Announcements

- ICES
- 4 CH assignments 1&2
- Content cutoff for final: Thu Nov 30

Goals

- Splines
- Num. integration

Review

Interpolation basis \( \phi_i \)

nodes \( x_i \)

\[ V = (\phi_i(x_j))_{ij} \quad V\tilde{\alpha} = \tilde{y} \]

\[ \max |f - p_{n-1}(x)| \leq C \max |g^{(m)}(x)| h^n \]

\( \sim \) "n-th order convergence"
Going piecewise: Simplest Case

Construct a piecewise linear interpolant at four points.

<table>
<thead>
<tr>
<th>$x_0, y_0$</th>
<th>$x_1, y_1$</th>
<th>$x_2, y_2$</th>
<th>$x_3, y_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_1 = a_1 x + b_1$</td>
<td>$f_2 = a_2 x + b_2$</td>
<td>$f_3 = a_3 x + b_3$</td>
<td></td>
</tr>
<tr>
<td>2 unk.</td>
<td>2 unk.</td>
<td>2 unk.</td>
<td>2 unk.</td>
</tr>
<tr>
<td>$f_1(x_0) = y_0$</td>
<td>$f_2(x_1) = y_1$</td>
<td>$f_3(x_2) = y_2$</td>
<td></td>
</tr>
<tr>
<td>2 eqn.</td>
<td>2 eqn.</td>
<td>2 eqn.</td>
<td>2 eqn.</td>
</tr>
</tbody>
</table>

Why three intervals?

2 end intervals, one middle
Piecewise Cubic (‘Splines’) 

\[ f_1(x) = a_1 x^3 + b_1 x^2 + c_1 x + d_1 \]

\[ f_2(x) = a_2 x^3 + b_2 x^2 + c_2 x + d_2 \]

\[ f_3(x) = a_3 x^3 + b_3 x^2 + c_3 x + d_3 \]

\( x_0, y_0 \)

\( x_1, y_1 \)

\( x_2, y_2 \)

\( x_3, y_3 \)

\[ f'_1(x_0) = y_0 \]

\[ f'_1(x_1) = y_1 \]

\[ f'_1'(x) = f'_2(x) \]

\[ f''_1(x) = f''_2(x) \]

\[ f''_1(x_0) = 0 \]

\[ f''_1(x_1) = 0 \]

\[ f''_1(x_2) = 0 \]

\[ f''_1(x_3) = 0 \]

\[ f'_2(x_0) = f'_2(x_1) \]

\[ f'_2(x_1) = y_1 \]

\[ f'_2(x_2) = y_2 \]

\[ f'_2(x_3) = y_3 \]

\[ f'_2'(x) = f'_3(x) \]

\[ f''_2(x) = f''_3(x) \]

\[ f''_2(x_0) = 0 \]

\[ f''_2(x_1) = 0 \]

\[ f''_2(x_2) = 0 \]

\[ f''_2(x_3) = 0 \]

'Natural' Spline
### Piecewise Cubic (‘Splines’): Accounting

<table>
<thead>
<tr>
<th></th>
<th>$x_0, y_0$</th>
<th>$x_1, y_1$</th>
<th>$x_2, y_2$</th>
<th>$x_3, y_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$f_1$</td>
<td>$a_1 x^3 + b_1 x^2 + c_1 x + d_1$</td>
<td>$a_2 x^3 + b_2 x^2 + c_2 x + d_2$</td>
<td>$a_3 x^3 + b_3 x^2 + c_3 x + d_3$</td>
<td></td>
</tr>
<tr>
<td>$f_2$</td>
<td>$a_1 x^3 + b_1 x^2 + c_1 x + d_1$</td>
<td>$a_2 x^3 + b_2 x^2 + c_2 x + d_2$</td>
<td>$a_3 x^3 + b_3 x^2 + c_3 x + d_3$</td>
<td></td>
</tr>
<tr>
<td>$f_3$</td>
<td>$a_1 x^3 + b_1 x^2 + c_1 x + d_1$</td>
<td>$a_2 x^3 + b_2 x^2 + c_2 x + d_2$</td>
<td>$a_3 x^3 + b_3 x^2 + c_3 x + d_3$</td>
<td></td>
</tr>
</tbody>
</table>

**# unknowns:** $4 \times N_{\text{intervals}}$

**# conditions:**

$$2 \times N_{\text{intervals}} + 2 \times N_{\text{middle nodes}} + 2$$

$$N_{\text{intervals}} - 1 = N_{\text{middle nodes}}$$

$$= 2 \times N_{\text{intervals}} + 2 (N_{\text{intervals}} - 1) + 2 = 4 \times N_{\text{intervals}}$$
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)
Derive the (absolute) condition number for numerical integration.

\[ f(x) = f(x) + e(x) \]

\[ \left| \int_a^b f(x) \, dx - \int_a^b f(x) \, dx \right| \leq \int_a^b |e(x)| \, dx \leq (b-a) \max_{x \in [a,b]} |e(x)| \]
Interpolatory Quadrature: Examples

\[ f(x) \approx p_{n-1}(x) = \sum_{i=1}^{n} f(x_i) l_i(x) \]

\[ \int_{a}^{b} f(x) \, dx \approx \sum_{i=1}^{n} f(x_i) \int_{a}^{b} l_i(x) \, dx \]

"quadrature rule": \[ \int_{a}^{b} f(x) \, dx \approx \sum_{i=1}^{n} f(x_i) \omega_i \]

By construction: integrates polynomials of up to degree \( n-1 \) exactly,
Interpolatory Quadrature: Computing Weights

How do the weights in interpolatory quadrature get computed?

Demo: Newton-Cotes weight finder [cleared]
\[ f(x) \cdot (b-a) \approx \sum_{a}^{b} f(x) \, dx \]
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 \( \frac{b-a}{6} \left( f(a) + 4f \left( \frac{a+b}{2} \right) + f(b) \right) \)
Interpolatory Quadrature: Accuracy

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

\[ \sum_i \omega_i f(x_i) = \int_a^b p_{n-1}(x) \, dx. \]

What can you say about the accuracy of the method?

\[
\left| \int_a^b f(x) \, dx - \sum_i \omega_i f(x_i) \right| \\
\leq \int_a^b \left| f(x) - p_{n-1}(x) \right| \, dx \\
\leq (b-a) \max_{x \in [a,b]} \left| f(x) - p_{n-1}(x) \right| \\
\leq Ch \max_{x \in [a,b]} \left| f^{(n)}(x) \right| h^n \\
\leq C \max_{x \in [a,b]} \left| f^{(n)} \right| h^{n+1}
\]
### Quadrature: Overview of Rules

<table>
<thead>
<tr>
<th>$n$</th>
<th>Deg.</th>
<th>Ex.Int.Deg. (w/odd)</th>
<th>Intp.Ord. $h^n$</th>
<th>Quad.Ord. (regular) $h^{n+1}$</th>
<th>Quad.Ord. (w/odd) $h^{n+1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>0</td>
<td>$(n-1)+1_{\text{odd}}$</td>
<td>1</td>
<td>2</td>
<td>3</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>1</td>
<td>2</td>
<td>3</td>
<td>3</td>
</tr>
<tr>
<td>3</td>
<td>2</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>5</td>
</tr>
<tr>
<td>4</td>
<td>3</td>
<td>3</td>
<td>4</td>
<td>5</td>
<td>5</td>
</tr>
</tbody>
</table>

- **$n$: 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 $x_1, \ldots, x_n$ (of degree $n - 1$)

Recall

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

What can you say about the stability of this method?

So, what quadrature weights make for bad stability bounds?

$$f(x) = f(x) + e(x)$$

$$| \omega_i f(x_i) - 3 \omega_i \hat{f}(x_i) | \leq 3 | \omega_i e(x_i) | \leq \left( \frac{3}{|\omega|} \right) \max_{x \in [a,b]} |e(x)|$$

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 (→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]