# Methods in Computational Science – Integration methods (ch.11)

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# Quadrature rules

$$\int_a^b f(x)\,dx \approx \sum_{i=0}^{q} f(x_i) w_i,$$

with $q+1$ *quadrature points* $x_i \in [a, b]$ and *quadrature weights* $w_i \in R$.

# Newton-Cotes quadrature

One approach to derive such quadrature rules is to interpolate the integrand at a set of
spaced quadrature points, and then to integrate the interpolating polynomial to determ
quadrature weights. Using Lagrange interpolation of degree $q$, we get

$$\int_a^b f(x)\,dx \approx \int_a^b \pi_q f(x)\,dx = \int_a^b \sum_{i=0}^{q} f(x_i)\lambda_i(x)\,dx$$
$$= \sum_{i=0}^{q} f(x_i)\int_a^b \lambda_i(x)\,dx = \sum_{i=0}^{q} f(x_i)w_i,$$

referred to as the *Newton-Cotes formulas*.

**Example 11.1.** The *trapezoidal rule* with quadrature points $x_0 = a$ and $x_1 = b$, and weights $w_0 = w_1 = 0.5(b-a)$, is recovered as the Newton-Cotes formula for $q = 1$.

# Quadrature error

$$\left|\int_a^b f(x)\,dx - \int_a^b \pi_q f(x)\,dx\right| = \left|\int_a^b (f(x) - \pi_q f(x))\,dx\right| \leq \int_a^b |f(x) - \pi_q f(x)|\,dx,$$

which by Theorem 9.2 is given by

$$\left|\int_a^b f(x)\,dx - \int_a^b \pi_q f(x)\,dx\right| \leq C(b-a)^{q+2}|\max_{[a,b]} |D^{q+1} f|,$$

with $C > 0$ an interpolation constant, assuming that $f \in C^{q+1}([a,b])$.

Therefore, Newton-Cotes quadrature exact for polynomials of order $q$.

# Quadrature on reference interval

The unit interval $\hat{I} = [0, 1]$ can be mapped to a general interval $I = [a, b]$ by an affine function $F : \hat{I} \to I$, defined by

$$x = F(\hat{x}) = a + (b - a)\hat{x},$$

and the corresponding mapped *measure* takes the form

$$dx = |F'|\, d\hat{x} = |b - a|\, d\hat{x},$$

where $F' = (b - a)$ is the Jacobian of the map $F$. Hence, quadrature rules on the unit interval, or reference interval, can be mapped to a general interval by multiplication with the Jacobian.

# Gauss quadrature

Newton-Cotes quadrature with $q + 1$ quadrature points

- Exact for polynomials of order $q$
- Equally spaced quadrature points.

Gauss quadrature with $q + 1$ quadrature points

- Exact for polynomials of order $2q + 1$
- Freely spaced quadrature points.

How to choose the quadrature points?

# Gauss quadrature

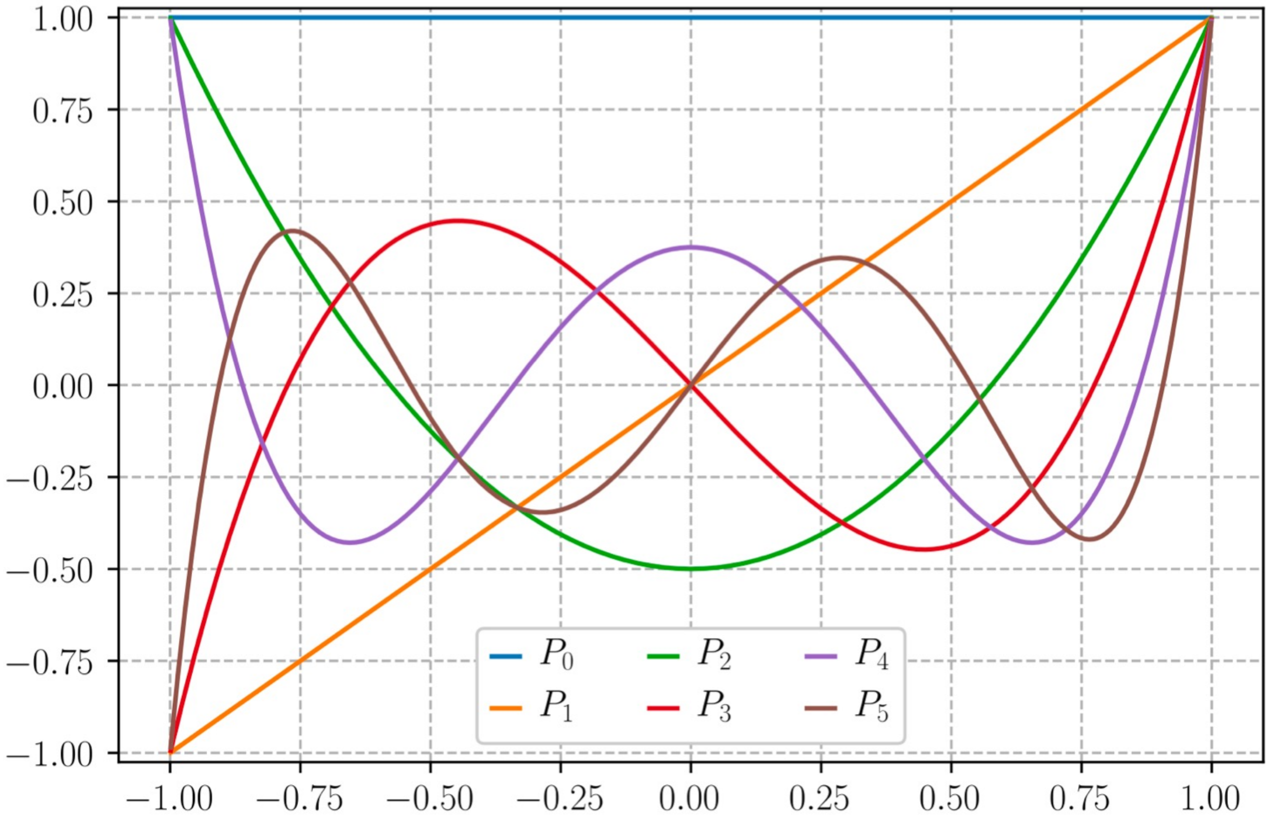
Select the $q + 1$ quadrature points $x_i \in [a, b]$ such that $\phi(x_i) = 0$, where $\phi(x)$ is an orthogonal polynomial, in the sense that

$$\int_a^b \phi(x) q(x)\, dx = 0, \quad \forall q \in \mathcal{P}^q([a, b]).$$

Therefore, $p(x_i) = r(x_i)$, and by interpolation of $r(x)$ using the Lagrange basis in $\mathcal{P}^q([a, b])$,

$$\begin{aligned}\int_a^b p(x)\, dx &= \int_a^b \phi(x) q(x)\, dx + \int_a^b r(x)\, dx = \int_a^b r(x)\, dx \\ &= \int_a^b \sum_{i=0}^{q} r(x_i) \lambda_i(x)\, dx = \sum_{i=0}^{q} r(x_i) \int_a^b \lambda_i(x)\, dx = \sum_{i=0}^{q} p(x_i) w_i.\end{aligned}$$

# First six Legendre polynomials over [-1,1]



# Gauss quadrature

To determine the quadrature points and weights without knowing the associated orthogonal polynomial in advance, let $\{\varphi_j(x)\}_{i=0}^{2q+1}$ be an arbitrary polynomial basis for $\mathcal{P}^{2q+1}([a,b])$ and let $\{c_i\}_{i=0}^{2q+1}$ be the coordinates of a polynomial $p \in \mathcal{P}^{2q+1}([a,b])$. Then,

$$\int_a^b p(x)\,dx - \sum_{j=0}^{q} p(x_j)w_j = \sum_{i=0}^{2q+1} c_i \left( \int_a^b \varphi_i(x)\,dx - \sum_{j=0}^{q} \varphi_i(x_j)w_j \right),$$

from which we can determine the quadrature points and weights from the system of equations

$$\sum_{j=0}^{q} \varphi_i(x_j)w_j = \int_a^b \varphi_i(x)\,dx, \quad i = 0, ..., 2q+1.$$

# Gauss quadrature

**Example 11.2.** To determine the Gauss quadrature rule on the interval $[-1, 1]$ such that all linear polynomials $p(x) = c_1 x + c_0$ are exact, we need one quadrature point. For any $c_0, c_1 \in R$,

$$\begin{aligned}\int_{-1}^{1} p(x)\,dx &= p(x_0)w_0,\\ \int_{-1}^{1} (c_1 x + c_0)\,dx &= (c_1 x_0 + c_0)w_0,\\ c_1 x_0 w_0 + c_0(w_0 - 2) &= 0,\end{aligned}$$

so that $x_0 = 0$ and $w_0 = 2$, which is the *midpoint rule*. Note the difference with respect to the trapezoidal rule which is also exact for linear polynomials, but requires two quadrature points. This is a Gauss-Legendre quadrature rule defined by the Legendre polynomial $P_1$, with one root at $x_0 = 0$, and the weight $w_0$ is the integral of the Lagrange basis function $\lambda_0 = 1$.

# Gauss quadrature

**Example 11.3.** The 2-point Gauss rule on the interval $[-1,1]$ is determined such that all cubic polynomials are exact, since $q = 1$ and $2q + 1 = 3$. For $c_0, ..., c_3$ arbitrary real numbers,

$$\int_{-1}^{1} p(x)\,dx = p(x_0)w_0 + p(x_1)w_1,$$

$$\int_{-1}^{1} \sum_{i=0}^{3} c_i x^i\,dx = w_0 \sum_{i=0}^{3} c_i x_0^i + w_1 \sum_{i=0}^{3} c_i x_1^i,$$

$$2c_2/3 + 2c_0 = (c_3 x_0^3 + c_2 x_0^2 + c_1 x_0 + c_0)w_0 + (c_3 x_1^3 + c_2 x_1^2 + c_1 x_1 + c_0)w_1,$$

which we can rearrange into

$$-c_3(x_0^3 w_0 + x_1^3 w_1) + c_2(2/3 - x_0^2 w_0 - x_1^2 w_1) - c_1(x_0 w_0 + x_1 w_1) + c_0(2 - w_0 - w_1) = 0.$$

Hence, the 2-point Gauss rule is given by $w_0 = w_1 = 1$, $x_0 = 1/\sqrt{3}$ and $x_1 = -1/\sqrt{3}$. This is a Gauss-Legendre quadrature rule defined by the Legendre polynomial $P_2$, with two roots at $x_0 = 1/\sqrt{3}$ and $x_1 = -1/\sqrt{3}$, and weights are the integrals of linear Lagrange basis functions.

# Quadrature rules

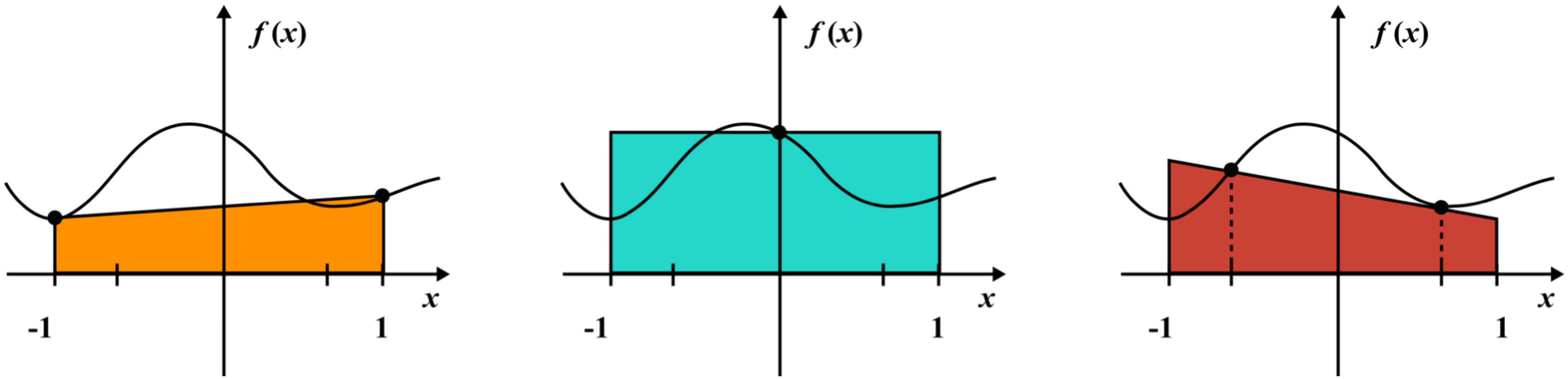



**Figure 11.2.** *Comparison between the trapezoidal rule (left), midpoint rule (center) and 2-point Gauss rule (right), for a function defined on the interval* $[-1, 1]$*, with the quadrature points marked.*

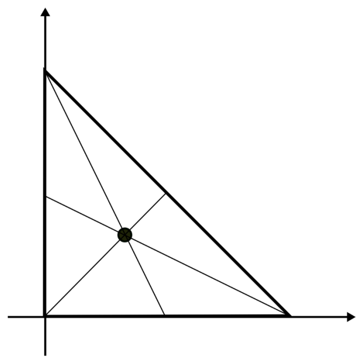
# Gauss quadrature for the reference triangle

**Example 11.4.** We seek a 1-point Gauss quadrature rule over the reference triangle, defined by the vertices $(0,0)$, $(1,0)$ and $(0,1)$. The linear functions are spanned by the three basis functions

$$\varphi_0(x) = 1, \quad \varphi_1(x) = x_1, \quad \varphi_2(x) = x_2,$$

for $x = (x_1, x_2) \in R^2$, which match the three degrees of freedom of a 1-point Gauss rule in terms of the weight $w_0$ and the two coordinates of the quadrature point $x_0 = (x_{0,1}, x_{0,2})$. By equation (11.4), the quadrature point and the weight are determined from

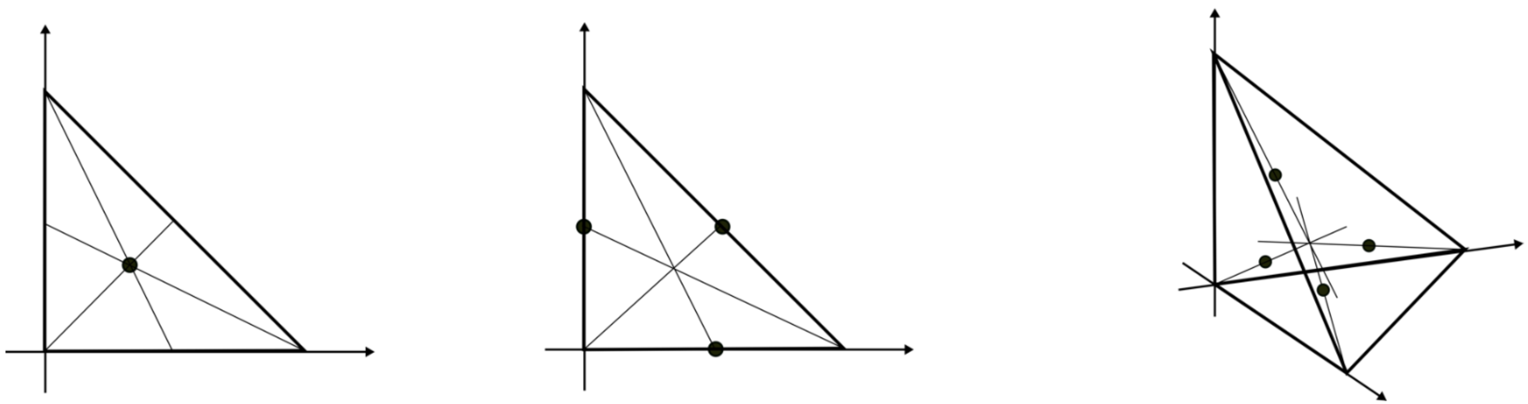
$$\begin{aligned} w_0 &= 1/2, \\ x_{0,1} w_0 &= 1/6, \\ x_{0,2} w_0 &= 1/6, \end{aligned}$$



with solution $x_0 = (1/3, 1/3)$ and $w_0 = 1/2$.

# Gauss quadrature on simplicies in 2D and 3D

**Example 11.5.** A 3-point rule which is exact for quadratic integrands is obtained by choosing the quadrature points as the midpoints of the three edges of the reference triangle, with weights $w_0 = w_1 = w_2 = 1/6$, motivated by the symmetry of the quadrature points.



# Quadrature over general domains

To approximate an integral over a general domain $\Omega \subset R^d$, we construct a coordinate map

$$F : \hat{\Omega} \to \Omega,$$

for $\hat{\Omega}$ a reference domain over which we want to use a quadrature rule,

$$\int_{\Omega} f(x)\, dx = \int_{\hat{\Omega}} f(F(\hat{x}))\, |\det(F')|\, d\hat{x} \approx |\det(F')| \sum_{i=0}^{q} f(F(\hat{x}_i))\, w_i,$$

where $F' \in R^{d \times d}$ is the Jacobian of the map $F$, which is constant for an affine map $F$. We can

# Quadrature over general domains

$$\Omega \approx \Omega^h = \sum_{j=1}^{M} \Omega_j^h,$$

after which we construct a coordinate map for each subdomain $\Omega_j^h$, $F_j : \hat{\Omega} \to \Omega_j^h$, to formulate a *composite quadrature rule* over the subdomains,

$$\int_\Omega f(x)\,dx \approx \sum_{j=1}^{M} \int_{\Omega_j^h} f(x)\,dx \approx \sum_{j=1}^{M} |\det(F_j')| \sum_{i=0}^{q} f(F_j(\hat{x}_i))w_i,$$

with $F_j'$ the Jacobian of the map $F_j$.

# Quadrature over general domains

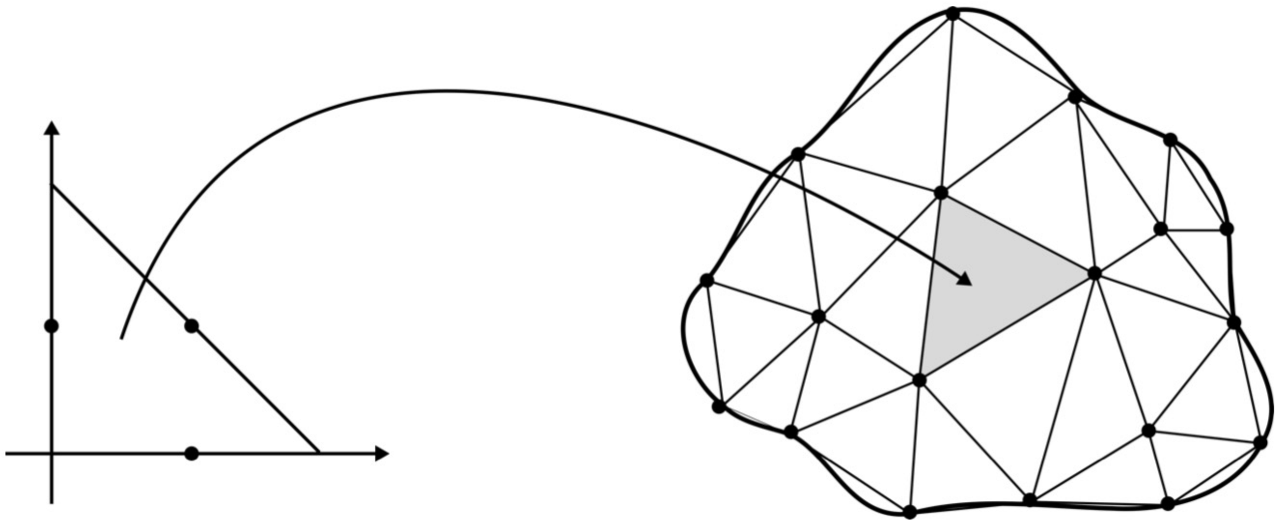


**Figure 11.4.** *Illustration of a composite quadrature rule for a general domain $\Omega \subset R^2$, based on discretization of $\Omega$ into a mesh of triangles $\Omega_j^h$ which all are mapped to the reference triangle $\hat{\Omega}$ where a 3-point quadrature rule is used to approximate the local integral.*

# Riemann integral of function $f \in C([a, b])$

$$s_N = \sum_{i=1}^{N} f(\bar{x}_i)\,(b-a)/N.$$

If the limit exists as $N \to \infty$, it defines the Riemann integral

$$\int_a^b f(x)\,dx = \lim_{N\to\infty} s_N,$$

and we say that the function $f(x)$ is Riemann integrable over the interval $[a, b]$.

# Riemann integral of function $f \in C([a, b])$

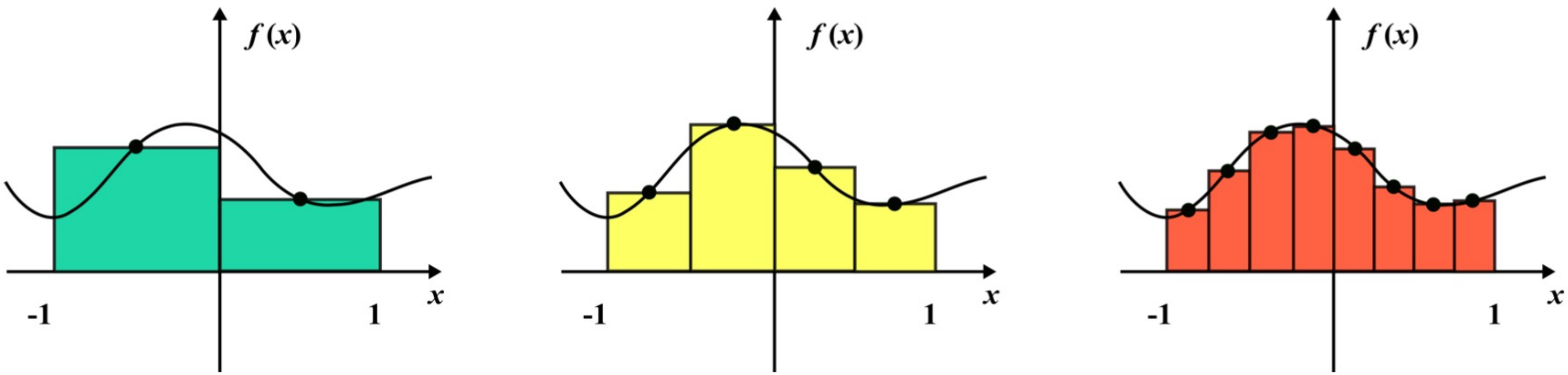



**Figure 11.5.** *Riemann sums $s_N$ based on composite midpoint rules on a progressively refined uniform partition of the interval $[-1, 1]$, converging towards the integral of the continuous function $f(x)$.*

# Fundamental theorem of calculus

Now consider a function $u(x)$ defined on a uniform partition of the interval $[a, b]$ into $N$ subintervals, with nodes

$$a = x_0 < x_1 < \dots < x_i < \dots < x_{N+1} = b.$$

We can express the difference $u(b) - u(a)$ as the *telescoping sum*

$$\begin{aligned} u(b) - u(a) &= (u(b) - u(x_N)) + (u(x_N) - u(x_{N-1})) + \dots + (u(x_1) - u(a)) \\ &= \frac{u(b) - u(x_N)}{\Delta x}\Delta x + \frac{u(N) - u(x_{N-1})}{\Delta x}\Delta x + \dots + \frac{u(x_1) - u(a)}{\Delta x}\Delta x, \end{aligned}$$

with $\Delta x = (b - a)/N$, which is a Riemann sum of secants of the function over the subintervals.

# Fundamental theorem of calculus

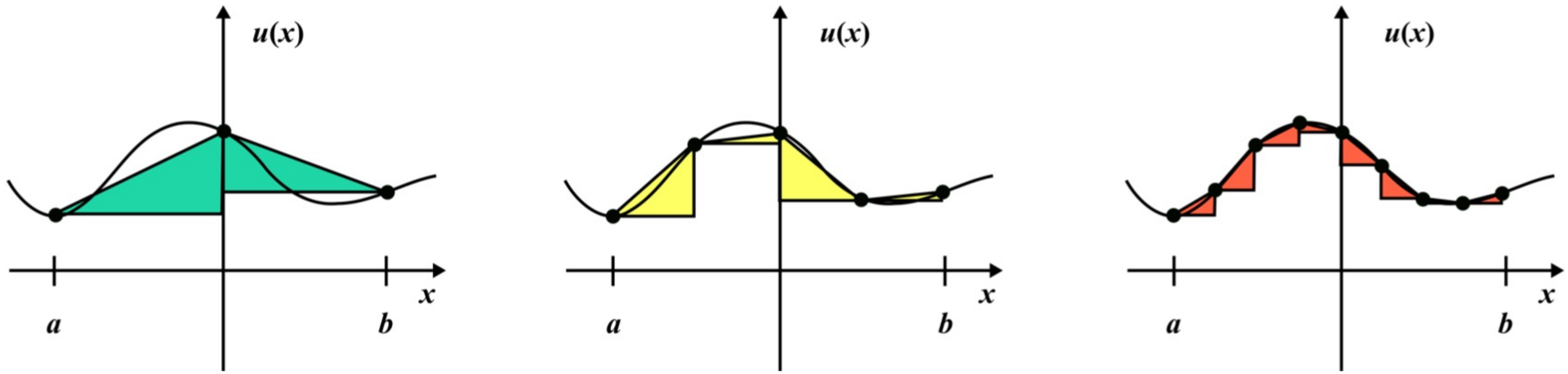



**Figure 11.6.** *Illustration of the proof of the fundamental theorem of calculus, where the difference $u(b) - b(a)$ is expressed in terms of a Riemann sum of the secants of the function $u(x)$ over a partition of the interval $[a, b]$ which undergoes uniform refinement.*

# Fundamental theorem of calculus

**Theorem 11.6 (Fundamental theorem of calculus).** *The differential equation*

$$u'(x) = f(x), \quad x \in [a, b],$$

*has a unique solution* $u(x)$*, given by the integral*

$$u(x) = u(a) + \int_a^x u'(y)\,dy = u(a) + \int_a^x f(y)\,dy,$$

*provided that* $f \in C([a, b])$*, which implies that* $u \in C^1([a, b])$*.*

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*provided that* $f \in C([a, b])$*, which implies that* $u \in C^1([a, b])$.

Partial integration then follows from the fundamental theorem of calculus and the product rule, by replacing the integrand with a product $u = vw$, for two functions $v, w \in C^1([a, b])$,

$$v(b)w(b) - v(a)w(a) = \int_a^b (v(x)w(x))'\,dx = \int_a^b v'(x)w(x)\,dx + \int_a^b v(x)w'(x)\,dx.$$

# Lebesgue integral

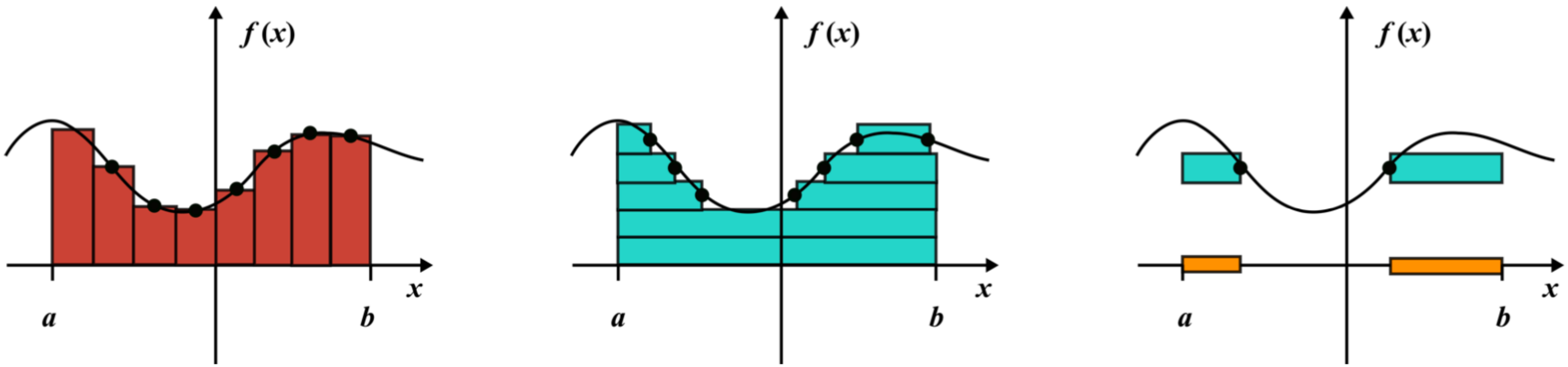


**Figure 11.7.** *Illustration of a Riemann sum for the function $f(x)$ over the interval $I = [a, b]$ (left), compared to the corresponding Lebesgue sum (center), and one slice of the range $[y_j, y_j + \Delta y]$ together with its associated subdomain $\{x \in I \mid f(x) > \bar{y}_j\}$ highlighted in green (right).*

# Lebesgue measure

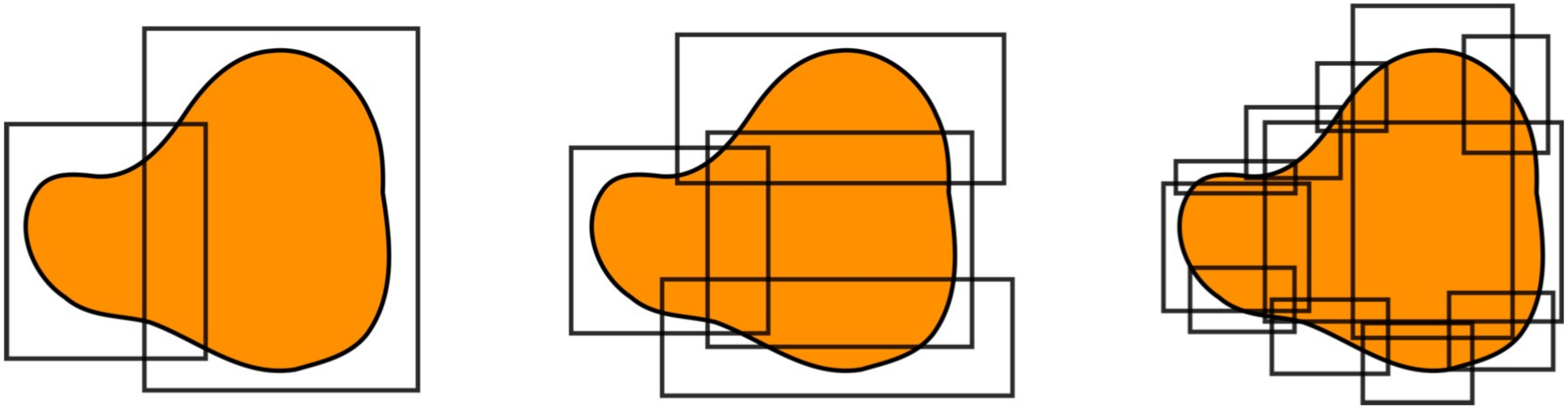

**Figure 11.8.** *The set $A \subset R^2$ with three covers of open boxes, for which the infimum of the area of the smallest possible cover defines the Lebesgue measure $\mu(A)$.*

# Lebesgue measure

$$\mu(A) = \inf\left\{\sum_{B\in\mathcal{C}} |B| : A \subset \bigcup_{B\in\mathcal{C}} B\right\},$$

where the open boxes $B \in \mathcal{C}$ are defined by the Cartesian product

$$B = \prod_{i=1}^{d} (a_i, b_i),$$

each with volume

$$|B| = \prod_{i=1}^{d} (b_i - a_i).$$

# Lebesgue space of integrable functions

All Lebesgue measurable subsets of $R^d$ form a *$\sigma$-algebra* $\Sigma$, which includes $R^d$ and is closed under complements and countable unions, that is,

$$A \in \Sigma \Rightarrow A^c \in \Sigma, \quad \{A_i\}_{i=1}^{\infty} \subset \Sigma \Rightarrow \cup_{i=1}^{\infty} A_i \in \Sigma.$$

The triple $(\Omega, \Sigma, \mu)$ then defines a *measure space*, where

$$\mu : \Sigma \to R^+.$$

Given a measure space $(\Omega, \Sigma, \mu)$, a function $f : \Omega \to R$ is *measurable*, if

$$\{x \in \Omega \,|\, f(x) > y\} \in \Sigma, \quad \forall y \in R,$$

and *Lebesgue integrable*, if

$$\int_{\Omega} |f(x)| \, d\mu(x) < \infty.$$

The Lebesgue space $L^1(\Omega)$ is defined as the vector space of all Lebesgue integrable functions.

# Lebesgue integrable functions

The Lebesgue space $L^1(\Omega)$ is defined as the vector space of all Lebesgue integrable functions, where we identify any two functions that only differ on a set of Lebesgue measure zero, which we refer to as *almost everywhere*. If a function is continuous almost everywhere it is Riemann integrable, and if both the Riemann integral and the Lebesgue integrals exist they take the same value. By convention, if $\Omega \subset R^d$ we use $dx$ instead of $d\mu(x)$ also for the Lebesgue integral, which makes the notation for the two integrals identical.

# Lebesgue integrable functions

So far we have met both $L^1$ and $L^2$ spaces, which we now extend to $L^p$ spaces, a class of Banach spaces which generalize the $l^p$ sequence spaces to functions, for which the norms are defined in terms of integrals instead of sums. We define the space $L^p(\Omega)$ to be the vector space of functions $f : \Omega \to R$ with finite $L^p$ norms, defined by

$$\|f\|_p = \|f\|_{L^p(\Omega)} = \left( \int_\Omega |f(x)|^p \, dx \right)^{1/p}$$

for the natural numbers $1 \leq p < \infty$, and

$$\|f\|_\infty = \|f\|_{L^\infty(\Omega)} = \operatorname{ess\,sup}_\Omega |f|.$$

# Lebesgue integrable functions

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The *essential supremum* is defined as the real number $c$ for which $|f| > c$ at most on subsets $\omega \subset \Omega$ of zero measure, that is, with zero integral,

$$\int_\omega dx = 0.$$

# Lebesgue integrable functions

**Example 11.7.** A point $d \in [a, b]$ has zero measure, which we can intuitively understand by formally interpreting an integral of over $d$ as an integral over the closed interval $\omega = [d, d]$,

$$\int_\omega dx = \int_{[d,d]} dx = \int_d^d 1\, dx = [x]_d^d = d - d = 0.$$

Hence, point evaluation in $L^p([a, b])$ is not well defined, instead $L^p([a, b])$ is a vector space of equivalence classes where functions are identified if they differ only on sets of measure zero.

**Example 11.8.** The functions $f$ and $g$ are identified as elements of the Banach space $L^p([-1, 1])$, since they only differ for the point $x = 0$ which has zero measure,

$$f(x) = \begin{cases} 0, & x < 0, \\ 1, & x \geq 0, \end{cases} \qquad g(x) = \begin{cases} 0, & x \leq 0, \\ 1, & x > 0. \end{cases}$$

# Vector fields

For a multidimensional domain $\Omega \subset R^d$, we can define both scalar functions $f : \Omega \to R$ and vector functions, or *vector fields*, $F : \Omega \to R^d$. The gradient $\nabla f$ and the Jacobian matrix $\nabla F$ are both defined in terms of the nabla operator $\nabla$, which we can formally express as the column vector

$$\nabla = (\partial/\partial x_1, ..., \partial/\partial x_d)^T,$$

so that $\nabla f = (\partial f/\partial x_i)$ is interpreted as a scalar multiplication, and $\nabla F = (\partial F_i/\partial x_j)$ an outer product. Similarly, the *divergence*

$$\text{div}(F) = \nabla \cdot F = (\partial F_i/\partial x_i),$$

can be interpreted as an inner product, whereas the *laplacian* and the *vector laplacian* are defined by

$$\Delta f = (\nabla \cdot \nabla) f = (\partial^2 f/\partial x_i^2),$$
$$\Delta F = (\nabla \cdot \nabla) F = (\partial^2 F_i/\partial x_j^2).$$

# Divergence theorem

**Theorem 11.11 (The divergence theorem).** *For any continuously differentiable vector field* $F : \Omega \to R^d$*, on a domain* $\Omega \subset R^d$ *with a piecewise smooth boundary* $\partial\Omega$ *and outward unit normal vector* $n : \partial\Omega \to R^d$*, the following relation holds,*

$$\int_\Omega \nabla \cdot F \, dx = \int_{\partial\Omega} F \cdot n \, ds.$$

# Divergence theorem

For a continuously differentiable function $g : \Omega \to R$, the product rule states that

$$\nabla \cdot (Fg) = (F \cdot \nabla)g + g(\nabla \cdot F),$$

and therefore by the divergence theorem,

$$\int_\Omega (F \cdot \nabla)g \, dx + \int_\Omega g(\nabla \cdot F) \, dx = \int_{\partial\Omega} g(F \cdot n) \, ds,$$

and if $F = \nabla f$, for some twice continuously differentiable function $f : \Omega \to R$, then

$$\int_\Omega \nabla f \cdot \nabla g \, dx + \int_\Omega g \Delta f \, dx = \int_{\partial\Omega} g(\nabla f \cdot n) \, ds,$$

both very useful formulas of partial integration in multiple dimensions.

# Variational formulation of Poisson's equation

$$-\Delta u(x) = f(x), \text{ for all } x \in \Omega$$
$$u(x) = 0, \text{ for all x} \in \partial\Omega$$

Multiply equation by test function $v(x)$ which satisfies the boundary conditions, and using the divergence theorem, we get

$$\int_{\Omega} -\Delta u v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx - \int_{\partial\Omega} \nabla u \cdot n v \, dx = \int_{\Omega} \nabla u \cdot \nabla v \, dx = \int_{\Omega} f v \, dx$$

$$a(u, v) = L(v)$$