# Scientific Computing: Numerical Integration

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# Outline

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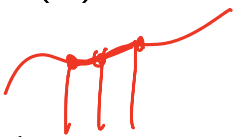
# Numerical Quadrature

- We want to numerically approximate a definite integral

$$J = \int_a^b f(x)dx.$$

- The function $f(x)$ may not have a closed-form integral, or it may itself not be in closed form.
- Recall that the integral gives the area under the curve $f(x)$, and also the **Riemann sum**:



$$\cancel{\lim_{n\to\infty}} \sum_{i=0}^{n} f(t_i)(x_{i+1} - x_i) = J, \text{ where } x_i \leq t_i \leq x_{i+1}$$

- A **quadrature formula** approximates the Riemann integral as a **discrete sum** over a set of $n$ nodes:

?

nodes

$\alpha$ = quadrature weight

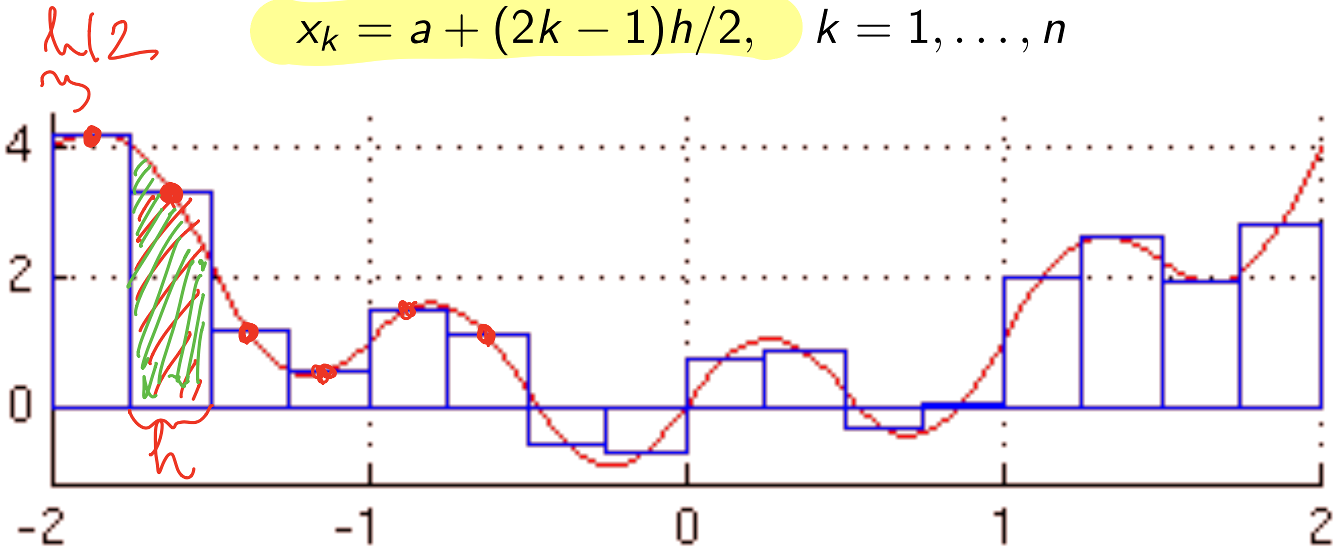
$$J \approx J_n = \sum_{i=1}^{n} \underline{\alpha_i} f(x_i)$$

?

# Midpoint Quadrature

Split the interval into $n$ intervals of width $h = (b - a)/n$ (**stepsize**), and then take as the nodes the midpoint of each interval:

$$x_k = a + (2k - 1)h/2, \quad k = 1, \ldots, n$$




$$J_n = h \sum_{k=1}^{n} f(x_k), \text{ and clearly } \lim_{n\to\infty} J_n = J$$

# Quadrature Error

- Focus on one of the sub intervals, and estimate the quadrature error using the midpoint rule assuming $f(x) \in C^{(2)}$:

$$\varepsilon^{(i)} = \left[ \int_{x_i - h/2}^{x_i + h/2} f(x)dx \right] - hf(x_i)$$

- Expanding $f(x)$ into a Taylor series around $x_i$ to first order,

$$f(x) = f(x_i) + f'(x_i)(\cancel{x} - x_i) + \frac{1}{2} f''\left[\eta(x)\right](x - x_i)^2,$$

The linear term integrates to zero, so we get

$$\int_{x_i - h/2}^{x_i + h/2} f'(x_i)(x - x_i) = 0 \quad \Rightarrow$$

$$\varepsilon^{(i)} = \frac{1}{2} \int_{x_i - h/2}^{x_i + h/2} f''\left[\eta(x)\right](x - x_i)^2 dx$$

# Composite Quadrature Error

- Using a generalized mean value theorem we can show

$$\varepsilon^{(i)} = f''\left[\xi\right] \frac{1}{2} \int_h (x - x_i)^2 dx = \frac{h^3}{24} f''\left[\xi\right] \quad \text{for some } \overset{x_i - \frac{h}{2}}{\cancel{a}} < \xi < \overset{x_i + \frac{h}{2}}{\cancel{b}}$$

- Now, combining the errors from all of the intervals together gives the **global error**

$$\varepsilon = \int_a^b f(x)dx - h \sum_{k=1}^{n} f(x_k) = J - J_n = \frac{h^3}{24} \sum_{k=1}^{n} f''\left[\xi_k\right]$$

- Use a discrete generalization of the mean value theorem to prove **second-order accuracy**

$$\varepsilon = \frac{h^3}{24} n \left(f''\left[\xi\right]\right) = \frac{b-a}{24} \cdot h^2 \cdot f''\left[\xi\right] \quad \text{for some } a < \xi < b$$

# Interpolatory Quadrature

Instead of integrating $f(x)$, integrate a polynomial interpolant $\phi(x) \approx f(x)$:

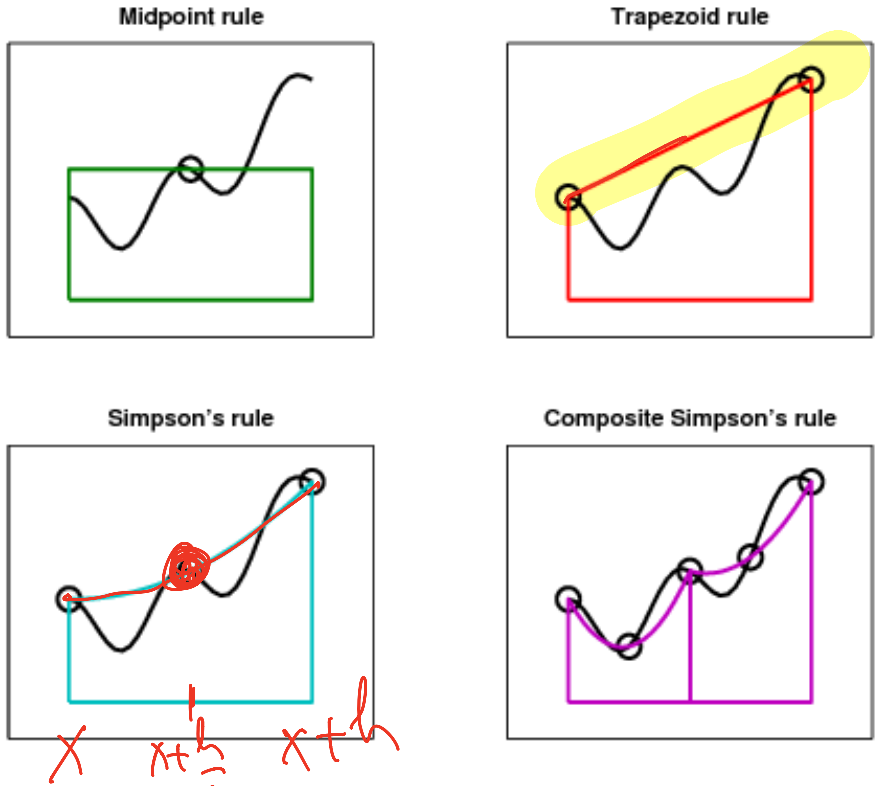
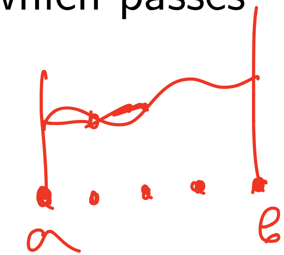



**Figure 6.2.** *Four quadrature rules.*

# Trapezoidal Rule

- Consider integrating an **interpolating function** $\phi(x)$ which passes through $n+1$ **nodes** $x_i$:



$$\phi(x_i) = y_i = f(x_i) \text{ for } i = 0, 2, \ldots, m.$$

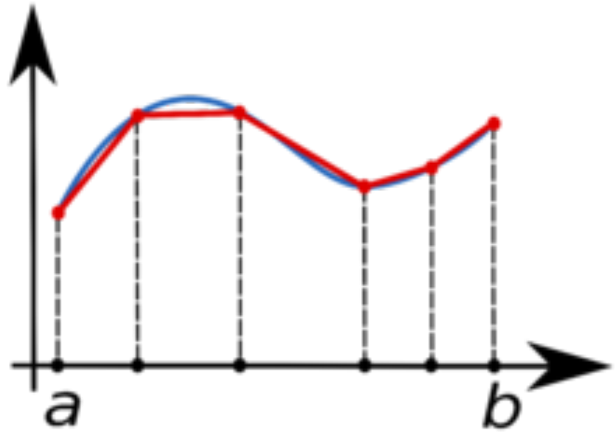
- First take the **piecewise linear interpolant** and integrate it over the sub-interval $I_i = [x_{i-1}, x_i]$:

$$\phi_i^{(1)}(x) = y_{i-1} + \frac{y_i - y_{i-1}}{x_i - x_{i-1}}(x - x_i)$$

to get the **trapezoidal formula** (the area of a trapezoid):

$$\int_{x \in I_i} \phi_i^{(1)}(x)dx = h\frac{f(x_{i-1}) + f(x_i)}{2}$$

# Composite Trapezoidal Rule




- Now add the integrals over all of the sub-intervals we get the **composite trapezoidal quadrature rule**:

$$\int_a^b f(x)dx \approx \frac{h}{2}\sum_{i=1}^{n}\left[f(x_{i-1})+f(x_i)\right]$$

$\alpha_0 = h/2$ $\alpha_n = h/2$

$$= \frac{h}{2}\left[f(x_0)+\underbrace{2f(x_1)+\cdots+2f(x_{n-1})}_{\alpha = h}+f(x_n)\right]$$

with similar error to the midpoint rule.

# Simpson's Quadrature Formula

- As for the midpoint rule, split the interval into $n$ intervals of width $h = (b-a)/n$, and then take as the nodes the endpoints and midpoint of each interval:

$$x_k = a + kh, \quad k = 0, \ldots, n$$
$$\bar{x}_k = a + (2k-1)h/2, \quad k = 1, \ldots, n$$

- Then, take the **piecewise quadratic interpolant** $\phi_i(x)$ in the sub-interval $I_i = [x_{i-1}, x_i]$ to be the parabola passing through the nodes $(x_{i-1}, y_{i-1})$, $(x_i, y_i)$, and $(\bar{x}_i, \bar{y}_i)$.
- Integrating this interpolant in each interval and summing gives the **Simpson quadrature rule**:

$\alpha_0 = h/6 = \alpha_n$

$$J_S = \frac{h}{6}\left[f(x_0) + 4f(\bar{x}_1) + 2f(x_1) + \cdots + 2f(x_{n-1}) + 4f(\bar{x}_n) + f(x_n)\right]$$

$\alpha_{mid} = 4/6 h = 2/3 h$ $\quad$ $\alpha_{node} = 2/6 h = 1/3 h$

$$\varepsilon = J - J_s = -\frac{(b-a)}{2880} \cdot h^4 f^{(4)}(\xi).$$

## Gauss Quadrature

- To reach **spectral accuracy** for **smooth functions**, instead of using higher-degree polynomial interpolants (recall Runge's phenomenon), let's try using $n$ **non-equispaced nodes**:

$$J \approx J_n = \sum_{i=0}^{n} w_i f(x_i)$$

take from existing codes

- It can be shown that there is a special set of $n+1$ nodes and weights, so that the quadrature formula is exact for polynomials of degree up to $m = 2n - 1$,

$$\int_a^b p_m(x)dx = \sum_{i=0}^{n} w_i p_m(x_i).$$

- This gives the **Gauss quadrature** based on the **Gauss nodes and weights**, usually pre-tabulated for the standard interval $[-1, 1]$:

$$\int_a^b f(x)dx \approx \frac{b-a}{2} \sum_{i=0}^{n} w_i f(x_i).$$

## Gauss Weights and Nodes

- The low-order Gauss formulas are: [-1, 1]

$$n=1:\int_{-1}^{1} f(x)dx \approx f\left(-\frac{1}{\sqrt{3}}\right)+f\left(\frac{1}{\sqrt{3}}\right)$$

$$n=2:\int_{-1}^{1} f(x)dx \approx \frac{5}{9}f\left(-\frac{\sqrt{15}}{5}\right)+\frac{8}{9}f(0)+\frac{5}{9}f\left(\frac{\sqrt{15}}{5}\right)$$

- The weights and nodes are either **tabulated** or calculated to numerical precision **on the fly**, for example, using eigenvalue methods.
- Gauss quadrature is **very accurate for smooth functions** even with few nodes.
- The MATLAB function integrate *quadl*($f$, $a$, $b$) uses (adaptive) Gauss-Lobatto quadrature. tolerance
- An alternative is to use Chebyshev nodes and weights, called **Clenshaw-Curtis quadrature** (exact for polynomials of degree $n$).

# Outline

# Asymptotic Error Expansions

- The idea in **Richardson extrapolation** is to use an error estimate formula to **extrapolate a more accurate answer** from less-accurate answers.
- Assume that we have a quadrature formula for which we have a theoretical error estimate:

order p

$$J_h = \sum_{i=1}^{n} \alpha_i f(x_i) = J + \alpha h^p + O\left(h^{p+1}\right)$$

e.g. $\alpha \sim f^{(4)}(\xi)$

- Recall the **big O notation**: $g(x) = O(h^p)$ if:

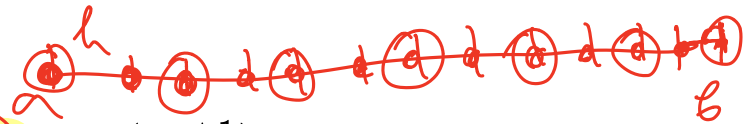
$$\exists (h_0, C) > 0 \text{ s.t. } |g(x)| < C\,|h|^p \text{ whenever } |h| < h_0$$

- For trapezoidal formula

$$\varepsilon = \frac{b-a}{24} \cdot h^2 \cdot f''[\xi] = O\left(h^2\right).$$

# Richardson Extrapolation

- Now repeat the calculation but with step size $2h$ (for equi-spaced nodes just skip the odd nodes):




$$\tilde{J}(h) = J + \alpha h^p + O\left(h^{p+1}\right)$$

$$\tilde{J}(2h) = J + \alpha 2^p h^p + O\left(h^{p+1}\right)$$

we also obtain $\alpha$

- Solve for $\alpha$ and obtain

$$J = \frac{2^p \tilde{J}(h) - \tilde{J}(2h)}{2^p - 1} + \boxed{O\left(h^{p+1}\right),}$$

which now has order of accuracy $p + 1$ instead of $p$.

- The composite trapezoidal quadrature gives $\tilde{J}(h)$ with order of accuracy $p = 2$, $\tilde{J}(h) = J + O\left(h^2\right)$.

## Romberg Quadrature

Not used as often

- Assume that we have evaluated $f(x)$ at $n = 2^m + 1$ equi-spaced nodes, $h = 2^{-m}(b-a)$, giving approximation $\tilde{J}(h)$.
- We can also easily compute $\tilde{J}(2h)$ by simply skipping the odd nodes. And also $\tilde{J}(4h)$ , and in general, $\tilde{J}(2^q h)$, $q = 0, \ldots, m$.
- We can keep applying **Richardson extrapolation recursively** to get **Romberg's quadrature**:
  Combine $\tilde{J}(2^q h)$ and $\tilde{J}(2^{q-1} h)$ to get a better estimate. Then combine the estimates to get an even better estimates, etc.

$$J_{r,0} = \tilde{J}\left(\frac{b-a}{2^r}\right), \quad r = 0, \ldots, m$$

$$J_{r,q+1} = \frac{4^{q+1} J_{r,q} - J_{r-1,q}}{4^{q+1} - 1}, \quad q = 0, \ldots, m-1, \quad r = q+1, \ldots, m$$

- The final answer, $J_{m,m} = J + O\left(h^{2(m+1)}\right)$ is much more accurate than the starting $J_{m,0} = J + O\left(h^2\right)$, for **smooth** functions.

# Adaptive (Automatic) Integration

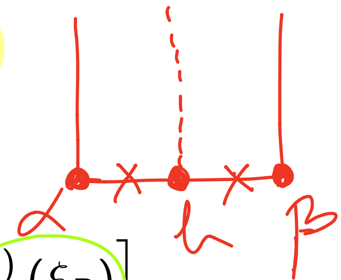
- We would like a way to control the error of the integration, that is, specify a **target error** $\varepsilon_{max}$ and let the algorithm figure out the correct step size $h$ to satisfy

$$|\varepsilon| \lesssim \varepsilon_{max},$$

  where $\varepsilon$ is an **error estimate**.
- Importantly, $h$ may **vary adaptively** in different parts of the integration interval:
  *Smaller step size when the function has larger derivatives.*
- The crucial step is obtaining an error estimate: Use the same idea as in Richardson extrapolation.

# Error Estimate for Simpson's Quadrature

- Assume we are using Simpson's quadrature and compute the integral $J(h)$ with step size $h$.
- Then also compute integrals for the left half and for the right half with step size $h/2$, $J(h/2) = J_L(h/2) + J_R(h/2)$.




$$J = J(h) - \frac{1}{2880} \cdot h^5 \cdot f^{(4)}(\xi) + O(h^6)$$

$$J = J(h/2) - \frac{1}{2880} \cdot \frac{h^5}{32} \cdot \left[ f^{(4)}(\xi_L) + f^{(4)}(\xi_R) \right].$$

$\left(\frac{h}{2}\right)^5$

- Now assume that the fourth derivative varies little over the interval, $f^{(4)}(\xi_L) \approx f^{(4)}(\xi_L) \approx f^{(4)}(\xi)$, to estimate:

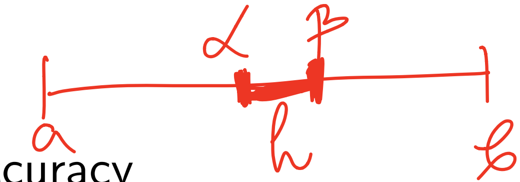
$$\frac{1}{2880} \cdot h^5 \cdot f^{(4)}(\xi) \approx \frac{16}{15} \left[ J(h) - J(h/2) \right]$$

$$J(h/2) - J \approx \varepsilon = \frac{1}{16} \left[ J(h) - J(h/2) \right].$$

# Adaptive Integration

- Now assume that we have split the integration interval $[a, b]$ into sub-intervals, and we are considering computing the integral over the sub-interval $[\alpha, \beta]$, with stepsize

$$h = \beta - \alpha.$$




- We need to compute this sub-integral with accuracy

$$|\varepsilon(\alpha, \beta)| = \frac{1}{16} \left|[J(h) - J(h/2)]\right| \leq \boxed{\varepsilon \frac{h}{b-a}}.$$

- An adaptive integration algorithm is $J \approx J(a, b, \epsilon)$ where the **recursive function** is:

$$\epsilon = \varepsilon \frac{h}{b-a}$$

$$J(\alpha, \beta, \epsilon) = \begin{cases} J(h/2) & \text{if } |J(h) - J(h/2)| \leq 16\varepsilon \\ J(\alpha, \frac{\alpha+\beta}{2}, \frac{\epsilon}{2}) + J(\frac{\alpha+\beta}{2}, \beta, \frac{\epsilon}{2}) & \text{otherwise} \end{cases}$$

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- In practice one also stops the refinement if $h < h_{min}$ and is more conservative e.g., use 10 instead of 16.

# Piecewise constant / linear basis functions

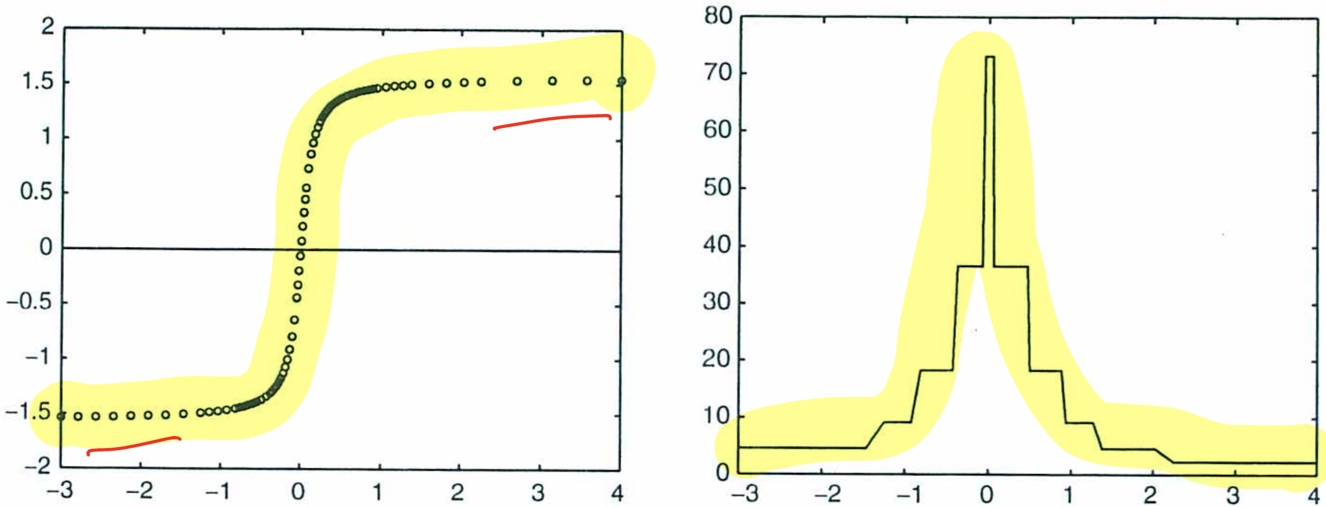



**Fig. 9.4.** Distribution of quadrature nodes (*left*); density of the integration stepsize in the approximation of the integral of Example 9.9 (*right*)

# Outline

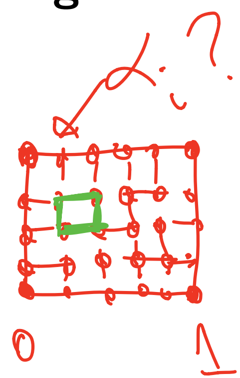
# Regular Grids in Two Dimensions

- A **separable integral** can be done by doing integration along one axes first, then another:

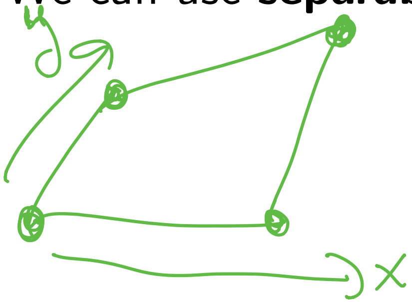
$$J = \int_{x=0}^{1} \int_{y=0}^{1} f(x,y)\,dx dy = \int_{x=0}^{1} dx \left[ \int_{y=0}^{1} f(x,y)\,dy \right]$$

- Consider evaluating the function at nodes on a **regular grid**

$$\mathbf{x}_{i,j} = \{x_i, y_j\}, \quad f_{i,j} = f(\mathbf{x}_{i,j}).$$



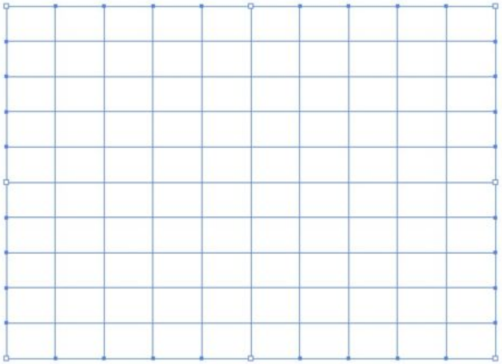

- We can use **separable basis** functions:

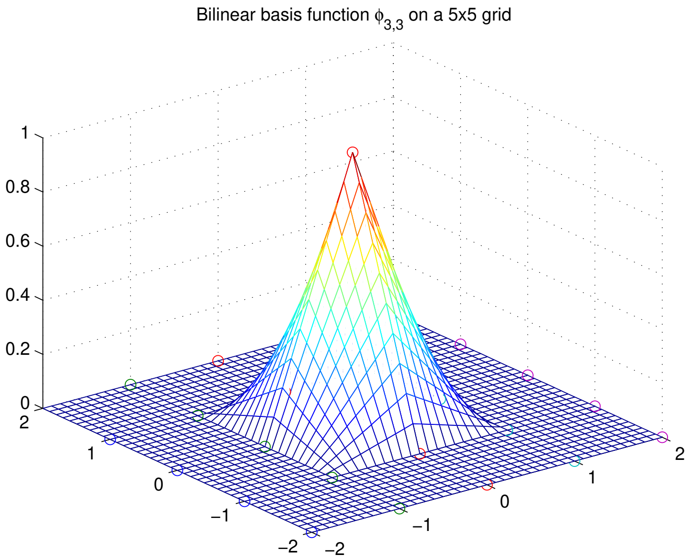



$$\phi_{i,j}(\mathbf{x}) = \phi_i(x)\phi_j(y).$$

$$\int_0^h \int_0^h (a+bx)(c+dy)$$

# Bilinear basis functions





# Piecewise-Polynomial Integration

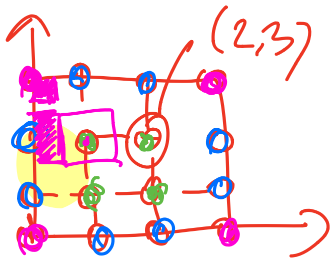
- Use a different interpolation function $\phi_{(i,j)} : \Omega_{i,j} \to \mathbb{R}$ in each rectange of the grid
$$\Omega_{i,j} = [x_i, x_{i+1}] \times [y_j, y_{j+1}],$$
and it is sufficient to look at a **unit reference rectangle** $\hat{\Omega} = [0,1] \times [0,1]$.
- Recall: The equivalent of piecewise linear interpolation in 1D is the **piecewise bilinear interpolation**
$$\phi_{(i,j)}(x,y) = \phi_{(i)}^{(x)}(x) \cdot \phi_{(j)}^{(y)}(y),$$
where $\phi_{(i)}^{(x)}$ and $\phi_{(j)}^{(y)}$ are linear function.
- The global interpolant can be written in the **tent-function basis**
$$\phi(x,y) = \sum_{i,j} f_{i,j} \phi_{i,j}(x,y).$$

# Bilinear Integration

- The composite **two-dimensional trapezoidal quadrature** is then:

$$J \approx \int_{x=0}^{1} \int_{y=0}^{1} \phi(x,y)dxdy = \sum_{i,j} f_{i,j} \int \int \phi_{i,j}(x,y)dxdy = \sum_{i,j} w_{i,j} f_{i,j}$$

- Consider one of the corners $(0,0)$ of the reference rectangle and the corresponding basis $\hat{\phi}_{0,0}$ restricted to $\hat{\Omega}$:




$$\hat{\phi}_{0,0}(\hat{x},\hat{y}) = (1-\hat{x})(1-\hat{y})$$

- Now integrate $\hat{\phi}_{0,0}$ over $\hat{\Omega}$:

$O(h^2)$

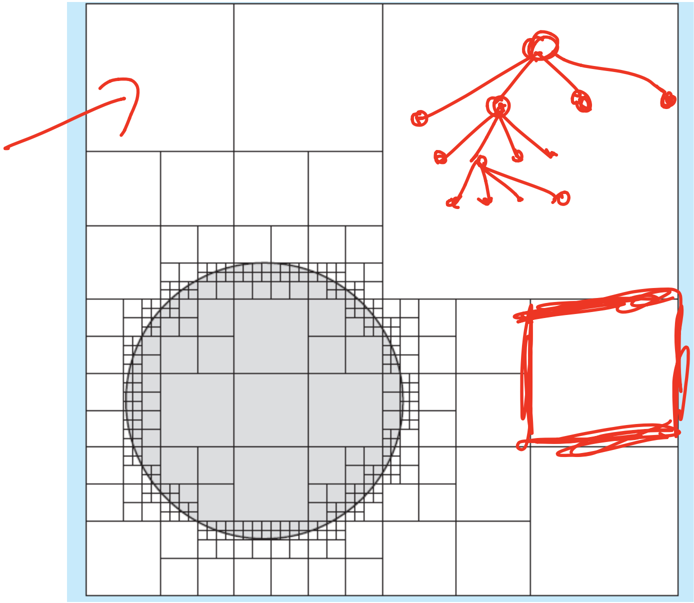
$$\int_{\hat{\Omega}} \hat{\phi}_{0,0}(\hat{x},\hat{y})d\hat{x}d\hat{y} = \frac{1}{4}.$$

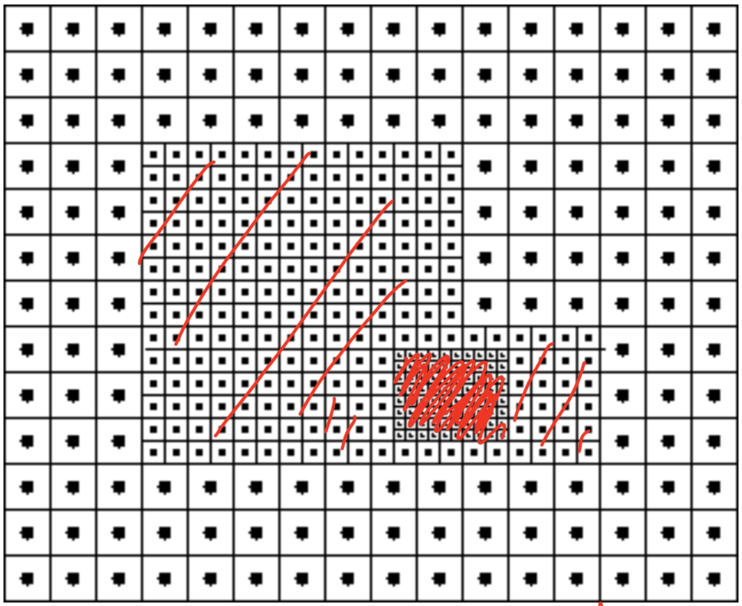
$J = h^2 \sum w_{i,j} f_{i,j}$

- Since each **interior node** contributes to 4 rectangles, its weight is 1. **Edge nodes** contribute to 2 rectangles, so their weight is 1/2. **Corners** contribute to only one rectangle, so their weight is 1/4.

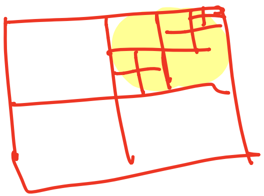
# Adaptive Meshes: Quadtrees and Block-Structured

Adaptive Mesh Refinement





Quadtree .

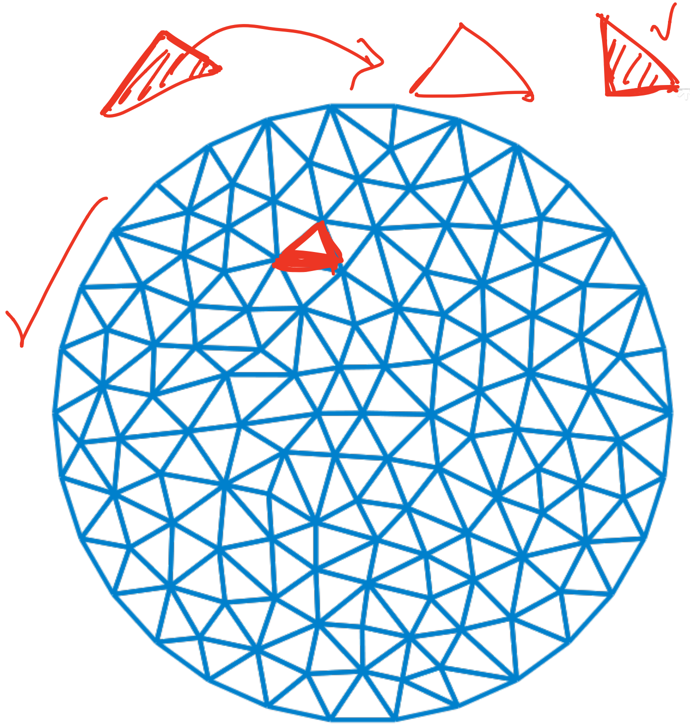


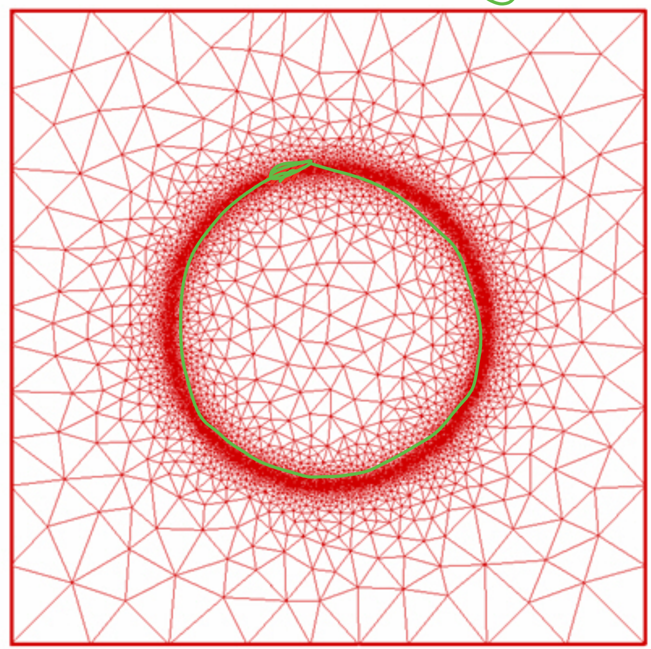
Block-structured refinement

# Irregular (Simplicial) Meshes

Any polygon can be triangulated into arbitrarily many **disjoint triangles**. Similarly **tetrahedral meshes** in 3D.

meshing software





# Outline

# In MATLAB

non-smooth or less accurate

smooth function, accurate integral

- The MATLAB function $quad(f, a, b, \varepsilon)$ uses adaptive Simpson quadrature to compute the integral.
- The MATLAB function $quadl(f, a, b, \varepsilon)$ uses adaptive Gauss-Lobatto quadrature.
- MATLAB says: "The function *quad* may be more efficient with low accuracies or nonsmooth integrands."
- In two dimensions, for separable integrals over rectangles, use

$$J = dblquad(f, x_{min}, x_{max}, y_{min}, y_{max}, \varepsilon)$$

$$J = dblquad(f, x_{min}, x_{max}, y_{min}, y_{max}, \varepsilon, \boxed{@quadl})$$

- There is also *triplequad*.

# Conclusions/Summary

- Numerical integration or quadrature approximates an integral via a discrete **weighted sum** of function values over a set of **nodes**.
- Integration is based on interpolation: Integrate the interpolant to get a good approximation.
- Piecewise polynomial interpolation over **equi-spaced nodes** gives the **trapezoidal and Simpson quadratures** for lower order, and higher order are generally not recommended.
- In higher dimensions we split the domain into **rectangles for regular grids** (separable integration), or **triangles/tetrahedra for simplicial meshes**.
- Integration in high dimensions $d$ becomes harder and harder because the number of nodes grows as $N^d$: **Curse of dimensionality**. Monte Carlo is one possible cure...