30 Non-independent variables: chain rule

Old, compressed version of topic 30 notes.

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 to \( x \) with \( y \) held constant.

This shows explicitly that \( x \) and \( y \) are independent variables.

Recall the chain rule: If \( w = f(x, y) \); and \( x = x(r, t), \ y = y(r, t) \)

\[
\begin{align*}
\frac{\partial w}{\partial r} \left|_t \right. &= \left( \frac{\partial w}{\partial x} \right)_y \left( \frac{\partial x}{\partial r} \right)_t + \left( \frac{\partial w}{\partial y} \right)_x \left( \frac{\partial y}{\partial r} \right)_t \\
\frac{\partial w}{\partial t} \left|_r \right. &= \left( \frac{\partial w}{\partial x} \right)_y \left( \frac{\partial x}{\partial t} \right)_r + \left( \frac{\partial w}{\partial y} \right)_x \left( \frac{\partial y}{\partial t} \right)_r
\end{align*}
\]

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.

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

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 $y = \text{constant}$ (example 1). \hspace{1cm} Slice $z = \text{constant}$ (example 2).

**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:

$$\left( \frac{\partial w}{\partial x} \right)_y \, dx + \left( \frac{\partial w}{\partial y} \right)_x \, dy$$

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 (**) above: $\left( \frac{\partial w}{\partial x} \right)_y = 2x + 4xz$, $\left( \frac{\partial w}{\partial y} \right)_x = 2y + 4yz$.

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 $dy$)

$$dw = 2x \, dx + 2y \, dy + 2z \, dz = w_x \, dx + w_y \, dy + w_z \, dz$$

$$dz = 2x \, dx + 2y \, dy \Rightarrow dy = \frac{1}{2y} dz - \frac{z}{y} \, dx$$

Substitute: $dw = 2x \, dx + 2y(\frac{1}{2y} dz - \frac{z}{y} \, dx) + 2z \, dz$

$$= (2x - 2x) \, dx + (1 + 2z) \, dz = 0 \, dx + (1 + 2z) \, dz$$

$$\Rightarrow \left( \frac{\partial w}{\partial x} \right)_z = 0, \left( \frac{\partial w}{\partial z} \right)_x = 1 + 2z.$$

**Example 3:** Let $w = x^3y - z^2t$, $xy = zt$. 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 \( \left( \frac{\partial t}{\partial x} \right)_{y,z} \) ⇒ differentiate \( xy = zt \) implicitly: \( y = z \left( \frac{\partial t}{\partial x} \right)_{y,z} \) ⇒ \( \left( \frac{\partial t}{\partial x} \right)_{y,z} = \frac{y}{z} . \)

\[ \Rightarrow \left( \frac{\partial w}{\partial x} \right)_{y,z} = 3x^2y - zy. \]

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

**answer:** Independent variables: \( x, y, z; \) dependent variables: \( t. \)

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

\( xy = zt \) ⇒ \( y \, dx + x \, dy = t \, dz + z \, dt \)

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

Substitute in \( dw: \)

\( dw = 3x^2y \, dx + x^3 \, dy - 2zt \, dz - z^2(\frac{y}{z} \, dx + \frac{x}{z} \, dy - \frac{t}{z} \, dz) \)

\[ = \left( 3x^2y - zy \right) \, dx + \left( x^3 - xz \right) \, dy + \left( -2zt + zt \right) \, dz . \]

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

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

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: \( \left( \frac{\partial U}{\partial p} \right)_T + T \left( \frac{\partial V}{\partial T} \right)_p + p \left( \frac{\partial V}{\partial p} \right)_T = 0. \) (**)  

**Example 5:** Express this law when \( V \) and \( T \) are the independent variables.

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

To simplify the notation we use the shorthand:

\( w_V = \left( \frac{\partial w}{\partial V} \right)_T, \ w_T = \left( \frac{\partial w}{\partial T} \right)_V. \)

i.e. in this notation \( V, T \) are always the independent variables.

We first work with an arbitrary function \( w: \)

\( dw = w_V \, dV + w_T \, dT. \) (eq. 1)

Our goal is to rewrite eq. 1 using \( dT \) and \( dp \) where our derivatives are all with respect to \( V \) and \( T. \)

We have: \( dp = p_V \, dV + p_T \, dT \Rightarrow dV = \frac{1}{p_V} \, dp - \frac{p_T}{p_V} \, dT \)
Substituting this into (eq. 1):

\[ dw = w_U \left( \frac{1}{p_U} \frac{dp}{dU} - \frac{p_T}{p_V} \frac{dT}{dU} \right) + w_T \frac{dT}{dU} = \frac{w_V}{p_V} \frac{dp}{dU} + \left( w_T - \frac{w_V p_T}{p_V} \right) \frac{dT}{dU} \]

Looking at the coefficients of \( dp \) and \( dT \):

\[ \left( \frac{\partial w}{\partial p} \right)_T = \frac{w_V}{p_V} \quad \text{and} \quad \left( \frac{\partial w}{\partial T} \right)_p = w_T - \frac{w_V p_T}{p_V}. \]

Now, replacing \( w \) by \( V \) and then \( U \) (and note \( V_T = 0 \) and \( V_V = 1 \)) we get:

\[ \left( \frac{\partial U}{\partial p} \right)_T = \frac{U_V}{p_V}, \quad \left( \frac{\partial U}{\partial T} \right)_p = V_T - \frac{V_T p_T}{p_V} = -\frac{p_T}{p_V}, \quad \left( \frac{\partial V}{\partial p} \right)_T = \frac{V_V}{p_V} = 1. \]

\[ \Rightarrow \text{equation (**) becomes } \frac{U_V}{p_V} + T \left( -\frac{p_T}{p_V} \right) + \frac{p}{p_V} = 0 \iff U_v - T p_T + p = 0 \]

\[ \Rightarrow \left( \frac{\partial U}{\partial V} \right)_T - T \left( \frac{\partial p}{\partial T} \right)_V + p = 0. \]

**Example 6:** Express the law (**) in terms of independent variables \( U \) and \( H \).

Now we’re changing both variables. This can be done using the Jacobian matrix method in example 7, but here we will do it using total differentials. Since the method is similar to example 5 we will offer fewer words of explanation.

Use the shorthand: \( w_U = \left( \frac{\partial w}{\partial U} \right)_H \) and \( w_H = \left( \frac{\partial w}{\partial H} \right)_U \).

We have:

\[ dw = w_U \, dU + w_H \, dH. \]  \hspace{1cm} (eq. 1)

We want to rewrite \( dU \) and \( dH \) in terms of \( dp \) and \( dT \) where our derivatives are all with respect to \( U \) and \( H \). We’ll use matrix methods.

\[ \begin{align*}
  dp &= p_U \, dU + p_H \, dH \\
  dT &= T_U \, dU + T_H \, dH
\end{align*} \quad \Rightarrow \quad \begin{pmatrix} dp \\ dT \end{pmatrix} = \begin{pmatrix} p_U & p_H \\ T_U & T_H \end{pmatrix} \begin{pmatrix} dU \\ dH \end{pmatrix} \]

\[ \Rightarrow \quad \begin{pmatrix} dU \\ dH \end{pmatrix} = \begin{pmatrix} p_U & p_H \\ T_U & T_H \end{pmatrix}^{-1} \begin{pmatrix} dp \\ dT \end{pmatrix} = \frac{1}{D} \begin{pmatrix} T_H & -p_H \\ -T_U & p_U \end{pmatrix} \begin{pmatrix} dp \\ dT \end{pmatrix}, \quad \text{where } D = \begin{vmatrix} p_U & p_H \\ T_U & T_H \end{vmatrix}. \]

\[ \Rightarrow \quad dU = \frac{T_H \, dp - p_H \, dT}{D} \quad \text{and} \quad dH = -\frac{T_U \, dp + p_U \, dT}{D}. \]

Substituting in (eq. 1) and organizing the terms we get:

\[ dw = \frac{(w_U T_H - w_H T_U)}{D} \, dp + \frac{(w_V p_H + w_H p_U)}{D} \, dT. \]

Looking at the coefficients:

\[ \left( \frac{\partial w}{\partial p} \right)_T = \frac{(w_U T_H - w_H T_U)}{D} \quad \text{and} \quad \left( \frac{\partial w}{\partial T} \right)_p = \frac{(w_U p_H + w_H p_U)}{D}. \]

Let \( w = U \) \Rightarrow \left( \frac{\partial U}{\partial p} \right)_T = \frac{(U_U T_H - U_H T_U)}{D} = \frac{T_H}{D}, \quad \text{since } U_U = 1 \text{ and } U_H = 0. \]

Let \( w = V \) \Rightarrow \left( \frac{\partial V}{\partial p} \right)_T = \frac{(V_U T_H - V_H T_U)}{D} \quad \text{and} \quad \left( \frac{\partial V}{\partial T} \right)_p = \frac{(V_U p_H + V_H p_U)}{D}. \]

Substituting in (**) gives:

\[ \frac{T_H}{D} + T \cdot \frac{-V_U p_H + V_H p_U}{D} + p \frac{V_U T_H - V_H T_H}{D} = 0 \]
Use the Jacobian to redo example 5.

Example 7:

The matrix is called the Jacobian matrix. We have to replace each term in the law by a derivative with independent variables \( x, y \) and \( V, T \).

- Step 1. Choose various \( w \): Old variables \( (x, y) \), new variables \( (r, t) \) to get all the pieces in formula (\( **) \).
- Step 2. Write in matrix form: \( (\frac{\partial w}{\partial r})_{t}, (\frac{\partial w}{\partial t})_{r} = (\frac{\partial w}{\partial x})_{y}, (\frac{\partial w}{\partial y})_{x}) \cdot (\frac{\partial x}{\partial r})_{t}, (\frac{\partial y}{\partial r})_{r}) \).

- Step 3. Decide which variables are \( (x, y) \) and which are \( (r, t) \): Old variables \( (x, y) \leftrightarrow (p, T) \), new variables \( (r, t) \leftrightarrow (V, T) \).

- Step 4. Substitute into formula in step 2: \( (\frac{\partial w}{\partial V})_{T}, (\frac{\partial w}{\partial T})_{V} = (\frac{\partial w}{\partial p})_{T}, (\frac{\partial w}{\partial T})_{p} \cdot (\frac{\partial p}{\partial V})_{T}, (\frac{\partial p}{\partial T})_{V} \).

- Step 5. Simplify the matrix: \( \frac{\partial T}{\partial V} = 0, \frac{\partial T}{\partial V} = 1 \)

\[ \frac{\partial w}{\partial V} = (\frac{\partial w}{\partial V})_{T}, (\frac{\partial w}{\partial T})_{V} = (\frac{\partial p}{\partial V})_{T}, (\frac{\partial p}{\partial T})_{V} \]

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

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

\( w = U \) \( \Rightarrow \) \( (\frac{\partial U}{\partial p})_{T}, (\frac{\partial U}{\partial T})_{p} \cdot A^{-1} \)

\[ = \frac{1}{|A|} \left( \begin{array}{cc} 1 & -\frac{\partial p}{\partial V} \\ 0 & 1 \end{array} \right) \cdot (\frac{\partial U}{\partial V})_{T}, (\frac{\partial U}{\partial T})_{V} \cdot (\frac{\partial p}{\partial V})_{T}, (\frac{\partial p}{\partial T})_{V} \cdot (\frac{\partial w}{\partial V})_{T} \cdot (\frac{\partial w}{\partial T})_{V} \).

\[ \Rightarrow \frac{\partial U}{\partial p}_{T} = \frac{1}{|A|} \frac{\partial U}{\partial p}_{T} \ \text{(This is for the first term in the law.)} \]

\( w = V \) \( \Rightarrow \) \( (\frac{\partial V}{\partial p})_{T}, (\frac{\partial V}{\partial T})_{p} \cdot A^{-1} \)

\[ = (1, 0) \cdot A^{-1} = \frac{1}{|A|} \left( \begin{array}{cc} 1 & -\frac{\partial p}{\partial V} \end{array} \right) \).

\[ \Rightarrow \frac{\partial V}{\partial p}_{T} = \frac{1}{|A|}, \frac{\partial V}{\partial T}_{p} = -\frac{1}{|A|} \frac{\partial p}{\partial V} \ \text{(This is for terms 2 and 3 in the law.)} \]
Step 8. Substitute into the law (★★):

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