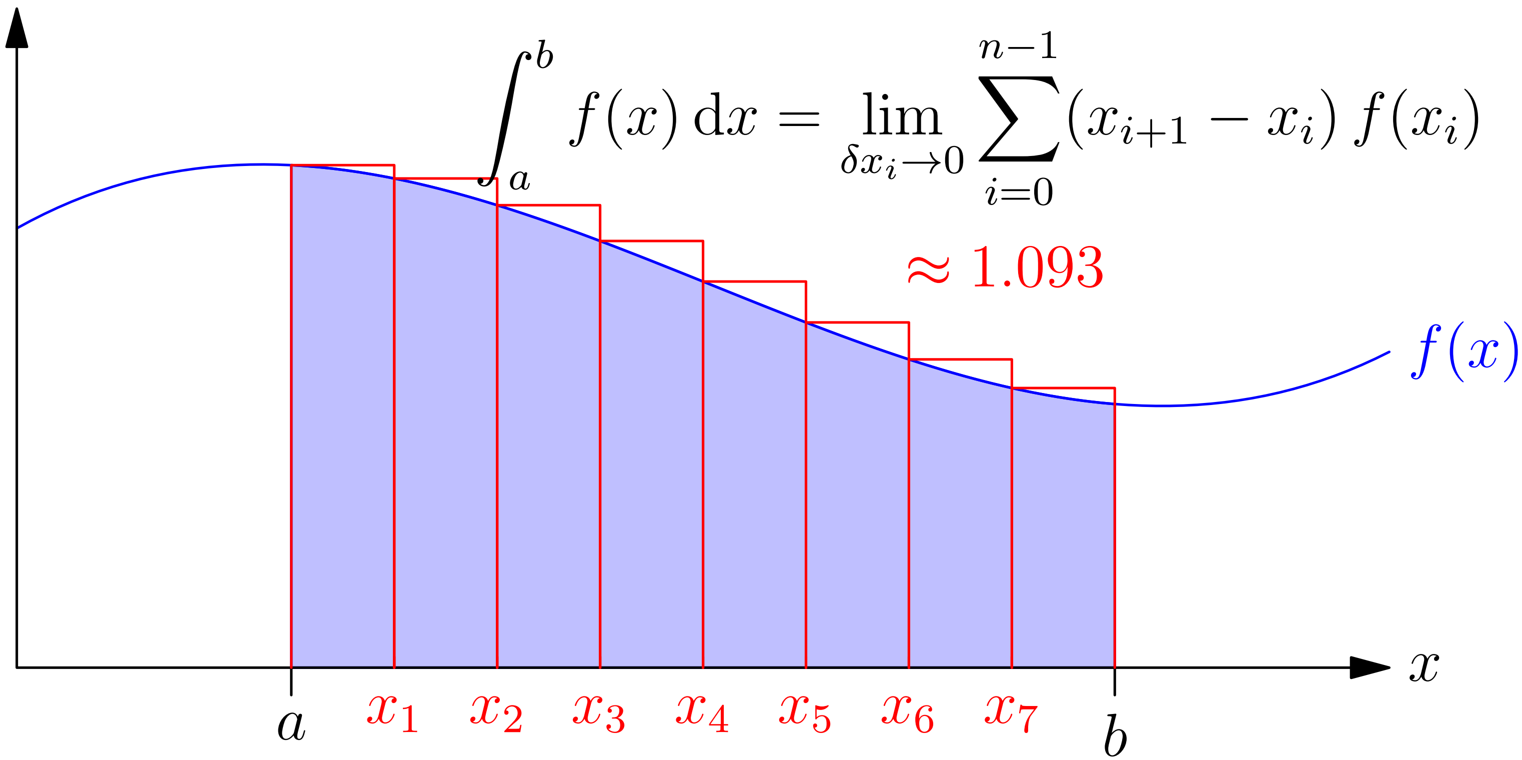
Advanced Machine Learning

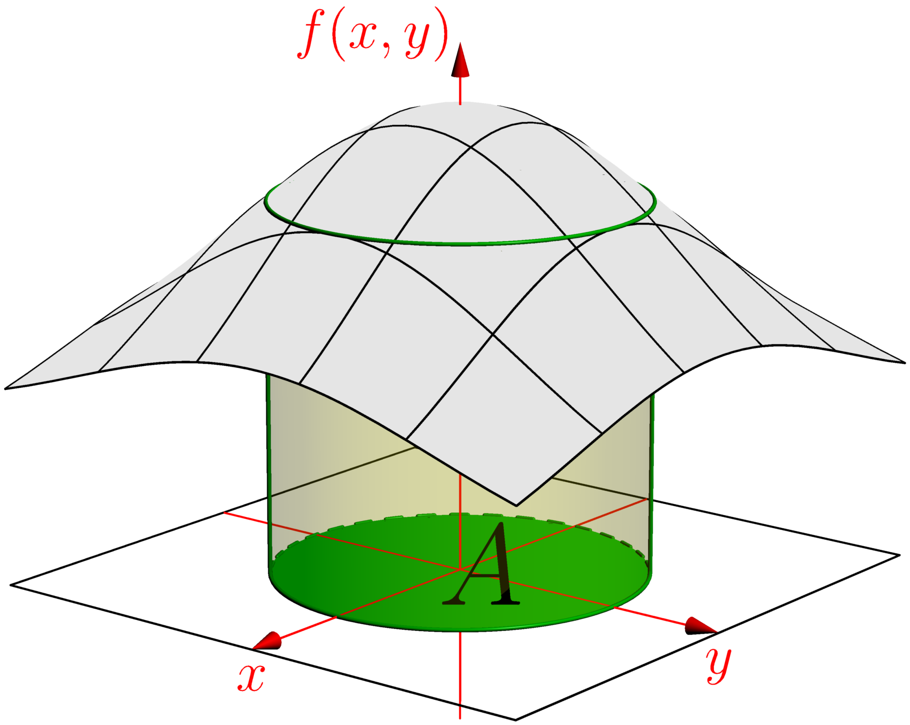
Integral Calculus



Riemann Integration, integration by parts, gaussian integrals

Outline

1. **Defining Integrals**
2. Doing Integrals
3. Gaussian Integrals



Riemann Integral

- Integrals represent area beneath a curve

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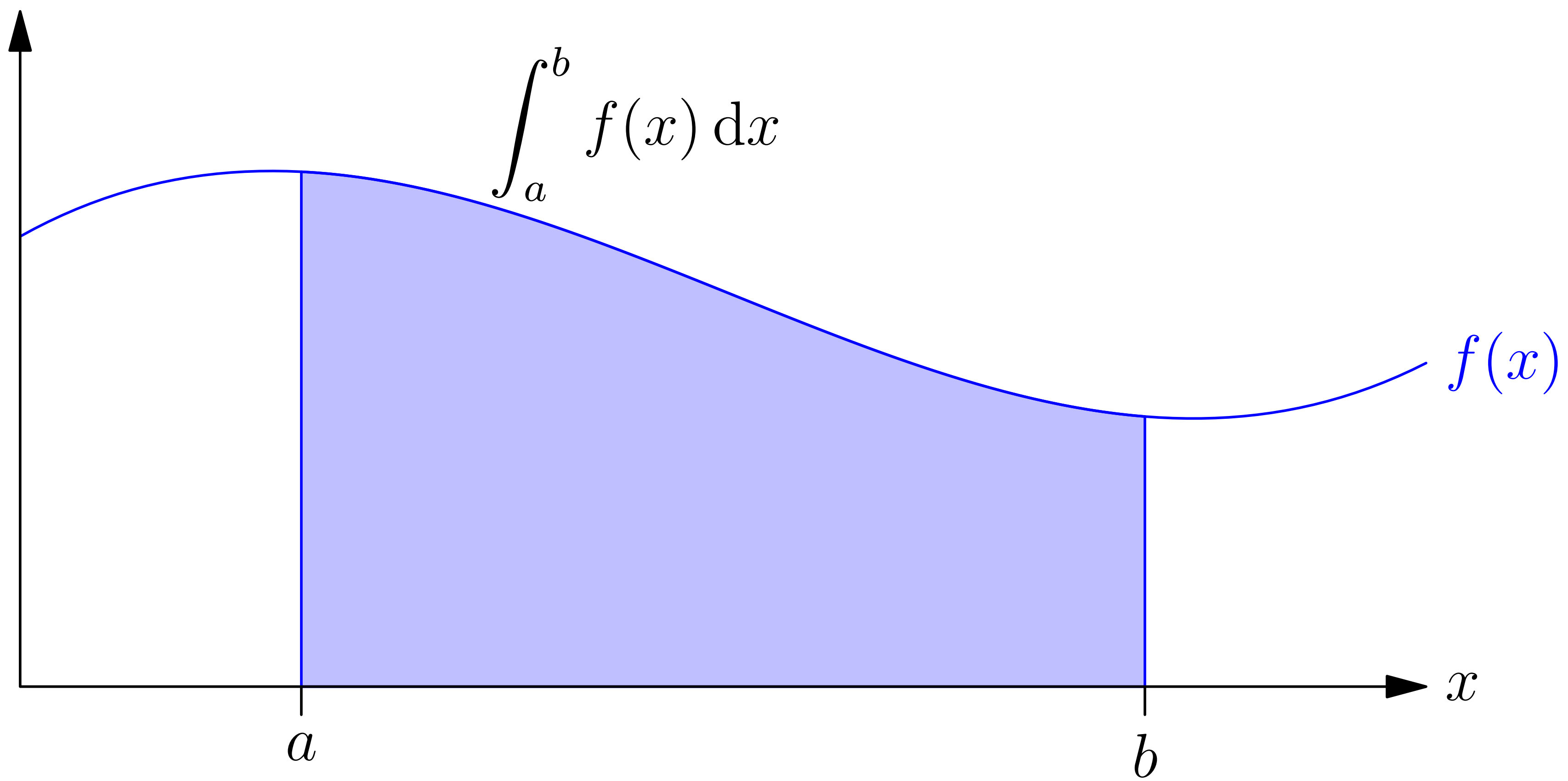

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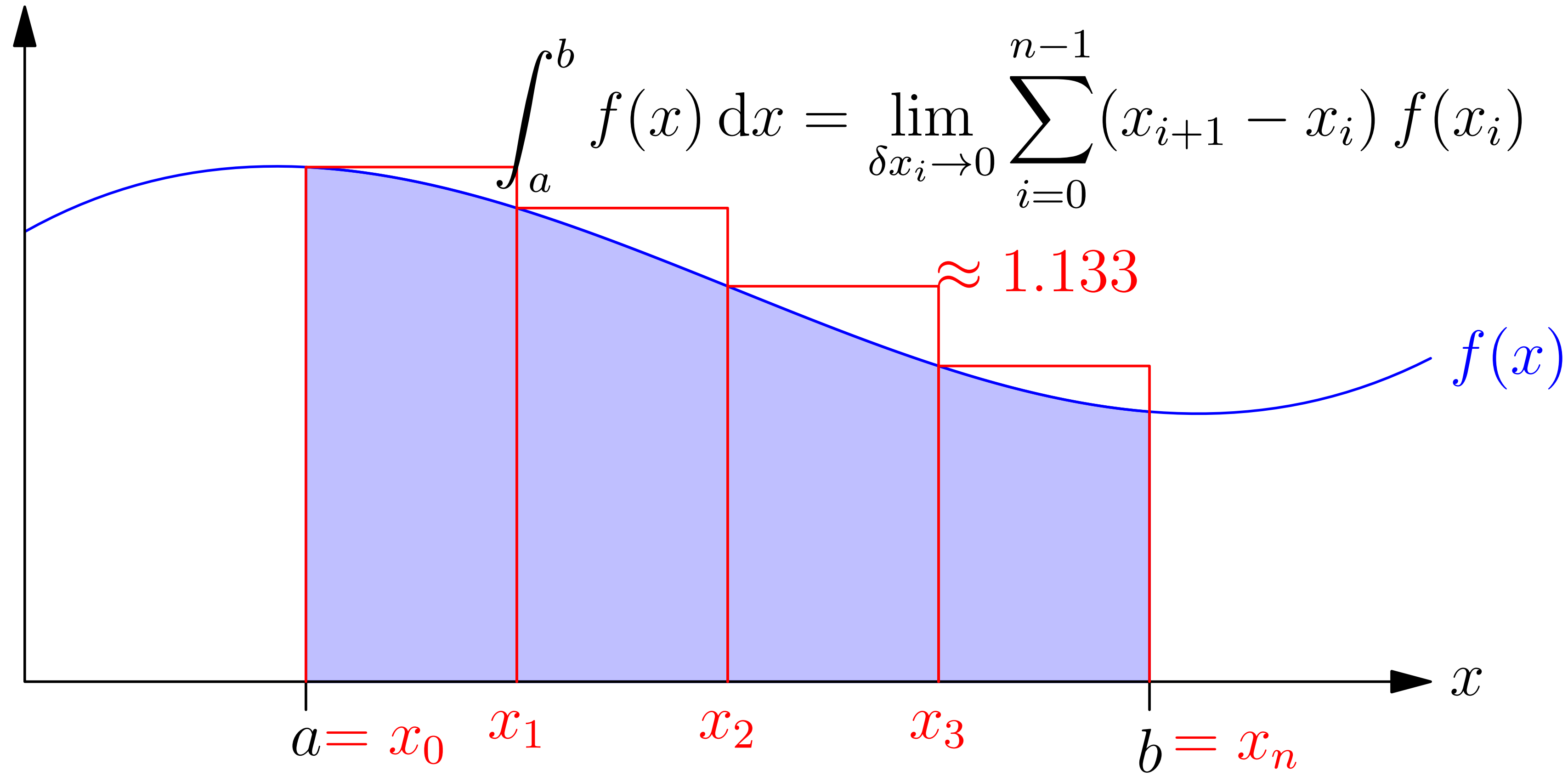

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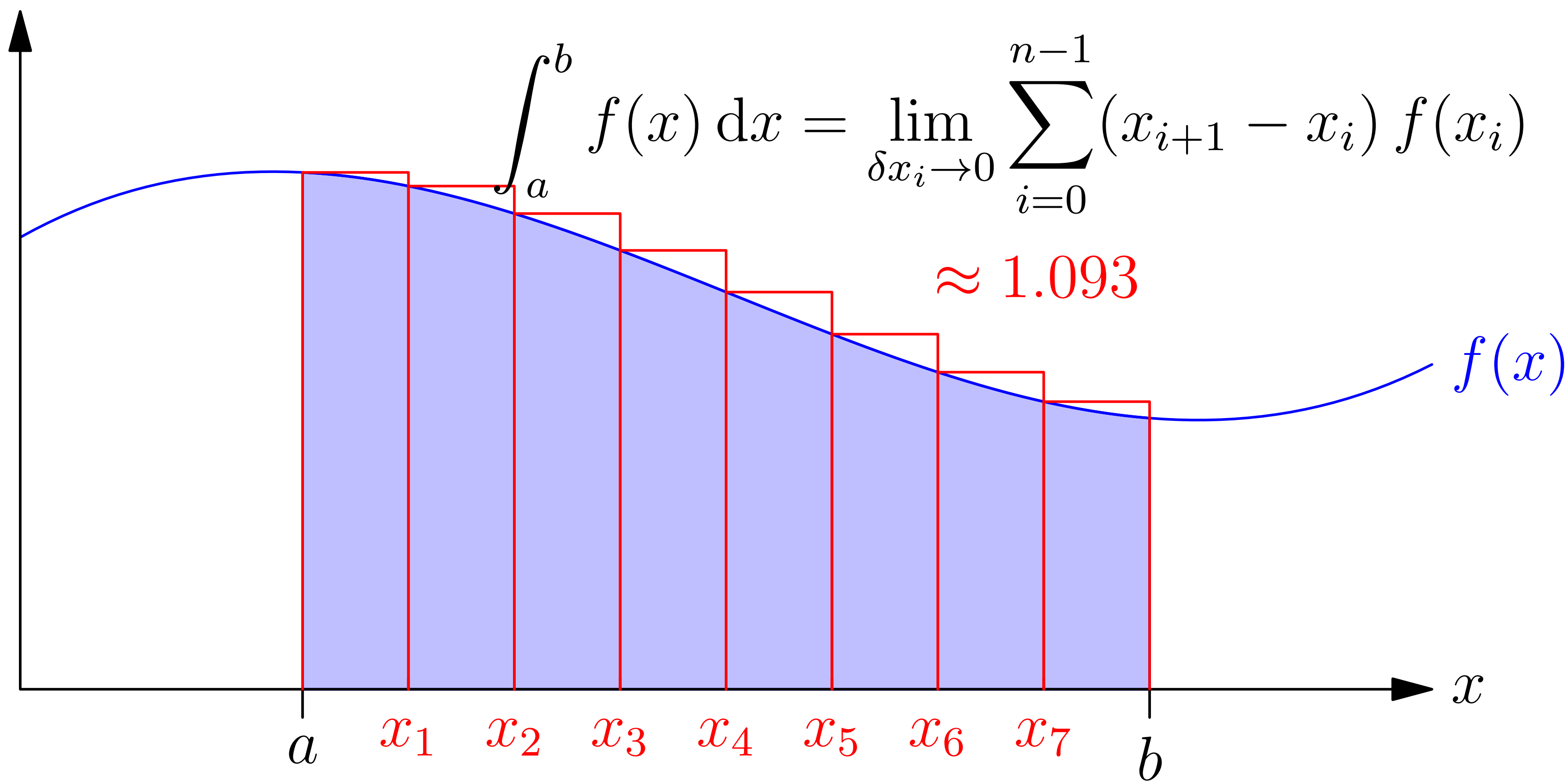

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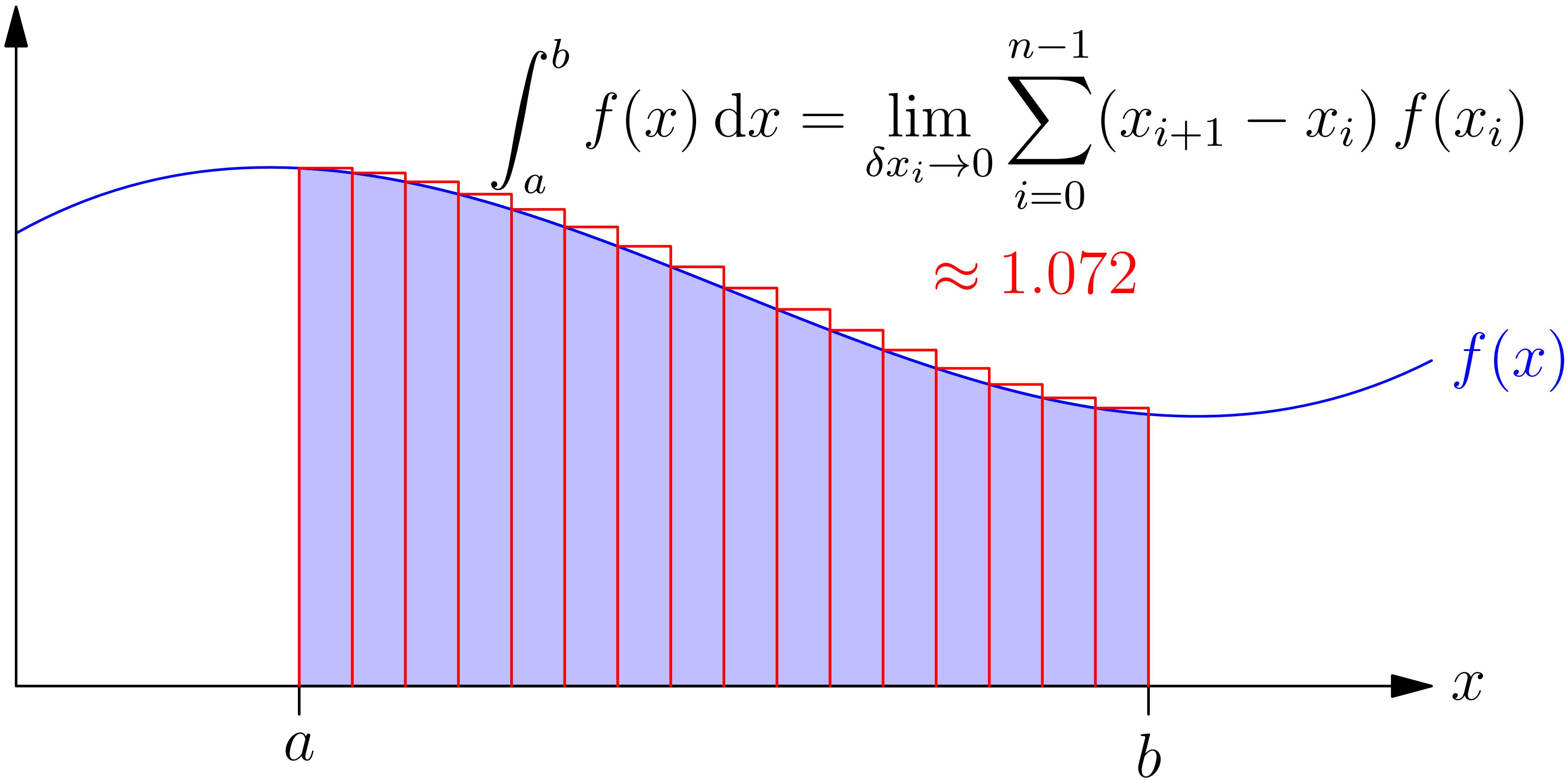

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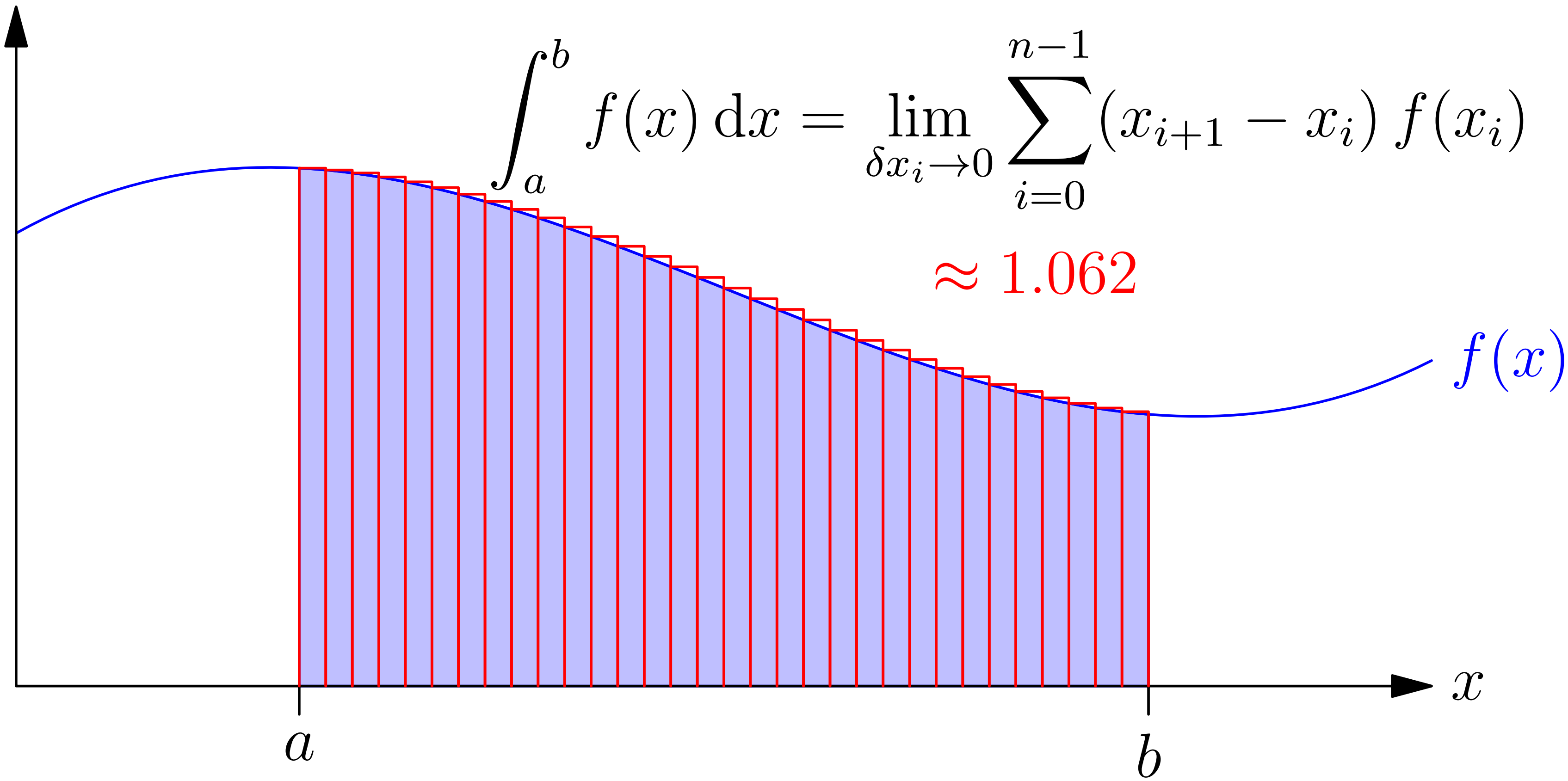

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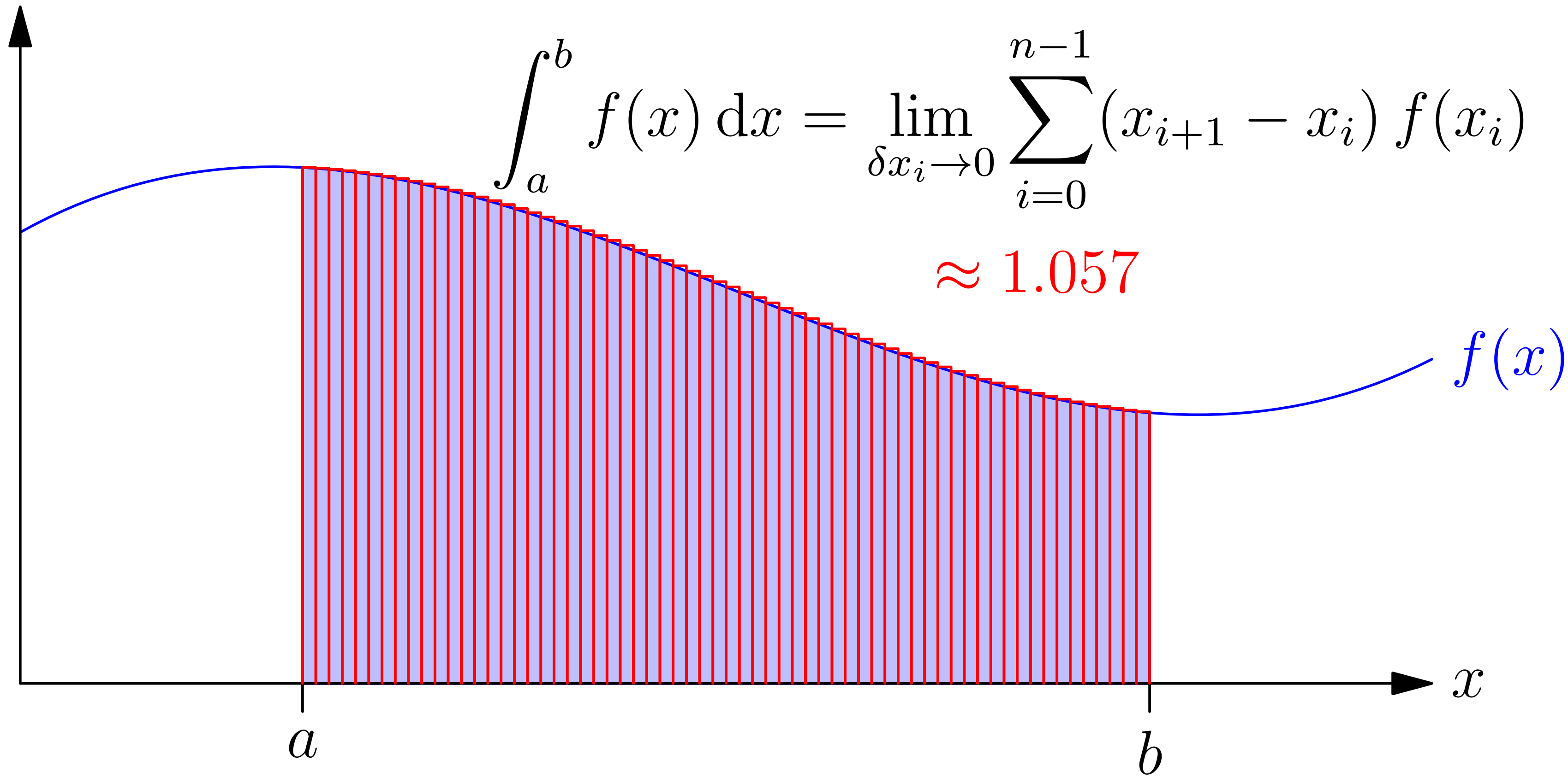

Linearity of Integration

- Integration is a linear operator

$$\int_a^b (r\,f(x) + s\,g(x))\,\mathrm{d}x = \lim_{\delta x_i \to 0} \sum_{i=0}^{n-1} (x_{i+1} - x_i)\,(r\,f(x_i) + s\,g(x_i))$$

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$$= \lim_{\delta x_i \to 0} \left(\sum_{i=0}^{n-1} (x_{i+1} - x_i)\,r\,f(x_i) + \sum_{i=0}^{n-1} (x_{i+1} - x_i)\,s\,g(x_i) \right)$$

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&= \lim_{\delta x_i \to 0} \left(\sum_{i=0}^{n-1} (x_{i+1} - x_i)\,r\,f(x_i) + \sum_{i=0}^{n-1} (x_{i+1} - x_i)\,s\,g(x_i) \right) \\
&= \lim_{\delta x_i \to 0} \left(r \sum_{i=0}^{n-1} (x_{i+1} - x_i)\,f(x_i) + s \sum_{i=0}^{n-1} (x_{i+1} - x_i)\,g(x_i) \right)
\end{aligned}$$

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&= r \int_a^b f(x)\,\mathrm{d}x + s \int_a^b f(x)\,\mathrm{d}x
\end{aligned}
$$

Fundamental Law of Calculus

- Let

$$I(a,x) = \int_a^x f(z)\,\mathrm{d}z = \lim_{\delta z_i \to 0} \sum_{i=0}^{n-1} (z_{i+1} - z_i) f(z_i)$$

- Now for small δx

$$I(a,x+\delta x) = \int_a^{x+\delta x} f(z)\,\mathrm{d}z = \lim_{\delta z_i \to 0} \sum_{i=0}^{n-1} (z_{i+1} - z_i) f(z_i) + \delta x\, f(x)$$

- Thus

$$\frac{\mathrm{d}I(a,x)}{\mathrm{d}x} = \lim_{\delta x \to 0} \frac{I(x+\delta x) - I(x)}{\delta x}$$

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The Other Way Around

- Consider

$$\int_a^b \frac{\mathrm{d}f(x)}{\mathrm{d}x}\mathrm{d}x = \int_a^b \lim_{\delta x \to 0} \frac{f(x+\delta x) - f(x)}{\delta x}\mathrm{d}x$$

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$$= \lim_{x_{i+1}-x_i \to 0} \sum_{i=0}^{n-1} (x_{i+1} - x_i) \frac{f(x_{i+1}) - f(x_i)}{x_{i+1} - x_i}$$

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&= (f(x_1) - f(x_0)) + (f(x_2) - f(x_1)) + (f(x_3) - f(x_2)) + \cdots \\
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- We can think of integration as an **anti-derivative** it undoes differentiation

Indefinite Integrals

- So far we have considered **definite integrals** where we integrate between two points (a and b)
- However, when think about integration as an anti-derivative, it is useful to think of a function $F(x) = \int f(x) \mathrm{d}x$
- So that $F'(x) = f(x)$
- However the function $F(x)$, $F(x) + 1$, $F(x) + \pi$, etc. all have the same derivative so $F(x)$ is only defined up to an additive constant
- Note that the definite integral is given by

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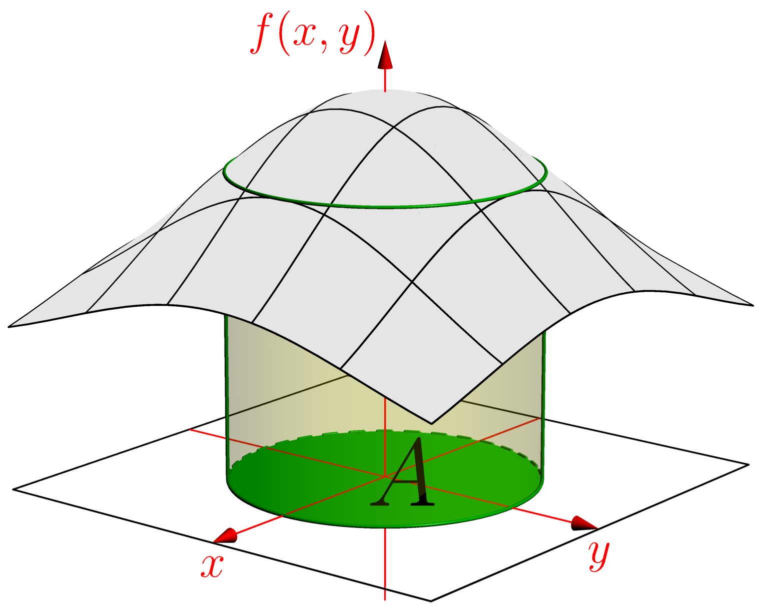
Multiple Integrals

- For functions involving many independent variables (e.g. $f(x,y)$, $f(x,y,z)$, $f(\boldsymbol{x})$) we can integrate over multiple dimensions

- For example

$$\iint_A f(x,y)\,\mathrm{d}x\,\mathrm{d}y$$



- It gets tedious writing multiple integral signs and I tend to write just one

$$\int \cdots \int f(x_1,x_2,\ldots,x_n)\,\mathrm{d}x_1\,\mathrm{d}x_2 \cdots \mathrm{d}x_n$$

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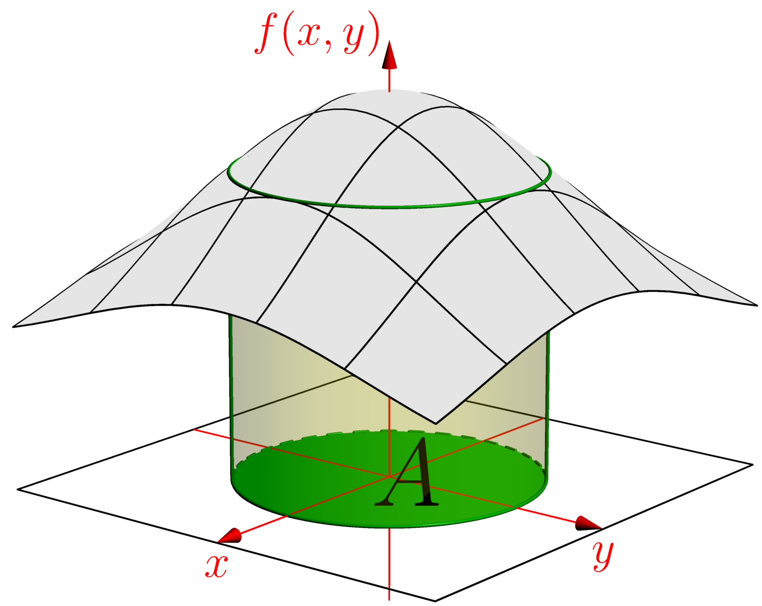

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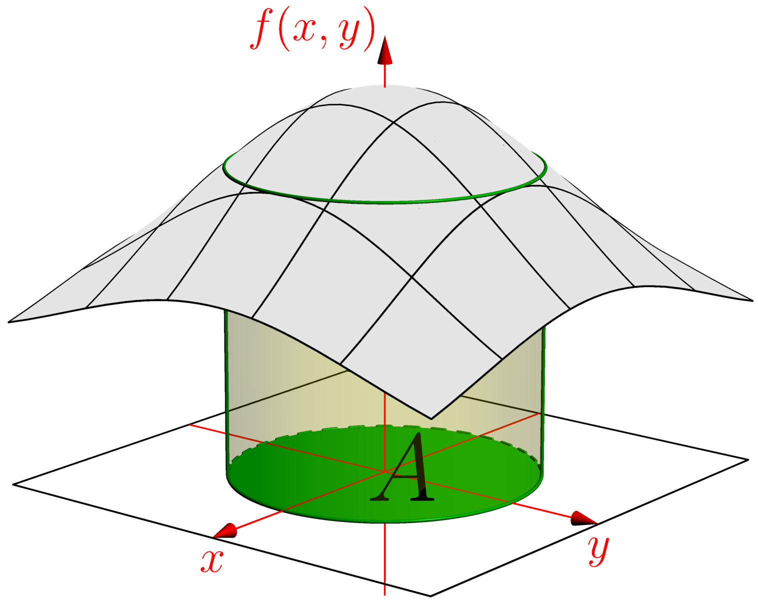

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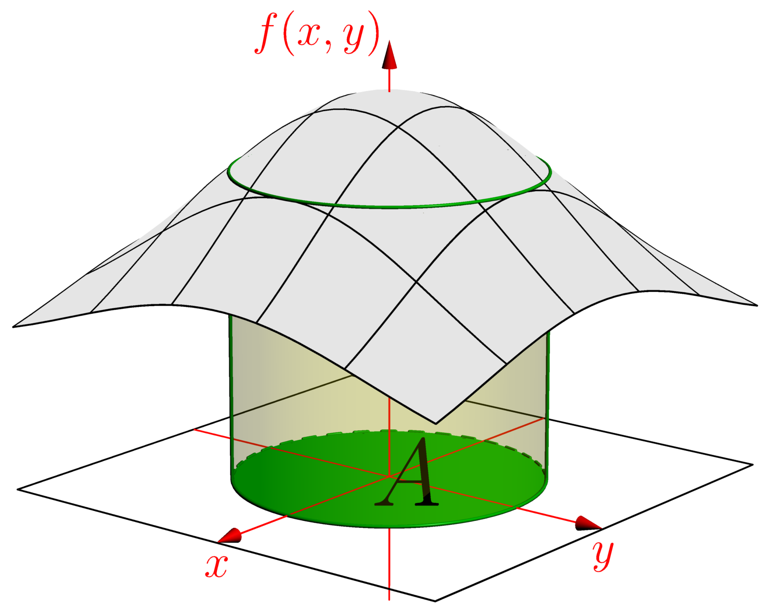

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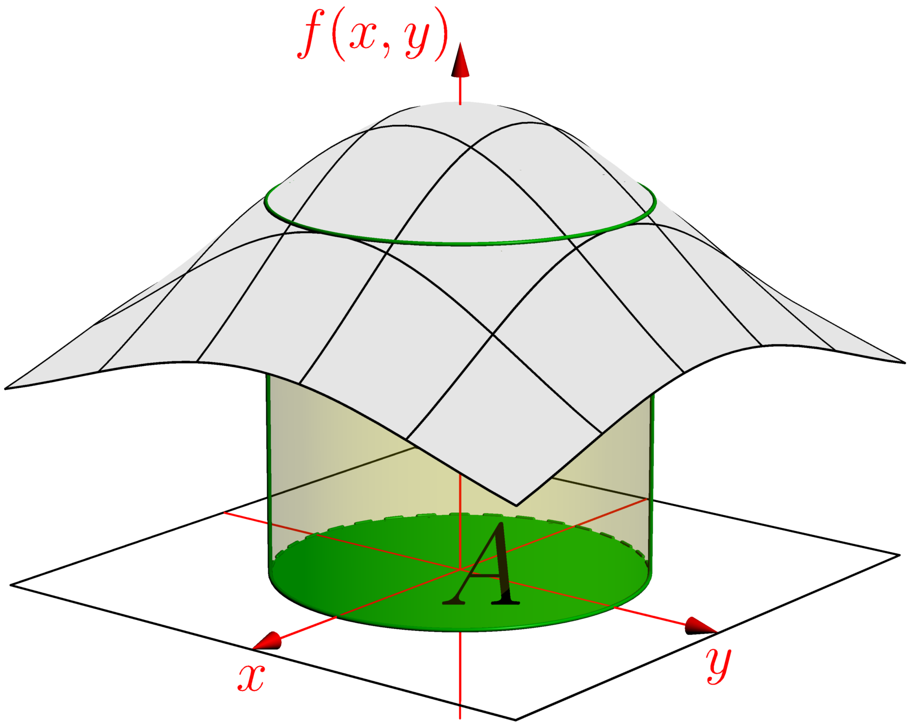
$$\int \cdots \int f(x_1,x_2,\ldots,x_n)\,\mathrm{d}x_1\,\mathrm{d}x_2\cdots\mathrm{d}x_n = \int f(\boldsymbol{x})\,\mathrm{d}\boldsymbol{x}$$

Outline

1. Defining Integrals
2. **Doing Integrals**
3. Gaussian Integrals



Performing Integration

- A key method for performing integrals is through knowledge of the anti-derivative
- If we know $F'(x) = f(x)$ then $F(x) + c = \int f(x)\,\mathrm{d}x$
- E.g. we know that $\mathrm{d}x^n/\mathrm{d}x = n x^{n-1}$ therefore

$$\int x^{n-1}\mathrm{d}x = \frac{1}{n}\int \frac{\mathrm{d}x^n}{\mathrm{d}x}\mathrm{d}x$$

and

$$\int_a^b x^{n-1}\mathrm{d}x = \frac{b^n}{n} - \frac{a^n}{n}$$

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- If we know $F'(x) = f(x)$ then $F(x) + c = \int f(x) \mathrm{d}x$

- E.g. we know that $\mathrm{d}x^n / \mathrm{d}x = n x^{n-1}$ therefore

$$\int x^{n-1} \mathrm{d}x = \frac{1}{n} \int \frac{\mathrm{d}x^n}{\mathrm{d}x} \mathrm{d}x = \frac{x^n}{n} + c$$

and

$$\int_a^b x^{n-1} \mathrm{d}x = \frac{b^n}{n} - \frac{a^n}{n}$$

Is Integration Straightforward?

- We saw due to the product and chain rules that we can differentiate almost anything

- Products and compositions

$$\int f(x)g(x)\mathrm{d}x = ? \qquad\qquad \int f(g(x))\mathrm{d}x = ?$$

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Integration by Parts

- Recall the product rule $\frac{\mathrm{d}f(x)g(x)}{\mathrm{d}x} = \frac{\mathrm{d}f(x)}{\mathrm{d}x}g(x) + f(x)\frac{\mathrm{d}g(x)}{\mathrm{d}x}$
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whether this is helpful depends on $f(x)$ and $g(x)$

Example of Integration by Parts

- Consider

$$\Pi(z) = \int_0^\infty x^z \mathrm{e}^{-x} \mathrm{d}x$$

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- Now
$\Pi(n) = n\Pi(n-1) = n(n-1)\Pi(n-2) = n(n-1)(n-2)\ldots 1 = n!$

Substitution

- We can make a transformation from x to u

$$\int_a^b f(x)\,\mathrm{d}x = \lim_{\delta x_i \to 0} \sum_{i=0}^{n-1} f(x_i)(x_{i+1} - x_i)$$

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⋆ where u_i is such that $x(u_i) = x_i$ or $u_i = u(x_i)$ where $u(x)$ is the inverse of $x(u)$

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$$= \int_{u(a)}^{u(b)} f(x(u)) \frac{\mathrm{d}x(u)}{\mathrm{d}u} \mathrm{d}u$$

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  - ⋆ using $\lim_{\delta u_i \to 0} \frac{x(u_{i+1}) - x(u_i)}{u_{i+1} - u_i} = \frac{\mathrm{d}x(u_i)}{\mathrm{d}u}$

Example of Integration by Substitution

- We consider $I(n) = \int\limits_0^\infty x^n \mathrm{e}^{-x^2/2} \mathrm{d}x$

- Let $u(x) = x^2/2$ or $x(u) = \sqrt{2u}$ so that

$$\frac{\mathrm{d}x(u)}{\mathrm{d}u} = \frac{1}{\sqrt{2u}} \qquad u(0) = 0 \qquad u(\infty) = \infty$$

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- $I(1) = 1$

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- $I(1) = 1$, $I(3) = 2 \times 1! = 2$, $I(5) = 2^2 \times 2! = 8$, but $I(0) = \Pi(-1/2)/\sqrt{2}$, $I(2) = \sqrt{2}\Pi(1/2) = \Pi(-1/2)/\sqrt{2}$

Changing Variables in Multidimensional Space

- When changing variables in many dimensions $\boldsymbol{x} \to \boldsymbol{u}$ the change of variables involves the Jacobian

$$\int f(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \int f(\boldsymbol{x}(\boldsymbol{u})) |\det(\mathrm{J})| \mathrm{d}\boldsymbol{u}, \qquad \boldsymbol{J} = \begin{pmatrix} \frac{\partial x_1}{\partial u_1} & \frac{\partial x_1}{\partial u_2} & \cdots & \frac{\partial x_1}{\partial u_n} \\ \frac{\partial x_1}{\partial u_2} & \frac{\partial x_2}{\partial u_2} & \cdots & \frac{\partial x_2}{\partial u_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial x_n}{\partial u_1} & \frac{\partial x_n}{\partial u_2} & \cdots & \frac{\partial x_n}{\partial u_n} \end{pmatrix}$$

- E.g. transforming from Cartesian coordinates (x,y) to polar coordinates (r,θ) then $x = r\cos(\theta)$ and $y = r\sin(\theta)$

$$|\det(\mathrm{J})| = \left| \det \begin{pmatrix} \frac{\partial r\cos(\theta)}{\partial r} & \frac{\partial r\cos(\theta)}{\partial \theta} \\ \frac{\partial r\sin(\theta)}{\partial r} & \frac{\partial r\sin(\theta)}{\partial \theta} \end{pmatrix} \right|$$

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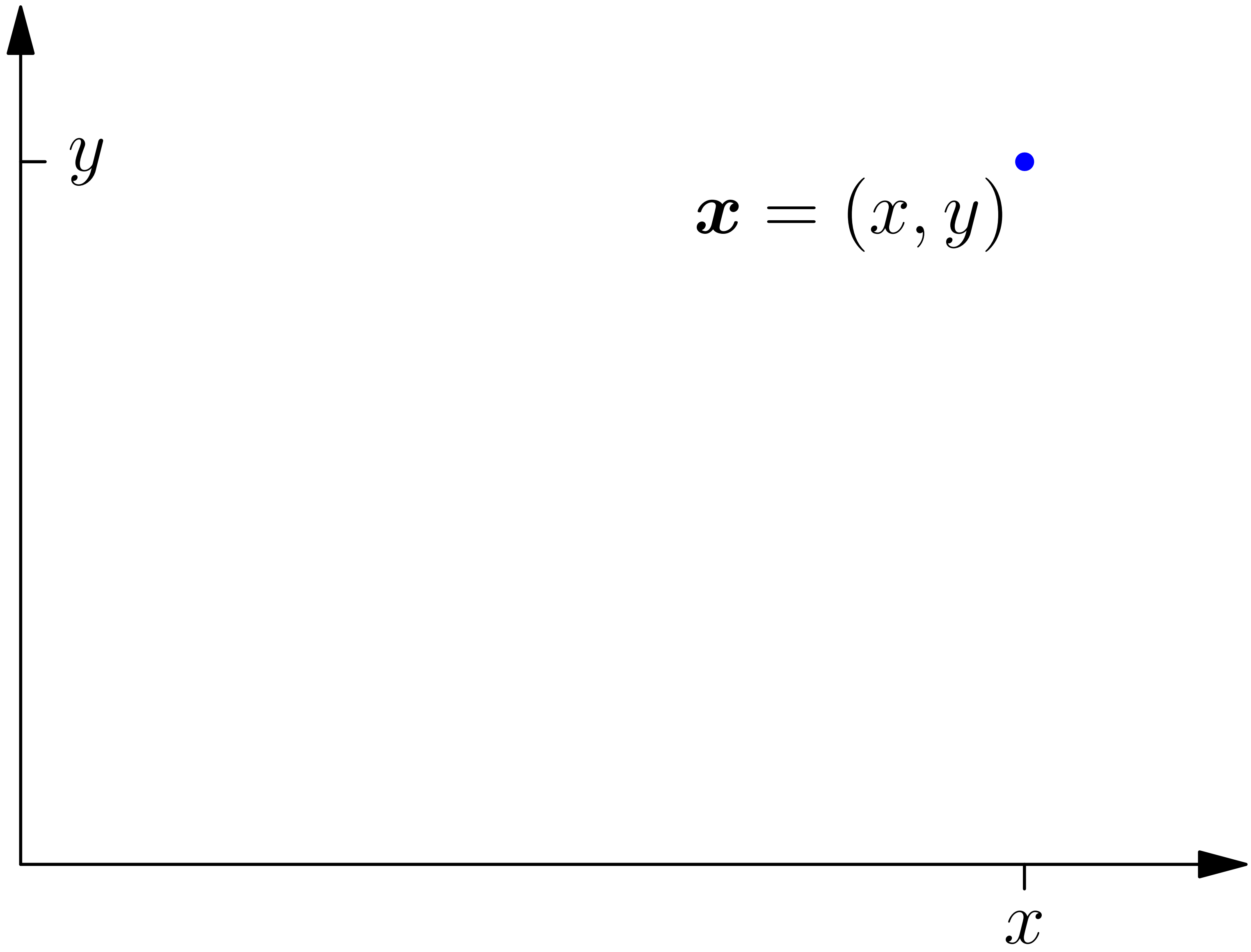
- That is, $\mathrm{d}x\mathrm{d}y = r\mathrm{d}r\mathrm{d}\theta$

Change of Variables in Pictures



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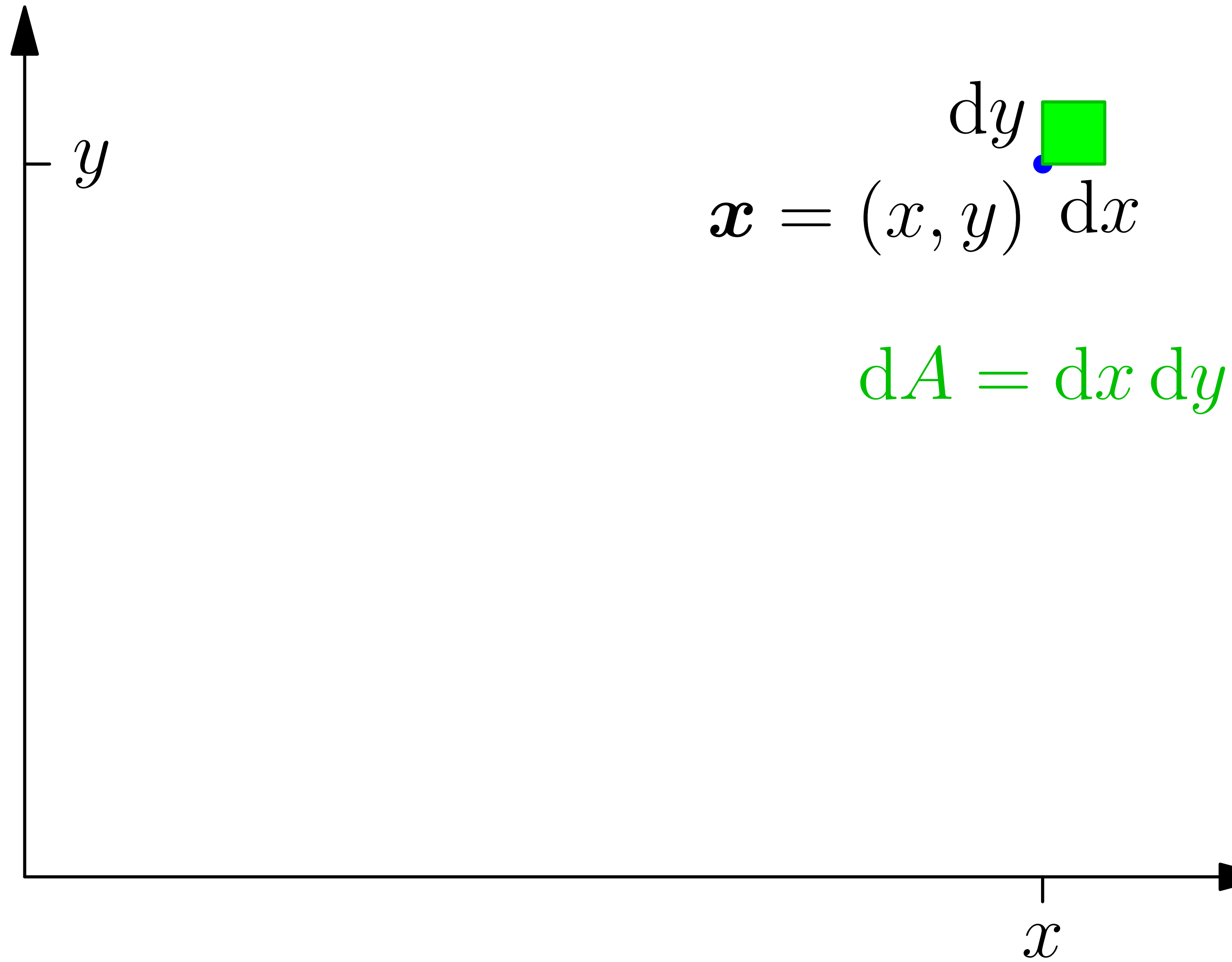

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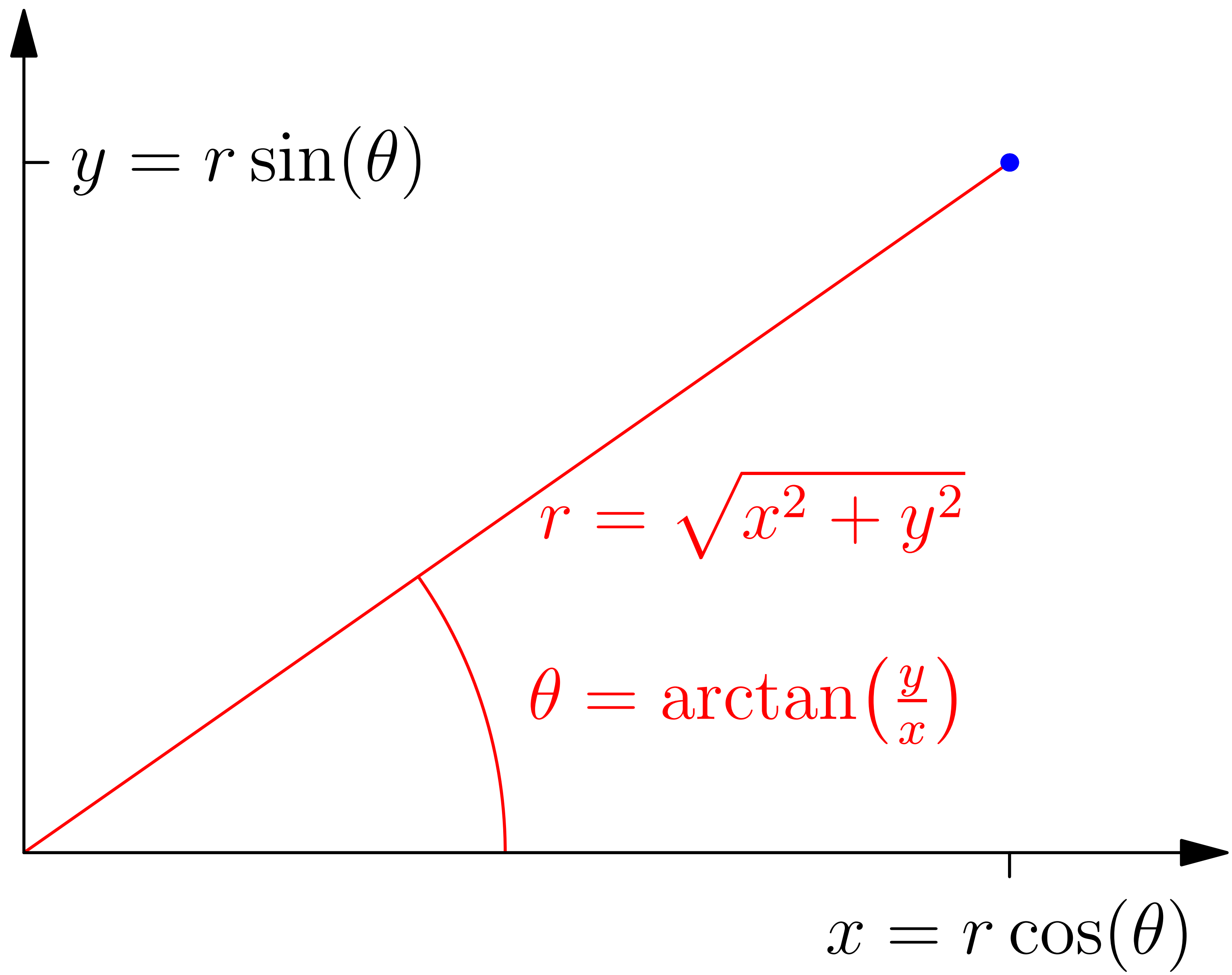

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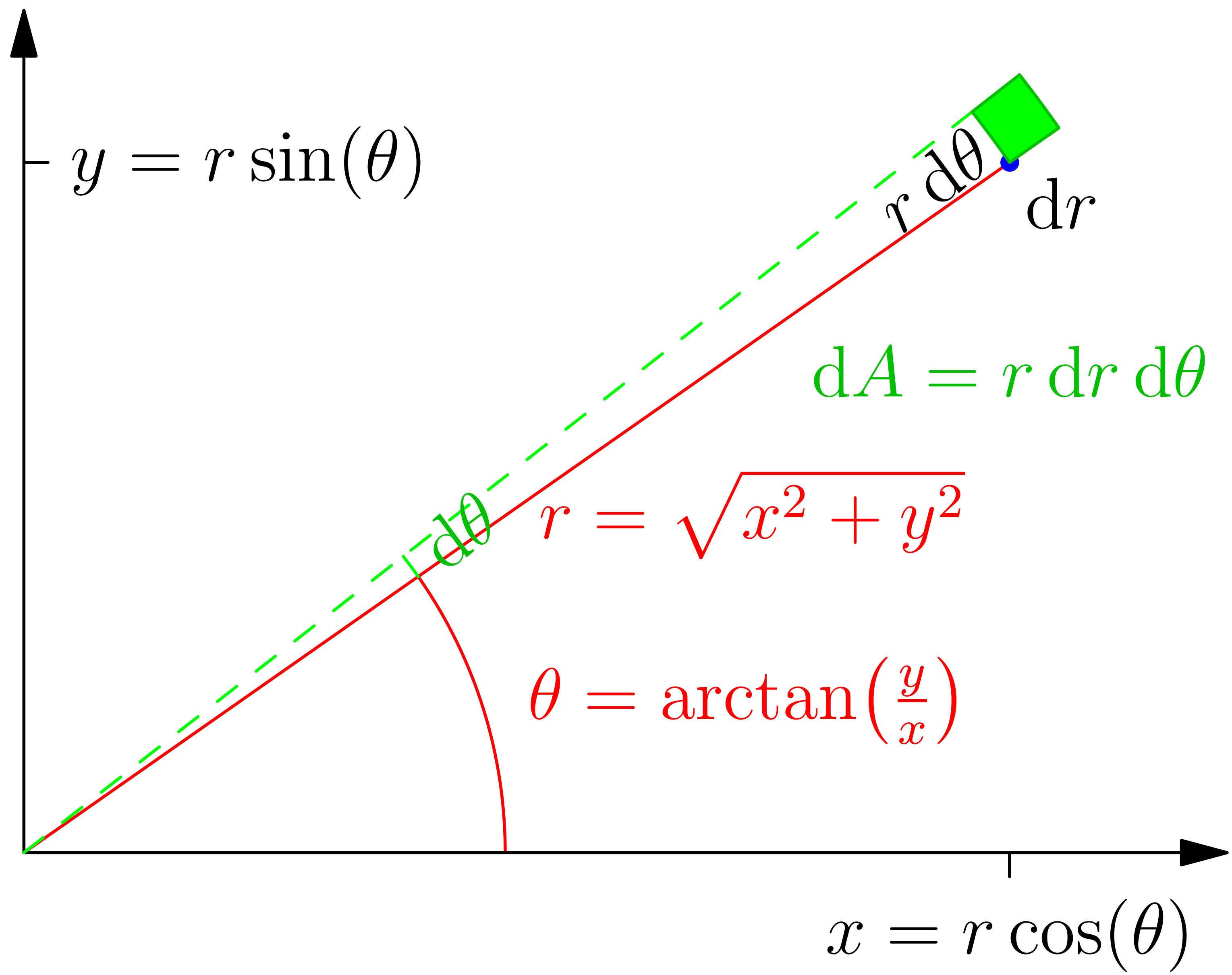

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Special Functions

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- We saw that $\Pi(z) = \int\limits_0^\infty x^z \mathrm{e}^{-x} \mathrm{d}x$ satisfies $\Pi(z) = z\Pi(z-1)$
- For integer n then $\Pi(n) = n!$, but for general z, the integal $\Pi(z)$ can't be written in terms of elementary functions
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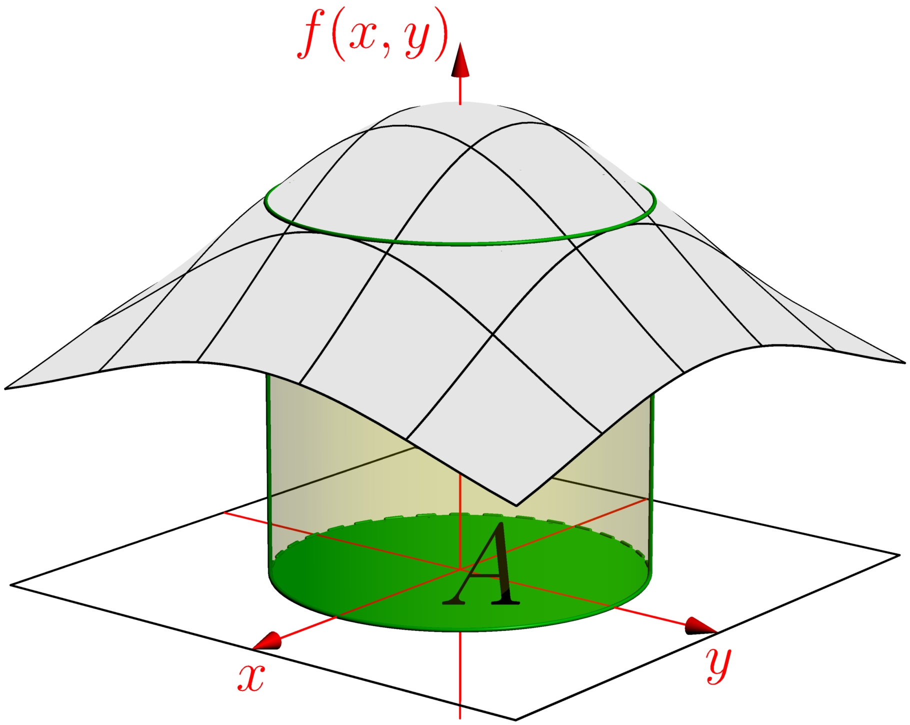
- Other special function defined by integrals exist (e.g. the Bessel , Aire, hypergeometric, elliptic, error functions, . . .)

Outline

1. Defining Integrals
2. Doing Integrals
3. **Gaussian Integrals**



Gaussian Integrals

- Gaussian integrals are integrals involving e^{-x^2}, e.g.

$$\int_{-\infty}^{\infty} \mathrm{e}^{-x^2} \mathrm{d}x \qquad\qquad \int_{-\infty}^{\infty} x^4 \mathrm{e}^{-a x^2 - b x} \mathrm{d}x$$

- They are important in computing integrals with respect to the normal distribution

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- The bad news is that they are quite tricky to do

The Gaussian Integral

- The integral over a Gaussian is surprisingly difficult

$$I_1 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2} \mathrm{d}x$$

- There is a nice trick which is to consider

$$I_1^2 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{e}^{-y^2/2} \mathrm{d}y = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-(x^2+y^2)/2} \mathrm{d}x \, \mathrm{d}y$$

- Making the change of variables $r = \sqrt{x^2 + y^2}$ and $\theta = \arctan(y/x)$ (so that $x = r\cos(\theta)$, $y = r\sin(\theta)$ and $x^2 + y^2 = r^2$)

$$I_1^2 = \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} r \, e^{-r^2/2} \mathrm{d}r = 2\pi \int_0^{\infty} r \, e^{-r^2/2} \mathrm{d}r$$

The Gaussian Integral

- The integral over a Gaussian is surprisingly difficult

$$I_1 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2} \mathrm{d}x$$

- There is a nice trick which is to consider

$$I_1^2 = \int_{-\infty}^{\infty} \mathrm{e}^{-x^2/2} \mathrm{d}x \int_{-\infty}^{\infty} \mathrm{e}^{-y^2/2} \mathrm{d}y = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \mathrm{e}^{-(x^2+y^2)/2} \mathrm{d}x\,\mathrm{d}y$$

- Making the change of variables $r = \sqrt{x^2 + y^2}$ and $\theta = \arctan(y/x)$ (so that $x = r\cos(\theta)$, $y = r\sin(\theta)$ and $x^2 + y^2 = r^2$)

$$I_1^2 = \int_0^{2\pi} \mathrm{d}\theta \int_0^{\infty} r\,e^{-r^2/2} \mathrm{d}r = 2\pi \int_0^{\infty} r\,e^{-r^2/2} \mathrm{d}r$$

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The Gaussian Integral Continued

- From before

$$I_1^2 = 2\pi \int_0^\infty r e^{-r^2/2} \mathrm{d}r$$

- Finally let $u = r^2/2$ so that $\mathrm{d}u/\mathrm{d}r = r$ or $\mathrm{d}u = r\,\mathrm{d}r$ we get

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- Incidentally, $I_1 = \sqrt{2}\Pi(-1/2)$ so $\Pi(-1/2) = \Gamma(1/2) = \sqrt{\pi}$

Normal Distribution

- We consider

$$I_2 = \int_{-\infty}^{\infty} \mathrm{e}^{-(x-\mu)^2/(2\sigma^2)} \mathrm{d}x$$

- Making the change of variables $z = (x - \mu)/\sigma$ so that $\mathrm{d}z = \mathrm{d}x/\sigma$ or $\mathrm{d}x = \sigma \mathrm{d}z$. Then

$$I_2 = \sigma \int_{-\infty}^{\infty} \mathrm{e}^{-z^2/2} \mathrm{d}z = \sigma I_1 = \sqrt{2\pi}\sigma$$

- Note that the *probability density function* (PDF) for a normally distributed random variable is given by

$$\mathcal{N}(x \mid \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \mathrm{e}^{-(x-\mu)^2/(2\sigma^2)}$$

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Multi-dimensional Gaussians

- Consider

$$I_3 = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}\|\boldsymbol{x}\|_2^2} \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

where $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^{\mathsf{T}}$

- Note that $\|\boldsymbol{x}\|_2^2 = x_1^2 + x_2^2 + \cdots + x_n^2$ and using $\mathrm{e}^{\sum_i a_i} = \prod_i \mathrm{e}^{a_i}$

$$I_3 = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}\sum_{i=1}^{n} x_i^2} \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

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Full Multi-variate Normal

- Consider

$$I_4 = \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^{\mathsf{T}}\boldsymbol{\Xi}^{-1}(\boldsymbol{x}-\mu)} \mathrm{d}x_1 \cdots \mathrm{d}x_n$$

- Let $\boldsymbol{\Xi}^{-1} = \mathbf{V}\boldsymbol{\Lambda}^{-1}\mathbf{V}^{\mathsf{T}}$ and make the change of variables $\boldsymbol{y} = \mathbf{V}^{\mathsf{T}}(\boldsymbol{x} - \boldsymbol{\mu})$
- The Jacobian $\mathbf{J}$ has elements (note that $\boldsymbol{x} = \mathbf{V}\boldsymbol{y} + \boldsymbol{\mu}$)

$$J_{ij} = \frac{\partial x_i}{\partial y_j} = \frac{\partial}{\partial y_j}\left(\sum_{k=1}^{n} V_{ik} y_k + \mu_i\right) = V_{ij}$$

- So that $\mathbf{J} = \mathbf{V}$ and consequently $|\det(\mathbf{J})| = |\det(\mathbf{V})| = 1$ then

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- Using the facts, that $\mathbf{\Xi} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\mathsf{T}$ then

$$\det(\mathbf{\Xi}) = \det(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^\mathsf{T})$$

- Recall $I_4 = \prod_i \sqrt{2\pi\lambda_i}$

- We note for an $n \times n$ matrix $\mathbf{M}$ then $\det(c\mathbf{M}) = c^n \det(\mathbf{M})$ so that

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- Finally, we get that for the PDF of a normal to integrate to 1

$$\mathcal{N}(\boldsymbol{x} \mid \boldsymbol{\mu}, \mathbf{\Xi}) = \frac{1}{\sqrt{\det(2\pi\mathbf{\Xi})}} \mathrm{e}^{-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu})^\mathsf{T}\mathbf{\Xi}^{-1}(\boldsymbol{x}-\mu)}$$

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- Making friends with integration will give you a super-power that not too many people share