Chemistry BC3252y
Problem Session 1
Monday, September 10, 2007

Partial Derivatives
Differential Equations (set 0)

Calculus: Partial derivatives

Single variable calculus

$y = y(x)$, derivative is dy/dx

dy/dx is the slope of the function $y(x)$

e.g. if $y = a + bx + cx^2 + k \ln x$,

then $dy/dx = b + 2cx + k/x$

(learn basics; use tables if you forget)

More variables

$z= z(x, y)$: what is the slope?

depends on direction!

Calculus: Partial derivatives

$z= z(x,y)$: what is the slope?

Specify direction: derivative with respect to y along the direction of constant x

slope = $(\partial z/\partial y)_x$

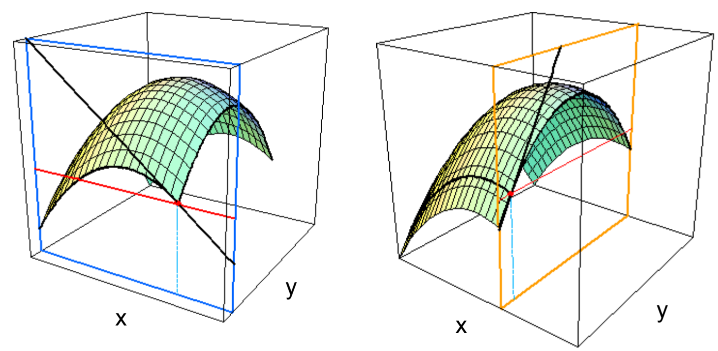
Mathematically, just treat x as a constant

If $z = axy + by^2$

then $(\partial z/\partial y)_x = ax + 2by$

and $(\partial z/\partial x)_y = ay$ [treating y as constant]

Calculus: Partial derivatives



$(\partial f/\partial x)_y$ $(\partial f/\partial y)_x$

figures from www.usd.edu/.../Graphics15/Chapter15_3/Pdy.gif

Calculus: derivatives to integrals

Suppose we know dy/dx. What is y(x)?

If dy/dx = ax, then dy = ax dx

Integrate both sides.

LHS: $\int dy = y$ RHS: $\int ax\,dx = \frac{1}{2}ax^2$

definite integral (with explicit limits)

$y_2 - y_1 = \frac{1}{2}a\,(x_2^2 - x_1^2)$

indefinite integral (include a constant)

$y = \frac{1}{2}ax^2 + C$

Calculus: Derivatives to integrals

Separate variables before integrating!

Anything involving y with dy,
anything involving x with dx.

Constants can be on either side.

Example: dy/dx = axy

$dy/y = ax\,dx \quad \rightarrow \ln y = \frac{1}{2}ax^2 + c$

$\rightarrow y = e^{\frac{1}{2}ax^2+c}$

Check: If $y = e^{\frac{1}{2}ax^2+c}$ What is dy/dx?

$dy/dx = (e^{\frac{1}{2}ax^2+c})(\frac{1}{2}a[2x]) = axy$ ok!

Calculus: Differential equations

dy = ax dx is a differential equation:

an equation involving differentials.

Differential: infinitesimal quantity

Every term in such equations must include a differential:

$dz = A\,dx + B\,dy$

The Classical Wave Equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$

Second order partial differential equation

Describes function u(x,t)

x = distance and t = time

What are units on v?

Use dimensional analysis!

The Classical Wave Equation

$$\frac{\partial^2 u}{\partial x^2} = \frac{1}{v^2}\frac{\partial^2 u}{\partial t^2}$$

Separating variables:

Can a product form $u(x,t) = X(x)T(t)$ work?

Substitute and see!

(Might there be other forms? Yes...

but we are looking for any solution.)

The Classical Wave Equation

$$\frac{1}{X(x)}\frac{\partial^2 X}{\partial x^2} = \frac{1}{v^2}\frac{1}{T(t)}\frac{\partial^2 T}{\partial t^2}$$

Everything on left depends on x; true for all x
Everything on right depends on t, true for all t
(v is a constant)
The ONLY was this equation can be correct for ALL (x, t) is that each side is equal to a constant!
So set each side equal to some constant k:
now have separate equations in x and t.

The Classical Wave Equation

$$\frac{d^2 X}{dx^2} = k\,X$$

No longer curly d's.
If X_1 and X_2 are solutions, then
$X_3 = c_1X_1 + c_2X_2$ is also a solution.

Verify by substitution.
Important general result!

The Classical Wave Equation

$$\frac{d^2 X}{dx^2} = k\,X$$

What must X(x) look like?
LHS = curvature
Suppose $k < 0$.
Then when $X > 0$, curves down,
when $X < 0$, curves up.
always curves back towards the x axis.

What are units on k?

The Classical Wave Equation

$$\frac{d^2X}{dx^2} = -\frac{1}{L^2}X$$

L is a length.
Verify that X = A sin(x/L + a) is a solution.

Two arbitrary constants A, a:
Always have two arbitrary constants in the general solution to a second order differential equation.
Boundary conditions will tell us what they are.

The Classical Wave Equation

$$\frac{d^2X}{dx^2} = k\,X$$

Suppose $k > 0$.
Then when $X < 0$, X(x) curves up,
when $X > 0$ X(x) curves down
(curvature away from axis).
Suppose X=1 when x=0;
what does X(x) look like?

The Classical Wave Equation

$$\frac{d^2X}{dx^2} = k\,X$$

Verify that **$X(x) = D \exp(-\frac{1}{2}kx + d)$** is a solution

Please read the rest on the answers to this problem set, posted on Courseworks.