Part IA: Mathematics for Natural Sciences B
Examples Sheet 13: The multivariable chain rule, exact differentials, and applications in thermodynamics

Model Solutions

Please send all comments and corrections to jmm232@cam.ac.uk.

The multivariable chain rule for first-order derivatives

1. Let $u \equiv u(x,y), v \equiv v(x,y)$ be functions of x, y, and let $f \equiv f_{xy}(x,y) \equiv f_{uv}(u,v)$ be a function which can be written in terms of x, y or in terms of u, v (so that f_{xy} represents the function f written in terms of x, y, and f_{uv} represents the function f written in terms of u, v).

(a) Using the limit definition of partial differentiation, show that:

$$\frac{\partial f_{xy}}{\partial x} = \frac{\partial f_{uv}}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f_{uv}}{\partial v}\frac{\partial v}{\partial x}, \qquad \text{and} \qquad \frac{\partial f_{xy}}{\partial y} = \frac{\partial f_{uv}}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial f_{uv}}{\partial v}\frac{\partial v}{\partial y}.$$

These formulae are called the *multivariable chain rules*. Learn them off by heart, and get your supervision partner to test you on them. [*Note: Normally, they are written without the subscripts and the dependence of f on (x,y) or (u,v) is left implicit! From now on, we will drop the coordinates - you can always write them in though, if you feel uncomfortable.*]

(b) Hence, prove that the differentials satisfy $df_{xy} = df_{uv}$. [*In lectures, you showed that if this is true, the multivariable chain rule follows. Hence, the multivariable chain rule is equivalent to the statement that 'differentials are independent of coordinate choice'.*]

Solution:

(a) We shall prove the first formula, and the second is proved similarly. We have:

$$\begin{aligned}
\frac{\partial f_{xy}}{\partial x} &= \lim_{h\to 0}\frac{f_{xy}(x+h,y) - f_{xy}(x,y)}{h} \\
&= \lim_{h\to 0}\frac{f_{uv}(u(x+h,y),v(x+h,y)) - f_{uv}(u(x,y),v(x,y))}{h} \\
&= \lim_{h\to 0}\left(\frac{f_{uv}(u(x+h,y),v(x+h,y)) - f_{uv}(u(x,y),v(x+h,y))}{h}\right) \\
&\qquad + \lim_{h\to 0}\left(\frac{f_{uv}(u(x,y),v(x,y)+v(x+h,y)-v(x,y)) - f_{uv}(u(x,y),v(x,y))}{h}\right).
\end{aligned}$$

The second term can be rewritten as:

$$\lim_{h\to 0}\left(\frac{f_{uv}(u(x,y),v(x,y)+v(x+h,y)-v(x,y)) - f_{uv}(u(x,y),v(x,y))}{v(x+h,y)-v(x,y)}\right)\cdot\lim_{h\to 0}\left(\frac{v(x+h,y)-v(x,y)}{h}\right).$$

Making the substitution $\Delta v = v(x+h,y) - v(x,y)$ in the first limit, we have $\Delta v \to 0$ as $h \to 0$, which gives:

$$\frac{\partial f_{uv}}{\partial v}\frac{\partial v}{\partial x},$$

as anticipated.

In the remaining term, we can use some Taylor expansion. We have:

$$u(x+h,y) = u(x,y) + h\frac{\partial u}{\partial x} + O(h^2).$$

Hence:

$$\begin{aligned}
&f_{uv}(u(x+h,y)v(x+h,y)) - f_{uv}(u(x,y),v(x+h,y)) \\
&\quad = f_{uv}\left(u(x,y) + h\frac{\partial u}{\partial x} + O(h^2), v(x+h,y)\right) - f_{uv}(u(x,y),v(x+h,y)) \\
&\quad = f_{uv}(u(x,y),v(x+h,y)) + h\frac{\partial u}{\partial x}\frac{\partial f_{uv}}{\partial u}(u(x,y),v(x+h,y)) + O(h^2) - f_{uv}(u(x,y),v(x+h,y)).
\end{aligned}$$

Dividing by h and taking the limit as $h \to 0$, we get the correct remaining term. Phew!

(b) The differentials are given respectively by:

$$df_{xy} = \frac{\partial f_{xy}}{\partial x}dx + \frac{\partial f_{xy}}{\partial y}dy,$$

and:

$$\begin{aligned}
df_{uv} &= \frac{\partial f_{uv}}{\partial u}du + \frac{\partial f_{uv}}{\partial v}dv \\
&= \frac{\partial f_{uv}}{\partial u}\left(\frac{\partial u}{\partial x}dx + \frac{\partial u}{\partial y}dy\right) + \frac{\partial f_{uv}}{\partial v}\left(\frac{\partial v}{\partial x}dx + \frac{\partial v}{\partial y}dy\right) \\
&= \left(\frac{\partial f_{uv}}{\partial x}\frac{\partial u}{\partial x} + \frac{\partial f_{uv}}{\partial x}\frac{\partial v}{\partial x}\right)dx + \left(\frac{\partial f_{uv}}{\partial y}\frac{\partial u}{\partial y} + \frac{\partial f_{uv}}{\partial y}\frac{\partial v}{\partial y}\right)dy.
\end{aligned}$$

Using the result from part (a), we see immediately that $df_{xy} = df_{uv}$, so that indeed the differential is 'coordinate independent'. In the lectures, you proved that if the differential is 'coordinate independent' then the multivariable chain rule follows (which is easier, but requires you to believe this non-trivial fact in the first place!).

2. Using the multivariable chain rule, show that if $f(u,v) = u^2 + v^2$, and $u(x,y) = x^3 - 2y, v(x,y) = 3y - 2x^2$, we have:

$$\frac{\partial f}{\partial x} = 2x\left(3x^4 - 6xy - 12y + 8x^2\right), \qquad \frac{\partial f}{\partial y} = 2\left(13y - 6x^2 - 2x^3\right).$$

Check your results by writing f in terms of x, y first, then taking partial derivatives.

➻ **Solution:** We have:

$$\begin{aligned}\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x} \\ &= 2u \cdot 3x^2 + 2v \cdot (-4x) \\ &= 2(x^3 - 2y) \cdot 3x^2 + 2(3y - 2x^2) \cdot (-4x) \\ &= 6x^5 - 12x^2y - 24xy + 16x^3 \\ &= 2x\left(3x^4 - 6xy - 12y + 8x^2\right).\end{aligned}$$

Checking the answer, we note that:

$$f(x,y) = (x^3 - 2y)^2 + (3y - 2x^2)^2 = x^6 - 4x^3y + 13y^2 - 12yx^2 + 4x^4.$$

Differentiating, we have:

$$\frac{\partial f}{\partial x} = 6x^5 - 12x^2y - 24xy + 16x^3 = 2x\left(3x^4 - 6xy - 12y + 8x^2\right),$$

as expected.

For the y-derivative, we have:

$$\begin{aligned}\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial y} \\ &= 2u \cdot (-2) + 2v \cdot (3) \\ &= -4(x^3 - 2y) + 6(3y - 2x^2) \\ &= 2\left(13y - 6x^2 - 2x^3\right),\end{aligned}$$

as required. Checking the answer, using the expression for $f(x,y)$ from above, we have:

$$\frac{\partial f}{\partial y} = -4x^3 + 26y - 12x^2 = 2\left(13y - 6x^2 - 2x^3\right),$$

as expected.

3. Let (x, y) be plane Cartesian coordinates, and let (r, θ) be plane polar coordinates. Let $f \equiv f(x, y)$ be a multivariable function whose expression in terms of Cartesian coordinates is $f(x, y) = e^{-xy}$.

(a) Compute $\partial f/\partial x$ and $\partial f/\partial y$.

(b) Compute $\partial f/\partial r$ and $\partial f/\partial \theta$, by: (i) writing f in terms of polar coordinates; (ii) using the multivariable chain rule.

(c) Using parts (a), (b), show directly in this case that the differential, df, is independent of coordinate choice. [*Hint: express dx and dy in terms of dr and $d\theta$.*]

Solution:

(a) We have:

$$\frac{\partial f}{\partial x} = -ye^{-xy}, \qquad \frac{\partial f}{\partial y} = -xe^{-xy}.$$

(b) (i) By first writing f in polar coordinates using $x = r\cos(\theta), y = r\sin(\theta)$, we have $f(r, \theta) = e^{-r^2\sin(\theta)\cos(\theta)} = e^{-\frac{1}{2}r^2\sin(2\theta)}$. Thus:

$$\frac{\partial f}{\partial r} = -r\sin(2\theta)e^{-\frac{1}{2}r^2\sin(2\theta)}, \qquad \frac{\partial f}{\partial \theta} = -r^2\cos(2\theta)e^{-\frac{1}{2}r^2\sin(2\theta)}.$$

(ii) Instead using the multivariable chain rule, we have:

$$\begin{aligned}\frac{\partial f}{\partial r} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial r} \\ &= -ye^{-xy}\cos(\theta) - xe^{-xy}\sin(\theta) \\ &= -2r\sin(\theta)\cos(\theta)e^{-\frac{1}{2}r^2\sin(2\theta)} \\ &= -r\sin(2\theta)e^{-\frac{1}{2}r^2\sin(2\theta)},\end{aligned}$$

which agrees with the previous result. Similarly, we have:

$$\begin{aligned}\frac{\partial f}{\partial \theta} &= \frac{\partial f}{\partial x}\frac{\partial x}{\partial \theta} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial \theta} \\ &= -ye^{-xy}\cdot(-r\sin(\theta)) - xe^{-xy}\cdot(r\cos(\theta)) \\ &= r^2(\sin^2(\theta) - \cos^2(\theta))e^{-\frac{1}{2}r^2\sin(2\theta)} \\ &= -r^2\cos(2\theta)e^{-\frac{1}{2}r^2\sin(2\theta)},\end{aligned}$$

which agrees with the previous result.

(c) We wish to show that:

$$df = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy = \frac{\partial f}{\partial r}dr + \frac{\partial f}{\partial \theta}d\theta.$$

Note that:

$$dx = \frac{\partial x}{\partial r}dr + \frac{\partial x}{\partial \theta}d\theta = \cos(\theta)dr - r\sin(\theta)d\theta, \qquad dy = \frac{\partial y}{\partial r}dr + \frac{\partial y}{\partial \theta}d\theta = \sin(\theta)dr + r\cos(\theta)d\theta.$$

Inserting into the above expression, we see that:

$$\left(\cos(\theta)\frac{\partial f}{\partial x} + \sin(\theta)\frac{\partial f}{\partial y}\right)dr + \left(-r\sin(\theta)\frac{\partial f}{\partial x} + r\cos(\theta)\frac{\partial f}{\partial y}\right)d\theta = \frac{\partial f}{\partial r}dr + \frac{\partial f}{\partial \theta}d\theta,$$

which we have verified explicitly in parts (a) and (b).

4. The function $f(x, y)$ satisfies the partial differential equation:

$$y\frac{\partial f}{\partial x} + x\frac{\partial f}{\partial y} = 0.$$

By transforming to the coordinates $(u, v) = (x^2 - y^2, 2xy)$, find the general solution of the equation.

➼ **Solution:** We have:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x} = 2x\frac{\partial f}{\partial u} + 2y\frac{\partial f}{\partial v},$$

so:

$$y\frac{\partial f}{\partial x} = 2xy\frac{\partial f}{\partial u} + 2y^2\frac{\partial f}{\partial v}.$$

Meanwhile, we also have:

$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial y} = -2y\frac{\partial f}{\partial u} + 2x\frac{\partial f}{\partial v},$$

so:

$$x\frac{\partial f}{\partial y} = -2xy\frac{\partial f}{\partial u} + 2x^2\frac{\partial f}{\partial v}.$$

The equation therefore gives:

$$2(x^2 + y^2)\frac{\partial f}{\partial v} = 0 \qquad \Leftrightarrow \qquad \frac{\partial f}{\partial v} = 0.$$

It follows that $f(u, v) = g(u)$, where g is an arbitrary function of u. In the original coordinates, $f(x, y) = g(x^2 - y^2)$, where g is an arbitrary function.

The multivariable chain rule for second-order derivatives

5. Let $f(u,v) = u^2\sinh(v)$, and let $u = x, v = x+y$.
   (a) By differentiating with respect to u, compute $\partial^2 f/\partial u^2$.
   (b) Using the multivariable chain rule, show that:
$$\frac{\partial^2 f}{\partial u^2} = \frac{\partial^2 f}{\partial x^2} - 2\frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 f}{\partial y^2},$$
   Hence compute the derivative in (a) by writing f in terms of x, y, differentiating, and using this relationship.
   (c) Repeat this exercise for the derivatives $\partial^2 f/\partial v^2$ and $\partial^2 f/\partial u \partial v$.

Solution:

(a) We obviously have:
$$\frac{\partial^2 f}{\partial u^2} = 2\sinh(v).$$

(b) First, note that $x = u$ and $y = v - x = v - u$. Hence, taking the first derivative, we have by the multivariable chain rule:
$$\frac{\partial f}{\partial u} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial u} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial u} = \frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}.$$
Now we treat $\partial f/\partial u$ as another function to which we can apply the multivariable chain rule (this is where the confusion usually starts). We have by the multivariable chain rule:
$$\begin{aligned}\frac{\partial^2 f}{\partial u^2} = \frac{\partial}{\partial u}\left(\frac{\partial f}{\partial u}\right) &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right)\frac{\partial x}{\partial u} + \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial u}\right)\frac{\partial y}{\partial u} \\ &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right) - \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial u}\right).\end{aligned}$$
Now, inserting the expression we already found for the first partial u-derivative in terms of (x,y), we have:
$$\begin{aligned}\frac{\partial^2 f}{\partial u^2} &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}\right) - \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial x} - \frac{\partial f}{\partial y}\right) \\ &= \frac{\partial^2 f}{\partial x^2} - 2\frac{\partial^2 f}{\partial x \partial y} + \frac{\partial^2 f}{\partial y^2},\end{aligned}$$
as required.

Writing f in terms of (x,y) then, we have $f(x,y) = x^2\sinh(x+y)$. Thus:
$$\frac{\partial^2 f}{\partial x^2} = 2\sinh(x+y) + 4x\cosh(x+y) + x^2\sinh(x+y), \qquad \frac{\partial^2 f}{\partial x \partial y} = 2x\cosh(x+y) + x^2\sinh(x+y),$$
$$\frac{\partial^2 f}{\partial y^2} = x^2\sinh(x+y).$$
Thus:
$$\begin{aligned}\frac{\partial^2 f}{\partial u^2} &= 2\sinh(x+y) + 4x\cosh(x+y) + x^2\sinh(x+y) - 4x\cosh(x+y) - 2x^2\sinh(x+y) + x^2\sinh(x+y) \\ &= 2\sinh(x+y) \\ &= 2\sinh(v),\end{aligned}$$
agreeing with what we found previously.

(c) We are now asked to laboriously repeat this exercise for the remaining two second derivatives, as useful practice. We first have:

$$\frac{\partial f}{\partial v} = \frac{\partial f}{\partial x}\frac{\partial x}{\partial v} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial v} = \frac{\partial f}{\partial y}.$$

Taking a second derivative, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial v^2} &= \frac{\partial}{\partial v}\left(\frac{\partial f}{\partial v}\right) \\
&= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial v}\right)\frac{\partial x}{\partial v} + \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial v}\right)\frac{\partial y}{\partial v} \\
&= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial v}\right) \\
&= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) \\
&= \frac{\partial^2 f}{\partial y^2}.
\end{aligned}$$

Comparing the derivatives computed both ways, we note for $f(u, v) = u^2 \sinh(v) = x^2 \sinh(x + y)$, we have:

$$\frac{\partial^2 f}{\partial v^2} = u^2 \sinh(v), \qquad \frac{\partial^2 f}{\partial y^2} = x^2 \sinh(x + y),$$

which indeed agree.

On the other hand, for the mixed derivative, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial u \partial v} &= \frac{\partial}{\partial u}\left(\frac{\partial f}{\partial v}\right) \\
&= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)\frac{\partial x}{\partial u} + \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right)\frac{\partial y}{\partial u} \\
&= \frac{\partial^2 f}{\partial x \partial y} - \frac{\partial^2 f}{\partial y^2}.
\end{aligned}$$

Comparing the derivatives computed both ways, we note for $f(u, v) = u^2 \sinh(v) = x^2 \sinh(x + y)$, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial u \partial v} &= 2u \cosh(v) = 2x \cosh(x + y), \\
\frac{\partial^2 f}{\partial x \partial y} - \frac{\partial^2 f}{\partial y^2} &= 2x \cosh(x + y) + x^2 \sinh(x + y) - x^2 \sinh(x + y) = 2x \cosh(x + y),
\end{aligned}$$

in perfect agreement.

6. Let $f(u,v)$ be a multivariable function of $u(x,y) = 1 + x^2 + y^2$, $v(x,y) = 1 + x^2y^2$, where (x,y) are plane Cartesian coordinates.

(a) Calculate $\partial f/\partial x, \partial f/\partial y, \partial^2 f/\partial x^2, \partial^2 f/\partial y^2, \partial^2 f/\partial x\partial y$ in terms of the derivatives of f with respect to u, v.

(b) For $f(u,v) = \log(uv)$, find $\partial^2 f/\partial x\partial y$ by: (i) using the expression derived in part (a); (ii) first expressing f in terms of x, y and then differentiating directly. Verify that your results agree.

Solution:

(a) Using the multivariable chain rule, we have:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x} = 2x\frac{\partial f}{\partial u} + 2xy^2\frac{\partial f}{\partial v},$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial y} = 2y\frac{\partial f}{\partial u} + 2yx^2\frac{\partial f}{\partial v}.$$

The second derivatives can be computed similarly. We have:

$$\begin{aligned}\frac{\partial^2 f}{\partial x^2} &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right)\\ &= \frac{\partial}{\partial x}\left(2x\frac{\partial f}{\partial u} + 2xy^2\frac{\partial f}{\partial v}\right)\\ &= 2\frac{\partial f}{\partial u} + 2x\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right) + 2y^2\frac{\partial f}{\partial v} + 2xy^2\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial v}\right).\end{aligned}$$

Note that $\partial f/\partial u, \partial f/\partial v$ are functions of $(u,v) = (u(x,y), v(x,y))$ so we can use the multivariable chain rule again on them. We get:

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right) = \frac{\partial^2 f}{\partial u^2}\frac{\partial u}{\partial x} + \frac{\partial^2 f}{\partial u\partial v}\frac{\partial v}{\partial x} = 2x\frac{\partial^2 f}{\partial u^2} + 2xy^2\frac{\partial^2 f}{\partial u\partial v}.$$

Similarly, we have:

$$\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial v}\right) = \frac{\partial^2 f}{\partial u\partial v}\frac{\partial u}{\partial x} + \frac{\partial^2 f}{\partial v^2}\frac{\partial v}{\partial x} = 2x\frac{\partial^2 f}{\partial u\partial v} + 2xy^2\frac{\partial^2 f}{\partial v^2}.$$

Putting everything together, we have:

$$\boxed{\frac{\partial^2 f}{\partial x^2} = 4x^2\frac{\partial^2 f}{\partial u^2} + 8x^2y^2\frac{\partial^2 f}{\partial u\partial v} + 4x^2y^4\frac{\partial^2 f}{\partial v^2} + 2\frac{\partial f}{\partial u} + 2y^2\frac{\partial f}{\partial v}.}$$

We now repeat the calculation for the second y-derivative. We have:

$$\begin{aligned}\frac{\partial^2 f}{\partial y^2} &= \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right)\\ &= \frac{\partial}{\partial y}\left(2y\frac{\partial f}{\partial u} + 2yx^2\frac{\partial f}{\partial v}\right)\\ &= 2\frac{\partial f}{\partial u} + 2y\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial u}\right) + 2x^2\frac{\partial f}{\partial v} + 2yx^2\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial v}\right).\end{aligned}$$

Using the multivariable chain rule to calculate the y-derivatives of $\partial f/\partial u$ and $\partial f/\partial v$, we have:

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial u}\right) = \frac{\partial^2 f}{\partial u^2}\frac{\partial u}{\partial y} + \frac{\partial^2 f}{\partial u\partial v}\frac{\partial v}{\partial y} = 2y\frac{\partial^2 f}{\partial u^2} + 2yx^2\frac{\partial^2 f}{\partial u\partial v},$$

$$\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial v}\right) = \frac{\partial^2 f}{\partial u\partial v}\frac{\partial u}{\partial y} + \frac{\partial^2 f}{\partial v^2}\frac{\partial v}{\partial y} = 2y\frac{\partial^2 f}{\partial u\partial v} + 2yx^2\frac{\partial^2 f}{\partial v^2}.$$

Putting everything together, we have:

$$\boxed{\frac{\partial^2 f}{\partial y^2} = 4y^2\frac{\partial^2 f}{\partial u^2} + 8y^2x^2\frac{\partial^2 f}{\partial u\partial v} + 4y^2x^4\frac{\partial^2 f}{\partial v^2} + 2\frac{\partial f}{\partial u} + 2x^2\frac{\partial f}{\partial v}}$$

Finally, we repeat the calculation for the mixed derivative. We have:

$$\begin{aligned}\frac{\partial^2 f}{\partial x\partial y} &= \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial y}\right)\\ &= \frac{\partial}{\partial x}\left(2y\frac{\partial f}{\partial u} + 2yx^2\frac{\partial f}{\partial v}\right)\\ &= 2y\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right) + 4xy\frac{\partial f}{\partial v} + 2yx^2\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial v}\right).\end{aligned}$$

Using the expressions we calculated previously for the x-derivative of $\partial f/\partial u, \partial f/\partial v$, we have:

$$\boxed{\frac{\partial^2 f}{\partial x\partial y} = 4xy\frac{\partial^2 f}{\partial u^2} + 8xy^3\frac{\partial^2 f}{\partial u\partial v} + 4x^3y^3\frac{\partial^2 f}{\partial v^2} + 4xy\frac{\partial f}{\partial v}.}$$

(b) Here, we have $f(u,v) = \log(uv)$. Hence,

$$\frac{\partial f}{\partial u} = \frac{1}{u}, \qquad \frac{\partial f}{\partial v} = \frac{1}{v}, \qquad \frac{\partial^2 f}{\partial u^2} = -\frac{1}{u^2}, \qquad \frac{\partial^2 f}{\partial u\partial v} = 0, \qquad \frac{\partial^2 f}{\partial v^2} = -\frac{1}{v^2}.$$

Inserting these expressions into the formula for $\partial^2 f/\partial x\partial y$ that we derived above, we have:

$$\frac{\partial^2 f}{\partial x\partial y} = -\frac{4xy}{u^2} - \frac{4x^3y^3}{v^2} + \frac{4xy}{v} = -\frac{4xy}{(1+x^2+y^2)^2} - \frac{4x^3y^3}{(1+x^2y^2)^2} + \frac{4xy}{1+x^2y^2}.$$

Alternatively, we can first write $f(u,v) = f(u(x,y), v(x,y)) = \log(1+x^2+y^2) + \log(1+x^2y^2)$. This gives:

$$\frac{\partial f}{\partial x} = \frac{2x}{1+x^2+y^2} + \frac{2xy^2}{1+x^2y^2},$$

and hence:

$$\frac{\partial^2 f}{\partial x\partial y} = -\frac{4xy}{(1+x^2+y^2)^2} - \frac{4x^3y^3}{(1+x^2y^2)^2} + \frac{4xy}{1+x^2y^2},$$

verifying our calculation.

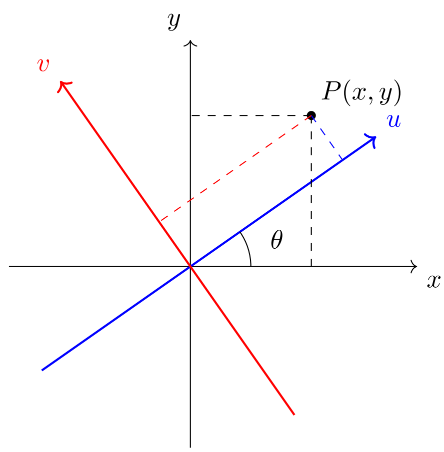
7. Let (x, y) be plane Cartesian coordinates, and let (u, v) be plane Cartesian coordinates which are rotated an angle θ anti-clockwise about the origin relative to the (x, y) coordinates. Let f be an arbitrary multivariable function of either (x, y) or (u, v). Show that:

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{\partial^2 f}{\partial u^2} + \frac{\partial^2 f}{\partial v^2}.$$

$(*)$ Comment on this result in relation to the *Laplacian*, $\nabla^2 = \nabla \cdot \nabla$, where $\cdot$ is the scalar product of vectors.

➡ **Solution:** Using some geometry, we see that the coordinate systems are related via the transformation:

$$u = \cos(\theta)x + \sin(\theta)y,$$
$$v = -\sin(\theta)x + \cos(\theta)y.$$



One way of easily getting this transformation is to imagine what the new coordinates of the points $(1, 0)$ and the points $(0, 1)$ will be in the (u, v) system. By linearity (rotations are linear maps), this generates the entire transformation.

This relationship implies:

$$\frac{\partial f}{\partial x} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial x} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial x} = \cos(\theta)\frac{\partial f}{\partial u} - \sin(\theta)\frac{\partial f}{\partial v},$$
$$\frac{\partial f}{\partial y} = \frac{\partial f}{\partial u}\frac{\partial u}{\partial y} + \frac{\partial f}{\partial v}\frac{\partial v}{\partial y} = \sin(\theta)\frac{\partial f}{\partial u} + \cos(\theta)\frac{\partial f}{\partial v}.$$

Taking a second derivative, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial x^2} &= \frac{\partial}{\partial x}\left(\cos(\theta)\frac{\partial f}{\partial u} - \sin(\theta)\frac{\partial f}{\partial v}\right) \\
&= \cos(\theta)\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial u}\right) - \sin(\theta)\frac{\partial}{\partial x}\left(\frac{\partial f}{\partial v}\right) \\
&= \cos(\theta)\left(\frac{\partial^2 f}{\partial u^2}\frac{\partial u}{\partial x} + \frac{\partial^2 f}{\partial u \partial v}\frac{\partial v}{\partial x}\right) - \sin(\theta)\left(\frac{\partial^2 f}{\partial u \partial v}\frac{\partial u}{\partial x} + \frac{\partial^2 f}{\partial v^2}\frac{\partial v}{\partial x}\right) \\
&= \cos(\theta)\left(\cos(\theta)\frac{\partial^2 f}{\partial u^2} - \sin(\theta)\frac{\partial^2 f}{\partial u \partial v}\right) - \sin(\theta)\left(\cos(\theta)\frac{\partial^2 f}{\partial u \partial v} - \sin(\theta)\frac{\partial^2 f}{\partial v^2}\right) \\
&= \cos^2(\theta)\frac{\partial^2 f}{\partial u^2} - 2\sin(\theta)\cos(\theta)\frac{\partial^2 f}{\partial u \partial v} + \sin^2(\theta)\frac{\partial^2 f}{\partial v^2}.
\end{aligned}$$

Similarly, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial y^2} &= \frac{\partial}{\partial y}\left(\sin(\theta)\frac{\partial f}{\partial u} + \cos(\theta)\frac{\partial f}{\partial v}\right) \\
&= \sin(\theta)\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial u}\right) + \cos(\theta)\frac{\partial}{\partial y}\left(\frac{\partial f}{\partial v}\right) \\
&= \sin(\theta)\left(\frac{\partial^2 f}{\partial u^2}\frac{\partial u}{\partial y} + \frac{\partial^2 f}{\partial u \partial v}\frac{\partial v}{\partial y}\right) + \cos(\theta)\left(\frac{\partial^2 f}{\partial u \partial v}\frac{\partial u}{\partial y} + \frac{\partial^2 f}{\partial v^2}\frac{\partial v}{\partial y}\right) \\
&= \sin^2(\theta)\frac{\partial^2 f}{\partial u^2} + 2\sin(\theta)\cos(\theta)\frac{\partial^2 f}{\partial u \partial v} + \cos^2(\theta)\frac{\partial^2 f}{\partial v^2}.
\end{aligned}$$

Summing the results we have obtained previously, we obtain the identity:

$$\frac{\partial^2 f}{\partial u^2} + \frac{\partial^2 f}{\partial v^2} = \frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2},$$

as required.

The *Laplacian* is defined as the scalar product of the gradient with itself, giving:

$$\nabla \cdot \nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) \cdot \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right) = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}.$$

We have shown that this is invariant under a rotation of the coordinate system. This is consistent with the fact that the scalar product of two vectors is invariant under a rotation of our coordinate system, since it only depends on the lengths and angles of the vectors involved (even though here, we have differential operators inside our vectors instead of numbers!).

8. Let (x, y) be plane Cartesian coordinates, and let (r, θ) be plane polar coordinates. Let f be a multivariable function. Show that:

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2}.$$

Hence determine all solutions of the partial differential equation:

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = 0$$

which are rotationally symmetric about the origin.

➡ **Solution:** Note that $r = \sqrt{x^2 + y^2}, \theta = \arctan(y/x)$. Hence we have:

$$\begin{aligned}
\frac{\partial f}{\partial x} &= \frac{\partial f}{\partial r}\frac{\partial r}{\partial x} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial x} \\
&= \frac{x}{\sqrt{x^2 + y^2}}\frac{\partial f}{\partial r} + \frac{(-y/x^2)}{1 + (y/x)^2}\frac{\partial f}{\partial \theta} \\
&= \cos(\theta)\frac{\partial f}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial f}{\partial \theta}.
\end{aligned}$$

Observe that we can take the second derivative in exactly the same way, giving:

$$\begin{aligned}
\frac{\partial^2 f}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial f}{\partial x}\right) &= \cos(\theta)\frac{\partial}{\partial r}\left(\frac{\partial f}{\partial x}\right) - \frac{\sin(\theta)}{r}\frac{\partial}{\partial \theta}\left(\frac{\partial f}{\partial x}\right) \\
&= \cos(\theta)\frac{\partial}{\partial r}\left(\cos(\theta)\frac{\partial f}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial f}{\partial \theta}\right) - \frac{\sin(\theta)}{r}\frac{\partial}{\partial \theta}\left(\cos(\theta)\frac{\partial f}{\partial r} - \frac{\sin(\theta)}{r}\frac{\partial f}{\partial \theta}\right) \\
&= \cos^2(\theta)\frac{\partial^2 f}{\partial r^2} + \frac{\sin(\theta)\cos(\theta)}{r^2}\frac{\partial f}{\partial \theta} - \frac{\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} + \frac{\sin^2(\theta)}{r}\frac{\partial f}{\partial r} - \frac{\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} \\
&\qquad + \frac{\sin(\theta)\cos(\theta)}{r^2}\frac{\partial f}{\partial \theta} + \frac{\sin^2(\theta)}{r^2}\frac{\partial^2 f}{\partial \theta^2} \\
&= \cos^2(\theta)\frac{\partial^2 f}{\partial r^2} + \frac{2\sin(\theta)\cos(\theta)}{r^2}\frac{\partial f}{\partial \theta} - \frac{2\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} + \frac{\sin^2(\theta)}{r}\frac{\partial f}{\partial r} + \frac{\sin^2(\theta)}{r^2}\frac{\partial^2 f}{\partial \theta^2}.
\end{aligned}$$

Proceeding in a similar way for the y-derivatives, we have:

$$\begin{aligned}
\frac{\partial f}{\partial y} &= \frac{\partial f}{\partial r}\frac{\partial r}{\partial y} + \frac{\partial f}{\partial \theta}\frac{\partial \theta}{\partial y} \\
&= \frac{y}{\sqrt{x^2 + y^2}}\frac{\partial f}{\partial r} + \frac{(1/x)}{1 + (y/x)^2}\frac{\partial f}{\partial \theta} \\
&= \sin(\theta)\frac{\partial f}{\partial r} + \frac{\cos(\theta)}{r}\frac{\partial f}{\partial \theta}.
\end{aligned}$$

Taking the second derivative, we have:

$$\begin{aligned}
\frac{\partial^2 f}{\partial y^2} = \frac{\partial}{\partial y}\left(\frac{\partial f}{\partial y}\right) &= \sin(\theta)\frac{\partial}{\partial r}\left(\frac{\partial f}{\partial y}\right) + \frac{\cos(\theta)}{r}\frac{\partial}{\partial \theta}\left(\frac{\partial f}{\partial y}\right) \\
&= \sin(\theta)\frac{\partial}{\partial r}\left(\sin(\theta)\frac{\partial f}{\partial r} + \frac{\cos(\theta)}{r}\frac{\partial f}{\partial \theta}\right) + \frac{\cos(\theta)}{r}\frac{\partial}{\partial \theta}\left(\sin(\theta)\frac{\partial f}{\partial r} + \frac{\cos(\theta)}{r}\frac{\partial f}{\partial \theta}\right) \\
&= \sin^2(\theta)\frac{\partial^2 f}{\partial r^2} - \frac{\sin(\theta)\cos(\theta)}{r^2}\frac{\partial f}{\partial \theta} + \frac{\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} + \frac{\cos^2(\theta)}{r}\frac{\partial f}{\partial r} \\
&\quad + \frac{\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} - \frac{\sin(\theta)\cos(\theta)}{r}\frac{\partial f}{\partial \theta} + \frac{\cos^2(\theta)}{r^2}\frac{\partial^2 f}{\partial \theta^2} \\
&= \sin^2(\theta)\frac{\partial^2 f}{\partial r^2} - \frac{2\sin(\theta)\cos(\theta)}{r^2}\frac{\partial f}{\partial \theta} + \frac{2\sin(\theta)\cos(\theta)}{r}\frac{\partial^2 f}{\partial r \partial \theta} + \frac{\cos^2(\theta)}{r}\frac{\partial f}{\partial r} + \frac{\cos^2(\theta)}{r^2}\frac{\partial^2 f}{\partial \theta^2}.
\end{aligned}$$

Summing the second derivatives, we obtain:

$$\frac{\partial^2 f}{\partial x^2} + \frac{\partial^2 f}{\partial y^2} = \frac{\partial^2 f}{\partial r^2} + \frac{1}{r}\frac{\partial f}{\partial r} + \frac{1}{r^2}\frac{\partial^2 f}{\partial \theta^2},$$

as requested.

When $f(x, y) = f(r, \theta)$ is rotationally symmetric about the origin, it has no θ dependence. Hence $f \equiv f(r)$. Therefore, using the polar form of the given equation, we have:

$$f''(r) + \frac{f'(r)}{r} = 0.$$

This is a first-order equation for $f'(r)$, with integrating factor $e^{\ln(r)} = r$. Hence:

$$\frac{d}{dr}\left(rf'(r)\right) = 0 \qquad \Rightarrow \qquad rf'(r) = c \qquad \Rightarrow \qquad f(r) = c\ln(r) + d.$$

Thus all rotationally symmetric solutions are given by $f(r, \theta) = A\ln(r) + B$ for constants A, B.

9. Consider a function $z(x, y)$ that satisfies $z(\lambda x, \lambda y) = \lambda^n z(x, y)$ for any real λ and a fixed integer n. Show that:

$$x\frac{\partial z}{\partial x} + y\frac{\partial z}{\partial y} = nz,$$

and

$$x^2\frac{\partial^2 z}{\partial x^2} + 2xy\frac{\partial^2 z}{\partial x \partial y} + y^2\frac{\partial^2 z}{\partial y^2} = n(n-1)z.$$

➾ **Solution:** Take the λ partial derivative of both sides. Then using the multivariable chain rule on the left, we have:

$$\frac{\partial z}{\partial x}(\lambda x, \lambda y)\frac{\partial(\lambda x)}{\partial \lambda} + \frac{\partial z}{\partial y}(\lambda x, \lambda y)\frac{\partial(\lambda y)}{\partial \lambda} = n\lambda^{n-1}z(x, y).$$

Simplifying, we have:

$$x\frac{\partial z}{\partial x}(\lambda x, \lambda y) + y\frac{\partial z}{\partial y}(\lambda x, \lambda y) = n\lambda^{n-1}z(x, y). \tag{$*$}$$

Taking $\lambda = 1$ gives the result.

Now taking a second derivative with respect to λ of ($*$), we have (using the multivariable chain rule again on the left hand side):

$$x\frac{\partial}{\partial \lambda}\left(\frac{\partial z}{\partial x}(\lambda x, \lambda y)\right) + y\frac{\partial}{\partial \lambda}\left(\frac{\partial z}{\partial y}(\lambda x, \lambda y)\right) = n(n-1)\lambda^{n-2}z(x, y)$$

$$x\left(\frac{\partial^2 z}{\partial x^2}(\lambda x, \lambda y)\frac{\partial(\lambda x)}{\partial \lambda} + \frac{\partial^2 z}{\partial x \partial y}(\lambda x, \lambda y)\frac{\partial(\lambda y)}{\partial \lambda}\right) + y\left(\frac{\partial^2 z}{\partial x \partial y}(\lambda x, \lambda y)\frac{\partial(\lambda x)}{\partial \lambda} + \frac{\partial^2 z}{\partial y^2}(\lambda x, \lambda y)\frac{\partial(\lambda y)}{\partial \lambda}\right) = n(n-1)\lambda^{n-2}z(x, y)$$

$$x^2\frac{\partial^2 z}{\partial x^2}(\lambda x, \lambda y) + 2xy\frac{\partial^2 z}{\partial x \partial y}(\lambda x, \lambda y) + y^2\frac{\partial^2 z}{\partial y^2}(\lambda x, \lambda y) = n(n-1)\lambda^{n-2}z(x, y).$$

Taking $\lambda = 1$, we establish:

$$x^2\frac{\partial^2 z}{\partial x^2} + 2xy\frac{\partial^2 z}{\partial x \partial y} + y^2\frac{\partial^2 z}{\partial y^2} = n(n-1)z(x, y),$$

as required.

Reciprocity and the cyclic relation

10. Three variables x, y, z are related by the implicit equation $f(x, y, z) = 0$ where f is some multivariable function.

(a) Derive the reciprocity relation:

$$\left(\frac{\partial y}{\partial x}\right)_z \left(\frac{\partial x}{\partial y}\right)_z = 1,$$

and the cyclic relation:

$$\left(\frac{\partial y}{\partial x}\right)_z \left(\frac{\partial x}{\partial z}\right)_y \left(\frac{\partial z}{\partial y}\right)_x = -1.$$

(b) Verify that these relationships hold if: (i) $f(x, y, z) = xyz + x^3 + y^4 + z^5$; (ii) $f(x, y, z) = xyz - \sinh(x + z)$.

➾ Solution:

(a) For the reciprocity relation, note that an implicit equation $f(x, y, z) = 0$ allows us to consider y to be a function of x and z. Thus, we have $f(x, y(x, z), z) = 0$. Taking the partial derivative with respect to x, we obtain:

$$\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x}\bigg|_z = 0.$$

Rearranging, we see that:

$$\frac{\partial y}{\partial x}\bigg|_z = -\frac{\partial f/\partial x}{\partial f/\partial y}.$$

On the other hand, we could also view x to be a function of y and z. Thus, we have $f(x(y, z), y, z) = 0$ being the defining the relation. Taking the partial derivative with respect to y, we obtain:

$$\frac{\partial f}{\partial x}\frac{\partial x}{\partial y}\bigg|_z + \frac{\partial f}{\partial y} = 0.$$

Rearranging, we see that:

$$\frac{\partial x}{\partial y}\bigg|_z = -\frac{\partial f/\partial y}{\partial f/\partial x}.$$

Multiplying these expressions together, we see that the reciprocity relation indeed holds.

We can similarly show that the cyclic chain rule holds. Considering the implicit relation between the variables through $f(x, y, z(x, y)) = 0$, $f(x, y(x, z), z) = 0$ and $f(x(y, z), y, z) = 0$ and differentiating with respect to y, x, z respectively, we have:

$$\frac{\partial f}{\partial y} + \frac{\partial f}{\partial z}\frac{\partial z}{\partial y}\bigg|_x = 0,$$

$$\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y}\frac{\partial y}{\partial x}\bigg|_z = 0,$$

$$\frac{\partial f}{\partial z} + \frac{\partial f}{\partial x}\frac{\partial x}{\partial z}\bigg|_y = 0.$$

Rearranging each of these equations, we obtain:

$$\frac{\partial z}{\partial y}\bigg|_x = -\frac{\partial f/\partial y}{\partial f/\partial z}, \qquad \frac{\partial y}{\partial x}\bigg|_z = -\frac{\partial f/\partial x}{\partial f/\partial y}, \qquad \frac{\partial x}{\partial z}\bigg|_y = -\frac{\partial f/\partial z}{\partial f/\partial x}.$$

Multiplying these results together, we obtain the cyclic chain rule, as required.

(b) We now verify that both relationships hold in two special cases:

(i) First, we have $f(x,y,z) = xyz + x^3 + y^4 + z^5 = 0$. We begin by viewing y as a function of x, z; then, taking the partial derivative with respect to x keeping z constant, we have:

$$yz + x\frac{\partial y}{\partial x}\bigg|_z z + 3x^2 + 4y^3\frac{\partial y}{\partial x}\bigg|_z = 0.$$

Rearranging, we have:

$$\frac{\partial y}{\partial x}\bigg|_z = -\frac{yz + 3x^2}{xz + 4y^3}.$$

Similarly, we can view x as a function of y, z; then, taking the partial derivative with respect to y keeping z constant, we have:

$$\frac{\partial x}{\partial y}\bigg|_z yz + xz + 3x^2\frac{\partial x}{\partial y}\bigg|_z + 4y^3 = 0.$$

Rearranging, we have:

$$\frac{\partial x}{\partial y}\bigg|_z = -\frac{xz + 4y^3}{yz + 3x^2}.$$

Thus, multiplying these expressions together we see that the reciprocity relation indeed holds.

Now regarding $xyz + x^3 + y^4 + z^5 = 0$ as defined y as a function of x, z, then x as a function of y, z, and then z as a function of x, y, we obtain the following derivatives by implicit differentiation:

$$yz + xz\frac{\partial y}{\partial x}\bigg|_z + 3x^2 + 4y^3\frac{\partial y}{\partial x}\bigg|_z = 0,$$

$$yz\frac{\partial x}{\partial z}\bigg|_y + xy + 3x^2\frac{\partial x}{\partial z}\bigg|_y + 5z^4 = 0,$$

$$xz + xy\frac{\partial z}{\partial y}\bigg|_x + 4y^3 + 5z^4\frac{\partial z}{\partial y}\bigg|_x = 0.$$

Rearranging, we have:

$$\frac{\partial y}{\partial x}\bigg|_z = -\frac{3x^2 + yz}{xz + 4y^3}, \qquad \frac{\partial x}{\partial z}\bigg|_y = -\frac{xy + 5z^4}{3x^2 + yz}, \qquad \frac{\partial z}{\partial y}\bigg|_z = -\frac{xz + 4y^3}{xy + 5z^4}.$$

Multiplying these together, we obtain -1, verifying the cyclic chain rule.

(ii) For $f(x,y,z) = xyz - \sinh(x+z) = 0$, it's a similar story. Calculating the necessary derivatives, we have:

$$yz + xz\frac{\partial y}{\partial x}\bigg|_z - \cosh(x+z) = 0,$$

$$yz\frac{\partial x}{\partial y}\bigg|_z + xz - \cosh(x+z)\frac{\partial x}{\partial y}\bigg|_z = 0,$$

$$yz\frac{\partial x}{\partial z}\bigg|_y + xy - \cosh(x+z)\frac{\partial x}{\partial z}\bigg|_y - \cosh(x+z) = 0,$$

$$xz + xy\frac{\partial z}{\partial y}\bigg|_x - \cosh(x+z)\frac{\partial z}{\partial y}\bigg|_x = 0.$$

Rearranging the first two relations, we have:

$$\left.\frac{\partial y}{\partial x}\right|_z = -\frac{yz - \cosh(x+z)}{xz}, \qquad \left.\frac{\partial x}{\partial y}\right|_z = -\frac{xz}{yz - \cosh(x+z)},$$

which indeed multiply to give one, verifying the reciprocity relation. On the other hand, rearranging the first, third and fourth relations, we have:

$$\left.\frac{\partial y}{\partial x}\right|_z = -\frac{yz - \cosh(x+z)}{xz}, \qquad \left.\frac{\partial x}{\partial z}\right|_y = -\frac{xy - \cosh(x+z)}{yz - \cosh(x+z)}, \qquad \left.\frac{\partial z}{\partial y}\right|_z = -\frac{xz}{xy - \cosh(x+z)}.$$

These multiply to give -1, verifying the cyclic chain rule in this case.

Exact differentials, and exact ordinary differential equations

11. Let $\omega = P(x,y)dx + Q(x,y)dy$ be a differential form.

(a) What does it mean to say that ω is *exact*? Define also a *potential function* for a given exact differential form.

(b) Show that $\partial P/\partial y = \partial Q/\partial x$ is a necessary condition for ω to be an exact differential form.

(c) $(*)$ Is the condition in part (b) sufficient for ω to be exact?

Solution:

(a) We say that ω is *exact* if there exists a *potential function* f satisfying $df = \omega$.

(b) If ω is exact, let f be a potential satisfying $df = \omega$. Then:

$$P(x,y)dx + Q(x,y)dy = \frac{\partial f}{\partial x}dx + \frac{\partial f}{\partial y}dy.$$

Comparing coefficients, we see that:

$$\frac{\partial f}{\partial x} = P(x,y), \qquad \frac{\partial f}{\partial y} = Q(x,y).$$

The symmetry of mixed partial derivatives now requires:

$$\frac{\partial P}{\partial y} = \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial^2 f}{\partial x \partial y} = \frac{\partial Q}{\partial x},$$

which is the required necessary condition for exactness.

(c) $(*)$ The condition in part (b) is necessary, but not always sufficient. To see why, let us suppose that $\partial P/\partial y = \partial Q/\partial x$. Then we seek a function $f(x,y)$ such that:

$$\frac{\partial f}{\partial x} = P(x,y), \qquad \frac{\partial f}{\partial y} = Q(x,y).$$

Integrating the first equation from some x_0 to some x, we have:

$$f(x,y) - f(x_0,y) = \int_{x_0}^{x} P(x,y)\,dx. \qquad (\dagger)$$

Similarly, we can integrate the second equation from some y_0 to some y, giving:

$$f(x,y) - f(x,y_0) = \int_{y_0}^{y} Q(x,y)\,dy.$$

Subtracting the first equation from the second, we see that:

$$f(x_0,y) - f(x,y_0) = \int_{y_0}^{y} Q(x,y)\,dy - \int_{x_0}^{x} P(x,y)\,dx.$$

Setting $x = x_0$, we see that:

$$f(x_0, y) = f(x_0, y_0) + \int_{y_0}^{y} Q(x, y)\, dy,$$

which on re-inserting into (†) reveals that $f(x, y)$ must be given (up to a constant, $f(x_0, y_0)$) by:

$$f(x, y) = \int_{x_0}^{x} P(x, y)\, dx + \int_{y_0}^{y} Q(x, y)\, dy + f(x_0, y_0).$$

The issue with this construction is that it assumes that the the interval $[x_0, x]$ lies inside the allowed x-range for every single y. Similarly, it assumes that the interval $[y_0, y]$ lies inside the allowed y-range for every single x. This is not always the case, for example if the differential only exists on a region with a hole at some singularity, for example:

$$\frac{xdy - ydx}{x^2 + y^2}$$

in the following question.

Crucially, the condition for the sufficiency of $\partial P/\partial y = \partial Q/\partial x$ is that $Pdx + Qdy$ must be defined on a *simply-connected domain*, which is a region that contains no holes (more specifically, any closed loop in the region can be continuously deformed to a point).

12. Determine whether the following differential forms are exact or not. In the cases where the differential forms are exact, find appropriate potential functions f.

(a) $ydx + xdy$, (b) $ydx + x^2dy$, (c) $(x+y)dx + (x-y)dy$, (d) $(*)$ $\dfrac{xdy - ydx}{x^2+y^2}$.

Solution:

(a) In the first case, we have:
$$\frac{\partial y}{\partial y} = 1 = \frac{\partial x}{\partial x},$$
so the differential form is exact. This implies that there exists some potential function f satisfying:
$$\frac{\partial f}{\partial x} = y, \qquad \frac{\partial f}{\partial y} = x.$$
By inspection, we may choose $f(x,y) = xy + c$.

(b) Note that:
$$\frac{\partial y}{\partial y} = 1 \neq 2x = \frac{\partial (x^2)}{\partial x},$$
so this differential form is not exact, and hence has no potential function.

(c) We have:
$$\frac{\partial}{\partial y}(x+y) = 1 = \frac{\partial}{\partial x}(x-y),$$
so this differential form is exact. This implies that there exists some potential function f satisfying:
$$\frac{\partial f}{\partial x} = x+y, \qquad \frac{\partial f}{\partial y} = x-y.$$
Integrating the first equation, we have $f(x,y) = \frac{1}{2}x^2 + xy + g(y)$, for an arbitrary function $g(y)$. Differentiating with respect to y and substituting into the second equation, we see that $g(y)$ must satisfy:
$$x + g'(y) = x - y.$$
Hence $g'(y) = -y$, giving $g(y) = -\frac{1}{2}y^2 + c$. Thus a potential function is:
$$f(x,y) = \frac{1}{2}x^2 + xy - \frac{1}{2}y^2 + c.$$

(d) $(*)$ This part is quite subtle, because it explores the case where $\partial P/\partial y = \partial Q/\partial x$ is necessary but not sufficient for exactness of the differential form. Certainly, we have:
$$\frac{\partial P}{\partial y} = \frac{y^2 - x^2}{(x^2+y^2)^2} = \frac{\partial Q}{\partial x},$$
so the usual condition for exactness is satisfied. However, if we attempt to integral $\partial f/\partial x = -y/(x^2+y^2)$, we get:
$$f(x,y) = -\arctan\left(\frac{x}{y}\right) + h(y).$$
This differentiates to:
$$\frac{\partial f}{\partial y} = \frac{x/y^2}{1 + (x/y)^2} + h'(y) = \frac{x}{x^2+y^2} + h'(y),$$
so that $h'(y) = 0$, and thus $h(y) =$ constant. It appears that $f(x,y) = -\arctan(x/y) + C$ is a suitable potential. However, this is not differentiable - it suffers a discontinuous jump as we pass round $y = 0$. We can find a potential, but not on the domain $\mathbb{R}^2 \backslash \{(0,0)\}$ where the differential is initially defined.

13. Find all values of the constant a for which the differential form:

$$\left(y^2 \sin(ax) + xy^2 \cos(ax)\right) dx + 2xy \sin(ax) dy$$

is exact. Find appropriate potential functions in the cases where the differential form is exact.

➾ **Solution:** For exactness, we require:

$$\frac{\partial}{\partial y}\left(y^2 \sin(ax) + xy^2 \cos(ax)\right) = 2y \sin(ax) + 2xy \cos(ax) = 2y \sin(ax) + 2axy \cos(ax) = \frac{\partial}{\partial x}\left(2xy \sin(ax)\right).$$

Hence, we see that the only case where the differential form is exact is when $a = 1$. In this case, a potential function f must satisfy:

$$df = \frac{\partial f}{\partial x} dx + \frac{\partial f}{\partial y} dy = \left(y^2 \sin(x) + xy^2 \cos(x)\right) dx + 2xy \sin(x) dy.$$

Comparing coefficients, we see that:

$$\frac{\partial f}{\partial x} = y^2 \sin(x) + xy^2 \cos(x), \qquad \frac{\partial f}{\partial y} = 2xy \sin(x).$$

Integrating the second equation (because it looks easier), we see that $f(x, y) = xy^2 \sin(x) + g(x)$, where $g(x)$ is an unknown function of x. Differentiating with respect to x and inserting into the first equation, we have:

$$y^2 \sin(x) + xy^2 \cos(x) + g'(x) = y^2 \sin(x) + xy^2 \cos(x),$$

which shows that $g'(x) = 0$, and hence $g(x)$ is independent of x. Thus all potential functions are $f(x, y) = xy^2 \sin(x) + c$, where c is an arbitrary constant.

14. Let $P(x,y,z)dx + Q(x,y,z)dy + R(x,y,z)dz$ be a differential form in three dimensions. Show that:

$$\frac{\partial P}{\partial y} = \frac{\partial Q}{\partial x}, \qquad \frac{\partial P}{\partial z} = \frac{\partial R}{\partial x}, \qquad \frac{\partial Q}{\partial z} = \frac{\partial R}{\partial y}$$

is a necessary condition for the differential form to be exact. It turns out that this is *also* a sufficient condition, under suitable criteria which you may assume hold. Hence, decide whether the following differential forms are exact or not, and find appropriate potential functions in the cases where the forms are exact:

(a) $xdx + ydy + zdz$, (b) $ydx + zdy + xdz$, (c) $2xy^3z^4dx + 3x^2y^2z^4dy + 4x^2y^3z^3dz$.

Solution: Let $f(x,y,z)$ be a potential function, satisfying $df = Pdx + Qdy + Rdz$. Then:

$$\frac{\partial f}{\partial x} = P, \qquad \frac{\partial f}{\partial y} = Q, \qquad \frac{\partial f}{\partial z} = R.$$

Differentiating the first equation with respect to y, z, the second equation with respect to x, z, and the third equation with respect to x, y, we generate six more equations for the second derivatives:

$$\frac{\partial^2 f}{\partial x \partial y} = \frac{\partial P}{\partial y}, \qquad \frac{\partial^2 f}{\partial x \partial z} = \frac{\partial P}{\partial z}, \qquad \frac{\partial^2 f}{\partial y \partial x} = \frac{\partial Q}{\partial x},$$

$$\frac{\partial^2 f}{\partial y \partial z} = \frac{\partial Q}{\partial z}, \qquad \frac{\partial^2 f}{\partial x \partial z} = \frac{\partial R}{\partial x}, \qquad \frac{\partial^2 f}{\partial y \partial z} = \frac{\partial R}{\partial y}.$$

Comparing the relevant mixed partial derivatives, the necessary condition given in the question follows.

For the given functions:

(a) We have $P = x, Q = y, R = z$, which gives:

$$\frac{\partial P}{\partial y} = \frac{\partial P}{\partial z} = 0, \qquad \frac{\partial Q}{\partial x} = \frac{\partial Q}{\partial z} = 0, \qquad \frac{\partial R}{\partial x} = \frac{\partial R}{\partial y} = 0.$$

In particular, the necessary condition derived at the start of the question is satisfied. If $f(x,y,z)$ is a potential, then we have:

$$\frac{\partial f}{\partial x} = x, \qquad \frac{\partial f}{\partial y} = y, \qquad \frac{\partial f}{\partial z} = z.$$

Integrating the first equation, we have $f(x,y,z) = \frac{1}{2}x^2 + g(y,z)$ for an unknown function $g(y,z)$. Differentiating and inserting into the second equation, we see that:

$$\frac{\partial g}{\partial y} = y \qquad \Rightarrow \qquad g(y,z) = \frac{1}{2}y^2 + h(z),$$

for an unknown function $h(z)$. Overall then, we have $f(x,y,z) = \frac{1}{2}x^2 + \frac{1}{2}y^2 + h(z)$. Differentiating again and inserting into the third equation, we see that:

$$h'(z) = z \qquad \Rightarrow \qquad h(z) = \frac{1}{2}z^2 + c,$$

where c is an arbitrary constant. Thus all potentials satisfy $f(x,y,z) = \frac{1}{2}x^2 + \frac{1}{2}y^2 + \frac{1}{2}z^2 + c$.

(b) This time, we have $P = y, Q = z, R = x$. This implies that:

$$\frac{\partial P}{\partial y} = 1 \neq 0 = \frac{\partial Q}{\partial x},$$

so this differential form is non-exact by the necessary condition derived at the start of the question.

(c) We have $P = 2xy^3z^4, Q = 3x^2y^2z^4, R = 4x^2y^3z^3$. Hence:

$$\frac{\partial P}{\partial y} = 6xy^2z^4 = \frac{\partial Q}{\partial x}, \qquad \frac{\partial P}{\partial z} = 8xy^3z^3 = \frac{\partial R}{\partial x}, \qquad \frac{\partial Q}{\partial z} = 12x^2y^2z^3 = \frac{\partial R}{\partial y},$$

so that indeed the differential form is exact. Let $f(x, y, z)$ be a potential function, satisfying:

$$\frac{\partial f}{\partial x} = 2xy^3z^4, \qquad \frac{\partial f}{\partial y} = 3x^2y^2z^4, \qquad \frac{\partial f}{\partial z} = 4x^2y^3z^3.$$

Integrating the first equation, we have $f(x, y, z) = x^2y^3z^4 + g(y, z)$. Differentiating and inserting into the second equation, we have:

$$3x^2y^2z^4 + \frac{\partial g}{\partial y} = 3x^2y^2z^4 \qquad \Rightarrow \qquad \frac{\partial g}{\partial y} = 0 \qquad \Rightarrow \qquad g(y, z) = h(z).$$

Thus we have $f(x, y, z) = x^2y^3z^4 + h(z)$. Differentiating and inserting into the third equation, we have:

$$4x^2y^3z^3 + h'(z) = 4x^2y^3z^3.$$

This shows $h(z)$ is a constant, and hence all potentials take the form $f(x, y, z) = x^2y^3z^4 + c$ for c an arbitrary constant.

15. Consider the first-order differential equation:

$$P(x,y)+Q(x,y)\frac{dy}{dx}=0. \tag{†}$$

Using the multivariable chain rule, show that $f(x,y(x)) = c$, for c and arbitrary constant, is an implicit solution of the equation if and only if $df = \mu\cdot(Pdx+Qdy)$, for some multivariable function $\mu(x,y)$, which is not identically zero. [*Hence, equation (†) can be solved implicitly if the differential $Pdx + Qdy$ is exact ($\mu = 1$), or can be made exact through multiplication by some 'integrating factor' - note this is* not *the same type of integrating factor we dealt with earlier in the course.*]

➠ **Solution:** Suppose that $f(x,y(x)) = c$ solves the equation. Then by the multivariable chain rule, we have:

$$\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}\frac{dy}{dx}=0.$$

Since y solves the equation, we have $dy/dx = -P/Q$. This gives:

$$\frac{\partial f}{\partial x}-\frac{P}{Q}\frac{\partial f}{\partial y}=0.$$

Rearranging, we see that:

$$\frac{\partial f/\partial x}{\partial f/\partial y}=\frac{P}{Q}.$$

If we choose $\mu = (\partial f/\partial y)/Q$, we see that $\partial f/\partial x = \mu P$ and $\partial f/\partial y = \mu Q$, so that $df = \mu(Pdx + Qdy)$, as required.

Conversely, suppose that $df = \mu(Pdx + Qdy)$. Then by the multivariable chain rule applied to $f(x,y(x)) = c$, we have:

$$0=\frac{\partial f}{\partial x}+\frac{\partial f}{\partial y}\frac{dy}{dx}=\mu P+\mu Q\frac{dy}{dx} \qquad \Rightarrow \qquad P+Q\frac{dy}{dx}=0,$$

as required.

16. Show that each of the following first-order differential equations is exact, and hence find their general solution:

(a) $2x + e^y + (xe^y - \cos(y))\dfrac{dy}{dx} = 0$, (b) $\dfrac{dy}{dx} = \dfrac{5x+4y}{8y^3-4x}$, (c) $\sinh(x)\sin(y) + \cosh(x)\cos(y)\dfrac{dy}{dx} = 0.$

Solution: We have:

(a) In this case, this equation corresponds to the differential form:

$$(2x + e^y)dx + (xe^y - \cos(y))dy.$$

Seeking a potential, we require:

$$\frac{\partial f}{\partial x} = 2x + e^y, \qquad \frac{\partial f}{\partial y} = xe^y - \cos(y).$$

By inspection, observe that $f(x,y) = x^2 + xe^y - \sin(y)$ is an appropriate potential. Thus the solution is:

$$x^2 + xe^y - \sin(y) = c,$$

for an arbitrary constant c.

(b) Rearranging to standard form, the equation becomes:

$$5x + 4y + (4x - 8y^3)\frac{dy}{dx} = 0$$

The equation corresponds to the differential form $(5x+4y)dx + (4x - 8y^3)dy$. Seeking a potential, we require:

$$\frac{\partial f}{\partial x} = 5x + 4y, \qquad \frac{\partial f}{\partial y} = 4x - 8y^3.$$

By inspection, observe that $f(x,y) = \frac{5}{2}x^2 + 4xy - 2y^4$ is an appropriate potential. Thus the solution is:

$$\frac{5}{2}x^2 + 4xy - 2y^4 = c,$$

for an arbitrary constant c.

(c) In this case, we seek a potential satisfying:

$$\frac{\partial f}{\partial x} = \sinh(x)\sin(y), \qquad \frac{\partial f}{\partial y} = \cosh(x)\cos(y).$$

Again, by inspection observe that $f(x,y) = \cosh(x)\sin(y)$ is an appropriate potential. Thus the solution of the equation is:

$$\cosh(x)\sin(y) = c,$$

for an arbitrary constant c.

17.

(a) Show that the differential form $Pdx + Qdy$ can be made exact through multiplication by the integrating factor $\mu(x)$ if and only if:

$$\frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right)$$

is independent of y.

(b) Hence, find a function μ for which the differential form:

$$\mu[(\cos(y) - \tanh(x)\sin(y))dx - (\cos(y) + \tanh(x)\sin(y))dy]$$

is exact.

(c) Using the result of part (b), solve the differential equation:

$$\frac{dy}{dx} = \frac{\cos(y) - \tanh(x)\sin(y)}{\cos(y) + \tanh(x)\sin(y)}.$$

➾ **Solution:** (a) Suppose that $\mu P dx + \mu Q dy$ is exact, where $\mu(x)$ is a function of x. Then:

$$\frac{\partial}{\partial y}(\mu P) = \frac{\partial}{\partial x}(\mu Q) \qquad \Rightarrow \qquad \mu(x)\frac{\partial P}{\partial y} = \mu'(x)Q + \mu(x)\frac{\partial Q}{\partial x}.$$

Rearranging, we see that:

$$\frac{\mu'(x)}{\mu(x)} = \frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right).$$

This implies the necessary condition that the quantity on the right hand side of the equation is independent of y (because the left hand side is independent of y, evidently). On the other hand, if this quantity is independent of y, we can integrate both sides of this equation to obtain an integrating factor:

$$\mu(x) \propto \exp\left(\int \frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) dx\right).$$

(b) Here, we have $P = \cos(y) - \tanh(x)\sin(y), Q = -\cos(y) - \tanh(x)\sin(y)$. Hence:

$$\frac{1}{Q}\left(\frac{\partial P}{\partial y} - \frac{\partial Q}{\partial x}\right) = -\frac{1}{\cos(y) + \tanh(x)\sin(y)}\left(-\sin(y) - \tanh(x)\cos(y) + \operatorname{sech}^2(x)\sin(y)\right).$$

Recall that $1 - \tanh^2(x) = \operatorname{sech}^2(x)$, hence we can rewrite this quotient as:

$$\frac{\tanh(x)\cos(y) + \tanh^2(x)\sin(y)}{\cos(y) + \tanh(x)\sin(y)} = \tanh(x),$$

so indeed this quotient is independent of x. This reveals that the integrating factor is $\mu(x) \propto \exp(\ln(\cosh(x))) = \cosh(x)$, using the integral of $\tanh(x) = \sinh(x)/\cosh(x)$. For this choice of $\mu(x)$, the differential form becomes:

$$(\cosh(x)\cos(y) - \sinh(x)\sin(y))\,dx - (\cosh(x)\cos(y) + \sinh(x)\sin(y))\,dy.$$

A potential for this differential form satisfies:

$$\frac{\partial f}{\partial x} = \cosh(x)\cos(y) - \sinh(x)\sin(y), \qquad \frac{\partial f}{\partial y} = -\cosh(x)\cos(y) - \sinh(x)\sin(y).$$

By inspection, note that $f(x,y) = \sinh(x)\cos(y) - \cosh(x)\sin(y)$ satisfies these equations. Thus the differential form has indeed been made exact.

(c) The equation can be rearranged to the standard form:

$$(\cos(y) - \tanh(x)\sin(y)) - (\cos(y) + \tanh(x)\sin(y))\,\frac{dy}{dx} = 0.$$

Multiplying through by $\cosh(x)$, we obtain an exact equation, with solution $\sinh(x)\cos(y) - \cosh(x)\sin(y) = c$, as required.

Applications in thermodynamics

18. A thermodynamic system can be modelled in terms of four fundamental variables, pressure p, volume V, temperature T, and entropy S. Only two of these variables are independent, so that any pair of them may expressed as functions of the remaining two variables. The *fundamental thermodynamic relation* tells us that for any given system, the differential of the internal energy U of the system is related to the differentials of the entropy and volume via:

$$dU = TdS - pdV.$$

(a) Give a physical interpretation of each of the terms in the fundamental thermodynamic relation.

(b) From the fundamental thermodynamic relation, prove Maxwell's first relation:

$$\left(\frac{\partial T}{\partial V}\right)_S = -\left(\frac{\partial p}{\partial S}\right)_V$$

(c) By defining an appropriate thermodynamic potential, show that $-SdT - pdV$ is an exact differential. Deduce Maxwell's second relation:

$$\left(\frac{\partial S}{\partial V}\right)_T = \left(\frac{\partial p}{\partial T}\right)_V$$

(d) Through similar considerations, derive the remaining Maxwell relations:

$$\left(\frac{\partial T}{\partial p}\right)_S = \left(\frac{\partial V}{\partial S}\right)_p, \qquad \left(\frac{\partial S}{\partial p}\right)_T = -\left(\frac{\partial V}{\partial T}\right)_p.$$

➾ Solution:

(a) dU is the 'infinitesimal' change in internal energy of a system under a transition between equilibrium states. The term $-pdV$ represents macroscopic mechanical energy transfer (if the system expands, it does work on the surroundings, transferring energy from the system to the environment). The term TdS represents energy transfer through heat, corresponding to the increase in microscopic energy from increased 'disorder' of a system (the entropy).

(b) This is obvious because $dU = TdS - pdV$ is an exact differential. Hence:

$$\left.\frac{\partial T}{\partial V}\right|_S = -\left.\frac{\partial p}{\partial S}\right|_V,$$

as required.

(c) Since $d(TS) = TdS + SdT$, we can write:

$$dU = d(TS) - SdT - pdV \qquad \Rightarrow \qquad d(U - TS) = -SdT - pdV.$$

This shows that $-SdT - pdV$ is exact with potential $F = U - TS$, the *Helmholtz free energy*. The Maxwell relation follows immediately from exactness.

(d) Since $d(pV) = pdV + Vdp$, we can write:

$$dU = TdS - d(pV) + Vdp \qquad \Rightarrow \qquad d(U + pV) = TdS + Vdp.$$

This shows that $TdS + Vdp$ is exact with potential $H = U + pV$, the *enthalpy*. The third Maxwell relation follows immediately from exactness. Similarly, using $d(TS) = TdS + SdT$, we have:

$$d(U + pV) = d(TS) - SdT + Vdp \qquad \Rightarrow \qquad d(U + pV - TS) = -SdT + Vdp.$$

This shows that $-SdT + Vdp$ is exact with potential $G = U + pV - TS$, the *Gibbs free energy*. The Maxwell relation follows immediately from exactness.

18. A classical monatomic ideal gas has equations of state:

$$pV = nRT, \qquad S = nR\log\left(\frac{VT^{3/2}}{\Phi_0}\right)$$

where n is the amount of substance in moles, which we consider constant, R is the gas constant, and Φ_0 is a constant which depends on the type of gas.

(a) Using the fundamental thermodynamic relation, show that the internal energy of the gas is $U = \frac{3}{2}nRT$.

(b) By appropriately expressing each pair of thermodynamic variables in terms of the remaining pair, verify Maxwell's relations for this thermodynamic system.

Solution:

(a) The fundamental thermodynamic relation $dU = T(S,V)dS - p(S,V)dV$ expects that T, p are expressed as functions of S, V. In our case, we can rearrange the second equation to give an equation for temperature in terms of S, V:

$$T(S,V) = \left(\frac{\Phi_0}{V}\right)^{2/3}\exp\left(\frac{2S}{3nR}\right).$$

Similarly we can rearrange the first equation to give an equation for pressure in terms of S, V (substituting for $T(S,V)$):

$$p(S,V) = \frac{nRT}{V} = nR\frac{\Phi_0^{2/3}}{V^{5/3}}\exp\left(\frac{2S}{3nR}\right).$$

Now using the fundamental thermodynamic relation, $dU = TdS - pdV$, we know that $\partial U/\partial S = T$ and $\partial U/\partial V = -p$. Hence we have the equations:

$$\frac{\partial U}{\partial S} = \left(\frac{\Phi_0}{V}\right)^{2/3}\exp\left(\frac{2S}{3nR}\right).$$

and:

$$\frac{\partial U}{\partial V} = -nR\frac{\Phi_0^{2/3}}{V^{5/3}}\exp\left(\frac{2S}{3nR}\right).$$

Integrating the first equation, we have:

$$U(S,V) = \frac{3nR}{2}\left(\frac{\Phi_0}{V}\right)^{2/3}\exp\left(\frac{2S}{3nR}\right) + g(V).$$

Differentiating and inserting into the second equation, we have:

$$-nR\frac{\Phi_0^{2/3}}{V^{5/3}}\exp\left(\frac{2S}{3nR}\right) + g'(V) = -nR\frac{\Phi_0^{2/3}}{V^{5/3}}\exp\left(\frac{2S}{3nR}\right),$$

which reveals that $g(V)$ is independent of V. Hence we have:

$$U = \frac{3nR}{2}\left(\frac{\Phi_0}{V}\right)^{2/3}\exp\left(\frac{2S}{3nR}\right) + c = \frac{3}{2}nRT + c.$$

Requiring the energy of the gas to vanish as $T \to 0$, the constant c is fixed to zero, as required.

(b) We have already expressed p, T in terms of S, V it is easy to check that:

$$\frac{\partial T}{\partial V} = -\frac{2}{3}\frac{\Phi_0^{2/3}}{V^{5/3}}\exp\left(\frac{2S}{3nR}\right) = -\frac{\partial p}{\partial S},$$

which verifies the first Maxwell relation.

For the second Maxwell relation, we express p, S in terms of T, V. This is the form used in the question (with $p = nRT/V$). Checking the relation then, we have:

$$\frac{\partial S}{\partial V} = \frac{nR}{V} = \frac{\partial p}{\partial T},$$

which verifies the second Maxwell relation.

For the third Maxwell relation, we express T, V in terms of p, S. Rearranging the first equation in the question, we have $V = nRT/p$, which we can substitute into the second equation in the question, giving:

$$S = nR\log\left(\frac{nRT^{5/2}}{\Phi_0 p}\right) \qquad \Rightarrow \qquad T(p,S) = \left(\frac{p\Phi_0}{nR}\right)^{2/5}\exp\left(\frac{2S}{5nR}\right).$$

This gives:

$$V(p,S) = \frac{nR}{p}\left(\frac{p\Phi_0}{nR}\right)^{2/5}\exp\left(\frac{2S}{5nR}\right).$$

Checking the relation, we note:

$$\frac{\partial T}{\partial p} = \frac{2}{5p}\left(\frac{p\Phi_0}{nR}\right)^{2/5} = \frac{\partial V}{\partial S}$$

which verifies the third Maxwell relation.

For the final Maxwell relation, we express S, V in terms of p, T. Rearranging the first equation in the question, we have $V = nRT/p$. Substituting into the second equation in the question, we have:

$$S(p,T) = nR\log\left(\frac{nRT^{5/2}}{p\Phi_0}\right).$$

Checking the relation, we have:

$$\frac{\partial S}{\partial p} = -\frac{nR}{p} = -\frac{\partial V}{\partial T},$$

which verifies the fourth and final Maxwell relation.

19.

(a) Using the fundamental thermodynamic relation, and the Maxwell relations, prove that:

$$\left(\frac{\partial U}{\partial V}\right)_T = T\left(\frac{\partial p}{\partial T}\right)_V - p.$$

(b) In a van der Waals gas, the equation of state is:

$$p = \frac{RT}{V-b} - \frac{a}{V^2},$$

where a, b, R are constants. Using part (a), derive a formula for U in terms of V, T, assuming that $U \to cT$, for some constant c, as $T \to \infty$.

Solution:

(a) Starting from the fundamental thermodynamic relation $dU = TdS - pdV$, we use the fact that S may be written as a function of V, T to obtain:

$$\begin{aligned} dU &= T\left(\left.\frac{\partial S}{\partial V}\right|_T dV + \left.\frac{\partial S}{\partial T}\right|_V dT\right) - pdV \\ &= \left.\frac{\partial S}{\partial T}\right|_V dT + \left(T\left.\left(\frac{\partial S}{\partial V}\right)\right|_T - p\right)dV. \end{aligned}$$

This implies that:

$$\left.\left(\frac{\partial U}{\partial V}\right)\right|_T = T\left.\left(\frac{\partial S}{\partial V}\right)\right|_T - p.$$

By the second Maxwell relation, the result in the question follows.

(b) The van der Waal's equation of state expresses p as a function of V, T which is exactly what we need for the first part to be applied. We have:

$$\left.\left(\frac{\partial U}{\partial V}\right)\right|_T = \frac{RT}{V-b} - \left(\frac{RT}{V-b} - \frac{a}{V^2}\right) = \frac{a}{V^2}.$$

Integrating both sides, we see that:

$$U(V,T) = -\frac{a}{V} + g(T),$$

where $g(T)$ is a function of temperature only. We are given that as $V \to \infty$, $U(V,T) \to cT$; this implies that $g(T) = cT$. Hence the internal energy of a van der Waal's gas is:

$$U(V,T) = cT - \frac{a}{V}.$$

20.

(a) Find an expression for $\left(\frac{\partial p}{\partial V}\right)_T - \left(\frac{\partial p}{\partial V}\right)_S$ in terms of $\left(\frac{\partial S}{\partial V}\right)_T$ and $\left(\frac{\partial S}{\partial p}\right)_V$.

(b) Hence, using the fundamental thermodynamic relation, show that:

$$\left(\frac{\partial \log(p)}{\partial \log(V)}\right)_T - \left(\frac{\partial \log(p)}{\partial \log(V)}\right)_S = \left(\frac{\partial (pV)}{\partial T}\right)_V \left[\frac{p^{-1}(\partial U/\partial V)_T + 1}{(\partial U/\partial T)_V}\right].$$

(c) Show that for a fixed amount of a classical monatomic ideal gas, $pV^{5/3}$ is a function of S. Hence, verify that the relation in part (b) holds for a classical monatomic ideal gas.

Solution:

(a) Regarding p as a function of V, T, we have:

$$dp = \left(\frac{\partial p}{\partial V}\right)\bigg|_T dV + \left(\frac{\partial p}{\partial T}\right)\bigg|_V dT.$$

Similarly regarding p as a function of V, S, we have:

$$dp = \left(\frac{\partial p}{\partial V}\right)\bigg|_S dV + \left(\frac{\partial p}{\partial S}\right)\bigg|_V dS.$$

Subtracting these equations we deduce that:

$$\left[\left(\frac{\partial p}{\partial V}\right)\bigg|_T - \left(\frac{\partial p}{\partial V}\right)\bigg|_S\right] dV = -\left(\frac{\partial p}{\partial T}\right)\bigg|_V dT + \left(\frac{\partial p}{\partial S}\right)\bigg|_V dS.$$

Expanding the differential dV, we have:

$$\left[\left(\frac{\partial p}{\partial V}\right)\bigg|_T - \left(\frac{\partial p}{\partial V}\right)\bigg|_S\right]\left[\left(\frac{\partial V}{\partial S}\right)\bigg|_T dS + \left(\frac{\partial V}{\partial T}\right)\bigg|_S dT\right] = -\left(\frac{\partial p}{\partial T}\right)\bigg|_V dT + \left(\frac{\partial p}{\partial S}\right)\bigg|_V dS.$$

Comparing coefficients of dS, we have:

$$\left(\frac{\partial p}{\partial V}\right)\bigg|_T - \left(\frac{\partial p}{\partial V}\right)\bigg|_S = \left(\frac{\partial p}{\partial S}\right)\bigg|_V \cdot \left(\frac{\partial S}{\partial V}\right)\bigg|_T = \frac{(\partial S/\partial V)|_T}{(\partial S/\partial p)|_V},$$

using reciprocity freely in the last step.

(b) Performing the differentiation on the left hand side, we have:

$$\left(\frac{\partial \log(p)}{\partial \log(V)}\right)_T - \left(\frac{\partial \log(p)}{\partial \log(V)}\right)_S = \frac{V}{p}\left(\frac{\partial p}{\partial V}\bigg|_T - \frac{\partial p}{\partial V}\bigg|_S\right) = \frac{V}{p}\frac{(\partial S/\partial V)|_T}{(\partial S/\partial p)|_V}. \qquad (*)$$

From the fundamental thermodynamic relation $dU = TdS - pdV$, we have:

$$dS = \frac{dU}{T} + \frac{pdV}{T} = \frac{1}{T}\left(\frac{\partial U}{\partial T}\bigg|_V dT + \frac{\partial U}{\partial V}\bigg|_T dV\right) + \frac{pdV}{T}.$$

This gives:

$$\left(\frac{\partial S}{\partial V}\right)\bigg|_T = \frac{1}{T}\frac{\partial U}{\partial V}\bigg|_T + \frac{p}{T},$$

allowing us to simplify the numerator.

For the denominator, note from the fundamental thermodynamic relation $dU = TdS - pdV$, we have:

$$dU = T\left(\frac{\partial S}{\partial T}\right)\bigg|_V dT + T\left(\frac{\partial S}{\partial V}\right)\bigg|_T dV - pdV,$$

giving $(\partial U/\partial T)|_V = T(\partial S/\partial T)|_V$. Regarding S as a function of both T, V and alternatively p, V gives both:

$$dS = \left(\frac{\partial S}{\partial T}\right)\bigg|_V dT + \left(\frac{\partial S}{\partial V}\right)\bigg|_T dV = \left(\frac{\partial S}{\partial p}\right)\bigg|_V dp + \left(\frac{\partial S}{\partial V}\right)\bigg|_p dV.$$

Expanding dp on the left hand side, we have:

$$\left(\frac{\partial S}{\partial T}\right)\bigg|_V dT + \left(\frac{\partial S}{\partial V}\right)\bigg|_T dV = \left(\frac{\partial S}{\partial p}\right)\bigg|_V \left[\left(\frac{\partial p}{\partial T}\right)\bigg|_V dT + \left(\frac{\partial p}{\partial V}\right)\bigg|_T dV\right] + \left(\frac{\partial S}{\partial V}\right)\bigg|_p dV.$$

Comparing coefficients of dT, we see that:

$$\left(\frac{\partial S}{\partial T}\right)\bigg|_V = \left(\frac{\partial S}{\partial p}\right)\bigg|_V \left(\frac{\partial p}{\partial T}\right)\bigg|_V.$$

This reveals that $(\partial S/\partial p)|_V = T^{-1}(\partial T/\partial p)|_V(\partial U/\partial T)|_V$, which on putting everything together gives in $(*)$:

$$\begin{aligned}\left(\frac{\partial \log(p)}{\partial \log(V)}\right)_T - \left(\frac{\partial \log(p)}{\partial \log(V)}\right)_S &= \frac{V}{p}\frac{p}{T}\frac{p^{-1}(\partial U/\partial V)|_T + 1}{T^{-1}(\partial T/\partial p)|_V(\partial U/\partial T)|_V} \\ &= \left(\frac{\partial(pV)}{\partial T}\right)\bigg|_V \frac{p^{-1}(\partial U/\partial V)_T + 1}{(\partial U/\partial T)_V},\end{aligned}$$

as required, phew!

(c) Using the results of Question 18, we have:

$$pV^{5/3} = nR\Phi_0^{2/3}\exp\left(\frac{2S}{3nR}\right),$$

which is indeed purely a function of S, i.e. $pV^{5/3} = f(S)$ for some f (which we have explicitly from Question 14). Taking logarithms, we have:

$$\log(p) = -\frac{5}{3}\log(V) + \log(f(S)).$$

Also regarding p as a function of V, T we have $pV = nRT$, which gives $\log(p) = -\log(V) + \log(nR) + \log(T)$. Thus the derivatives required in part (b) are:

$$\frac{\partial \log(p)}{\partial \log(V)}\bigg|_T = -1, \qquad \frac{\partial \log(p)}{\partial \log(V)}\bigg|_S = -\frac{5}{3},$$

so the left-hand side is $-1 + 5/3 = 2/3$.

Recall also that $U = \frac{3}{2}nRT$. Hence, on the right hand side, we have:

$$\frac{\partial U}{\partial V}\bigg|_T = 0, \qquad \frac{\partial U}{\partial T}\bigg|_V = \frac{3}{2}nR.$$

We also have:

$$\frac{\partial(pV)}{\partial T}\bigg|_V = nR.$$

Putting everything together then, we see that the right-hand side is $2/3$, in perfect agreement.