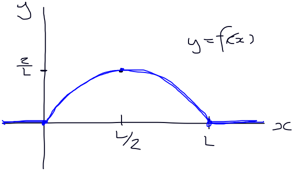
Application of Integration: Probability

Example: QM particle (e.g. "in a box", or hydrogen's electron)

- the **wave function** $\psi(x)$ describes the particle's state
- $f(x) = |\psi(x)|^2 =$ **probability density function** for the position X of the particle



What does this mean? The probability of finding the particle in the interval $[x_1, x_2]$ is $P(x_1 \leq X \leq x_2) = \int_{x_1}^{x_2} f(x)\, dx$.

(And what does *that* mean? The proportion of $N \gg 1$ measurements of the particle <u>in the same state</u> which find it in $[x_1, x_2]$ tends to $P(x_1 \leq X \leq x_2) = \int_{x_1}^{x_2} f(x) dx$, as $N \to \infty$.)

Probability Density Functions

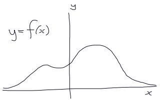
A random variable X is a **continuous random variable** if its possible values range over some interval, $a < x < b$ (possibly $a = -\infty$ and/or $b = \infty$), of real numbers:
position of QM particle, morning commute time, light bulb life,..

The **probability density function**, $f(x)$ of X, defined for $a < x < b$, satisfies: the probability X lies within $[x_1, x_2]$ is

$$\boxed{P(x_1 \leq X \leq x_2) = \int_{x_1}^{x_2} f(x)dx}$$

for each $a < x_1 < x_2 < b$.

- $P(x_1 \leq X \leq x_2) \geq 0 \implies \boxed{f(x) \geq 0}$
- $P(a < X < b) = 1 \implies \boxed{\int_a^b f(x)dx = 1}$ (f is "normalized")



Ex: the probability density function for position X of a QM particle in a 1D box $0 \le x \le L$, at energy $E_n = \frac{\hbar^2\pi^2}{2mL^2}n^2$ $(n = 1, 2, 3, \ldots)$ is

$$f(x) = \psi_n^2(x) = \left\{ \begin{array}{cc} A\sin^2(\frac{n\pi}{L}x) & 0 \le x \le L \\ 0 & x < 0,\ x > L \end{array} \right\}.$$

- Find A:

$$1 = \int_{-\infty}^{\infty} f(x)dx = \int_0^L A\sin^2(\tfrac{n\pi}{L}x)dx = A\int_0^L \tfrac{1}{2}(1 - \cos(2\tfrac{n\pi}{L}x))dx$$
$$= A(\tfrac{1}{2}x - \tfrac{L}{4n\pi}\sin(2\tfrac{n\pi}{L}x))|_0^L = A\tfrac{L}{2} \implies A = \tfrac{2}{L}.$$

This is called "normalizing" a probability density function.

- How likely is the particle to be found in the left $1/4$ of the box?

$$P(0 < X < \tfrac{L}{4}) = \int_0^{\frac{L}{4}} f(x)dx = \tfrac{2}{L}(\tfrac{1}{2}x - \tfrac{L}{4n\pi}\sin(2\tfrac{n\pi}{L}x))|_0^{\frac{L}{4}}$$
$$= \tfrac{1}{4} - \tfrac{1}{n\pi}\sin(\tfrac{n\pi}{2})$$

The (Cumulative) Distribution Function

If X is a continuous random variable taking values in an interval (a, b), with density function $f(x)$, then its **(cumulative) distribution function** is

$$\boxed{F(x) = P(X < x) = \int_a^x f(t)dt}$$

- $F(a) = 0, \quad F(b) = 1$
- since $f(x) \geq 0$, F is an increasing function (strictly speaking, non-decreasing)
- we can recover f from F via Fundamental Theorem of Calculus

  $f(x) = \frac{d}{dx}F(x)$

  and $P(x_1 < X < x_2) = \int_{x_1}^{x_2} f(x)dx = F(x_2) - F(x_1)$

Concept check:
$P(X > x) = \int_x^b f(t)dt = 1 - F(x) = 1 - P(X < x) = 1 - \int_a^x f(t)dt$

The Mean of a Probability Density Function

Let X be a continuous random variable with probability density function $f(x)$. Then the
"average value of X in the long-run" $=$ the **mean of** f:

$$\boxed{\mu = \bar{x} = \int_a^b x\, f(x)\, dx}$$

Ex: The probability density function for the electron-proton distance r in the hydrogen atom ground state (1s orbital) is

$$f(r) = 4\pi r^2\, \psi_{100}^2(r) = \frac{4}{a_0^3} r^2 e^{-\frac{2r}{a_0}}, \quad r \geq 0 \quad (a_0 = \text{Bohr radius})$$

What is the "most probable" location of the electron (max of f) ?

$r_{max} = a_0$

What is the "expected" (mean) location of the electron?

$\bar{r} = \int_0^\infty r\, \frac{4}{a_0^3} r^2 e^{-\frac{2r}{a_0}}\, dr = \frac{3}{2} a_0$