

Announcements

- ICES
- 4CM assignments 1&2
- Content cutoff for Final:
Thu Nov 30

Review



Interpolation basis φ_i
nodes x_i

$$V = (\varphi_i(x_j))_{ij} \quad V\vec{\alpha} = \vec{y}$$

$$\max |f - p_{n-1}(x)| \leq C \max |f^{(n)}(x)| h^n$$

↪ "n-th order convergence"

Goals

- Splines
- num. integration

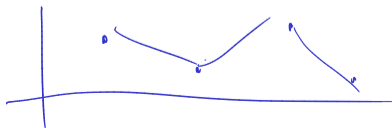
Going piecewise: Simplest Case

Construct a piecewise linear interpolant at four points.

x_0, y_0	$f_1 = a_1x + b_1$	x_1, y_1	$f_2 = a_2x + b_2$	x_2, y_2	$f_3 = a_3x + b_3$	x_3, y_3
	2 unk.		2 unk.		2 unk.	
	$f_1(x_0) = y_0$		$f_2(x_1) = y_1$		$f_3(x_2) = y_2$	
	$f_1(x_1) = y_1$		$f_2(x_2) = y_2$		$f_3(x_3) = y_3$	
	2 eqn.		2 eqn.		2 eqn.	

Why three intervals?

2 end intervals, one middle



Piecewise Cubic ('Splines')

(x_0, y_0)

$$f_1 = a_1x^3 + b_1x^2 + c_1x + d_1$$

(x_1, y_1)

$$f_2 = a_2x^3 + b_2x^2 + c_2x + d_2$$

(x_2, y_2)

$$f_3 = a_3x^3 + b_3x^2 + c_3x + d_3$$

(x_3, y_3)

4 unk.

$$\begin{cases} f_1(x_0) = y_0 \\ f_1(x_1) = y_1 \end{cases}$$

4 unk.

$$\begin{cases} f_2(x_1) = y_1 \\ f_2(x_2) = y_2 \end{cases}$$

4 unk.

$$\begin{cases} f_3(x_2) = y_2 \\ f_3(x_3) = y_3 \end{cases}$$

$$f_1'(x_1) = f_2'(x_1)$$

$$f_2'(x_2) = f_3'(x_2)$$

$$f_1''(x_1) = f_2''(x_1)$$

$$f_2''(x_2) = f_3''(x_2)$$

$$f_1''(x_0) = 0$$

$$f_3''(x_3) = 0$$

'natural' spline

Piecewise Cubic ('Splines'): Accounting

x_0, y_0		x_1, y_1		x_2, y_2		x_3, y_3
	f_1		f_2		f_3	
	$a_1x^3 + b_1x^2 + c_1x + d_1$		$a_2x^3 + b_2x^2 + c_2x + d_2$		$a_3x^3 + b_3x^2 + c_3x + d_3$	

unknowns: $4 N_{\text{intervals}}$

conditions: $2 N_{\text{intervals}} + 2 N_{\text{middle nodes}} + 2$
 $N_{\text{intervals}} - 1 = N_{\text{middle nodes}}$

$\rightarrow = 2 N_{\text{intervals}} + 2 (N_{\text{intervals}} - 1) + 2 = 4 N_{\text{intervals}}$

Outline

Introduction to Scientific Computing

Systems of Linear Equations

Linear Least Squares

Eigenvalue Problems

Nonlinear Equations

Optimization

Interpolation

Numerical Integration and Differentiation

Numerical Integration

Quadrature Methods

Accuracy and Stability

Gaussian Quadrature

Composite Quadrature

Numerical Differentiation

Richardson Extrapolation

Initial Value Problems for ODEs

Boundary Value Problems for ODEs

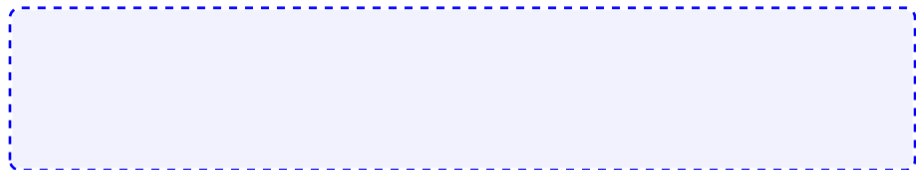
Partial Differential Equations and Sparse Linear Algebra

Fast Fourier Transform

Additional Topics

Numerical Integration: About the Problem

What is numerical integration? (Or **quadrature**?)



What about existence and uniqueness?



Numerical Integration: About the Problem

What is numerical integration? (Or **quadrature**?)

Given a , b , f , compute (approximately!)

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

What about existence and uniqueness?

- ▶ Answer exists e.g. if f is integrable in the Riemann or Lebesgue senses.
- ▶ Answer is unique if f is e.g. piecewise continuous and bounded. (this also implies existence)

Conditioning

Derive the (absolute) condition number for numerical integration.

$$\hat{f}(x) = f(x) + e(x)$$

$$\left| \int_a^b f(x) dx - \int_a^b \hat{f}(x) dx \right|$$

$$= \left| \int_a^b e(x) dx \right| \leq \int_a^b |e(x)| dx \leq (b-a) \max_{x \in (a,b]} |e(x)|$$

Interpolatory Quadrature: Examples

$$f(x) \approx p_{n-1}(x) = \sum_{i=1}^n f(x_i) \hat{l}_i(x)$$

$$\int_a^b f(x) dx \approx \sum_{i=1}^n f(x_i) \underbrace{\int_a^b \hat{l}_i(x) dx}_{w_i}$$

Lagrange poly

ⁿ quadrature rule $\int_a^b f(x) dx \approx \sum_{i=1}^n f(x_i) w_i$

↑ nodes ↑ weights,

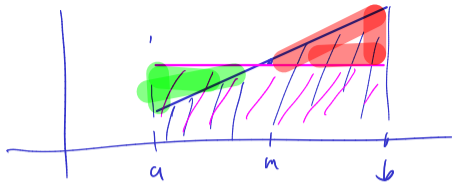
By construction: integrates polynomials of up to degree $n-1$ exactly

Interpolatory Quadrature: Computing Weights

How do the weights in interpolatory quadrature get computed?

$$\begin{aligned} & \quad \quad \quad | \cdot, x_1, \dots, x_n \\ b-a & \Rightarrow \int_a^b 1 dx = \omega_1 \cdot 1 + \dots + \omega_n \cdot 1 \\ \left[\frac{1}{2} x^2 \right]_a^b & \Rightarrow \int_a^b x dx = \omega_1 \cdot x_1 + \dots + \omega_n \cdot x_n \\ & \quad \quad \quad \vdots \\ \left[\frac{1}{n} x^n \right]_a^b & \Rightarrow \int_a^b x^{n-1} dx = \omega_1 \cdot x_1^{n-1} + \dots + \omega_n \cdot x_n^{n-1} \\ \vec{w} & = \underbrace{V^T}_{\text{"method of undetermined coefficients"}} \vec{\omega} \end{aligned}$$

Demo: Newton-Cotes weight finder [cleared]



$$f(m) \cdot (b-a) \approx \int_a^b f(x) dx$$

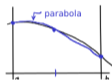
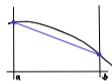
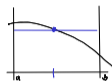
Examples and Exactness

To what polynomial degree are the following rules exact?

Midpoint rule $(b-a)f\left(\frac{a+b}{2}\right)$

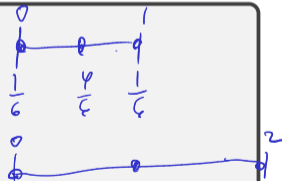
Trapezoidal rule $\frac{b-a}{2}(f(a) + f(b))$

Simpson's rule $\frac{b-a}{6} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right)$



$$b-a = \int_a^b 1 \approx \sum w_i$$

Observed: symmetric nodes & odd node count: extra degree of polynomial integrate exactly



Interpolatory Quadrature: Accuracy

Let p_{n-1} be an interpolant of f at nodes x_1, \dots, x_n (of degree $n-1$)

Recall

$$\sum_i w_i f(x_i) = \int_a^b p_{n-1}(x) dx.$$

What can you say about the accuracy of the method?

$$\begin{aligned} & \left| \int_a^b f(x) dx - \int_a^b p_{n-1}(x) dx \right| \\ & \leq \int_a^b |f(x) - p_{n-1}(x)| dx \\ & \leq (b-a) \max_{x \in (a,b)} |f(x) - p_{n-1}(x)| \\ & \leq Ch \max_{x \in (a,b)} |f^{(n)}(x)| h^n \\ & \leq C \max |f^{(n)}| h^{n+1} \end{aligned}$$

Quadrature: Overview of Rules

"Newton-Cotes" rules

	n	Deg.	Ex.Int.Deg. (w/odd)	Intp.Ord. h^n	Quad.Ord. (regular) h^{n+1}	Quad.Ord. (w/odd) h^{n+2}
		$n - 1$	$(n-1)+1_{\text{odd}}$	n	$n + 1$	$(n+1)+1_{\text{odd}}$
Midp.	1	0	1	1	2	3
Trapz.	2	1	1	2	3	3
Simps.	3	2	3	3	4	5
S. 3/8	4	3	3	4	5	5

- ▶ n : number of points
- ▶ "Deg.": Degree of polynomial used in interpolation ($= n - 1$)
- ▶ "Ex.Int.Deg.": Polynomials of up to (and including) this degree *actually* get integrated exactly. (including the odd-order bump)
- ▶ "Intp.Ord.": Order of Accuracy of Interpolation: $O(h^n)$
- ▶ "Quad.Ord. (regular)": Order of accuracy for quadrature predicted by the error result above: $O(h^{n+1})$
- ▶ "Quad.Ord. (w/odd)": Actual order of accuracy for quadrature given 'bonus' degrees for rules with odd point count

Observation: Quadrature gets (at least) 'one order higher' than interpolation—even more for odd-order rules. (i.e. more accurate)

Interpolatory Quadrature: Stability

Let p_n be an interpolant of f at nodes x_1, \dots, x_n (of degree $n - 1$)

Recall

$$\sum_i w_i f(x_i) = \int_a^b p_n(x) dx$$

What can you say about the stability of this method?

$$\sum w_i = b - a$$

$$\hat{f}(x) = f(x) + e(x)$$

$$\left| \sum w_i f(x_i) - \sum w_i \hat{f}(x_i) \right| \leq \sum |w_i e(x_i)| \leq \left(\sum |w_i| \right) \max_{x \in [a, b]} |e(x)|$$

when bigger:

So, what quadrature weights make for bad stability bounds?

negative weights

About Newton-Cotes

What's not to like about Newton-Cotes quadrature?

Demo: Newton-Cotes weight finder [cleared] (again, with many nodes)



About Newton-Cotes

What's not to like about Newton-Cotes quadrature?

Demo: Newton-Cotes weight finder [cleared] (again, with many nodes)

In fact, Newton-Cotes must have at least one negative weight as soon as $n \geq 11$.

More drawbacks:

- ▶ All the fun of high-order interpolation with monomials and equispaced nodes (i.e. convergence not guaranteed)
- ▶ Weights possibly non-negative (\rightarrow stability issues)
- ▶ Coefficients determined by (possibly ill-conditioned) Vandermonde matrix
- ▶ Thus hard to extend to arbitrary number of points.

Gaussian Quadrature

So far: nodes chosen from outside.

Can we gain something if we let the quadrature rule choose the nodes, too? **Hope:** More design freedom \rightarrow Exact to higher degree.



[Demo: Gaussian quadrature weight finder \[cleared\]](#)