Mathematics for Biochemistry

LECTURE 14

Functions of more variables 2

Content:

- multiple integrals
- examples of multiple integrals

Functions of several variables:

Multiple integrals (as „antipole“ of partial derivatives):

The multiple integral is a generalization of the definite integral to functions of more than one real variable, for example, $f(x, y)$ or $f(x, y, z)$.
Integrals of a function of two variables over a region in R^2 are called double integrals, and integrals of a function of three variables over a region of R^3 are called triple integrals.
General form of a multiple integral:

$$\int \cdots \int_{\mathbf{D}} f(x_1, x_2, \ldots, x_n) \, dx_1 \cdots dx_n$$

The domain *D* of integration is either represented symbolically for every argument over each integral sign, or is abbreviated by a variable at the rightmost integral sign.

$$\int\limits_{x_1} \cdots \int\limits_{x_n} f(x_1, x_2, \ldots, x_n) \, dx_1 \cdots dx_n$$

Functions of several variables:

Multiple integrals:

Basic rule: the so called changing the order of integration (or reversing the order of integration).

In the case of a double integral: $\iint_D f(x,y)\,dA$

We can integrate with respect to x first: $\iint_D f(x,y)\,dA = \int_{\square}^{\square} \left(\int_{\square}^{\square} f(x,y)\,dx \right) dy,$

... or with respect to y first: $\iint_D f(x,y)\,dA = \int_{\square}^{\square} \left(\int_{\square}^{\square} f(x,y)\,dy \right) dx.$

We often say that the first integral is in *dxdy* order and the second integral is in *dydx* order.

Limits (bounds) of integration (boxes □) can be numbers and sometimes also functions.

Comment: In some situations, we know the limits of integration the *dxdy* order and need to determine the limits of integration for the equivalent integral in *dydx* order (or vice versa).

Functions of several variables:

Multiple integrals – simple example:

Let $R = [0,2] \times [0,1]$. Evaluate the double integral

$$\iint_R xe^y \, dA$$

using both possible orders of integration,
we can write this double integral as either of the iterated integrals

$$\int_0^2 \int_0^1 xe^y dy\, dx, \int_0^1 \int_0^2 xe^y dx\, dy.$$

The former integral is equal to

$$\int_0^2 xe^y \Big|_{y=0}^{y=1} dx = \int_0^2 x(e-1)\, dx = \frac{(e-1)x^2}{2}\Big|_0^2 = 2(e-1).$$

The latter integral is equal to

$$\int_0^1 e^y \frac{x^2}{2}\Big|_{x=0}^{x=2} dy = \int_0^1 2e^y\, dy = 2e^y\Big|_0^1 = 2(e-1).$$

As expected, these two iterated integrals are equal to each other.

Functions of several variables:

Multiple integrals – simple example:

Sometimes it is easier to integrate with respect to one variable first instead of the other variable. For example, let $R = [0, \pi] \times [0, 1]$, and evaluate the double integral

$$\iint_R x \cos(xy)\, dA.$$

Which variable is it easier to integrate with respect to first? If we want to integrate with respect to x, we will need to perform an integration by parts. However, if we integrate with respect to y, we need only use a quick u-substitution, $u = xy$. Then $du = x\,dy$, and we get

$$\iint_R x\cos(xy)\,dA = \int_0^{\pi}\int_0^{1} x\cos(xy)\,dy\,dx = \int_0^{\pi}\left(\sin(xy)\Big|_{y=0}^{y=1}\right)dx =$$

$$= \int_0^{\pi} \sin x\,dx = -\cos x\Big|_0^{\pi} = 2.$$

While in principle it does not matter which variable you integrate with respect to first, in practice it can be computationally easier to integrate with respect to one variable first instead of using the other variable.

Functions of several variables:

Multiple integrals – double integrals:

Properties of double integrals (valid also for triple, etc.):

- For two functions f and g over a region D,

$$\int\int_D [f(x,y)+g(x,y)]\,dxdy = \int\int_D f(x,y)dxdy + \int\int_D g(x,y)dxdy$$

- For constant c,

$$\int\int_D cf(x,y)dxdy = c\int\int_D f(x,y)dxdy.$$

- If $D = D_1 \bigcup D_2$, where D_1 and D_2 do not overlap except perhaps on their boundaries, then

$$\int\int_D f(x,y)dxdy = \int\int_{D_1} f(x,y)dxdy + \int\int_{D_2} f(x,y)dxdy$$

Multiple integrals – double integrals over general regions:

A plane region D is said to be of type I if

$$D = \{(x, y) | a \leq x \leq b, g_1(x) \leq y \leq g_2(x)\},$$

where g_1 and g_2 are continuous on $[a, b]$.

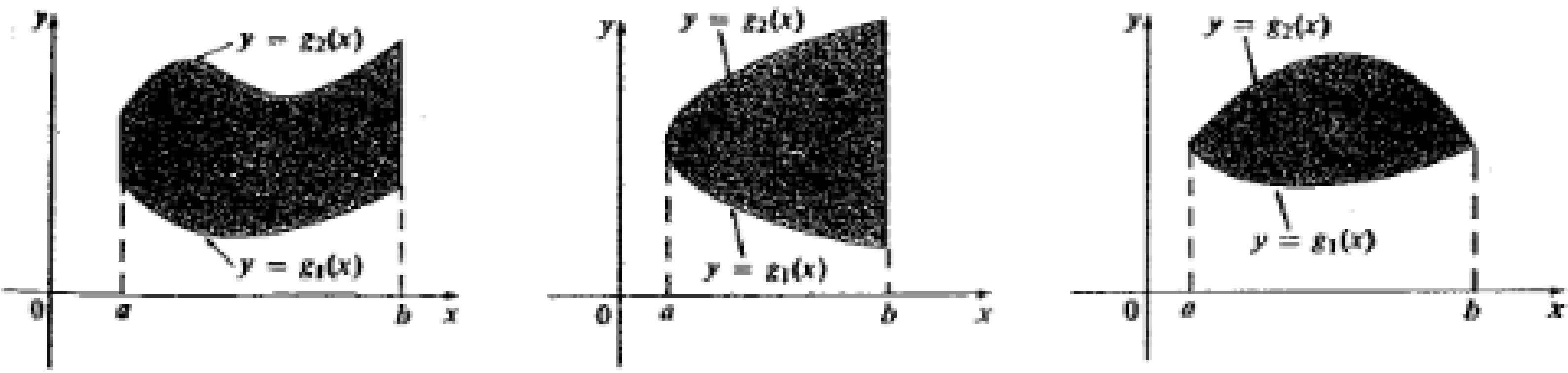


Figure Some type I regions

If f is continuous on a type I region

$$D = \{(x, y) | a \leq x \leq b, g_1(x) \leq y \leq g_2(x)\},$$

then

$$\int\int_D f(x, y)dxdy = \int_a^b \int_{g_1(x)}^{g_2(x)} f(x, y)dydx = \int_a^b \left[\int_{g_1(x)}^{g_2(x)} f(x, y)dy\right] dx$$

Multiple integrals – double integrals over general regions:

Example . Evaluate $\int\int_D (x+2y)dxdy$, where

$$D = \{(x,y) | -1 \le x \le 1, 2x^2 \le y \le 1+x^2\}.$$

Solution. Note that D is a region of type I. We have

$$\begin{aligned}
\int\int_D (x+2y)dxdy &= \int_{-1}^{1}\int_{2x^2}^{1+x^2}(x+2y)dydx \\
&= \int_{-1}^{1}\left[\int_{2x^2}^{1+x^2}(x+2y)dy\right]dx \\
&= \int_{-1}^{1}(xy+y^2)\Big|_{2x^2}^{1+x^2}dx \\
&= \int_{-1}^{1}\left[x(1+x^2)+(1+x^2)^2-(x\cdot 2x^2+4x^4)\right]dx \\
&= \int_{-1}^{1}(-3x^4-x^3+2x^2+x+1)dx \\
&= \left[-\frac{3}{5}x^5-\frac{x^4}{4}+\frac{2x^3}{3}+\frac{x^2}{2}+x\right]\Big|_{-1}^{1} = \frac{32}{15}.
\end{aligned}$$

Double integrals - example (so called Gaussian integral): (1/3)

In lecture nr.9 (slide nr. 6) we have mentioned that solutions of some indefinite integrals do not exist, when we describe the primitive functions by means of elementary functions.

One of this functions was also the exp($-x^2$), used often in statistics. But in the case of an unbounded (improper) integral, the solution can be found by means of a double integral.

So, we try to find the solution of the following (Gaussian) integral:

$$I = \int_{-\infty}^{\infty} e^{-x^2}\, dx$$

We can formulate a square of the searched integral I:

$$I^2 = \left(\int_{-\infty}^{\infty} e^{-x^2}\, dx\right)^2 = \int_{-\infty}^{\infty} e^{-x^2}\, dx \int_{-\infty}^{\infty} e^{-y^2}\, dy$$

where the dummy variable y has been substituted for x in the last integral. This is now a double integral, which can be rewritten:

$$I^2 = \left(\int_{-\infty}^{\infty} e^{-x^2}\,dx\right)^2 = \int_{-\infty}^{\infty} e^{-x^2}\,dx \int_{-\infty}^{\infty} e^{-y^2}\,dy$$

The product of two integrals can be expressed as a double integral:

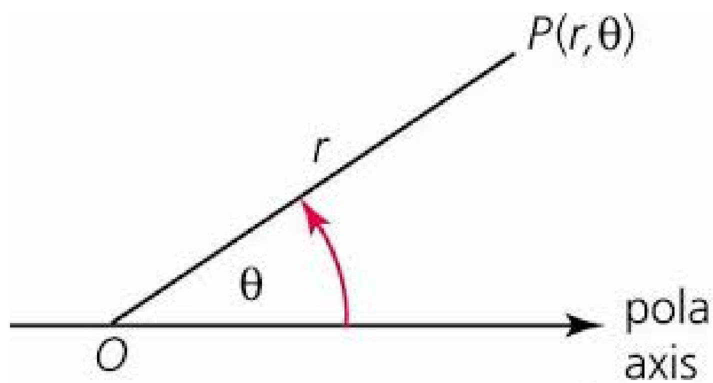
$$I^2 = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{-(x^2+y^2)}\,dx\,dy$$

The differential *dxdy* represents an element of area in Cartesian coordinates. An alternative representation of the last integral can be expressed in plane polar coordinates *r*, *θ*.

These two coordinate systems are related by following relations:

$$x = r\cos\theta, \qquad y = r\sin\theta \qquad r^2 = x^2 + y^2$$

The element of area in polar coordinates is given by *rdrdθ* (exactly: *dr·rdθ*), so that the double integral becomes:



$$I^2 = \int_0^{\infty} \int_0^{2\pi} e^{-r^2}\, r\,dr\,d\theta$$

$$I^2 = \int_0^\infty \int_0^{2\pi} e^{-r^2}\, r\, dr\, d\theta$$

Integration over θ gives a factor 2π. The integral over r can be done after the substitution $u = r^2$, $du = 2r\,dr$:

$$I^2 = 2\pi \int_0^\infty e^{-r^2}\, r\, dr = 2\pi \tfrac{1}{2} \int_0^\infty e^{-u}\, du = \pi$$

Finally, we can write:

$$\int_{-\infty}^{\infty} e^{-x^2}\, dx = \sqrt{\pi}$$

This nice and simple solution we were not able to obtain by means of the solution of indefinite integral of one variable...

Double integrals – next examples:

Using again a double integral in plane polar coordinates (*r*, *θ*),
we can write (element of area in polar coordinates is given by *rdrdθ*):

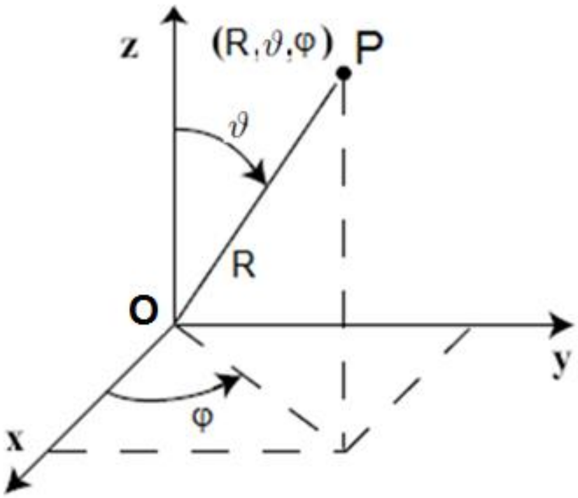
$$S = \int_0^R \int_0^{2\pi} r dr d\theta = 2\pi \int_0^R r dr = 2\pi \left[\frac{r^2}{2} \right]_0^R = \boxed{\pi R^2}$$

This gave us the well known formula for circle area evaluation.

Coming back to the spherical coordinate system (R, ϑ, φ):

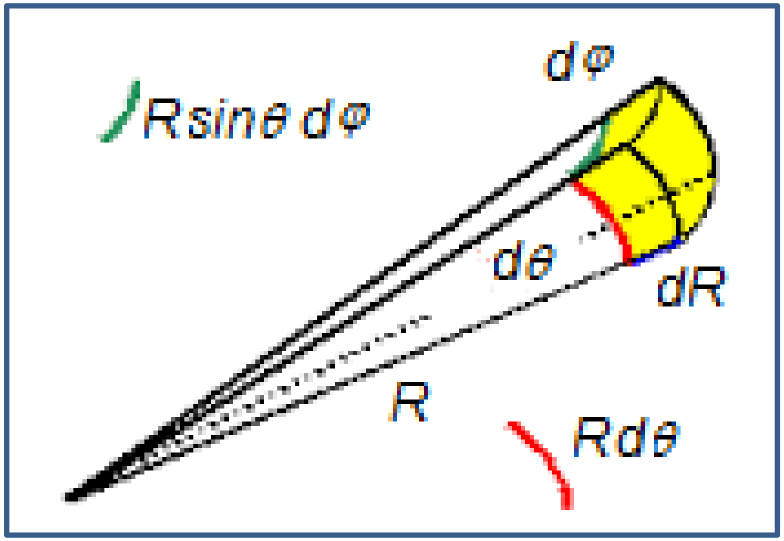
$$S = \int_0^{\pi} \int_0^{2\pi} R^2 \sin\vartheta d\vartheta d\varphi = 2\pi R^2 \int_0^{\pi} \sin\vartheta d\vartheta =$$

$$= 2\pi R^2 \left[-\cos\vartheta \right]_0^{\pi} = 2\pi R^2 [1+1] = \boxed{4\pi R^2}$$



This gave us the well known formula for a sphere surface evaluation.

Triple integral – example:



Staying with the spherical coordinate system (R, ϑ, φ):

$$V=\int_0^{\pi}\int_0^{2\pi}\int_0^{a} R^2 \sin\vartheta d\vartheta d\varphi dR = 2\pi\int_0^{\pi}\int_0^{a} R^2 \sin\vartheta d\vartheta dR =$$

$$=2\pi\int_0^{a}\left[-\cos\vartheta\right]_0^{\pi} R^2 dR = 4\pi\int_0^{a} R^2 dR =$$

$$=4\pi\left[\frac{R^3}{3}\right]_0^{a} = \boxed{\frac{4}{3}\pi a^3}$$

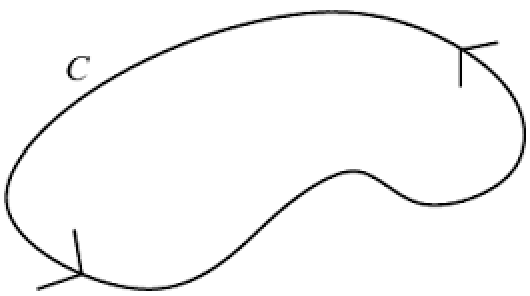
This gave us the well known formula for a sphere volume evaluation.

Integrals – additional comments:

In various text-books and scientific papers you can find notation of integrals with a circle crossing the symbols of integrals. These show integrals evaluated along closed curves or surfaces.

$$\oint_C A\,dl$$

- so called circulation integral (curve integral - along the closed curve *C*), *A* is the integrated function, *dl* is the element of the curve



$$\oiint_S E\,ds$$

- so called flux integral (surface integral - over the closed surface *S*), *E* is the integrated function, *ds* is the element of the surface