Chapter 5: Basic Calculus

Derivatives

Derivatives can be evaluated in *Mathematica* using many different commands. The *D* command requires three arguments inside the square brackets: the function, the variable and the number of derivatives. The last two arguments must be in a list.

```
Clear[f]
f = Sin[x];
firstDer = D[f, {x, 1}];
Print["1st derivative of f = ", firstDer]
1st derivative  of f = Cos[x]
```

```
secDer = D[f, {x, 2}];
Print["2nd derivative of f = ", secDer]
2nd derivative  of f = -Sin[x]
```

From Calculus Early Transcendentals, 4th Edition by James Stewart:

Chapter 3 Review: Calculate y'

1. **$y = (x + 2)^8 (x + 3)^6$**
2. **y =** $\sqrt[3]{x} + \dfrac{1}{\sqrt[3]{x}}$
3. **y =** $\dfrac{x}{\sqrt{9-4x}}$
4. **y =** $\dfrac{e^x}{1+x^2}$

Answers: Chapter 3 Review

Problem 1:

Define a function called *f1* and check that the output matches the function:

```
f1 = (x + 2) ^8 * (x + 3) ^6
```

$(2+x)^8\,(3+x)^6$

Take the first derivative of *f1* to get *y'*:

```
ans1 = D[f1, {x, 1}]
```

$6\,(2+x)^8\,(3+x)^5+8\,(2+x)^7\,(3+x)^6$

Simplify this answer using *Simplify*:

```
Simplify[ans1]
```

$2\,(2+x)^7\,(3+x)^5\,(18+7\,x)$

Problem 2:

```
f2 = x^(1 / 3) + 1 / x^(1 / 3)
```

$\frac{1}{x^{1/3}}+x^{1/3}$

```
ans2 = D[f2, {x, 1}]
```

$-\frac{1}{3\,x^{4/3}}+\frac{1}{3\,x^{2/3}}$

```
Simplify[ans2]
```

$\frac{-1+x^{2/3}}{3\,x^{4/3}}$

Problem 3:

```
f3 = x / Sqrt[9 - 4 * x]
```

$\frac{x}{\sqrt{9-4\,x}}$

```
ans3 = D[f3, {x, 1}]
```

$\frac{1}{\sqrt{9-4\,x}}+\frac{2\,x}{(9-4\,x)^{3/2}}$

```
Simplify[ans3]
```
$$\frac{9-2x}{(9-4x)^{3/2}}$$

Problem 4:

```
f4 = Exp[x] / (1 + x^2)
```
$$\frac{e^x}{1+x^2}$$

```
ans4 = D[f4, {x, 1}]
```
$$-\frac{2e^x x}{(1+x^2)^2}+\frac{e^x}{1+x^2}$$

```
Simplify[ans4]
```
$$\frac{e^x(-1+x)^2}{(1+x^2)^2}$$

Partial Derivatives

Another way of evaluating derivatives is to use the palettes. The symbol $\partial_x f$ will evaluate the partial derivative of the function *f* with respect to the variable *x*:

```
∂x f
Cos[x]
```

Try this command on a function containing two variables, *x* and *y*:

```
g = Sin[x] - Cos[y];
∂x g;
Print["The partial derivative of g with respect to x = ",
 %]
The partial derivative of g with respect to x = Cos[x]

∂y g;
Print["The partial derivative of g with respect to y = ",
 %]
The partial derivative of g with respect to y = Sin[y]
```

You can also evaluate the derivative of a function with respect to several variables using the palettes. The expression $\partial_x \, \partial_y \, h$ will allow you to evaluate the partial derivative of *h* with respect to *y* and the partial derivative of the result with respect to *x*.

```
h = x^2 y^4;
∂x ∂y h
8 x y^3
```

The expression above can also be written as $\partial_{y,x} h$ where the list of variables after the ∂ symbol gives the order of differentiation:

```
∂y,x h
8 x y^3
```

From Calculus Early Transcendentals, 4th Edition by James Stewart:

Chapter 14: Example 1

If f (x, y) = $x^3 + x^2 y^3 - 2y^2$, find f_x (2, 1) and f_y (2, 1)

Answers: Chapter 14

<u>Note</u>: f_x and f_y represent the derivative of *f* with respect to *x* and *y*, respectively.
Clear all variables and define a function called *f*:

```
Clear[f, x, y]
f = x^3 + x^2 * y^3 - 2 * y^2
x^3 - 2 y^2 + x^2 y^3
```

Take the derivative with respect to *x*:

```
ans1 = D[f, {x, 1}]
3 x^2 + 2 x y^3
```

Substitute the values of (x,y) = (2,1) into the answer:

```
ans2 = ans1 /. {x → 2, y → 1}
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```

Take the derivative with respect to *y*:

```
ans3 = D[f, {y, 1}]
```
$-4 y + 3 x^2 y^2$

Substitute the values of (x,y) = (2,1) into the answer:

```
ans4 = ans3 /. {x → 2, y → 1}
```
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From Physical Chemistry A Molecular Approach, by Donald McQuarrie and John D. Simon:

Example H-1
Evaluate the two first partial derivatives of the molar pressure *P* for the van der Waals equation:

$$\mathbf{P} = \frac{R\,T}{V - b} - \frac{a}{V^2}$$

P depends on *T* and *V* so *P* = *P (T, V)*. Define an equation for *P*:

```
P = R * T / (V - b) - a / V^2
```
$$-\frac{a}{V^2} + \frac{R\,T}{-b + V}$$

Using *D*, take the partial derivative of *P* with respect to *T* at constant *V*:

```
der1 = D[P, {T, 1}];
Print["(∂P/∂T)V = ", der1]
```
$$\left(\frac{\partial P}{\partial T}\right)_V = \frac{R}{-b + V}$$

Using $\partial_V\, P$, take the partial derivative of *P* with respect to *V* at constant *T*:

```
der2 = ∂V P;
Print["(∂P/∂V)T = ", der2]
```
$$\left(\frac{\partial P}{\partial V}\right)_T = \frac{2\,a}{V^3} - \frac{R\,T}{(-b + V)^2}$$

Infinite Series

The Taylor series of the function *f* at $x_o = c$ can be expressed as:

$$f(\text{x}) = \sum \frac{f^{(n)}(c)}{n!}(x - c)^n = f(c) + \frac{f'(c)}{1!}x + \frac{f''(c)}{2!}x^2 + \ldots$$

If $c = 0$, we have the Maclauren series:

$$f(\text{x}) = \sum \frac{f^{(n)}(0)}{n!}x^n = f(0) + \frac{f'(0)}{1!}x + \frac{f''(0)}{2!}x^2 + \ldots$$

The command *Series* will execute a Taylor series for any function. The command requires four arguments: the function, the variable, the initial value of the variable and the order of the expansion. The last three arguments must be in a list.

For example, execute the Taylor series for $c = 1$ to the 5th order for the function:
$f(x) = \ln x$

```
Series[Log[x], {x, 1, 5}]
```

$$(x-1) - \frac{1}{2}(x-1)^2 + \frac{1}{3}(x-1)^3 - \frac{1}{4}(x-1)^4 + \frac{1}{5}(x-1)^5 + O[x-1]^6$$

Now execute the Maclauren series for $c = 0$ to the 4th order for the function:

$$g(x) = \frac{1}{(1+x)^2}$$

```
Series[1 / (1 + x)^2, {x, 0, 4}]
```

$$1 - 2x + 3x^2 - 4x^3 + 5x^4 + O[x]^5$$

From Calculus Early Transcendentals, 4th Edition by James Stewart:

Chapter 11.10:

Find the Taylor series for *f*(x) centered at the given value of *c:*

$f(x) = 1 + x + x^2$, c = 2

$f(x) = e^x$, c = 3

Answers: Chapter 11.10

Clear all variables and define a function called *f1*:

```
Clear[f1, f2, x]
f1 = 1 + x + x^2
```

$1 + x + x^2$

Take the Taylor series with $a = 2$ to the 4th order:

```
ans1 = Series[f1, {x, 2, 4}]
```

$7 + 5 (x - 2) + (x - 2)^2 + O[x - 2]^5$

Try a different order to see if the answer changes:

```
ans2 = Series[f1, {x, 2, 2}]
```

$7 + 5 (x - 2) + (x - 2)^2 + O[x - 2]^3$

Define a function called *f2* and take the Taylor series with $a = 3$ to the 4th order:

```
f2 = Exp[x]
```

e^x

```
ans3 = Series[f2, {x, 3, 4}]
```

$e^3 + e^3 (x - 3) + \frac{1}{2} e^3 (x - 3)^2 + \frac{1}{6} e^3 (x - 3)^3 + \frac{1}{24} e^3 (x - 3)^4 + O[x - 3]^5$

Try a different order to see if the answer changes:

```
ans4 = Series[f2, {x, 3, 6}]
```

$e^3 + e^3 (x - 3) + \frac{1}{2} e^3 (x - 3)^2 + \frac{1}{6} e^3 (x - 3)^3 +$
$\frac{1}{24} e^3 (x - 3)^4 + \frac{1}{120} e^3 (x - 3)^5 + \frac{1}{720} e^3 (x - 3)^6 + O[x - 3]^7$

From Physical Chemistry A Molecular Approach, by Donald McQuarrie and John D. Simon:

Problem H-7

Evaluate $\left(\frac{\partial U}{\partial V}\right)_T$ for an ideal gas and for a van der Waals gas.

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

Ideal gas: $P = \frac{RT}{V}$

van der Waals gas: $P = \frac{RT}{V - b} - \frac{a}{V^2}$

Answers: Problem H-7

For an ideal gas:

Define an equation for the molar pressure *P* of an ideal gas:

```
Clear[R, T, V, P]
Pideal = R * T / V
```

$\frac{R\,T}{V}$

Using $\partial_T\ Pideal$, take the partial derivative of *Pideal* with respect to *T* at constant *V*:

```
derIdeal = ∂T Pideal
```

$\frac{R}{V}$

Evaluate $T\left(\frac{\partial P}{\partial T}\right)_V - P$ to get $\left(\frac{\partial U}{\partial V}\right)_T$ and print out the answer:

```
ans1 = T * derIdeal - P;
Print["(∂U/∂V)T = ", ans1]
```

$(\frac{\partial U}{\partial V})_T = -P + \frac{R\,T}{V}$

Recall that the molar pressure *P* was defined as *Pideal*. Use the substitution command /. and print out the actual answer:

```
ans2 = ans1 /. P → Pideal;
Print["(∂U/∂V)T = ", ans2, " for an ideal gas"]
```

$(\frac{\partial U}{\partial V})_T = 0$ for an ideal gas

The internal energy *U* of an ideal gas is independent of *V* at constant *T*.

For a van der Waals gas:

Define an equation for the molar pressure *P* of a van der Waals gas:

```
Clear[R, T, V, P, a, b]
Pvdw = R * T / (V - b) - a / V^2
```

$$-\frac{a}{V^2} + \frac{R\ T}{-b + V}$$

Using $\partial_T\ Pvdw$, take the partial derivative of *Pvdw* with respect to *T* at constant *V*:

```
dervdw = ∂T Pvdw
```

$$\frac{R}{-b + V}$$

Evaluate $T\left(\frac{\partial P}{\partial T}\right)_V$ - *P* to get $\left(\frac{\partial U}{\partial V}\right)_T$ and print out the answer:

```
ans3 = T * dervdw - P;
Print["(∂U/∂V)T = ", ans3]
```

$$\left(\frac{\partial U}{\partial V}\right)_T = -P + \frac{R\ T}{-b + V}$$

Recall that the molar pressure *P* was defined as *Pvdw*. Use the substitution command /. and print out the actual answer:

```
ans4 = ans3 /. P → Pvdw;
Print["(∂U/∂V)T = ", ans4, " for a van der Waals gas"]
```

$\left(\frac{\partial U}{\partial V}\right)_T = \frac{a}{V^2}$ for a van der Waals gas

The internal energy *U* of a van der Waals gas is dependent on *V* at constant *T*.