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Today’s Undergraduate Colloquium

Mathematics Undergraduate Colloquium
Wednesday, November 1 12:55 - 1:45 LCB 225

Christel Hohenegger will present The scallop theorem”

Abstract: Bacteria and other small swimming organisms can’t coast. Once they stop moving their flagella, they come to a complete stop instantaneously. They live in a world where inertia doesn’t matter. We, on the other hand, live and swim in an inertia dominated world. The scallop theorem is a beautiful and simple geometric argument explaining why if inertia does not matter, you can’t swim with a single hinge or via reciprocal motion. While the scallop theorem tells us what does not work, it does not explain the rich swimming behavior observed in nature. To answer this question, applied mathematicians use a combination of model, analysis and simulation starting from the famous Navier-Stokes equations.
Gaussian Quadrature

• Recall our general quadrature formula

\[ \int_a^b f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i) \quad (1) \]

where the \( w_i \) are the weights and the \( x_i \) are the knots.

• Note that today we start with \( i = 1 \) instead of \( i = 0 \).

• If the knots are evenly spaced we have a Newton-Cotes Formula.

• In Gaussian Quadrature we pick both the weights and the knots so as to obtain exactness for polynomials of degree as high as possible.

• Moreover, we generalize the formula (1) to include the possibility of having a positive weight function \( w(x) > 0 \). Thus we consider the more general formula

\[ \int_a^b w(x)f(x)dx \approx \sum_{i=1}^{n} w_i f(x_i) \quad (2) \]

We want this formula to be exact when \( f \) (and not the whole integrand \( w(x)f(x) \)) is a polynomial of degree as high as possible.

\[ \square \]

Note that

\[ w_i \neq w(x_i) \]
• One application of having a weight function is to accommodate improper integrals. For example, we could use
  
  – **Legendre**, ordinary integrals as before:
    \[
    I = \int_{-1}^{1} f(x) \, dx, \quad w(x) = 1, \quad [a, b] = [-1, 1]
    \]

  – **Chebychev**, the integrand is singular at the end points:
    \[
    I = \int_{-1}^{1} \frac{1}{\sqrt{1-x^2}} f(x) \, dx, \quad w(x) = \frac{1}{\sqrt{1-x^2}}, \quad [a, b] = [-1, 1]
    \]

  – **Laguerre**, the interval is semi-infinite:
    \[
    I = \int_{0}^{\infty} e^{-x} f(x) \, dx, \quad w(x) = e^{-x}, \quad [a, b] = [0, \infty)
    \]

  – **Hermite**, we are integrating over the whole real line:
    \[
    I = \int_{-\infty}^{\infty} e^{-x^2} f(x) \, dx, \quad w(x) = e^{-x^2}, \quad (a, b) = (-\infty, \infty)
    \]
Method of Undetermined Coefficients

• As we did for Simpson’s Rule, we can use the method of undetermined coefficients to obtain a system of equations for the knots and the weights.

However, that system is nonlinear!

• For example, consider the case $n = 2$, $[a, b] = [-1, 1]$ and $w(x) = 1$.

\[ \int_{-1}^{1} f(x)dx \approx w_1 f(x_1) + w_2 f(x_2) \]

which is exact if $f$ is a polynomial of degree up to 3.

• We get the nonlinear $4 \times 4$ system:

\[
\begin{align*}
  f(x) &= 1 & & \int_{-1}^{1} 1dx = 2 = w_1 + w_2 \\
  f(x) &= x & & \int_{-1}^{1} xdx = 0 = w_1 x_1 + w_2 x_2 \\
  f(x) &= x^2 & & \int_{-1}^{1} x^2dx = 2/3 = w_1 x_1^2 + w_2 x_2^2 \\
  f(x) &= x^3 & & \int_{-1}^{1} x^3dx = 0 = w_1 x_1^3 + w_2 x_2^3 \quad (3)
\end{align*}
\]

• In general, nonlinear systems can be very hard to solve.

• However, it is easy to check that the system
(3) has the solution

\[
\begin{align*}
  w_1 &= 1 \\
  w_2 &= 1 \\
  x_1 &= -\frac{\sqrt{3}}{3} \\
  x_2 &= \frac{\sqrt{3}}{3}
\end{align*}
\]

- This is pretty remarkable!
- Carl Friedrich Gauss (1777-1855) managed to solve problems like (3) in great generality.
- How he did this is our next topic.
- So, again, we want to find weights \( w_i \) and knots \( x_i, i = 1, \ldots, n \) such that the formula

\[
\int_a^b w(x)f(x)dx \approx \sum_{i=1}^n w_i f(x_i)
\]

is exact for polynomials \( f \) of degree as high as possible.

How high is possible?

\[2n - 1\]
• Let $p$ be a polynomial of degree $2n - 1$.

• The nonlinear system is linear in the coefficients $w_i$, so we need to break the polynomial $p$ into 2 pieces:

$$p(x) = Q_n(x)q(x) + r(x)$$

where $Q_n$ is a polynomial of degree $n$ that we will determine suitably.

• $q$ is the **quotient** and $r$ is the **remainder**. Both are polynomials of degree $n - 1$.

• Given $Q_n$ we can compute $q$ and $r$ by **long division**.

• Example:

\[
\begin{align*}
  n &= 2 \\
  Q_2(x) &= x^2 - \frac{1}{3} \\
  p(x) &= x^3 + 2x^2 + 3x + 4 \\
  &\quad \overline{x^2 - \frac{1}{3}} \quad \overline{x + 2} = q \\
  &\quad \underline{x^3} \quad \underline{- \frac{x}{3}} \\
  &\quad 2x^2 + \frac{10}{3}x + 4 \\
  &\quad \underline{2x^2} \quad \underline{- \frac{2}{3}} \\
  &\quad \frac{10}{3}x + \frac{14}{3}
\end{align*}
\]
How do we pick $Q_n$? We have

$$I = \int_a^b w(x)p(x)dx$$

$$= \int_a^b w(x)(Q_n(x)q(x) + r(x))dx$$

$$= \int_a^b w(x)Q_n(x)q(x)dx + \int_a^b w(x)r(x)dx$$

make this zero

So $Q_n$ must be a polynomial that is orthogonal to all lower degree polynomials with respect to the **inner product**:

$$(f, g) = \int_a^b w(x)f(x)g(x)dx$$

- We could compute these polynomials by the Gram-Schmidt process, but we can do better and will return to this issue.

- Choosing $Q_n$ this way our integral simplifies
\[ I = \int_a^b w(x)r(x)dx \]
\[ = \sum_{i=1}^n w_i p(x_i) \]
\[ = \sum_{i=1}^n w_i \left( Q_n(x_i)q(x_i) + r(x + i) \right) \]

- To simplify this further **pick the** \( x_i \) **to be the roots of** \( Q_n \). **We get**

\[ I = \int_a^b w(x)r(x)dx = \sum_{i=1}^n w_i r(x_i) \]

- But note that

\[ r(x) = \sum_{i=1}^n r(x_i)L_i(x) \]

(where the \( L_i \) are the Lagrange basis functions) and that hence

\[ I = \int_a^b w(x) \sum_{i=1}^n r(x_i)L(x_i) \]
\[ = \sum_{i=1}^n r(x_i) \int_a^b w(x)L_i(x)dx \]
\[ =: w_i \]
• So we pick the $x_i$ to be the roots of $Q_n$, i.e.,

$$Q_n(x_i) = 0, \quad i = 1, \ldots, n$$

and

$$w_i = \int_a^b w(x)L_i(x)dx.$$

• putting it all together we get

\[
I = \int_a^b w(x)p(x)dx \\
= \int_a^b w(x)(Q_n(x)q(x) + r(x))dx dx \\
= \int_a^b w(x)r(x)dx \\
= \int_a^b w(x)\sum_{i=1}^n r(x_i)L_i(x)dx \\
= \sum_{i=1}^n r(x_i)\int_a^b w(x)L_i(x)dx \\
= \sum_{i=1}^n w_i r(x_i) \\
= \sum_{i=1}^n w_i (Q_n(x_i)q(x_i) + r_i(x)) \\
= \sum_{i=1}^n w_i p_i(x)
\]

for all polynomials $p$ of degree up to $2n - 1$. 
Roots of Orthogonal Polynomials

What if the roots of $Q_n$ are not simple and in $(a, b)$?

- They are simple and in $(a, b)$. We can see this as follows:

- Suppose $Q_n$ changes sign at points $z_1, z_2, \ldots, z_k$ in $(a, b)$. Since $Q_n$ is a polynomial of degree $n$ we know that $k \leq n$ and we want to show that $k \geq n$, which implies that $k = n$.

- Consider the integral

\[ Z = \int_{a}^{b} w(x)Q_n(x)(x-z_1)(x-z_2)\times\ldots\times(x-z_k). \]

- We know that $Z \neq 0$ since the integrand never changes sign. (This is where the positivity of $w$ becomes important).

- On the other hand, $Z$ is the inner product of $Q_n$ and a polynomial of degree $k$. Thus $k$ must be at least $n$ since $Q_n$ is orthogonal to all polynomials of degree less than $n$.

- This implies our result: there are $n$ simple roots of $Q_n$ in $(a, b)$.
Numerical Example

- Suppose we want to compute

\[ I = \int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, dx \]

where \( f \) is a well-behaved function that is well approximated by a polynomial.

- Using the above ideas with the weight function

\[ w(x) = \frac{1}{\sqrt{1 - x^2}} \]

we get the formulas

\[ \int_{-1}^{1} \frac{f(x)}{\sqrt{1 - x^2}} \, dx = \sum_{i=1}^{n} w_i f(x_i) + R_n \]

where

\[ x_i = \cos \left( \frac{(2i - 1)\pi}{2n} \right), \quad n = 1 \text{, dots, } n \]

\[ w_i = \frac{\pi}{n} \]

\[ R_n = \frac{\pi}{(2n)!} \frac{2^{2n-1}}{2n-1} f^{(2n)}(\xi). \]

- The following Table lists the factor \( A_n \) multiplying the derivative for small values of \( n \):

Math 5610 Fall 2017 Notes of 11/1/17 page 12
\[ n \quad A_n \]

1 \[ \frac{\pi}{4} \]

2 \[ \frac{\pi}{192} \]

3 \[ \frac{\pi}{23,040} \]

4 \[ \frac{\pi}{5,160,960} \]

5 \[ \frac{\pi}{1,857,445,600} \]

- It is evident that 4 or 5 points suffice to get the integral accurately for most applications.

- By comparison, if we were to use an open Newton-Cotes Formula we would need to evaluate at millions of points just to get a modest accuracy of \(10^{-3}\) or so.
There are many formulas in Abramowitz/Stegun, here are just a few examples.

Examples of Orthogonal Polynomials

Legendre Polynomials

\[(f, g) = \int_{-1}^{1} f(x)g(x)dx, \quad w(x) = 1, \quad [a, b] = [-1, 1]\]

\[p_0 = 1\]
\[p_1 = x\]
\[p_2 = -1/2 + 3/2x^2\]
\[p_3 = 5/2x^3 - 3/2x\]
\[p_4 = 3/8 + 35/8x^4 - 15/4x^2\]
\[p_5 = 63/8x^5 - 35/4x^3 + 15/8x\]
\[p_6 = -5/16 + 231/16x^6 - 315/16x^4 + 105/16x^2\]
\[p_7 = 429/16x^7 - 693/16x^5 + 315/16x^3 - 35/16x\]
\[p_8 = 35/128 + 6435/128x^8 - 3003/32x^6 + 3465/64x^4 - 315/32x^2\]
Legendre Polynomials.
Chebychev Polynomials

\[(f, g) = \int_{-1}^{1} \frac{1}{\sqrt{1 - x^2}} f(x) g(x) \,dx, \quad w(x) = \frac{1}{\sqrt{1 - x^2}}, \quad [a, b] = [-1, 1]\]

\[p_0 = 1\]
\[p_1 = x\]
\[p_2 = 2x^2 - 1\]
\[p_3 = 4x^3 - 3x\]
\[p_4 = 8x^4 - 8x^2 + 1\]
\[p_5 = 16x^5 - 20x^3 + 5x\]
\[p_6 = 32x^6 - 48x^4 + 18x^2 - 1\]
\[p_7 = 64x^7 - 112x^5 + 56x^3 - 7x\]
\[p_8 = 128x^8 - 256x^6 + 160x^4 - 32x^2 + 1\]
Chebychev Polynomials.

\[ \prod_{i=0}^{n} (x - x_i) \quad -1 \leq x_i \leq 1 \]
Laguerre Polynomials

\[ (f, g) = \int_{0}^{\infty} e^{-x} f(x) g(x) dx, \quad w(x) = e^{-x}, \quad [a, b) = [0, \infty) \]

\[
\begin{align*}
p_0 &= 1 \\
p_1 &= 1 - x \\
p_2 &= 1 - 2x + 1/2x^2 \\
p_3 &= 1 - 3x + 3/2x^2 - 1/6x^3 \\
p_4 &= 1 - 4x + 3x^2 - 2/3x^3 + 1/24x^4 \\
p_5 &= 1 - 5x + 5x^2 - 5/3x^3 + 5/24x^4 - 1/120x^5 \\
p_6 &= 1 - 6x + 15/2x^2 - 10/3x^3 + 5/8x^4 - 1/20x^5 + 1/720x^6 \\
p_7 &= 1 - 7x + 21/2x^2 - 35/6x^3 + 35/24x^4 - 7/40x^5 + 7/720x^6 - 1/5040x^7 \\
p_8 &= 1 - 8x + 14x^2 - 28/3x^3 + 35/12x^4 - 7/15x^5 + 7/180x^6 - 1/630x^7 + 1/40320x^8
\end{align*}
\]
Laguerre Polynomials.
Hermite Polynomials

\[(f, g) = \int_{-\infty}^{\infty} e^{-x^2} f(x)g(x)dx, \quad w(x) = e^{-x^2}, \quad (a, b) = (-\infty, \infty)\]

\[p_0 = 1\]
\[p_1 = 2x\]
\[p_2 = 4x^2 - 2\]
\[p_3 = 8x^3 - 12x\]
\[p_4 = 16x^4 - 48x^2 + 12\]
\[p_5 = 32x^5 - 160x^3 + 120x\]
\[p_6 = 64x^6 - 480x^4 + 720x^2 - 120\]
\[p_7 = 128x^7 - 1344x^5 + 3360x^3 - 1680x\]
\[p_8 = 256x^8 - 3584x^6 + 13440x^4 - 13440x^2 + 1680\]
Hermite Polynomials.
\[ \int_a^b f(x) \, dx = \sum_{i=1}^n w_i f(x_i) + E \]

\[ w_i, x_i = ? \]

\[ E = 0 \text{ if } f \text{ is polynomial of degree up to } 2n-1 \]

\[ p(x) = \sum_{i=0}^{2n-1} a_i x^i = q(x) \Theta_n(x) + r(x) \]

\[ \deg Q_n = n \]

\[ q: \text{ quotient} \quad \deg q = n - 1 \]

\[ Q_n: \text{ divisor} \quad \deg Q_n = n \]

\[ a_n: \text{ remainder} \quad \deg r = n - 1 \]
\[
\int_a^b p(x) \, dx = \int_a^b q(x) \, dx + r(x) \, dx
\]

\[
= \int_a^b q(x) \, dx + \int_a^b r(x) \, dx
\]

\[
= 0
\]

\[
= \int_a^b r(x) \, dx
\]

\[
= \sum_{i=1}^n w_i \, L_i(x) \, dx
\]

\[
= \sum_{i=1}^n w_i \, r(x_i) \quad W_i = \int_a^b L_i(x) \, dx
\]

\[
= \sum_{i=1}^n \left( \sum_{i=1}^n w_i \, (q(x_i) \, q(x_i) + r(x_i)) \right)
\]

\[
= \sum_{i=1}^n w_i \, p(x_i)
\]