Numerical Methods for PDEs

Integral Equation Methods, Lecture 2
Numerical Quadrature

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April 28, 2003

Outline

Easy technique for computing integrals

- Piecewise constant approach

Gaussian Quadrature

- Convergence properties
- Essential role of orthogonal polynomials
- Multidimensional Integrals

Techniques for singular kernels

- Adaptation and variable transformation
- Singular quadrature.

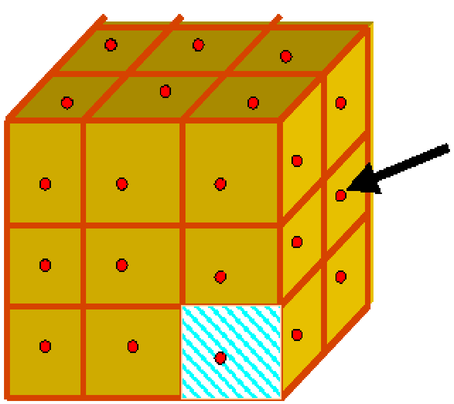
3D Laplace's Equation

Basis Function Approach

Centroid Collocation

Put collocation points at panel centroids

$$\Psi\left(x_{c_i}\right) = \sum_{j=1}^{n} \alpha_j \underbrace{\int_{panel\ j} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'}_{A_{i,j}}$$



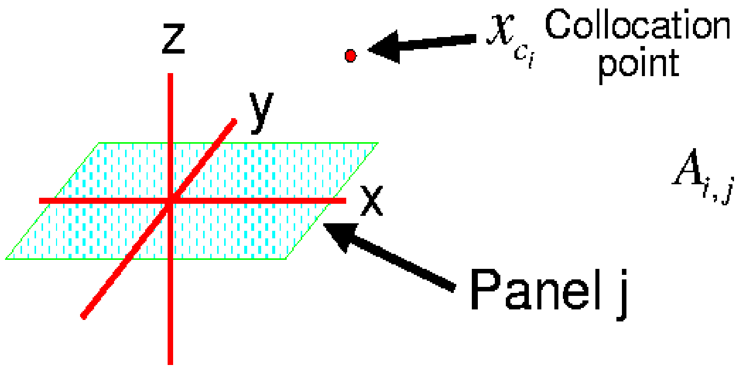
x_{c_i} Collocation point

$$\begin{bmatrix} A_{1,1} & \cdots & \cdots & A_{1,n} \\ \vdots & \ddots & & \vdots \\ \vdots & & \ddots & \vdots \\ A_{n,1} & \cdots & \cdots & A_{n,n} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \vdots \\ \vdots \\ \alpha_n \end{bmatrix} = \begin{bmatrix} \Psi\left(x_{c_1}\right) \\ \vdots \\ \vdots \\ \Psi\left(x_{c_n}\right) \end{bmatrix}$$

3D Laplace's Equation

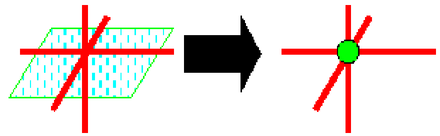
Basis Function Approach

Calculating Matrix Elements



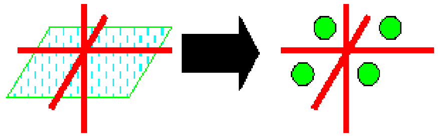
$$A_{i,j} = \int_{panel\ j} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

One point quadrature Approximation



$$A_{i,j} \approx \frac{Panel\ \ Area}{\left\| x_{c_i} - x_{centroid_j} \right\|}$$

Four point quadrature Approximation



$$A_{i,j} \approx \sum_{j=1}^{4} \frac{0.25 * Area}{\left\| x_{c_i} - x_{point_j} \right\|}$$

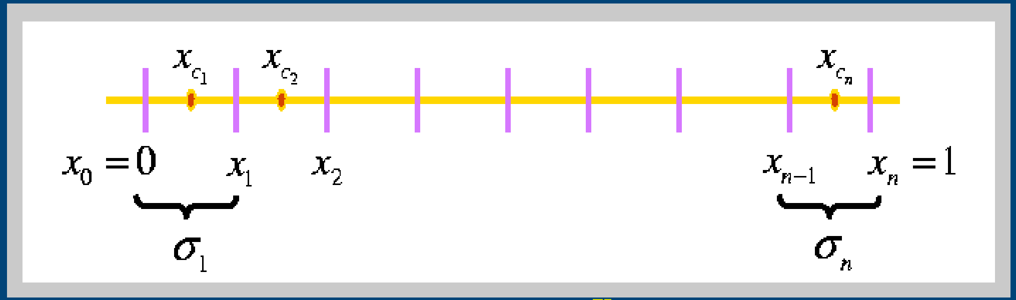
Normalized 1D Problem

Basis Function Approach

Collocation Discretization of 1D Equation

$$\Psi(x) = \int_0^1 g(x, x')\sigma(x')dS' \qquad x \in [0,1]$$

<u>Centroid collocated piecewise constant scheme</u>

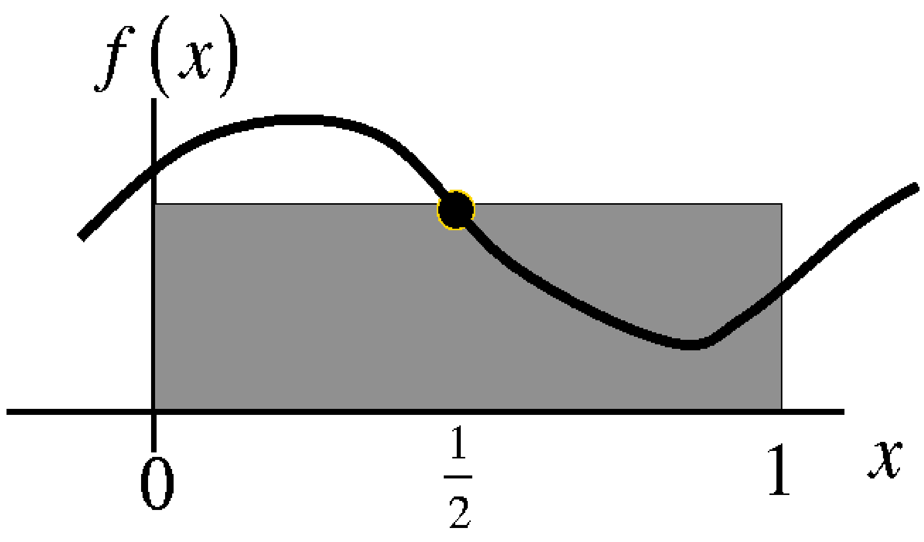


$$\Psi(x_{c_i}) = \sum_{j=1}^{n} \sigma_j \underbrace{\int_{x_{j-1}}^{x_j} g(x_{c_i}, x')dS'}_{\textit{to be evaluated}}$$

Normalized 1D Problem

Simple Quadrature Scheme

$$\int_0^1 f(x)dx \simeq f\left(\frac{1}{2}\right)$$



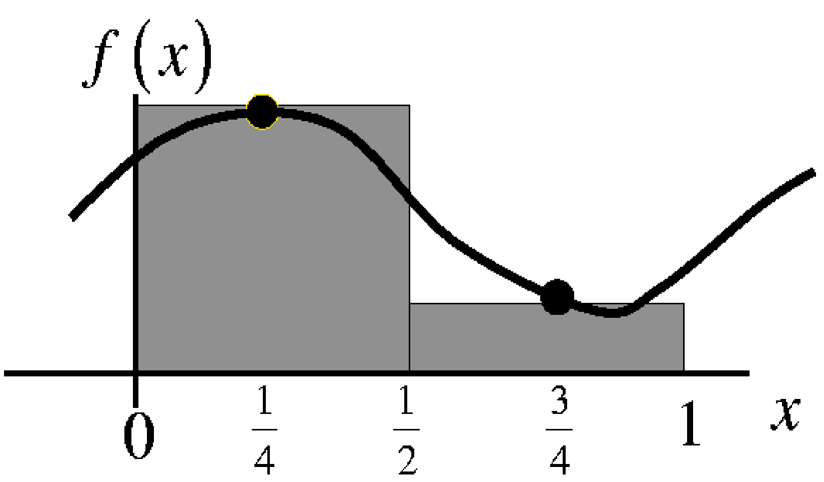
Area under the curve is approximated by a rectangle

Normalized 1D Problem

Simple Quadrature Scheme

Improving the Accuracy

$$\int_0^1 f(x)dx \simeq \frac{1}{2} f\left(\frac{1}{4}\right) + \frac{1}{2} f\left(\frac{3}{4}\right)$$



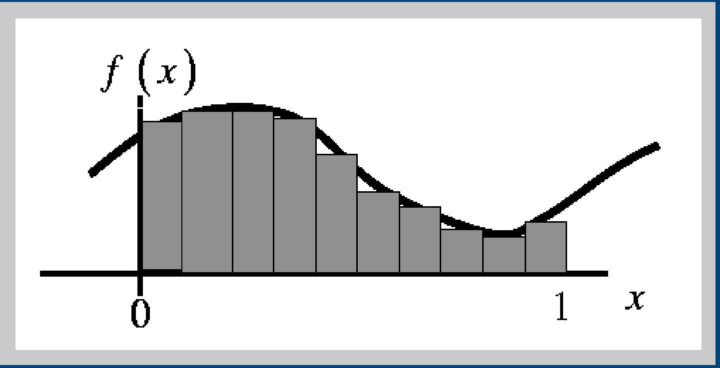
Area under the curve is approximated by two rectangles

Normalized 1D Problem

Simple Quadrature Scheme

General n-Point Formula

$$\int_0^1 f(x)dx \simeq \sum_{i=1}^{n} \frac{1}{n} f\left(\frac{i-\frac{1}{2}}{n}\right)$$



Key questions about the method:

How fast do the errors decay with n?

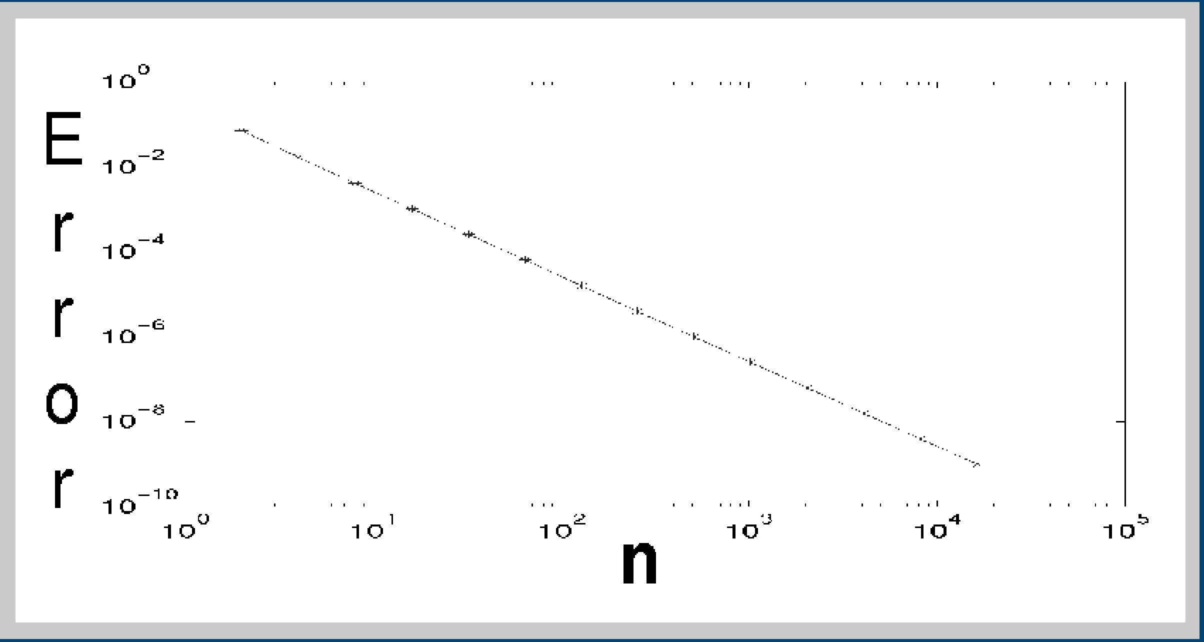
Are there better methods?

Normalized 1D Problem

Simple Quadrature Scheme

Numerical Example

$$\int_0^1 sin(x)dx \simeq \sum_{i=1}^{n} \frac{1}{n} sin\left(\frac{i-\frac{1}{2}}{n}\right)$$



Normalized 1D Problem

General Quadrature Scheme

General 1D Form

$$\int_0^1 f(x)dx \simeq \sum_{i=1}^{n} \underbrace{w_i}_{weight} \underbrace{f(x_i)}_{Evaluation\ Point}$$

Free to pick the **evaluation points**.

Free to pick the **weights** for each point.

An n-point formula has 2n degrees of freedom!

Normalized 1D Problem

General Quadrature Scheme

Point-Weight Selection Criteria

Result should be exact if $f(x)$ is a polynomial

$$f(x) = a_0 + a_1 x + a_2 x^2 + \cdots + a_l x^l = p_l(x)$$

Select x_i's and w_i's such that

$$\int_0^1 p_l(x)dx = \sum_{i=1}^{n} w_i p_l(x_i)$$

for ANY polynomial upto (and including) l^{th} order

With $2n$ degrees of freedom, $l = 2n - 1$

Normalized 1D Problem

General Quadrature Scheme

Why the Exactness Criteria?

Consider the Taylor series for $f(x)$

$$f(x) = f(0) + \frac{\partial f(0)}{\partial x} x + \cdots + \frac{1}{l!} \frac{\partial^l f(0)}{\partial x^l} x^l + R_{l+1}$$

R_{l+1} is the **remainder**

$$R_{l+1} = \frac{1}{(l+1)!} \frac{\partial^{l+1} f(\tilde{x})}{\partial x^{l+1}} x^{l+1}$$

where $\tilde{x} \in [0, x]$

Normalized 1D Problem

General Quadrature Scheme

Estimating the Error

Using the Taylor series results and the exactness criteria

$$\int_0^1 f(x)dx - \sum_{i=1}^n w_i f(x_i) = \underbrace{\frac{1}{(l+1)!}\int_0^1 \frac{\partial^{l+1} f(\tilde{x}(x))}{\partial x^{l+1}} x^{l+1} dx}_{Remainder}$$

Assuming derivatives of $f(x)$ are bounded on $[0,1]$

$$\left| \int_0^1 f(x)dx - \sum_{i=1}^n w_i f(x_i) \right| \leq \frac{K}{(l+1)!}$$

Convergence is **very** fast!!

Normalized 1D Problem

General Quadrature Scheme

Meeting the Exactness Criteria

Exactness condition requires

$$\int_0^1 p_l(x)dx = \int_0^1 (a_0 + a_1 x + a_2 x^2 + \cdots + a_l x^l)dx = \sum_{i=1}^{n} w_i p_l(x_i)$$

for any set of $l+1$ coefficients $a_0, a_1, \ldots, a_l$

Equivalently

$$\int_0^1 a_0 dx + \int_0^1 a_1 x dx + \int_0^1 a_2 x^2 dx + \cdots + \int_0^1 a_l x^l dx = \sum_{i=1}^{n} w_i p_l(x_i)$$

Normalized 1D Problem

General Quadrature Scheme

Meeting the Exactness Criteria

Exactness condition will be satisfied if and only if

$$\int_0^1 dx = \sum_{i=1}^{n} w_i \cdot 1$$

$$\int_0^1 x\,dx = \sum_{i=1}^{n} w_i \cdot x_i$$

$$\vdots$$

$$\int_0^1 x^l dx = \sum_{i=1}^{n} w_i \cdot {x_i}^l$$

Normalized 1D Problem

General Quadrature Scheme

Meeting the Exactness Criteria

Reorganizing exactness equations

$$\begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_1^l & x_2^l & \cdots & x_n^l \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} - \begin{bmatrix} 1 \\ \vdots \\ \vdots \\ \int_0^1 x^l \, dx \end{bmatrix} = 0$$

Nonlinear, since x_i's and w_i's are unknowns

Normalized 1D Problem

General Quadrature Scheme

Computing the Points and Weights

Could use **Newton's Method**

$$F(y) = 0 \Rightarrow J_F\left(y^k\right)\left(y^{k+1} - y^k\right) = -F\left(y^k\right)$$

The nonlinear function for Newton is then

$$F\begin{pmatrix} w \\ x \end{pmatrix} = \begin{bmatrix} 1 & 1 & \cdots & 1 \\ x_1 & x_2 & \cdots & x_n \\ \vdots & \vdots & \ddots & \vdots \\ x_1^l & x_2^l & \cdots & x_n^l \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} - \begin{bmatrix} 1 \\ \vdots \\ \vdots \\ \int_0^1 x^l \, dx \end{bmatrix} = 0$$

Normalized 1D Problem

General Quadrature Scheme

Computing the Points and Weights

Newton Method Jacobian reveals problem

$$
J_F\begin{pmatrix} w \\ x \end{pmatrix} = \overbrace{\begin{bmatrix} 1 & 1 & \cdots & 1 & 0 & 0 & \cdots & 0 \\ x_1 & x_2 & \cdots & x_n & w_1 & w_2 & \cdots & w_n \\ \vdots & \vdots & \ddots & \vdots & \vdots & \vdots & \ddots & \vdots \\ x_1^l & x_2^l & \cdots & x_n^l & l w_1 x_1^{l-1} & \cdots & \cdots & l w_1 x_n^{l-1} \end{bmatrix}}^{2n}
$$

Columns become linearly dependent for high order

Normalized 1D Problem

General Quadrature Scheme

Use Different Polynomials

Exactness criteria will be satisfied if and only if

$$\int_0^1 c_0(x)\,dx = \sum_{i=1}^{n} w_i c_0(x_i)$$

$$\int_0^1 c_1(x)\,dx = \sum_{i=1}^{n} w_i c_1(x_i)$$

$$\vdots$$

$$\int_0^1 c_l(x)\,dx = \sum_{i=1}^{n} w_i c_l(x_i)$$

BUT

Each c_i polynomial must

- Contain an x^i term
- Be linearly independent

Normalized 1D Problem

General Quadrature Scheme

Orthogonal Polynomials

For the normalized integral, two poynomials are said to be **orthogonal** if

$$\int_0^1 c_i(x)c_j(x)dx = 0 \quad for\ j \neq i$$

The above integral is often referred to as an inner product and ascribed the notation

$$(c_i, c_j) = \int_0^1 c_i(x)c_j(x)dx$$

The connection between polynomial inner products and vector inner products can be seen by sampling.

Normalized 1D Problem

General Quadrature Scheme

Exploiting the Different Polynomials

Consider rewriting the exactness criteria

$$\underbrace{\begin{aligned}\int_0^1 c_0(x)\,dx &= \sum_{i=1}^{n} w_i c_0(x_i)\\ &\vdots\\ \int_0^1 c_{n-1}(x)\,dx &= \sum_{i=1}^{n} w_i c_{n-1}(x_i)\end{aligned}}_{\text{Low order terms}} \qquad \underbrace{\begin{aligned}\int_0^1 c_n(x)\,dx &= \sum_{i=1}^{n} w_i c_n(x_i)\\ &\vdots\\ \int_0^1 c_{2n-1}(x)\,dx &= \sum_{i=1}^{n} w_i c_{2n-1}(x_i)\end{aligned}}_{\text{High Order Terms}}$$

Recall that $l(\#\ polys) = 2n - 1(\#\ of\ coefficients)$

Normalized 1D Problem

General Quadrature Scheme

Exploiting the Different Polynomials

Can write the higher order terms differently

$$\int_0^1 c_n(x)dx = \sum_{i=1}^n w_i c_n(x_i) \Rightarrow \int_0^1 c_n(x)c_0(x)dx = \sum_{i=1}^n w_i c_n(x_i)c_0(x_i)$$

$$\vdots$$

$$\vdots$$

$$\int_0^1 c_{2n-1}(x)dx = \sum_{i=1}^n w_i c_{2n-1}(x_i) \Rightarrow \int_0^1 c_n(x)c_{n-1}(x)dx = \sum_{i=1}^n w_i c_n(x_i)c_{n-1}(x_i)$$

The products $c_n(x)c_j(x)$ are linearly independent!

Normalized 1D Problem

General Quadrature Scheme

Using Orthogonality and Roots

Use orthogonal polynomials

$$\cancel{\int_0^1 c_n(x)\, c_0(x)\, dx} = \sum_{i=1}^{n} w_i c_n(x_i)\, c_0(x_i)$$

$$\vdots$$

$$\cancel{\int_0^1 c_n(x)\, c_{n-1}(x)\, dx} = \sum_{i=1}^{n} w_i c_n(x_i)\, c_{n-1}(x_i)$$

Pick the x_i's to be n roots of $c_n(x)$

The higher order constraints are exactly satisfied!

Normalized 1D Problem

General Quadrature Scheme

Satisfying the Lower Order Constraints

An abbreviated exactness equation

$$\begin{array}{c} \uparrow \\ n \\ \downarrow \end{array}\begin{bmatrix} 1 & 1 & \cdots & 1 \\ c_0(x_1) & \cdots & \cdots & c_0(x_n) \\ \vdots & \vdots & \ddots & \vdots \\ c_{n-1}(x_1) & \cdots & \cdots & c_{n-1}(x_n) \end{bmatrix} \begin{bmatrix} w_1 \\ w_2 \\ \vdots \\ w_n \end{bmatrix} = \begin{bmatrix} 1 \\ \vdots \\ \vdots \\ \int_0^1 c_{n-1}(x)\,dx \end{bmatrix}$$

Now **linear**, as x_i's are known!

Rows are sampled orthogonal polynomials!

Normalized 1D Problem

Gaussian Quadrature Summary

Algorithm Steps

1. Construct $n+1$ orthogonal polynomials
$$\int_0^1 c_i(x)c_j(x)dx = 0 \quad for\ j \neq i$$
2. Compute n **roots**, $x_i,\ i = 1, \ldots, n$ of the n^{th} order orthogonal polynomial such that $c_n(x_i) = 0$
3. Solve a linear system for the **weights** w_i
4. Approximate the integral as a sum
$\int_0^1 f(x)dx = \sum_{i=1}^{n} w_i f(x_i)$

Normalized 1D Problem

Gaussian Quadrature Summary

Accuracy Result

$$\int_0^1 f(x)dx \simeq \sum_{i=1}^{n} w_i f(x_i)$$

Key properties of the method

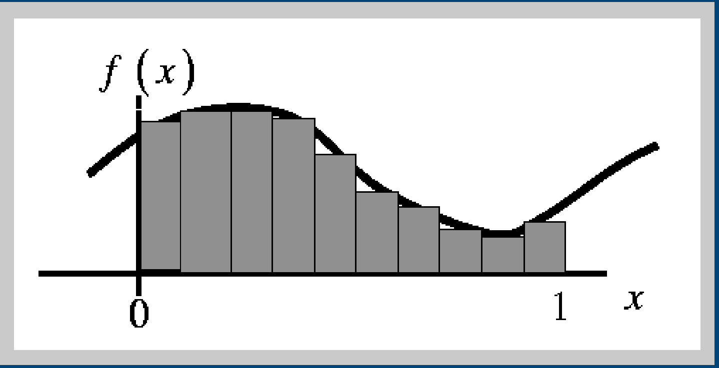
- An n-point Gauss quadrature rule is **exact** for polynomials of order $2n - 1$
- Error is proportional to $\left(\frac{1}{2n}\right)^{2n}$

Normalized 1D Problem

Simple Quadrature Scheme

General n-Point Formula

$$\int_0^1 f(x)dx \simeq \sum_{i=1}^{n} \frac{1}{n} f\left(\frac{i-\frac{1}{2}}{n}\right)$$

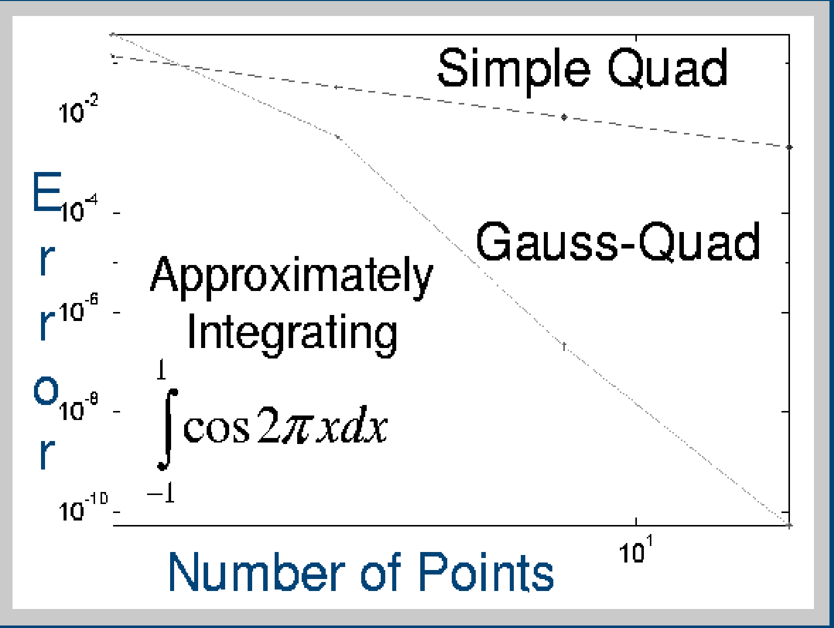


Key property of the method

- Error is proportional to $\frac{1}{n^2}$

Normalized 1D Problem

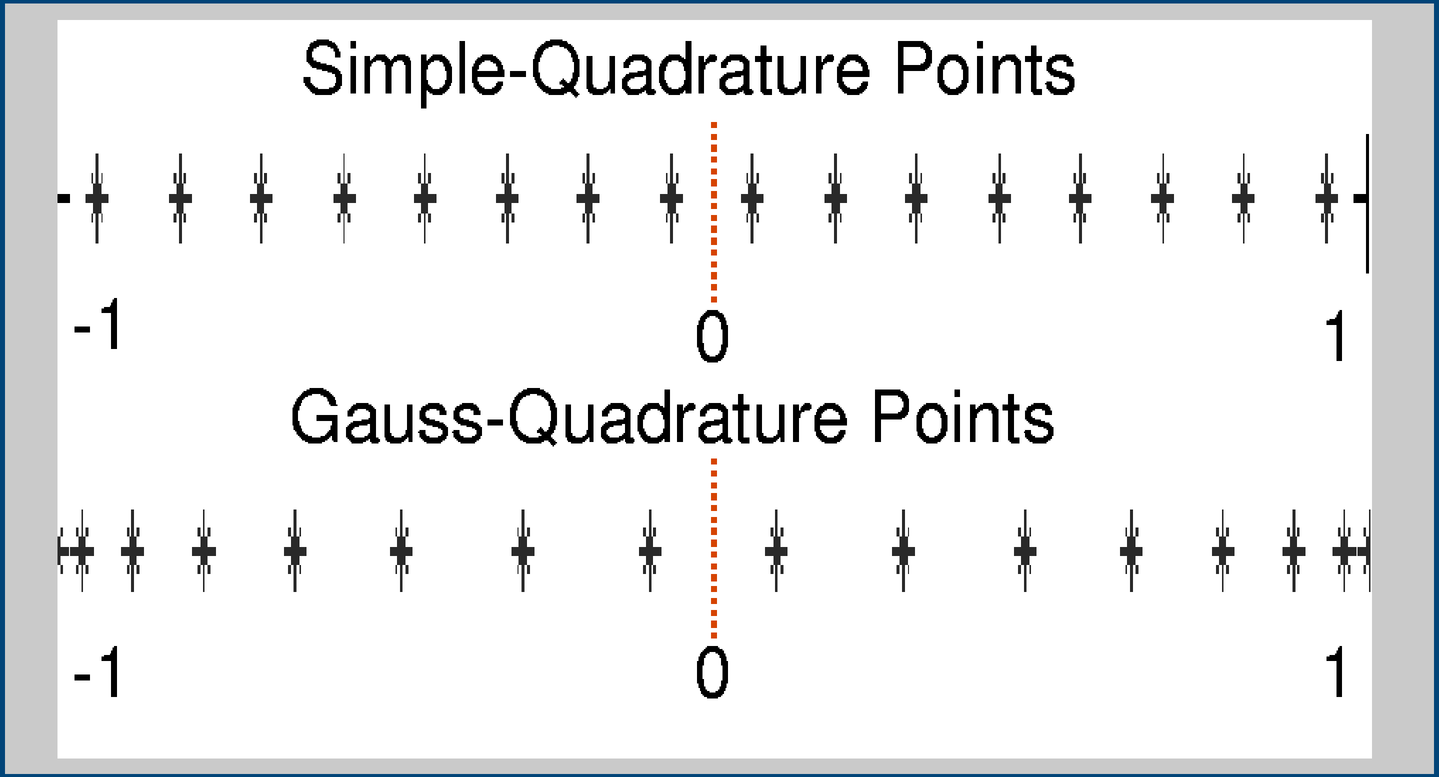
Comparing Simple Quad and Gauss Quad



Normalized 1D Problem

Comparing Simple Quad and Gauss Quad

Evaluation Point Placement

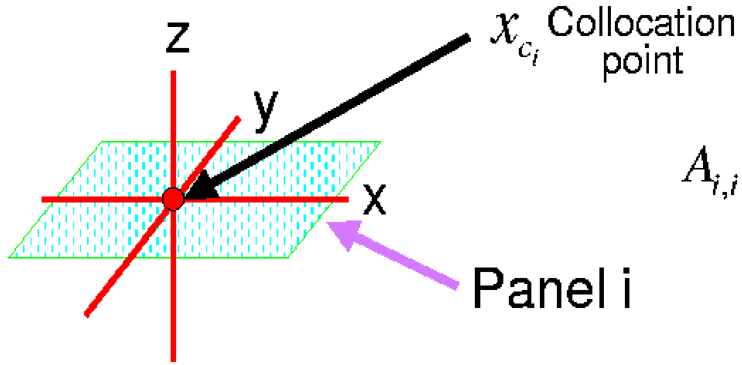


Notice the clustering at interval ends

The Singular Kernel Problem

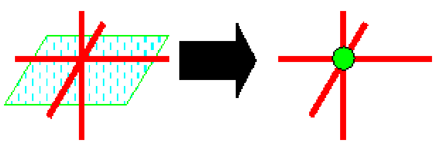
3D Laplace Example

Calculating the "Self-Term"



$$A_{i,i} = \int_{panel\ i} \frac{1}{\left\| x_{c_i} - x' \right\|} dS'$$

One point quadrature Approximation



$$A_{i,i} \approx \cancel{\frac{Panel\ \ Area}{\underbrace{\left\| x_{c_i} - x_{c_i} \right\|}_{0}}}$$

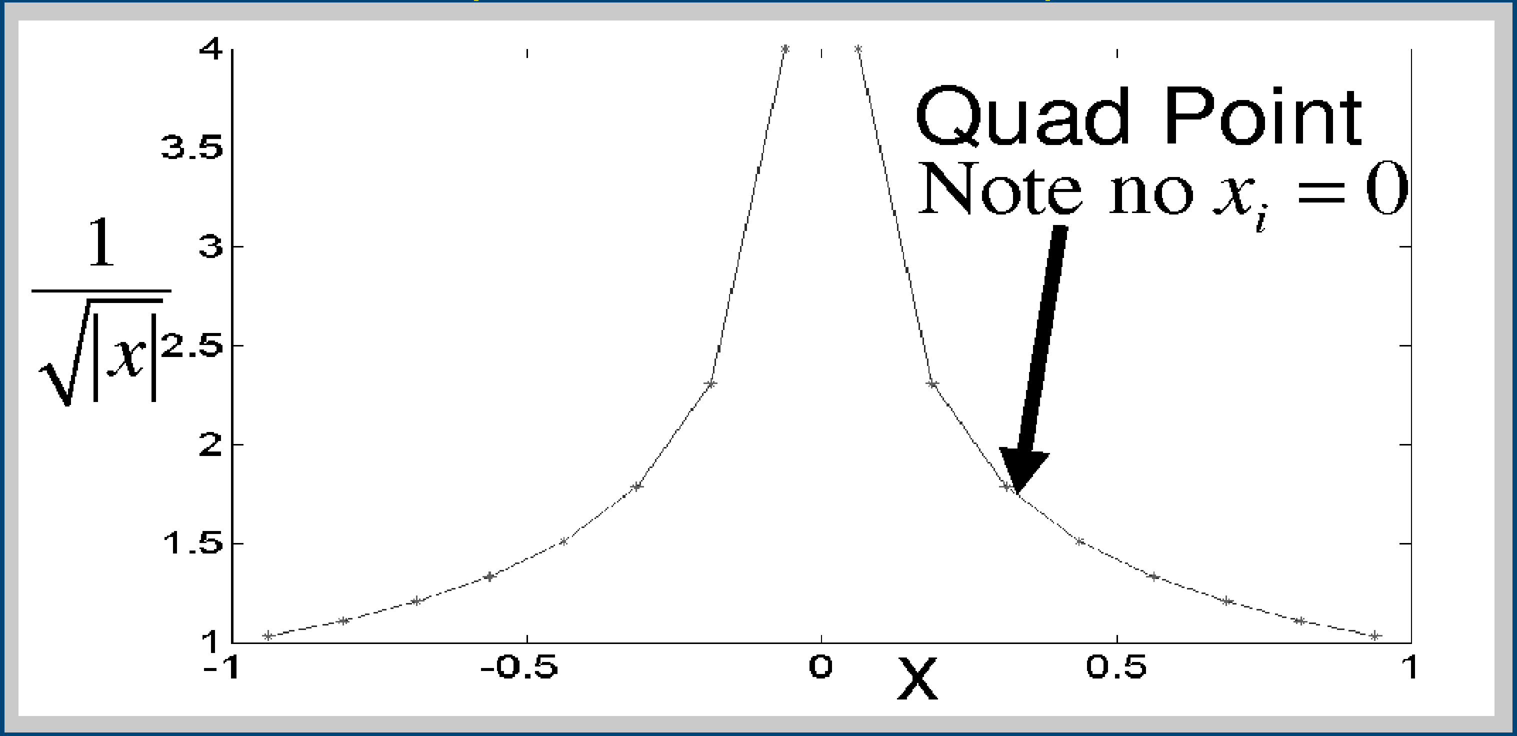
$$\boxed{A_{i,i} = \int_{panel\ i} \frac{1}{\left\| x_{c_i} - x' \right\|} dS' \text{ is an integrable singularity}}$$

The Singular Kernel Problem

Symmetrized 1D Example

Example

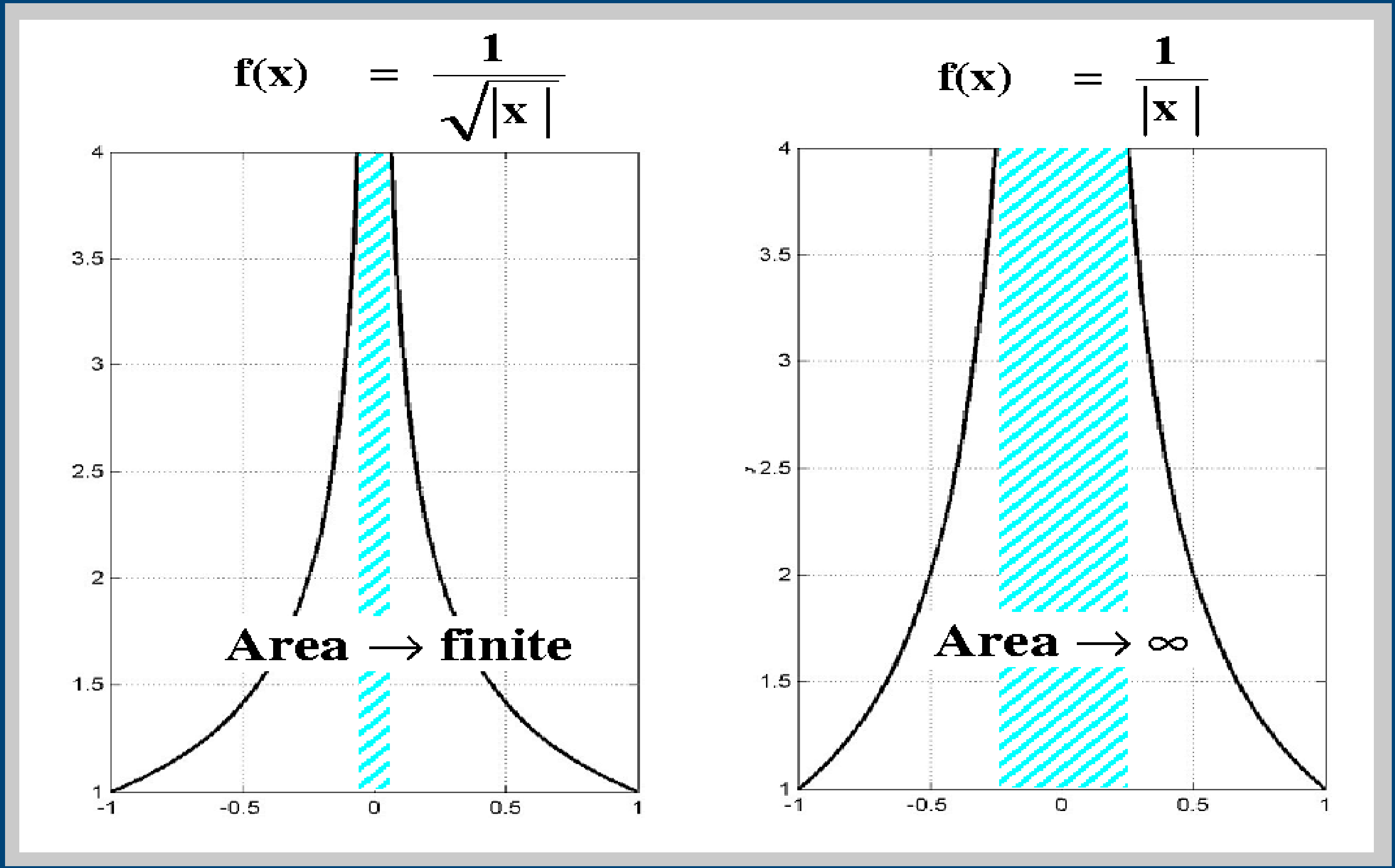
$$\int_{-1}^{1} \frac{1}{\sqrt{|x|}} dx \simeq \sum_{i=1}^{n} w_i \frac{1}{\sqrt{|x_i|}}$$



The Singular Kernel Problem

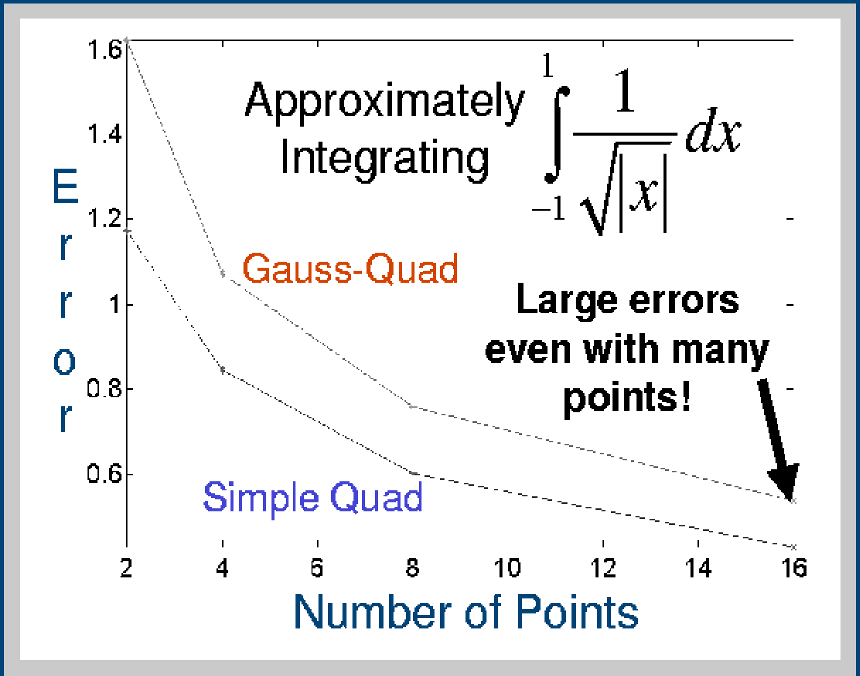
Symmetrized 1D Example

Integrable and Nonintegrable Singularities



The Singular Kernel Problem

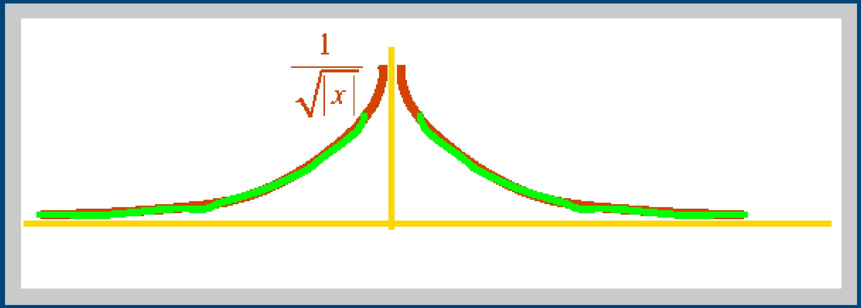
Comparing Quadrature Schemes



The Singular Kernel Problem

Improved Techniques

Subinterval (Adaptive) Quadrature



Subdivide the integration interval

$$\int_{-1}^{1} \frac{1}{\sqrt{|x|}}dx = \int_{-1}^{-0.1} \frac{1}{\sqrt{|x|}}dx + \int_{-0.1}^{0} \frac{1}{\sqrt{|x|}}dx + \int_{0}^{0.1} \frac{1}{\sqrt{|x|}}dx + \int_{0.1}^{1} \frac{1}{\sqrt{|x|}}dx$$

Use Gauss quadrature in each subinterval

- Polynomials fit subintervals better
- Expensive if many subintervals used.

The Singular Kernel Problem

Improved Techniques

Change of Variables - for Simple Cases

Change variables to eliminate singularity

$$y^2 = x$$

$$\Rightarrow 2ydy = dx$$

$$\int_{-1}^{1} \frac{1}{\sqrt{|x|}}dx = 2\int_{0}^{1} \frac{1}{\sqrt{|y^2|}}2ydy = 2\int_{0}^{1} 2dy$$

Apply Gauss quadrature on desingularized intergrand

The Singular Kernel Problem

Improved Techniques

Singular Quadrature - Complicated Cases

Integrand has known singularity $s(x)$

$\int_{-1}^{1} f(x)s(x)dx$ where $f(x)$ is smooth

Develop a quadrature formula exact for

$\int_{-1}^{1} p_l(x)s(x)dx$ where $p_l(x)$ is polynomial of order l

Calculate weights like Gauss quadrature

The Singular Kernel Problem

Improved Techniques

Singular Quadrature Weights

$$
\begin{bmatrix}
1 & 1 & \cdots & 1 \\
c_0(x_1) & \cdots & \cdots & c_0(x_n) \\
\vdots & \vdots & \ddots & \vdots \\
c_{n-1}(x_1) & \cdots & \cdots & c_{n-1}(x_n)
\end{bmatrix}
\begin{bmatrix}
w_1 \\ w_2 \\ \vdots \\ w_n
\end{bmatrix}
=
\begin{bmatrix}
\int_{1}^{1} s(x)\,dx \\
\vdots \\
\int_{-1}^{1} c_{n-1}(x)\,s(x)\,dx
\end{bmatrix}
$$

Need (analytic) formulas for integral of $c(x)s(x)$

Summary

Easy technique for computing integrals

Piecewise constant approach

Gaussian quadrature

Faster convergence

Essential role of orthogonal polynomials

Techniques for singular kernels

Adaptation and Variable Transformation

Singular quadrature

What about multiple dimensions?