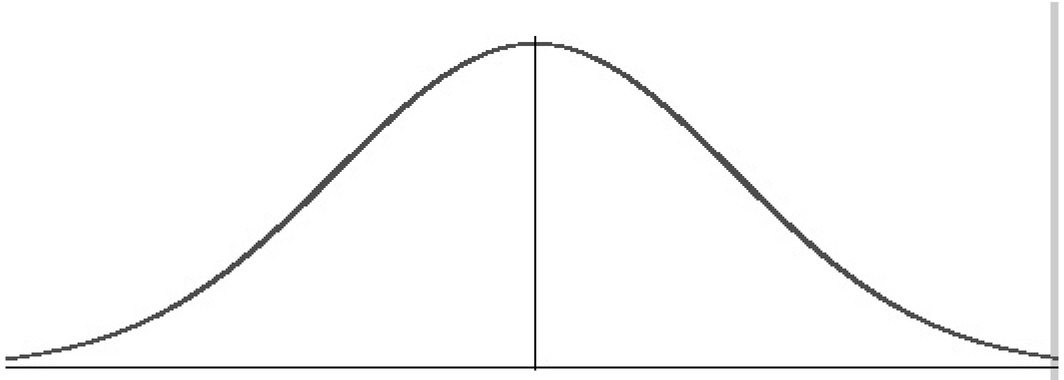
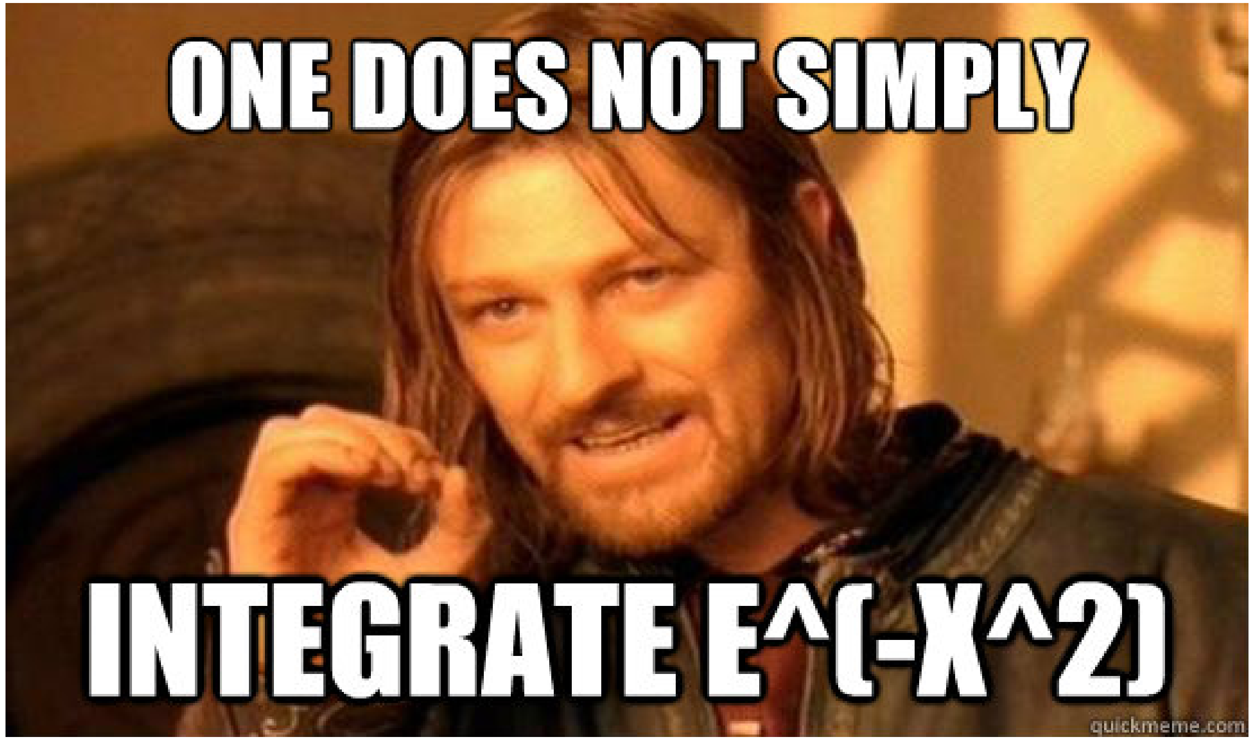
Application 1 of multivariate calculus to probability/statistics: the Gaussian integral

The normal distribution (also called the Gaussian distribution) has probability density function proportional to e^{-x^2}, i.e. $p(x) = \frac{1}{Z}e^{-x^2}$ for some Z. We need to choose the constant of proportionality Z so that the total probability is 1, i.e.

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





The problem is, we cannot write down the antiderivative of e^{-x^2} - it is not an elementary function. But multiple integration will help us in a surprising, clever way.

First, we need to show that the improper integral $Z = \int_{-\infty}^{\infty} e^{-x^2}\,dx$ converges.

It will be enough to show that $Z' = \int_{1}^{\infty} e^{-x^2}\,dx$ converges, because then

$$Z = \int_{-\infty}^{-1} e^{-x^2}\,dx + \int_{-1}^{1} e^{-x^2}\,dx + \int_{1}^{\infty} e^{-x^2}\,dx = Z' + \int_{-1}^{1} e^{-x^2}\,dx + Z'.$$

We show that Z' converges using the (non-examinable) technique of integral estimation by inequalities:

e^{-x^2} is a non-negative function, so FTC1 says that $F(R) = \int_{1}^{R} e^{-x^2}\,dx$ is an increasing function (in R).

So, using some theorems from analysis, we know that, if there is a number M such that $M \geq F(R) = \int_{1}^{R} e^{-x^2}\,dx$ for every $R > 1$, then $\lim_{R\to\infty} F(R)$ exists, i.e. Z' converges.

For all $x \geq 1$, we have $e^{-x^2} \leq e^{-x}$, so $\int_{1}^{R} e^{-x^2}\,dx \leq \int_{1}^{R} e^{-x}\,dx = e^{-1} - e^{-R} \leq e^{-1}$,

so e^{-1} is the upper bound M that we want.

Reminder: we wish to evaluate $Z = \int_{-\infty}^{\infty} e^{-x^2}\,dx$.

Consider the double integral $\iint_{\mathbb{R}^2} e^{-x^2}e^{-y^2}\,dA$. The integrand is always positive, so we can calculate this improper integral using an iterated integral:

$$\iint_{\mathbb{R}^2} e^{-x^2}e^{-y^2}\,dA = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-x^2}e^{-y^2}\,dy\,dx = \int_{-\infty}^{\infty} e^{-x^2} Z\,dx = Z^2$$

But we can also calculate this double integral using polar coordinates (yes, you can use change of variables on improper integrals):

$$\iint_{\mathbb{R}^2} e^{-x^2}e^{-y^2}\,dA = \int_0^{2\pi}\int_0^{\infty} e^{-r^2} r\,dr\,d\theta$$

inner integral independent of θ, and substitution $u = r^2$

$$= 2\pi\int_0^{\infty}\frac{e^{-u}}{2}\,du = \pi \lim_{R\to\infty}\int_0^R e^{-u}\,du = \pi\left(\lim_{R\to\infty} 1 - e^{-R}\right) = \pi.$$

So $Z^2 = \pi$, i.e. $Z = \sqrt{\pi}$.

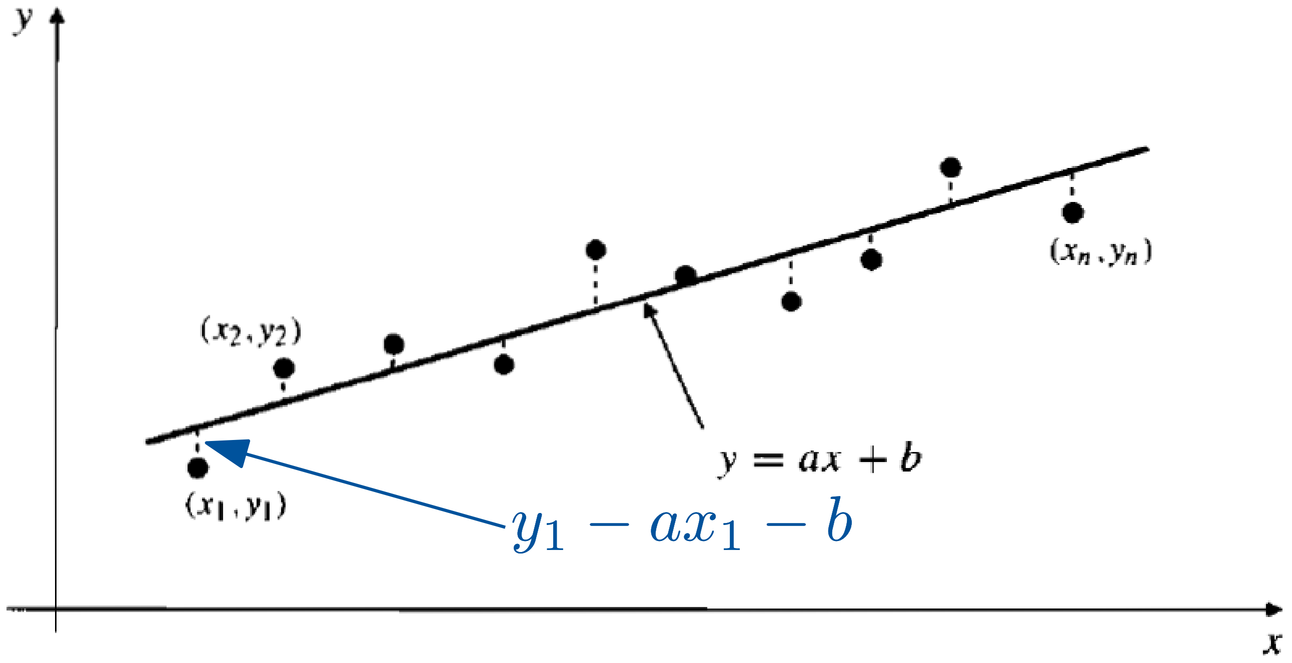
Application 2 of multivariate calculus to probability/statistics: linear regression

Suppose two physical quantities x and y (e.g. temperature and pressure) are related by $y = ax + b$, for some unknown constants a and b. To estimate a and b, we can do an experiment to find some data $(x_1, y_1), \ldots, (x_n, y_n)$, then plot the data and draw a line that "best" fits the data. Mathematically, this means we want to maximise (or minimise) some function $f(a, b)$, where f measures "how well (or how badly) the line fits the data" - what this means will depend on the physical situation.

One common and convenient scheme is least squares, where we minimise the error function

$$f(a,b) = \sum_{i=1}^{n} (y_i - ax_i - b)^2$$

the sum of squares of the vertical distances from the data points to the line (dotted lines in the diagram).



Reminder: given data points $(x_1, y_1), \ldots, (x_n, y_n)$, we wish to minimise the error function $f(a, b) = \sum_{i=1}^{n} (y_i - ax_i - b)^2$.

(The notation is confusing: a, b are the unknowns, and x_i, y_i are known numbers.)

The domain for (a, b) is all of $\mathbb{R}^2$, which has no boundary. So, if a minimum for f exists, it must be at a critical point (because f is differentiable everywhere, so it has no singular points).

At a critical point:

$$\frac{\partial f}{\partial a} = 0 \Rightarrow \sum_{i=1}^{n} 2(y_i - ax_i - b)(-x_i) = 0 \Rightarrow \left(\sum_{i=1}^{n} x_i^2\right) a + \left(\sum_{i=1}^{n} x_i\right) b = \sum_{i=1}^{n} x_i y_i$$

$$\frac{\partial f}{\partial b} = 0 \Rightarrow \sum_{i=1}^{n} 2(y_i - ax_i - b)(-1) = 0 \Rightarrow \left(\sum_{i=1}^{n} x_i\right) a + \left(\sum_{i=1}^{n} 1\right) b = \sum_{i=1}^{n} y_i$$

Divide each equation on the far right hand side by n, and use the mean value notation $\bar{x} = \frac{1}{n}\sum_{i=1}^{n} x_i$:

$$\overline{x^2}a + \overline{x}b = \overline{xy}$$
$$\overline{x}a + b = \overline{y}$$

Combine into a matrix equation:

$$\begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}$$

So $\begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} \overline{x^2} & \overline{x} \\ \overline{x} & 1 \end{pmatrix}^{-1} \begin{pmatrix} \overline{xy} \\ \overline{y} \end{pmatrix}$, which means $a = \dfrac{\overline{xy} - \overline{x}\,\overline{y}}{\overline{x^2} - (\overline{x})^2}$; $\quad b = \dfrac{\overline{x^2}\overline{y} - \overline{x}\,\overline{xy}}{\overline{x^2} - (\overline{x})^2}$.

To conclude that these values of (a, b) really minimises $f(a, b) = \displaystyle\sum_{i=1}^{n} (y_i - ax_i - b)^2$, we need to show that f achieves a minimum on $\mathbb{R}^2$. A precise proof is complicated. The main idea: as (a, b) "moves away from the origin", $f(a, b) \to \infty$ (and $\mathbb{R}^2$ has no boundary so we do not need to consider (a, b) moving towards a boundary point that is not in the domain).