18.02A Topic 30: Non-independent variables, chain rule.
Read: TB: 19.6, SN: N.1-N.3

We'll get increasingly fancy.

We use the notation that fully specifies the role of all the variables:
$\left(\frac{\partial w}{\partial x}\right)_y$ is the partial of w with respect ot x with y held constant.
This shows explicitly that x and y are independent variables.

Recall the **chain rule**: If $w = f(x, y)$; and $x = x(u, v)$, $y = y(u, v)$

$$\Rightarrow \begin{array}{ccc} \left(\frac{\partial w}{\partial u}\right)_v & = & \left(\frac{\partial w}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial w}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v \\ \left(\frac{\partial w}{\partial v}\right)_u & = & \left(\frac{\partial w}{\partial x}\right)_y \left(\frac{\partial x}{\partial v}\right)_u + \left(\frac{\partial w}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_u \end{array}$$

Example 1: Given $w = x^2 + y^2 + z^2$ constrained by the relation $z = x^2 + y^2$
compute $\left(\frac{\partial w}{\partial x}\right)_y$:

Method 1: Implicit differentiation
Differentiate the formula for w (x is the variable, y is a constant and z is a function of x).

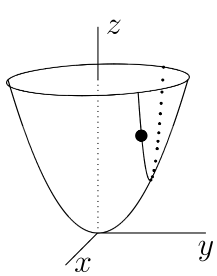
$$\Rightarrow \left(\frac{\partial w}{\partial x}\right)_y = 2x + 2z \left(\frac{\partial z}{\partial x}\right)_y.$$

Need to find $\left(\frac{\partial z}{\partial x}\right)_y$ $\Rightarrow$ differentiate the constraint relation implicitly.

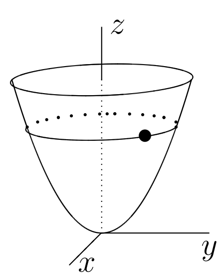
$$\Rightarrow \left(\frac{\partial z}{\partial x}\right)_y = 2x \Rightarrow \boxed{\left(\frac{\partial w}{\partial x}\right)_y = 2x + 2z(2x).}$$

Formalizing method 1: Let w_x, w_y, w_z be the 'formal' derivatives of w. That is, the derivatives when x, y and z are thought of as independent:
I.e., $w_x = 2x$, $w_y = 2y$, $w_z = 2z$ $\Rightarrow$

$$\left(\frac{\partial w}{\partial x}\right)_y = w_x \left(\frac{\partial x}{\partial x}\right)_y + w_y \left(\frac{\partial y}{\partial x}\right)_y + w_z \left(\frac{\partial z}{\partial x}\right)_y = w_x \cdot 1 + w_y \cdot 0 + w_z \left(\frac{\partial z}{\partial x}\right)_y$$



Slice y = constant (example 1).



Slice z = constant (example 2).

(continued)

Method 2: Total differentials:
$dw = w_x\,dx + w_y\,dy + w_z\,dz = 2x\,dx + 2y\,dy + 2z\,dz$
(This is the usual approximation formula made infinitesimal).
If we used the constraint to eliminate z so that $w = w(x, y)$ then we'd have the formula:
$(\star) \quad dw = \left(\frac{\partial w}{\partial x}\right)_y dx + \left(\frac{\partial w}{\partial y}\right)_x dy$
This can be hard, instead we use the constraint to remove dz.
Constraint $\Rightarrow\ dz = 2x\,dx + 2y\,dy$
$\Rightarrow\ dw = 2x\,dx + 2y\,dy + 2z(2x\,dx + 2y\,dy) = (2x + 4xz)\,dx + (2y + 4yz)\,dy$
Compare this with $(\star)$ above: $\left(\frac{\partial w}{\partial x}\right)_y = 2x + 4xz, \quad \left(\frac{\partial w}{\partial y}\right)_x = 2y + 4yz.$
Note, we get both differentials at once.

Example 2: For the same functions find $\left(\frac{\partial w}{\partial x}\right)_z$
Now x and z are the independent variables, and y is an intermediate variable.
Method 1: $\left(\frac{\partial w}{\partial x}\right)_z = 2x + 2y\left(\frac{\partial y}{\partial x}\right)_z = w_x \cdot 1 + w_y\left(\frac{\partial y}{\partial z}\right)_x + w_z \cdot 0.$
Constraint: $0 = 2x + 2y\left(\frac{\partial y}{\partial x}\right)_z \ \Rightarrow\ \left(\frac{\partial y}{\partial x}\right)_z = -\frac{x}{y} \ \Rightarrow\ \left(\frac{\partial w}{\partial x}\right)_z = 2x + 2y(-\frac{x}{y}) = 0.$
(Not surprising: z constant $\Rightarrow\ x^2 + y^2$ is constant $\Rightarrow\ w = x^2 + y^2 + z^2$ is constant.)
Method 2: (remove dy)
$dw = 2x\,dx + 2y\,dy + 2z\,dz = w_x\,dx + w_y\,dy + w_z\,dz$
$dz = 2x\,dx + 2y\,dy \ \Rightarrow\ dy = \frac{1}{2y}\,dz - \frac{x}{y}\,dx$
Substitute: $dw = 2x\,dx + 2y(\frac{1}{2y}\,dz - \frac{x}{y}\,dx) + 2z\,dz$
$\qquad = (2x - 2x)\,dx + (1 + 2z)\,dz = 0\,dx + (1 + 2z)\,dz$
$\Rightarrow\ \left(\frac{\partial w}{\partial x}\right)_z = 0, \ \left(\frac{\partial w}{\partial z}\right)_x = 1 + 2z.$

Example 3: Let $w = x^3y - z^2t, \quad xy = zt$. Find $\left(\frac{\partial w}{\partial x}\right)_{y,z}$.
__**answer:**__ Variable: x; Constants: y, z; Function of x: t.
$\Rightarrow\ \left(\frac{\partial w}{\partial x}\right)_{y,z} = 3x^2y - z^2\left(\frac{\partial t}{\partial x}\right)_{y,z}.$
Need $\left(\frac{\partial t}{\partial x}\right)_{y,z} \Rightarrow$ differentiate $xy = zt$ implicitly: $\quad y = z\left(\frac{\partial t}{\partial x}\right)_{y,z} \ \Rightarrow\ \left(\frac{\partial t}{\partial x}\right)_{y,z} = \frac{y}{z}.$
$\Rightarrow\ \left(\frac{\partial w}{\partial x}\right)_{y,z} = 3x^2y - zy.$

(continued)

Example 4: Let $w = x^3y - z^2t$, $\quad xy = zt$. Find $\left(\dfrac{\partial w}{\partial x}\right)_{y,z}$, $\left(\dfrac{\partial w}{\partial y}\right)_{x,z}$, $\left(\dfrac{\partial w}{\partial z}\right)_{x,y}$ using differentials.

answer: Independent variables: x, y, z; $\quad$ dependendent variables: t.

$w = z^3y - z^2t \ \Rightarrow\ dw = 3x^2y\,dx + x^3\,dy - 2zt\,dz - z^2\,dt.$

$xy = zt \ \Rightarrow\ y\,dx + x\,dy = t\,dz + z\,dt$

Solve for dt: $\quad dt = \frac{y}{z}\,dx + \frac{x}{z}\,dy - \frac{t}{z}\,dz$

Substitute in dw:

$$\begin{aligned} dw &= 3x^2y\,dx + x^3\,dy - 2zt\,dz - z^2\left(\tfrac{y}{z}\,dx + \tfrac{x}{z}\,dy - \tfrac{t}{z}\,dz\right) \\ &= (3x^2y - zy)\,dx + (x^3 - xz)\,dy + (-2zt + zt)\,dz \end{aligned}.$$

$$\Rightarrow\ \left(\frac{\partial w}{\partial x}\right)_{y,z} = 3x^2 - zy, \quad \left(\frac{\partial w}{\partial y}\right)_{x,z} = x^3 - xz, \quad \left(\frac{\partial w}{\partial z}\right)_{x,y} = -2zt + zt$$

(Reason: if $w = f(x,y,z)$ then $dw = \left(\dfrac{\partial w}{\partial x}\right)_{y,z} dx + \left(\dfrac{\partial w}{\partial y}\right)_{x,z} dy + \left(\dfrac{\partial w}{\partial z}\right)_{x,y} dz$.)

Thermodynamic variables: p, V, T, U, S, H (pressure, volume, temperature, internal energy, entropy, enthalpy). Any two can be independent and then the others are dependent.

When p, T are independent have the law: $\quad \left(\dfrac{\partial U}{\partial p}\right)_T + T\left(\dfrac{\partial V}{\partial T}\right)_p + p\left(\dfrac{\partial V}{\partial p}\right)_T = 0. \quad (\star\star)$

Example 5: Express this law when V and T are the independent variables.

answer: We need to express $\left(\dfrac{\partial U}{\partial p}\right)_T$, $\left(\dfrac{\partial V}{\partial p}\right)_T$, $\left(\dfrac{\partial V}{\partial T}\right)_p$ in terms of derivatives with independent variables V, T.

To help with the algebra we use the shorthand: $\quad p_V = \left(\frac{\partial p}{\partial V}\right)_T$, $\quad U_T = \left(\frac{\partial U}{\partial T}\right)_V$ etc.

(i.e. V, T are always the independent variables.)

Dependent variables are U and p so we look at dU and dp:

$$\begin{aligned} dU &= \left(\tfrac{\partial U}{\partial V}\right)_T dV + \left(\tfrac{\partial U}{\partial T}\right)_V dT &= U_V\,dV + U_T\,dT. \\ dp &= \left(\tfrac{\partial p}{\partial V}\right)_T dV + \left(\tfrac{\partial p}{\partial T}\right)_V dT &= p_V\,dV + p_T\,dT. \end{aligned}$$

Second eq. $\Rightarrow\ dV = \frac{1}{p_V}\,dp - \frac{p_T}{p_V}\,dT \quad \Rightarrow\ \boxed{\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{p_V}}$ and $\boxed{\left(\frac{\partial V}{\partial T}\right)_p = \frac{-p_T}{p_V}.}$

Substitute for dV: $\quad dU = \frac{1}{p_V}U_V\,dp + \left(-U_V\frac{p_T}{p_V} + U_T\right)dT \quad \Rightarrow\ \boxed{\left(\frac{\partial U}{\partial p}\right)_T = \frac{1}{p_V}U_V.}$

Using the boxed formulas we can restate the law as: $\quad \frac{1}{p_V}\left(\frac{\partial U}{\partial V}\right)_T - \frac{p_T}{p_V} + p\cdot\frac{1}{p_V} = 0.$

(continued)

Fanciest version (Jacobian): As before: $w = f(x, y)$; $x = x(u, v)$, $y = y(u, v)$
In matrix form the chain rule is:

$$\left(\left(\frac{\partial w}{\partial u}\right)_v, \left(\frac{\partial w}{\partial v}\right)_u\right) = \left(\left(\frac{\partial w}{\partial x}\right)_y, \left(\frac{\partial w}{\partial y}\right)_x\right) \begin{pmatrix} \left(\frac{\partial x}{\partial u}\right)_v & \left(\frac{\partial x}{\partial v}\right)_u \\ \left(\frac{\partial y}{\partial u}\right)_v & \left(\frac{\partial y}{\partial v}\right)_u \end{pmatrix}$$
$$= \left(\left(\frac{\partial w}{\partial x}\right)_y, \left(\frac{\partial w}{\partial y}\right)_x\right) \begin{pmatrix} x_u & x_v \\ y_u & y_v \end{pmatrix}$$

The matrix is called the **Jacobian matrix**.
(This is easy to derive using total differentials.)

Example 6: Use the Jacobian to redo example 5.
We do this in small steps.
Step 1. Chain rule:

$$\left(\frac{\partial w}{\partial u}\right)_v = \left(\frac{\partial w}{\partial x}\right)_y \left(\frac{\partial x}{\partial u}\right)_v + \left(\frac{\partial w}{\partial y}\right)_x \left(\frac{\partial y}{\partial u}\right)_v, \quad \left(\frac{\partial w}{\partial v}\right)_u = \left(\frac{\partial w}{\partial x}\right)_y \left(\frac{\partial x}{\partial v}\right)_u + \left(\frac{\partial w}{\partial y}\right)_x \left(\frac{\partial y}{\partial v}\right)_u.$$

Step 2. Write in matrix form: $\left(\left(\frac{\partial w}{\partial u}\right)_v, \left(\frac{\partial w}{\partial v}\right)_u\right) = \left(\left(\frac{\partial w}{\partial x}\right)_y, \left(\frac{\partial w}{\partial y}\right)_x\right) \begin{pmatrix} \left(\frac{\partial x}{\partial u}\right)_v & \left(\frac{\partial x}{\partial v}\right)_u \\ \left(\frac{\partial y}{\partial u}\right)_v & \left(\frac{\partial y}{\partial v}\right)_u \end{pmatrix}.$

Step 3. Decide which variables are (x, y) and which are (u, v):
Old variables $(x, y) \leftrightarrow (p, T)$, new variables $(u, v) \leftrightarrow (V, T)$.

Step 4. Substitute into formula in step 2: $\left(\left(\frac{\partial w}{\partial V}\right)_T, \left(\frac{\partial w}{\partial T}\right)_V\right) = \left(\left(\frac{\partial w}{\partial p}\right)_T, \left(\frac{\partial w}{\partial T}\right)_p\right) \begin{pmatrix} \left(\frac{\partial p}{\partial V}\right)_T & \left(\frac{\partial p}{\partial T}\right)_V \\ \left(\frac{\partial T}{\partial V}\right)_T & \left(\frac{\partial T}{\partial T}\right)_V \end{pmatrix}.$

Step 5. Simplify the matrix: $\left(\frac{\partial T}{\partial V}\right)_T = 0$, $\left(\frac{\partial T}{\partial T}\right)_V = 1$

$$\Rightarrow \left(\left(\frac{\partial w}{\partial V}\right)_T, \left(\frac{\partial w}{\partial T}\right)_V\right) = \left(\left(\frac{\partial w}{\partial p}\right)_T, \left(\frac{\partial w}{\partial T}\right)_p\right) \begin{pmatrix} \left(\frac{\partial p}{\partial V}\right)_T & \left(\frac{\partial p}{\partial T}\right)_V \\ 0 & 1 \end{pmatrix}.$$

Step 6. Call the matrix A, find A^{-1}: $A^{-1} = \frac{1}{|A|} \begin{pmatrix} 1 & -\left(\frac{\partial p}{\partial T}\right)_V \\ 0 & \left(\frac{\partial p}{\partial V}\right)_T \end{pmatrix}.$

Step 7. Choose various w to get all the pieces in formula $(\star\star)$:

$$w = U \Rightarrow \left(\left(\frac{\partial U}{\partial p}\right)_T, \left(\frac{\partial U}{\partial T}\right)_p\right) = \left(\left(\frac{\partial U}{\partial V}\right)_T, \left(\frac{\partial U}{\partial T}\right)_V\right) \cdot A^{-1}$$
$$= \frac{1}{|A|}\left(\left(\frac{\partial U}{\partial V}\right)_T, -\left(\frac{\partial U}{\partial V}\right)_T \left(\frac{\partial p}{\partial T}\right)_V + \left(\frac{\partial U}{\partial T}\right)_V \left(\frac{\partial p}{\partial V}\right)_T\right).$$

$$w = V \Rightarrow \left(\left(\frac{\partial V}{\partial p}\right)_T, \left(\frac{\partial V}{\partial T}\right)_p\right) = \left(\left(\frac{\partial V}{\partial V}\right)_T, \left(\frac{\partial V}{\partial T}\right)_V\right) \cdot A^{-1}$$
$$= (1, 0) \cdot A^{-1}$$
$$= \frac{1}{|A|}\left(1, -\left(\frac{\partial p}{\partial T}\right)_V\right).$$

I.e. $\left(\frac{\partial U}{\partial p}\right)_T = \frac{1}{|A|}\left(\frac{\partial U}{\partial V}\right)_T$, $\left(\frac{\partial V}{\partial p}\right)_T = \frac{1}{|A|}$, $\left(\frac{\partial V}{\partial T}\right)_p = -\frac{1}{|A|}\left(\frac{\partial p}{\partial T}\right)_V.$

Step 8. Substitute into the law $(\star\star)$:

$$\frac{1}{|A|}\left(\left(\frac{\partial U}{\partial V}\right)_T - T\left(\frac{\partial p}{\partial T}\right)_V + p\right) = 0 \Rightarrow \boxed{\left(\frac{\partial U}{\partial V}\right)_T - T\left(\frac{\partial p}{\partial T}\right)_V + p = 0.}$$