}) & f_{yy}(\mathbf{p}) \end{pmatrix}$ is the Hessian matrix (if you haven't seen this before, it's ok - just compare your solution with mine).

For the function $f(x, y) = \arctan(x + 2y)$, we begin by calculating all partial derivatives up to second order.

$$\begin{align}
f_x(x, y) &= \frac{1}{1 + (x + 2y)^2} \tag{6.2}\\
f_y(x, y) &= \frac{1}{1 + (x + 2y)^2} \cdot 2 \tag{6.3}\\
f_{xx}(x, y) &= -\frac{1}{1 + (x + 2y)^2} \cdot 2(x + 2y) \tag{6.4}\\
f_{yy}(x, y) &= -\frac{2}{1 + (x + 2y)^2} \cdot 4(x + 2y) \tag{6.5}\\
f_{xy}(x, y) &= -\frac{2}{1 + (x + 2y)^2} \cdot 2(x + 2y) = f_{yx}(x, y) \tag{6.6}
\end{align}$$

where (6.6) follows from Clairaut's theorem. We evaluate these derivatives at the point $\mathbf{p} = (1, 0)$, which give

$$\begin{align}
f_x(1, 0) &= \frac{1}{2} \tag{6.7}\\
f_y(1, 0) &= 1 \tag{6.8}\\
f_{xx}(1, 0) &= -1 \tag{6.9}\\
f_{yy}(1, 0) &= -4 \tag{6.10}\\
f_{xy}(1, 0) &= -2 = f_{yx}(1, 0). \tag{6.11}
\end{align}$$

We then work to simplify equation (6.1):

$$\begin{align}
P_2(x, y) &= \frac{1}{2} + \left(\frac{1}{2}, -1\right)\begin{pmatrix} x - 1 \\ y \end{pmatrix} + \frac{1}{2}(x - 1, y)\begin{pmatrix} -1 & -2 \\ -2 & -4 \end{pmatrix}\begin{pmatrix} x - 1 \\ y \end{pmatrix} \tag{6.12}\\
&= \frac{\pi}{4} + \frac{1}{2}(x - 1) + y - \frac{1}{2}(x - 1, y)\begin{pmatrix} (x - 1) + 2y \\ 2(x - 1) + 4y \end{pmatrix} \tag{6.13}\\
&= \frac{\pi}{4} + \frac{1}{2}(x - 1) + y - \frac{1}{2}\left((x - 1)^2 + 2y(x - 1) + 2y(x - 1) + 4y^2\right) \tag{6.14}\\
&= \frac{\pi}{4} + \frac{1}{2}(x - 1) + y - \frac{1}{2}(x - 1)^2 + 2y(x - 1) + 2y^2 \tag{6.15}\\
&= \frac{\pi}{4} + \frac{1}{2}x - \frac{1}{2} + y - \frac{1}{2}x^2 - \frac{1}{2} + x + 2yx - 2y + 2y^2 \tag{6.16}\\
&= \frac{\pi}{4} - 1 + \frac{3}{2}x + 3y - \frac{1}{2}x^2 - 2xy - 2y^2 \tag{6.17}
\end{align}$$

which is the second order Taylor polynomial of $f(x, y)$ about the point $\mathbf{p} = (1, 0)$.

7. Let $q(x,y,z) = \ln(x^2 + \cos(y) + e^{z^2} + 2)$. Find the second order Taylor polynomial of q about $(1, 3\pi/4, 0)$.

Solution: The Taylor polynomial will have 3 variables, so we must find all derivatives of q in the 3 variables. Begin by calculating all first-order partial derivatives. One should find

$$\frac{\partial q}{\partial x} = \frac{2x}{x^2 + \cos y + e^{z^2} + 2} \tag{7.1}$$

$$\frac{\partial q}{\partial y} = -\frac{\sin y}{x^2 + \cos y + e^{z^2} + 2} \tag{7.2}$$

$$\frac{\partial q}{\partial z} = \frac{2ze^{z^2}}{x^2 + \cos y + e^{z^2} + 2} \tag{7.3}$$

Upon evaluating (7.1)-(7.3) at $(1, 3\pi/4, 0)$, $\cos(3\pi/4) = -\frac{\sqrt{2}}{2} = -\sin(3\pi/4)$ and $e^0 = 1$, so the gradient at the point is

$$\nabla q(1, 3\pi/4, 0) = \left\langle \frac{4}{8-\sqrt{2}}, -\frac{\sqrt{2}}{8-\sqrt{2}}, 0 \right\rangle \tag{7.4}$$

(I will quickly note that $q(1, 3\pi/4, 0) = \ln[(8-\sqrt{2})/2]$) The next part is to determine the second-order partials and to form the Hessian matrix. Note that our function is C^2, so we can interchange partials by Clairaut's theorem. One quick observation is that any additional partial derivative involving first-order in z will evaluate to zero, so we need not calculate

$$\frac{\partial^2 q}{\partial z \partial x} = \frac{\partial^2 q}{\partial z \partial y} = 0 \tag{7.5}$$

but not q_{zz}, as you will see will be non-zero. This is because the z constant in (7.3) will always evaluate to zero up to first-order in z. Continuing,

$$\frac{\partial^2 q}{\partial x^2} = \frac{2}{x^2 + \cos y + e^{z^2} + 2} - \frac{2x}{(x^2 + \cos y + e^{z^2} + 2)^2} \cdot 2x \tag{7.6}$$

$$\left.\frac{\partial^2 q}{\partial x^2}\right|_{(1,3\pi/4,0)} = \frac{2}{(8-\sqrt{2})/2} - \frac{4}{(8-\sqrt{2})^2/4} = \frac{4\sqrt{2}}{(8-\sqrt{2})^2} \equiv A \tag{7.7}$$

$$\frac{\partial^2 q}{\partial x \partial y} = -\frac{2x}{(x^2 + \cos y + e^{z^2} + 2)^2}(-\sin y) \tag{7.8}$$

$$\left.\frac{\partial^2 q}{\partial x \partial y}\right|_{(1,3\pi/4,0)} = \frac{2\frac{\sqrt{2}}{2}}{(8-\sqrt{2})^2/4} = \frac{4\sqrt{2}}{(8-\sqrt{2})^2} \equiv A \tag{7.9}$$

$$\frac{\partial^2 q}{\partial y^2} = -\frac{\cos y}{x^2 + \cos y + e^{z^2} + 2} - \left[-\frac{\sin y}{(x^2 + \cos y + e^{z^2} + 2)^2} \cdot (-\sin y)\right] \tag{7.10}$$

$$\left.\frac{\partial^2 q}{\partial y^2}\right|_{(1,3\pi/4,0)} = -\frac{-\sqrt{2}/2}{(8-\sqrt{2})/2} - \frac{(\sqrt{2}/2)^2}{(8-\sqrt{2})^2/4} = \frac{\sqrt{2}}{(8-\sqrt{2})} - \frac{2}{(8-\sqrt{2})^2} = \frac{8\sqrt{2}-4}{(8-\sqrt{2})^2} \equiv B \tag{7.11}$$

$$\frac{\partial^2 q}{\partial z^2} = \frac{2e^{z^2}}{x^2+\cos y+e^{z^2}+2} + \frac{2ze^{z^2}\cdot e^{z^2}2z}{x^2+\cos y+e^{z^2}+2} - \frac{2ze^{z^2}}{(x^2+\cos y+e^{z^2}+2)^2}\cdot e^{z^2}2z \tag{7.12}$$

$$\left.\frac{\partial^2 q}{\partial z^2}\right|_{(1,3\pi/4,0)} = \frac{2}{(8-\sqrt{2})/2} + 0 + 0 = \frac{4}{8-\sqrt{2}} \equiv C \tag{7.13}$$

These are the only unique values in the Hessian since $Hq(1,3\pi/4,0)$ is symmetric (only 6 unique values in the upper-triangle). Therefore we find

$$Hq(1,3\pi/4,0) = \begin{pmatrix} \frac{4\sqrt{2}}{(8-\sqrt{2})^2} & \frac{4\sqrt{2}}{(8-\sqrt{2})^2} & 0 \\ \frac{4\sqrt{2}}{(8-\sqrt{2})^2} & \frac{8\sqrt{2}-4}{(8-\sqrt{2})^2} & 0 \\ 0 & 0 & \frac{4}{8-\sqrt{2}} \end{pmatrix} \tag{7.14}$$

$$= \begin{pmatrix} A & A & 0 \\ A & B & 0 \\ 0 & 0 & C \end{pmatrix} \tag{7.15}$$

where I have used A, B, C as constant placeholds as defined in (7.7), (7.9), (7.11), and (7.13). The three-dimensional quadratic Taylor expansion at a point $P = (\alpha, \beta, \gamma)$ is given by

$$P_2(x,y,z) = q(\alpha,\beta,\gamma) + \nabla q(\alpha,\beta,\gamma)(\mathbf{x}-P) + \frac{1}{2}(\mathbf{x}-P)^T Hq(\alpha,\beta,\gamma)(\mathbf{x}-P) \tag{7.16}$$

Plugging in our expression for the Hessian, the quadratic term *only* is

$$\frac{1}{2}(\mathbf{x}-P)^T Hq(\alpha,\beta,\gamma)(\mathbf{x}-P) = \frac{1}{2}\begin{pmatrix} x-\alpha & y-\beta & z-\gamma \end{pmatrix} \begin{pmatrix} A & A & 0 \\ A & B & 0 \\ 0 & 0 & C \end{pmatrix} \begin{pmatrix} x-\alpha \\ y-\beta \\ z-\gamma \end{pmatrix} \tag{7.17}$$

$$= \frac{1}{2}\begin{pmatrix} x-\alpha & y-\beta & z-\gamma \end{pmatrix} \begin{pmatrix} A(x-\alpha)+A(y-\beta) \\ A(x-\alpha)+B(y-\beta) \\ C(z-\gamma) \end{pmatrix} \tag{7.18}$$

$$= \frac{1}{2}\left[A(x-\alpha)^2 + 2A(x-\alpha)(y-\beta) + B(y-\beta)^2 + C(z-\gamma)^2\right] \tag{7.19}$$

We can now put together the polynomial using our constants, our gradient (7.4), and our Hessian expansion (7.19):

$$\begin{aligned} P_2^q(x,y,z) = {} & \ln[(8-\sqrt{2})/2] + \frac{4}{8-\sqrt{2}}(x-1) - \frac{\sqrt{2}}{8-\sqrt{2}}(y-3\pi/4) \\ & + \frac{A}{2}(x-1)^2 + A(x-1)(y-3\pi/4) + \frac{B}{2}(y-3\pi/4)^2 + \frac{C}{2}z^2 \end{aligned} \tag{7.20}$$

$$\begin{aligned} &= \ln[(8-\sqrt{2})/2] + \frac{4}{8-\sqrt{2}}(x-1) - \frac{\sqrt{2}}{8-\sqrt{2}}(y-3\pi/4) \\ &+ \frac{2\sqrt{2}}{(8-\sqrt{2})^2}(x-1)^2 + \frac{4\sqrt{2}}{(8-\sqrt{2})^2}(x-1)(y-3\pi/4) + \frac{4\sqrt{2}-2}{(8-\sqrt{2})^2}(y-3\pi/4)^2 + \frac{2}{8-\sqrt{2}}z^2 \end{aligned} \tag{7.21}$$

8. Consider a particle in an infinitely deep potential well of width L along $[0, L]$. The time-dependent wavefunction is given by $\psi(x,t) = \sum_{n=1}^{\infty} c_n \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) e^{-\frac{iE_n t}{\hbar}}$ where the c_n are coefficients, $E_n = \frac{n^2\pi^2\hbar^2}{2mL^2}$ is the energy of the particle at the n-th excitation, $\sqrt{\frac{2}{L}}$ yields probabilistic normalization, and m is the mass of the particle. Show that $\psi(x,t)$ satisfies the Schrödinger equation on the domain $0 \leq x \leq L$,

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x,t).$$

Solution: We begin by mentioning the linearity of the derivative operator on functions. For two functions $f : \mathbb{R} \to \mathbb{R}$ and $g : \mathbb{R} \to \mathbb{R}$ and a real constant a, then $\frac{d}{dx}(f + ag) = \frac{df}{dx} + a\frac{dg}{dx}$. This single variable definition extends to multivariable partial derivatives as well.

We show that $\psi(x,t)$ satisfies the Schrödinger equation by calculating the partial derivatives in t and x. We can seperate ψ into positional and temporal components, $\psi(x,t) = \sum_{n=1}^{\infty} \varphi_n(x) e^{-\frac{iE_n t}{\hbar}}$, where the $\varphi_n(x)$ are 'stationary states' given by $\varphi_n(x) = c_n\sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$. We find that

$$\begin{aligned}
\frac{\partial \psi}{\partial t} &= \frac{\partial}{\partial t}\left(\sum_{n=1}^{\infty} \varphi_n(x)\, e^{-\frac{iE_n t}{\hbar}}\right) && (8.1)\\
&= \sum_{n=1}^{\infty} \varphi_n(x) \left(\frac{\partial}{\partial t} e^{-\frac{iE_n t}{\hbar}}\right) && (8.2)\\
&= \sum_{n=1}^{\infty} \varphi_n(x)\, e^{-\frac{iE_n t}{\hbar}} \cdot \frac{-iE_n}{\hbar}. && (8.3)
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{\partial^2 \psi}{\partial x^2} &= \frac{\partial}{\partial t}\left(\sum_{n=1}^{\infty} \varphi_n(x)\, e^{-\frac{iE_n t}{\hbar}}\right) && (8.4)\\
&= \sum_{n=1}^{\infty} c_n\sqrt{\frac{2}{L}}\left(\frac{\partial^2}{\partial x^2}\sin\left(\frac{n\pi x}{L}\right)\right) && (8.5)\\
&= \sum_{n=1}^{\infty} c_n\sqrt{\frac{2}{L}}\left(-\frac{n^2\pi^2}{L^2}\sin\left(\frac{n\pi x}{L}\right)\right) && (8.6)\\
&= -\sum_{n=1}^{\infty} \frac{n^2\pi^2}{L^2}\varphi_n(x)e^{-\frac{iE_n t}{\hbar}}. && (8.7)
\end{aligned}$$

Plugging (8.3) and (8.6) into the Schrödinger equation yields

$$i\hbar\left(\sum_{i=1}^{\infty} \varphi_n(x)\, e^{-\frac{iE_n t}{\hbar}} \cdot \frac{-iE_n}{\hbar}\right) = -\frac{\hbar^2}{2m}\left(-\sum_{n=1}^{\infty}\frac{n^2\pi^2}{L^2}\varphi_n(x)e^{-\frac{iE_n t}{\hbar}}\right) \qquad (8.8)$$

which must be true for every n. After distributing the factors of i and $\hbar$ and recalling that $i^2 = -1$, we substitute $E_n = \dfrac{n^2\pi^2\hbar^2}{2mL^2}$ and find that

$$\sum_{n=1}^{\infty} \varphi_n(x) e^{-\frac{iE_n t}{\hbar}} E_n = \sum_{n=1}^{\infty} \frac{\hbar^2}{2m} \cdot \frac{n^2\pi^2}{L^2} \varphi_n(x) e^{-\frac{iE_n t}{\hbar}} \tag{8.9}$$

$$\implies \sum_{n=1}^{\infty} \varphi_n(x) e^{-\frac{iE_n t}{\hbar}} E_n = \sum_{n=1}^{\infty} \varphi_n(x) e^{-\frac{iE_n t}{\hbar}} E_n \tag{8.10}$$

$$\implies \psi(x,t) = \psi(x,t) \tag{8.11}$$

hence $\psi(x,t)$ satisfied the Schrödinger equation.