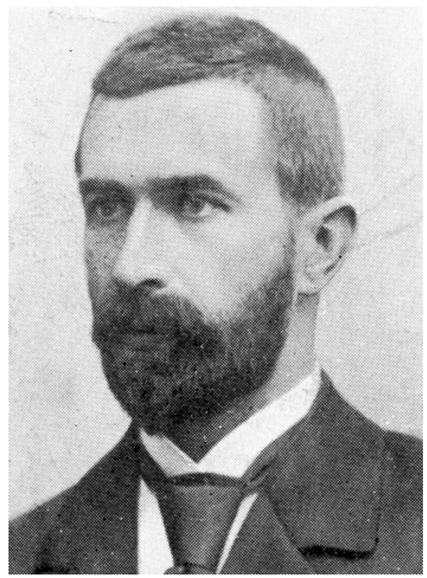
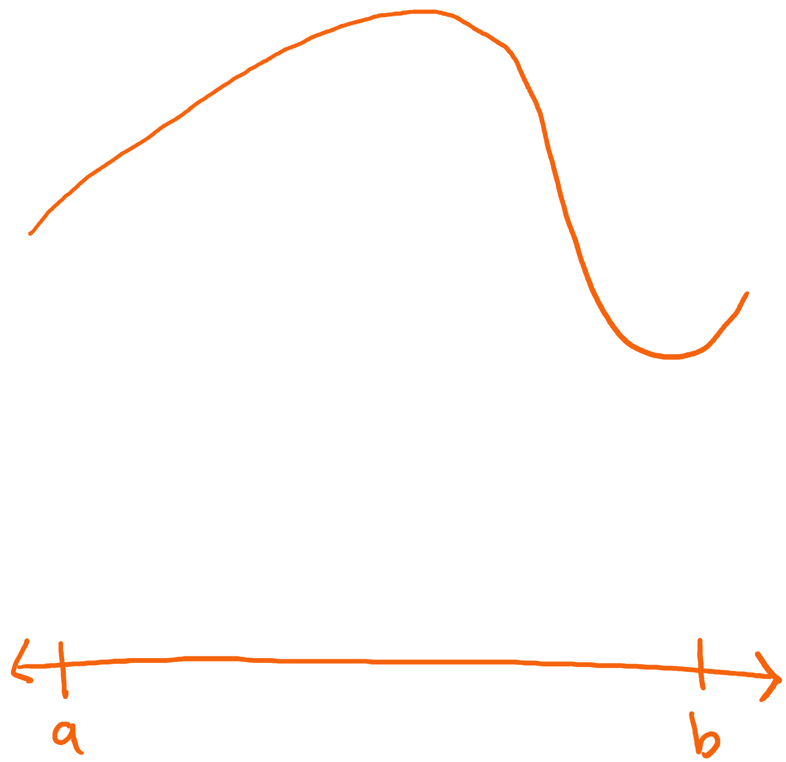
Adaptive Quadrature for Nyström



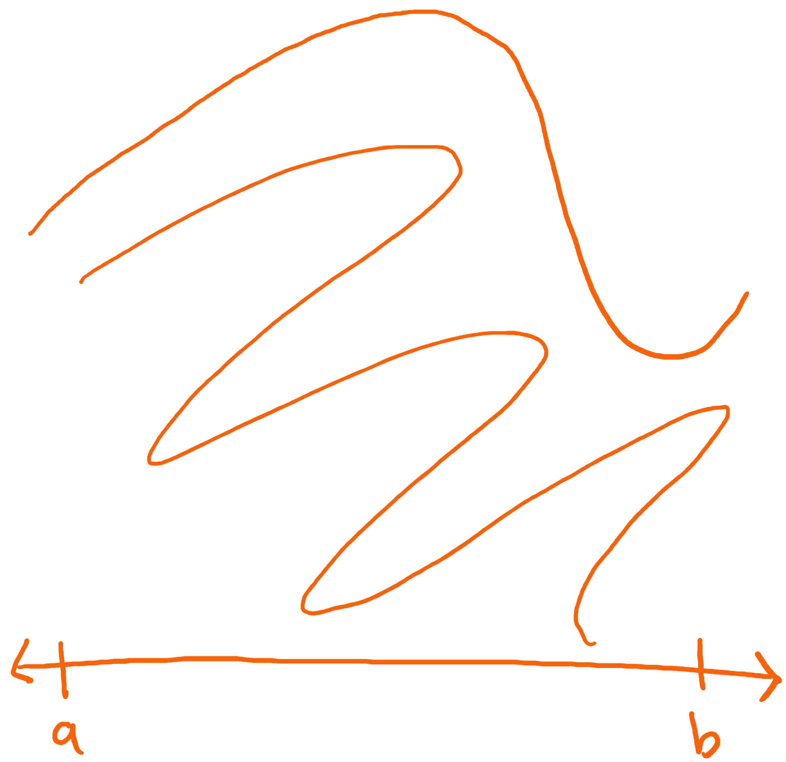
Yuchen Su

12/6/17

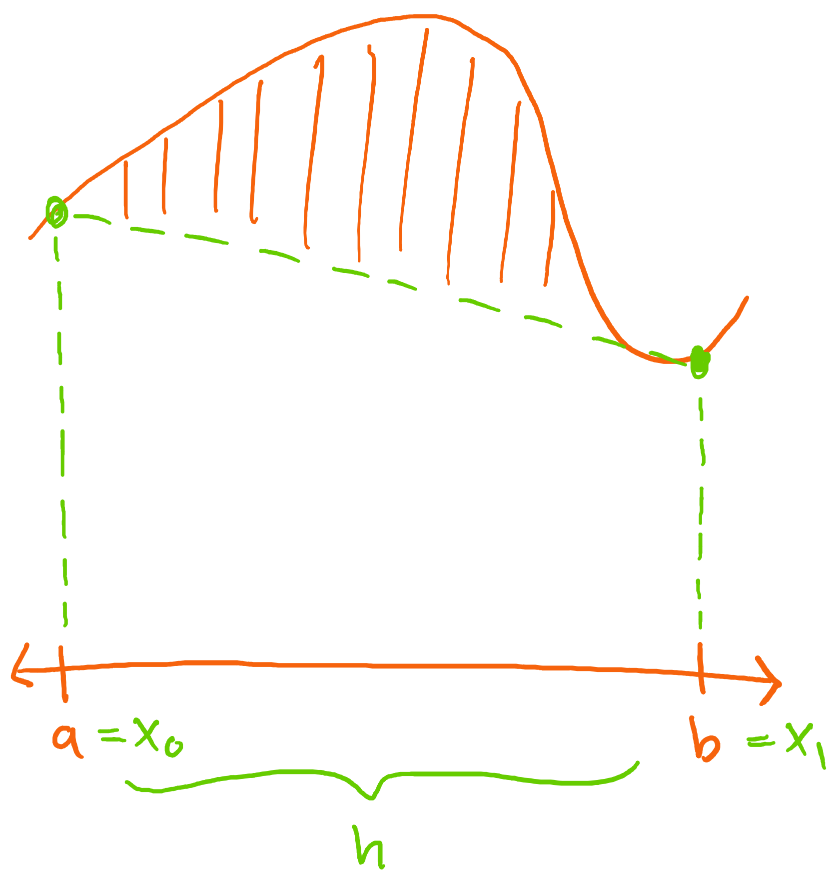
Quadrature



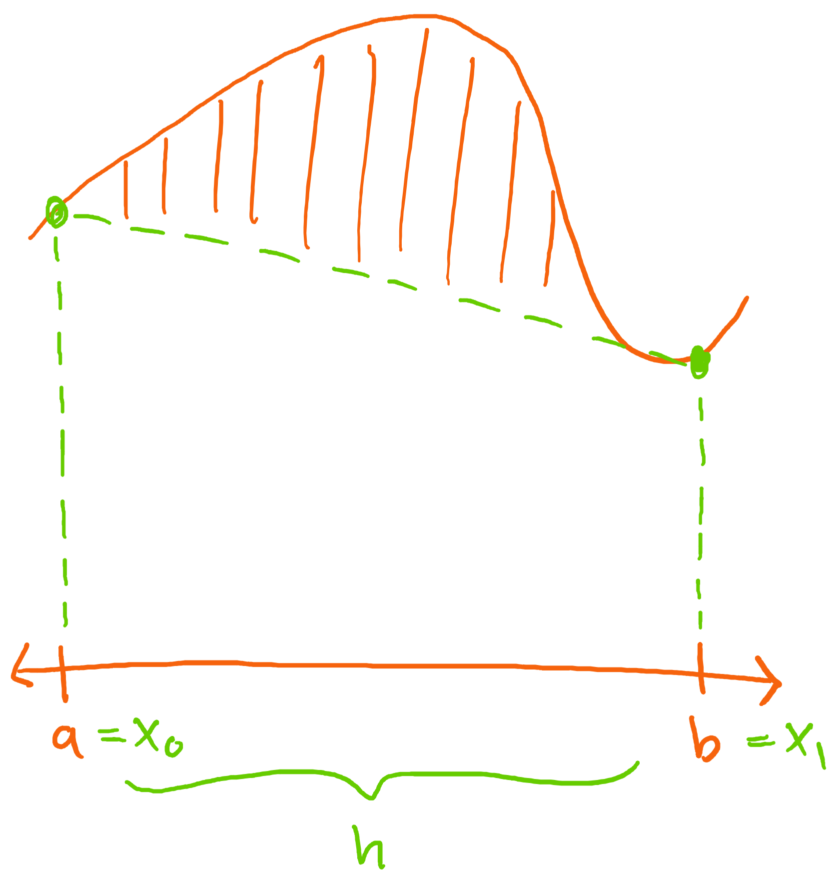
Quadrature



Quadrature

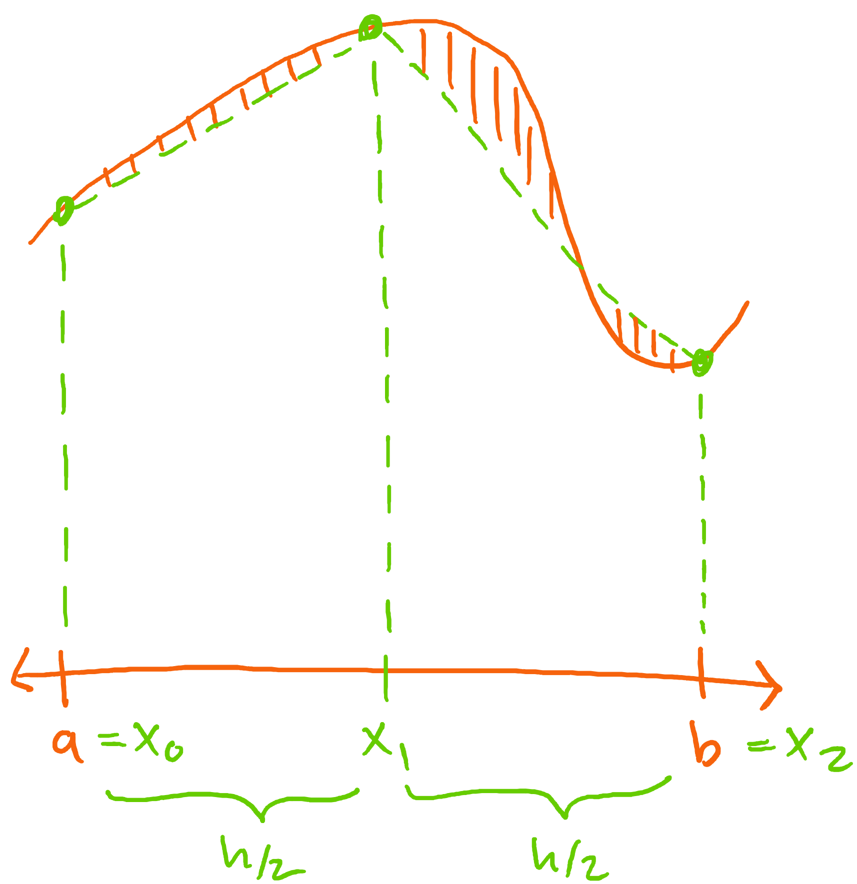


Quadrature

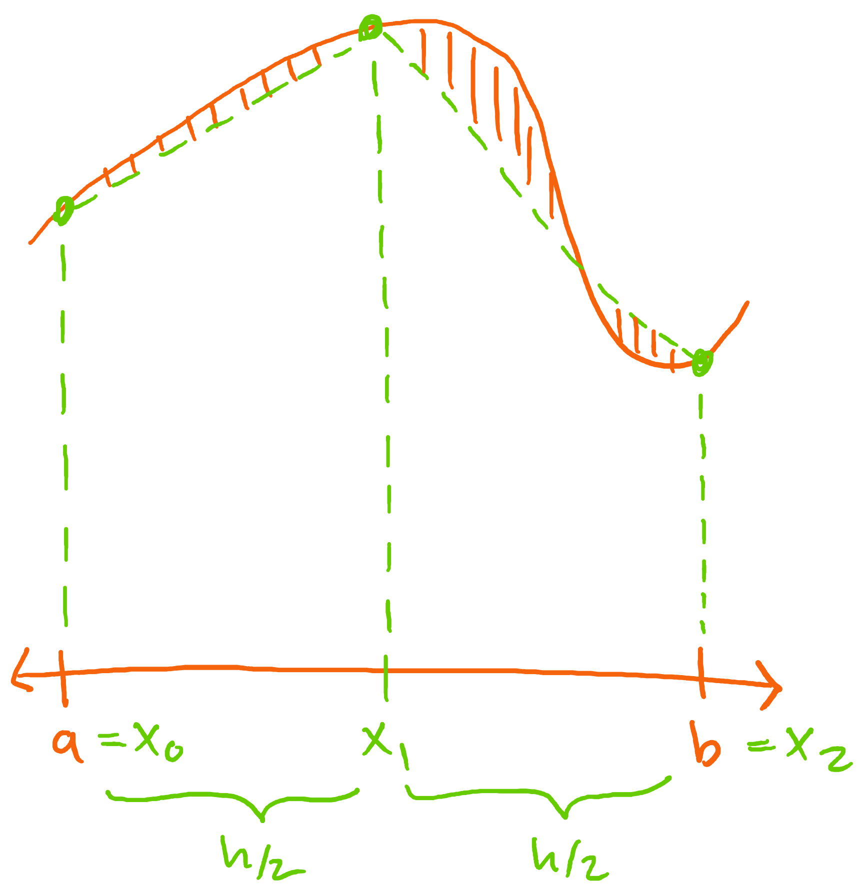


$$\int_a^b f(x)dx \approx Q_n = \sum_{i=0}^{n} w_i f(x_i)$$

Quadrature

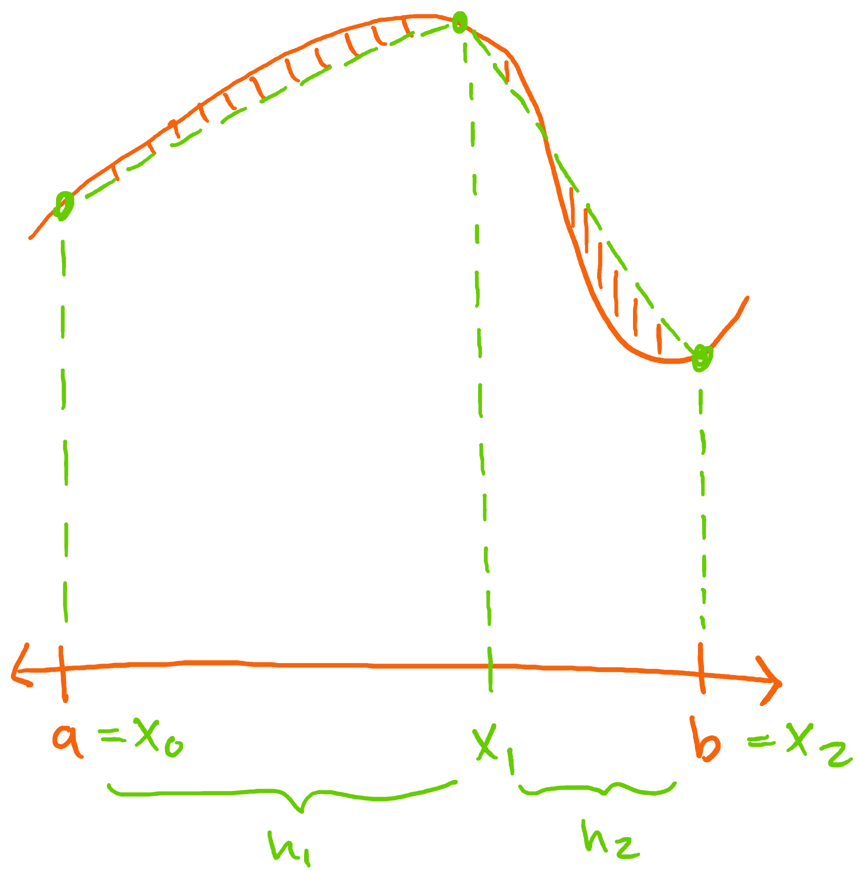


Quadrature



Composite Newton-Cotes

Quadrature



Composite Gaussian

Error Estimation

When should we be satisfied with our Quadrature?

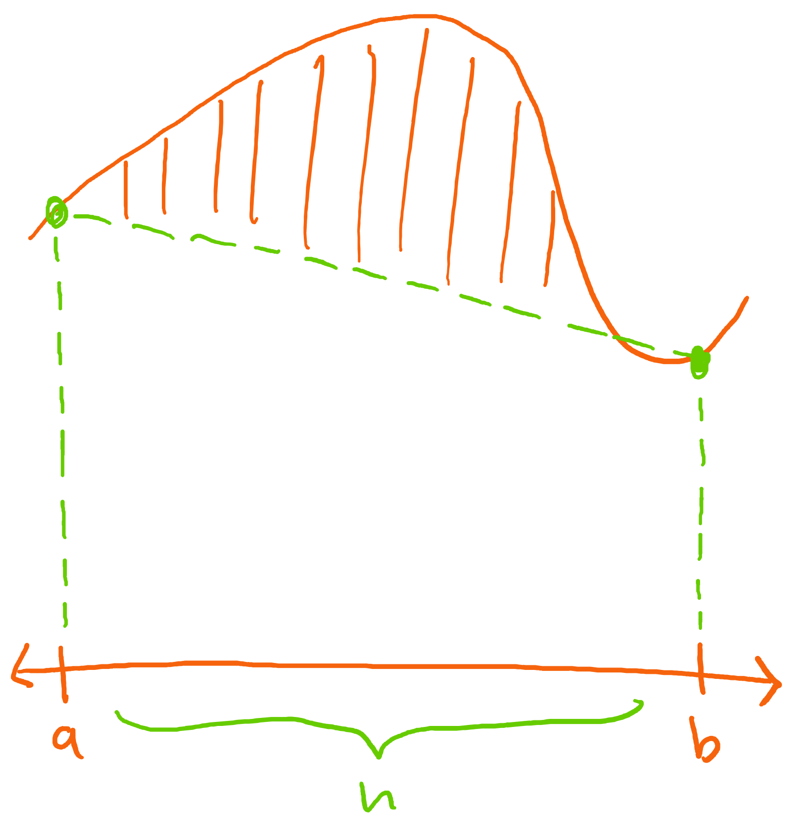
Error Estimation

When should we be satisfied with our Quadrature?

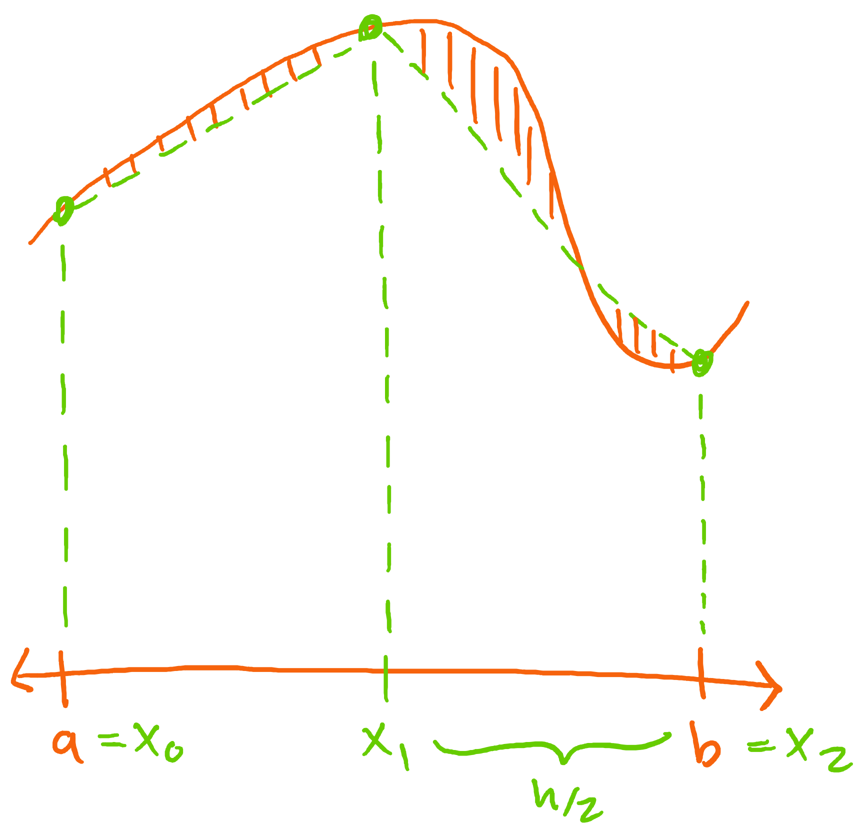
Consider error:

$$\epsilon_n \approx |Q_n - \int_a^b f(x)dx|$$

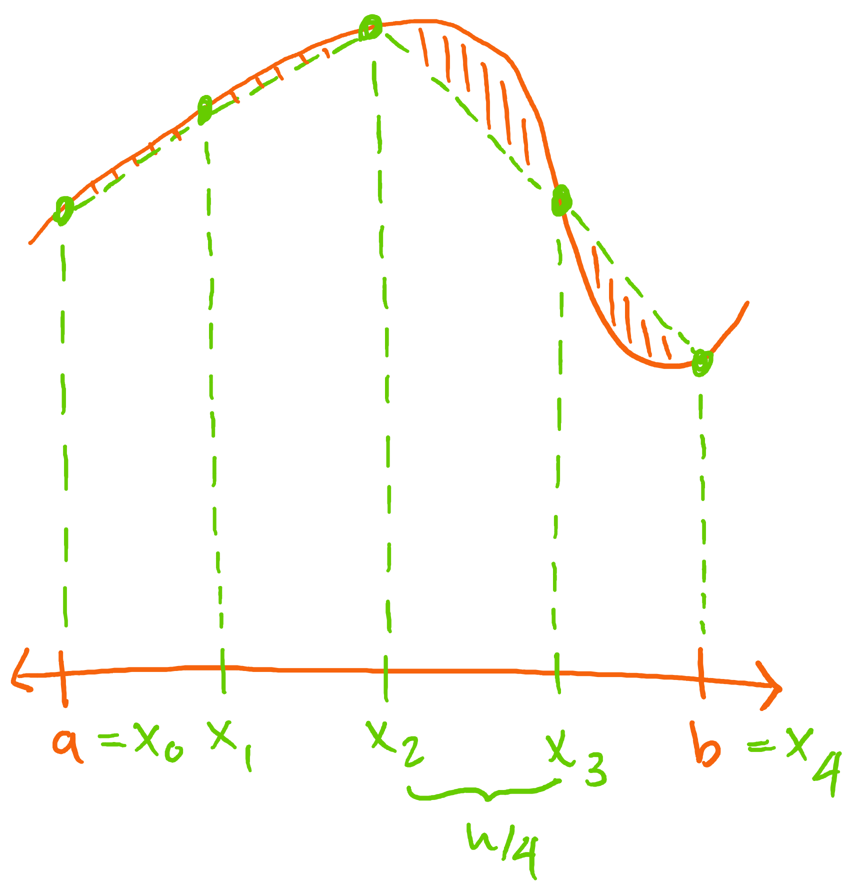
Automatic Quadrature



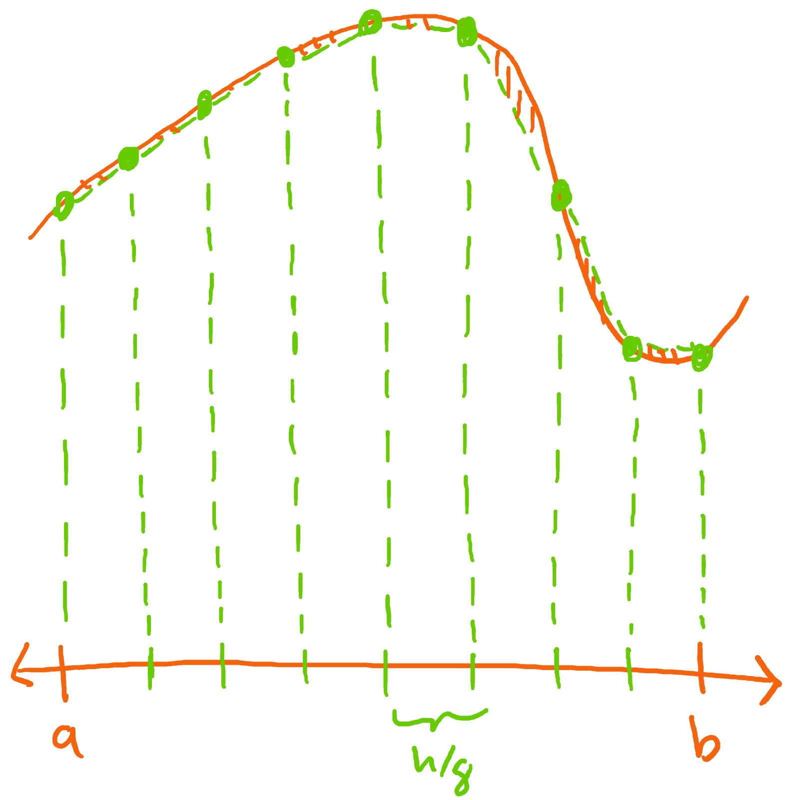
Automatic Quadrature



Automatic Quadrature



Automatic Quadrature



Automatic Quadrature

Algorithm:

1. Set an error tolerance τ
2. Compute $Q_n = Quad(f(x), [a,b], n, \tau)$
3. If $\varepsilon_n > \tau$
   - Increase n
   - Loop to Step 2

Automatic Quadrature

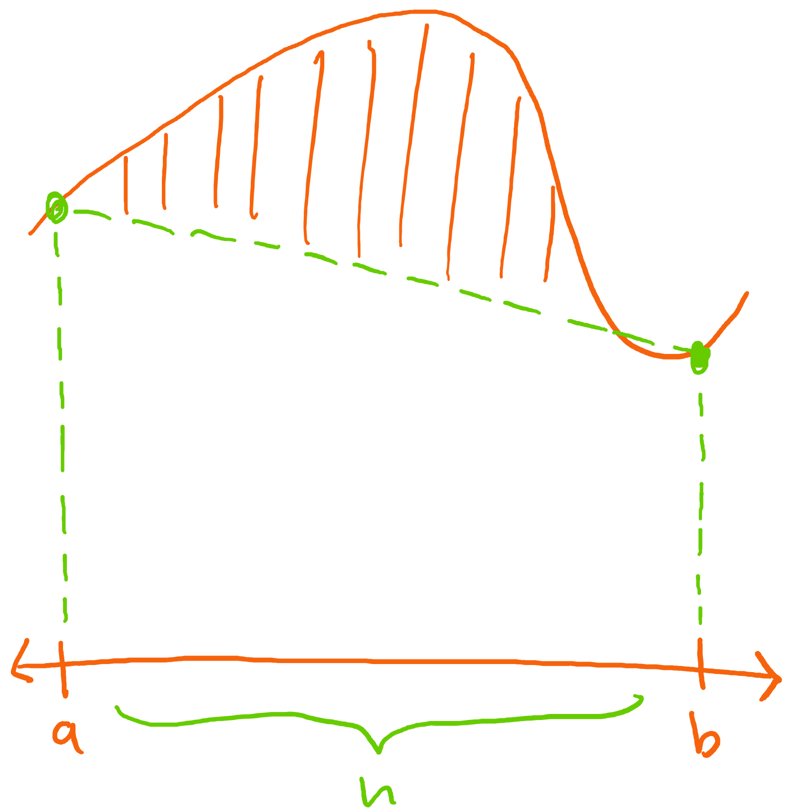
This seems unintelligent

Automatic Quadrature

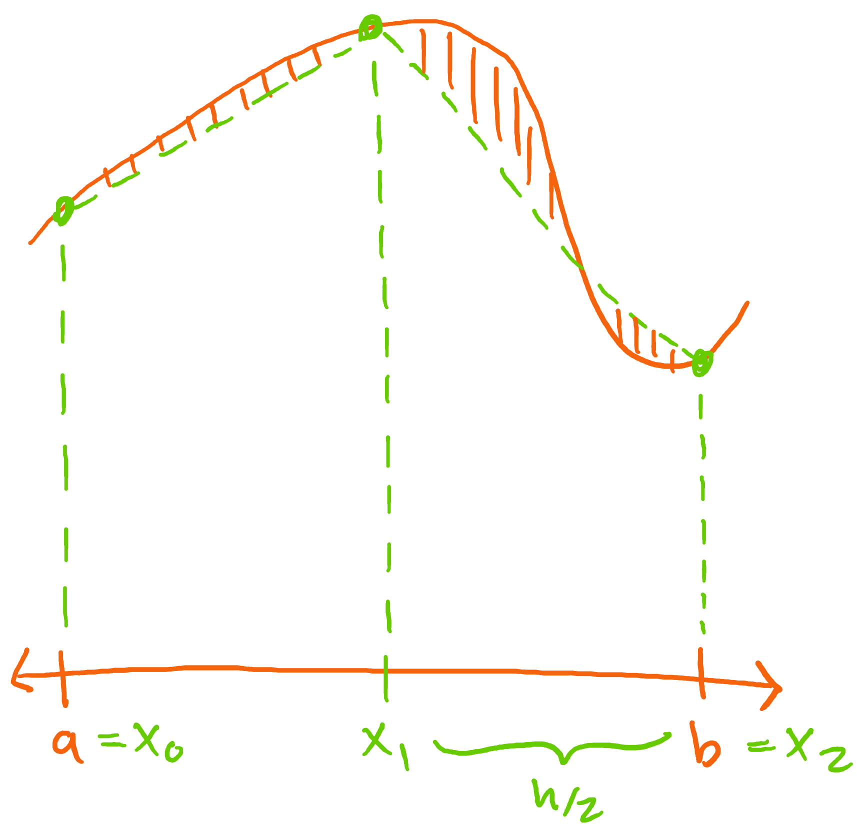
This seems unintelligent

Can we do better?

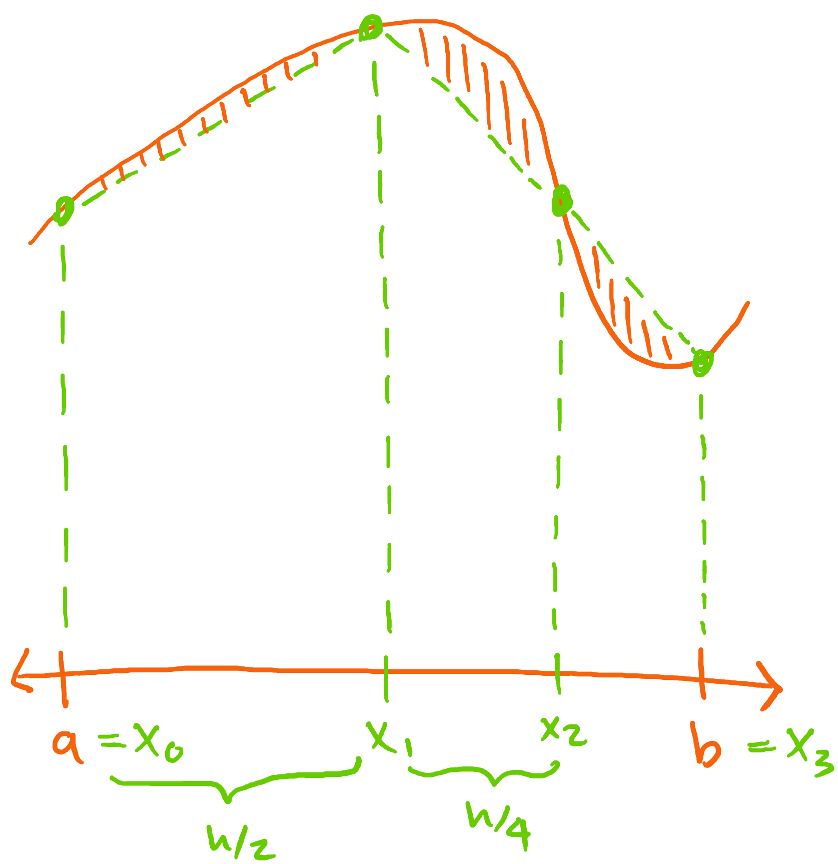
Adaptive Quadrature



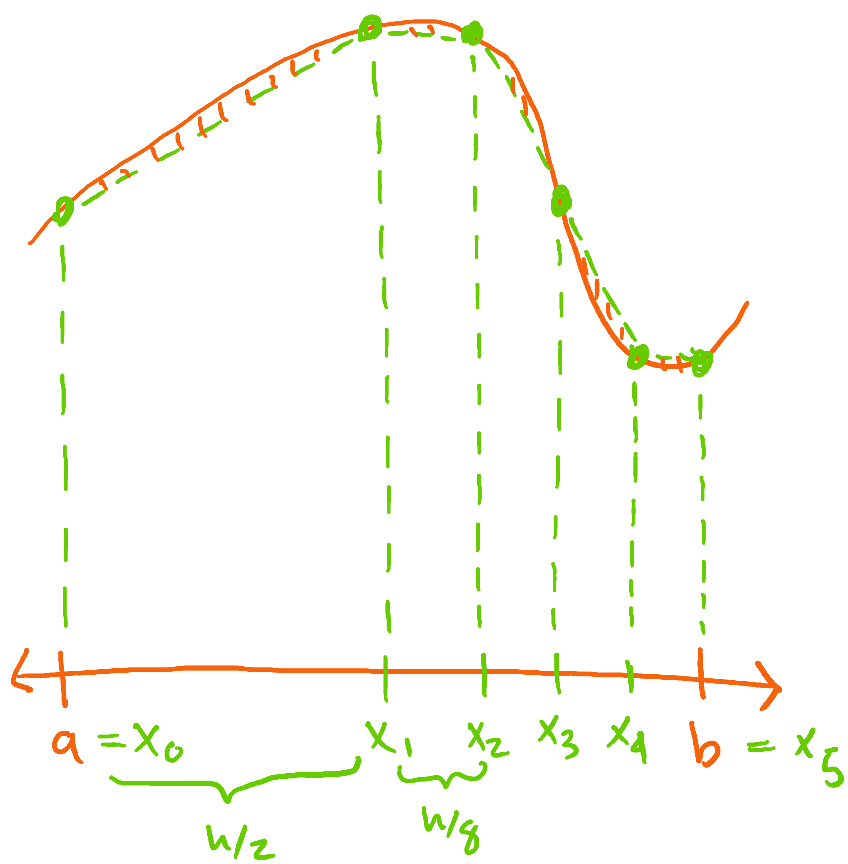
Adaptive Quadrature



Adaptive Quadrature



Adaptive Quadrature



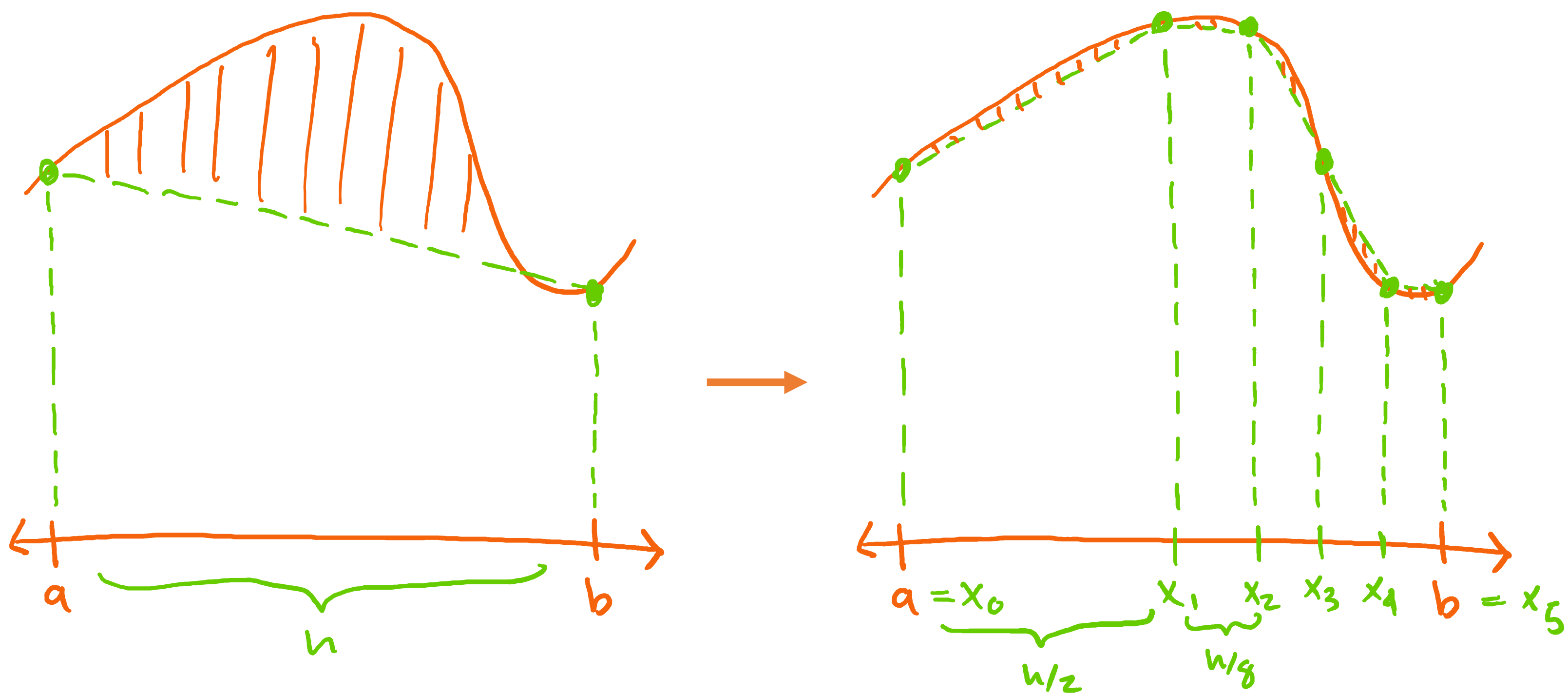
Adaptive Quadrature

Algorithm:

1. Set an error tolerance τ, n usually 1
2. Compute $Q_n^{(i)} = Quad(f(x), [a, b], n, \tau)$
3. If $\varepsilon_n > \tau$
   - Let $m = \frac{a+b}{2}$
   - Compute $Q_n^{(i+1)} = Quad(f(x), [a, m], n, \frac{\tau}{2}) + Quad(f(x), [m, b], n, \frac{\tau}{2})$

Amazing Quadrature

Can we make this jump directly?



Error Estimation

Main approaches:

Error $\sim$

1. $|Q_n^{(i_1)} - Q_n^{(i_2)}|$
2. $|Q_{n_1} - Q_{n_2}|$
3. $|f^n(\xi)|$
4. $|\tilde{c_n}|$

Gonnet – *A Review of Error Estimation in Adaptive Quadrature*, ACM Computing Surveys (2012)

Nyström Method

Consider the Fredholm equation of the second kind

$$\varphi - A\varphi = f$$

Where the integral operator is

$$(A\varphi)(x) = \int_G K(x, y)\varphi(y)dy, \quad x \in G$$

Nyström Method

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Where the integral operator is

$$(A\varphi)(x) = \int_G K(x,y)\varphi(y)dy, \quad x \in G$$

If we approximate A by some quadrature rule

$$(A_n\varphi)(x) = \sum_{k=1}^{n} w_k^{(n)} K(x, x_k^{(n)})\varphi(x_k^{(n)})$$

We can solve the system at the quadrature points

$$\varphi_n - A_n\varphi_n = f_n$$

↓

$$(\mathbf{I} - \mathbf{KW})\varphi = \mathbf{f}$$

Nyström Method

Once we have the density at the quadrature points

$$\varphi = (\mathbf{I} - \mathbf{KW})^{-1}\mathbf{f}$$

Use Nyström interpolation to get density for all $x \in G$

$$\varphi_n(x) = f(x) + \sum_{k=1}^{n} w_k^{(n)} K(x, x_k^{(n)})\varphi(x_k^{(n)})$$

Nyström Method

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$$\varphi_n(x) = f(x) + \sum_{k=1}^{n} w_k^{(n)} K(x, x_k^{(n)})\varphi(x_k^{(n)})$$

For example if $\mathbf{x} \in \mathbb{R}^{\mathbf{m}}$, we may interpolate by:

$$\varphi_{\mathbf{n}} = \mathbf{f}_{\mathbf{n}} + \mathbf{KW}\varphi$$

where $\mathbf{K} \in \mathbb{R}^{m \times n}$, $\mathbf{W} \in \mathbb{R}^{n \times n}$

Nyström Error Estimate

$$||\varphi_n - \varphi|| \leq C(||(A_n - A)\varphi|| + ||f_n - f||)$$

Corollary 10.11, Kress – LIE (2nd ed.)

Nyström Error Estimate

$$||\varphi_n - \varphi|| \leq C(||(A_n - A)\varphi|| + ||f_n - f||)$$

$$||A_n\varphi_n - A_f\varphi_f||$$

Corollary 10.11, Kress – LIE (2nd ed.)

Example 1

Consider the following second kind integral equation

$$\varphi(x) - \frac{1}{2}\int_{-1}^{1}(x+1)e^{-xy}\varphi(y)dy = g(x)$$

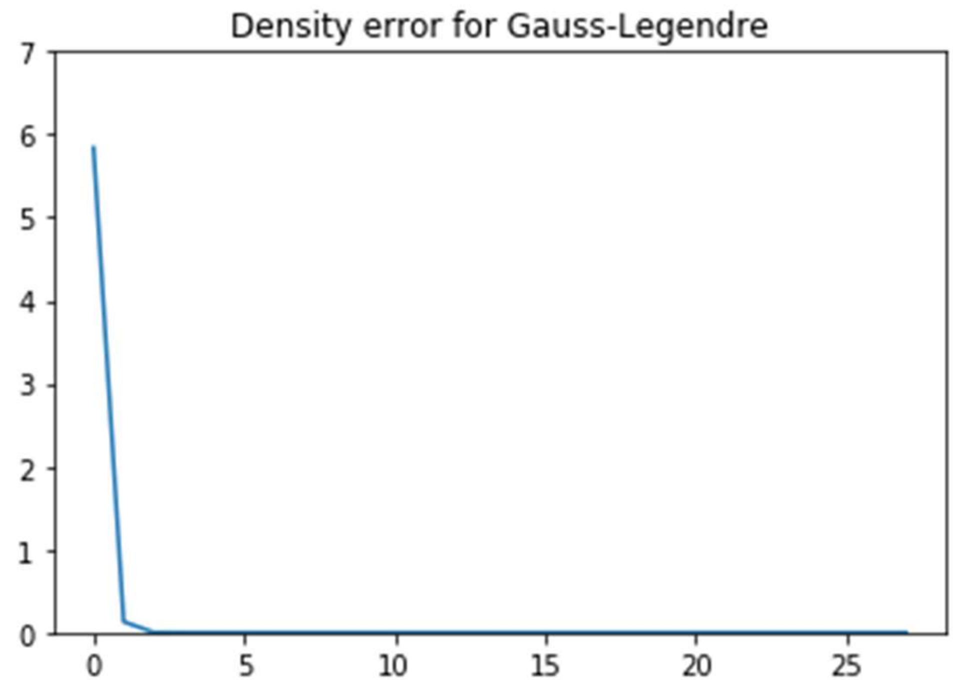
Where

$$g(x) = e^{-x} - \frac{1}{2}\left(e^{x+1} - e^{-(x+1)}\right)$$

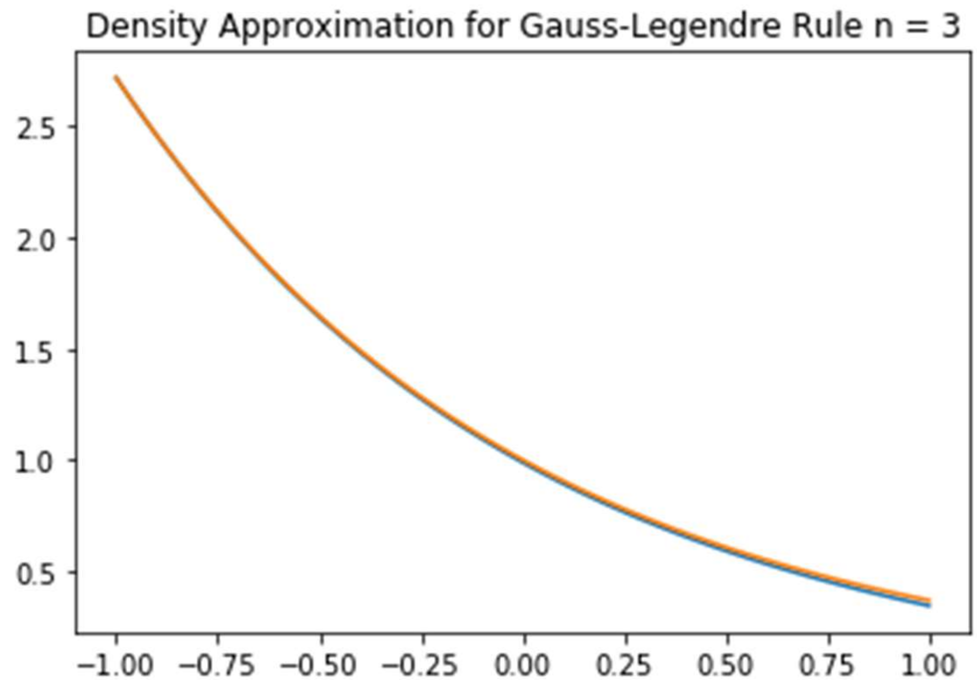
We can compute the solution as

$$\varphi(x) = e^{-x}$$

Ex 1 Density Error: Gauss-Legendre

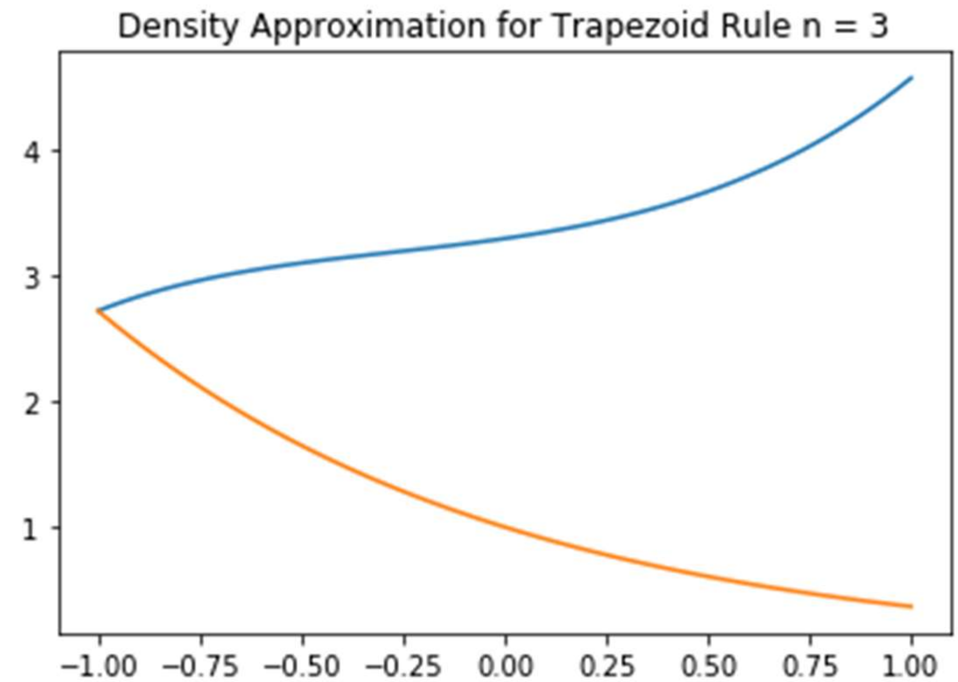


Ex 1 Density Approx: Gauss-Legendre

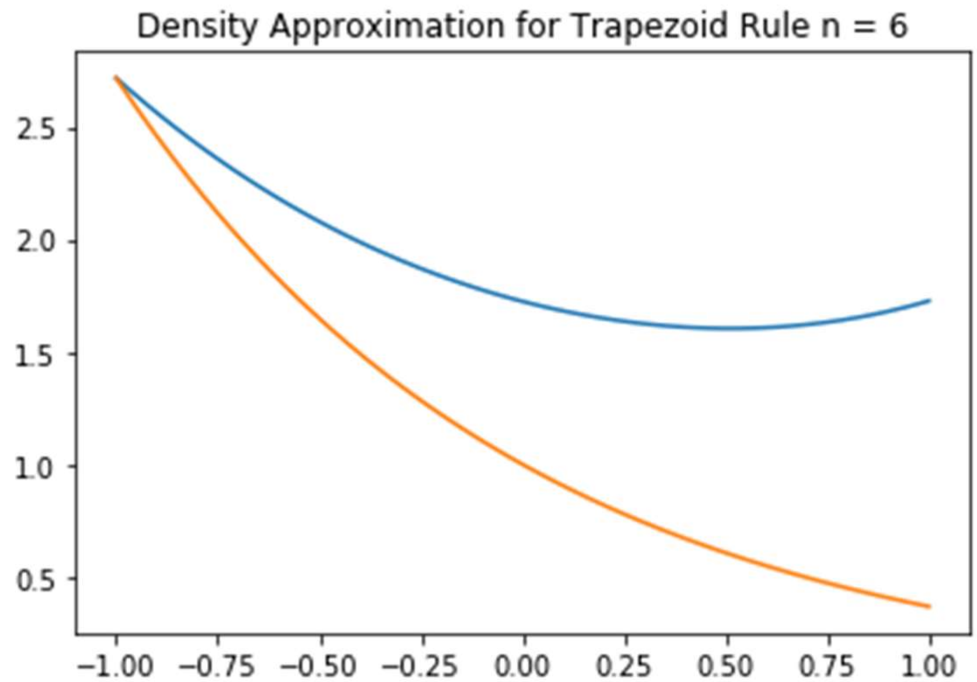


Ex 1 Density Error: Trapezoid Rule

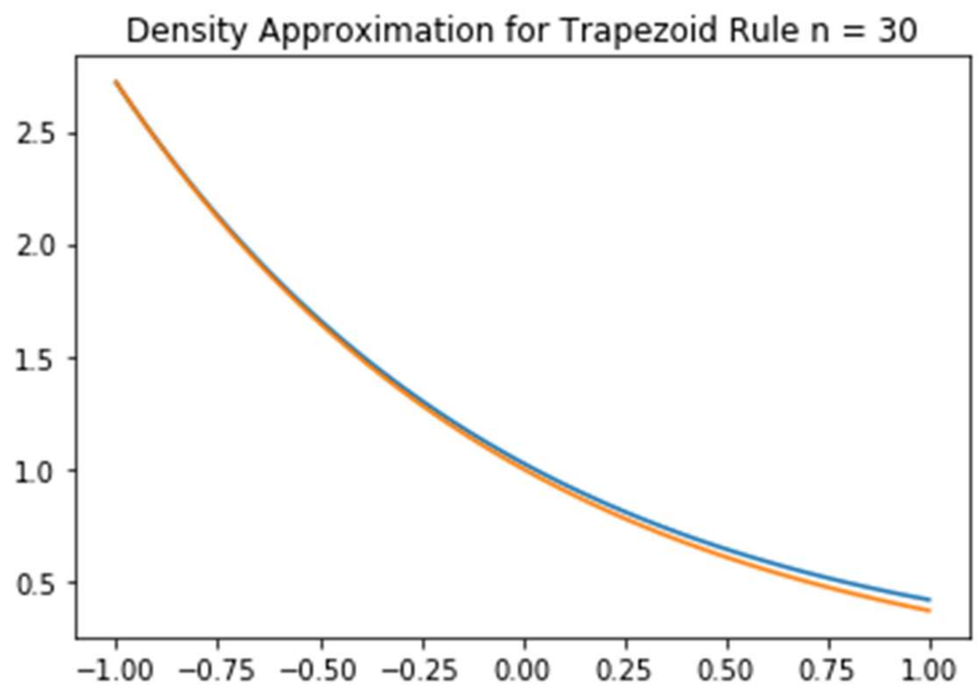
Ex 1 Density Approx: Trapezoid Rule



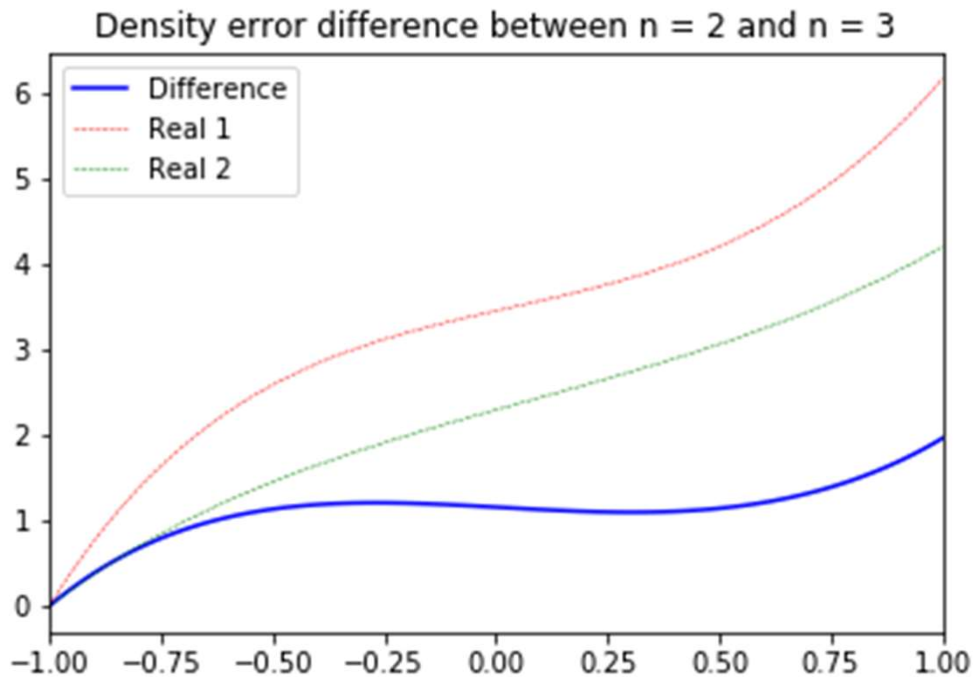
Ex 1 Density Approx: Trapezoid Rule



Ex 1 Density Approx: Trapezoid Rule



Ex 1: Trapezoid Rule Differences



Example 2

Consider the following second kind integral equation

$$\varphi(x) - \frac{1}{2}\int_{-1}^{1} |x-y| f(y)dy = g(x)$$

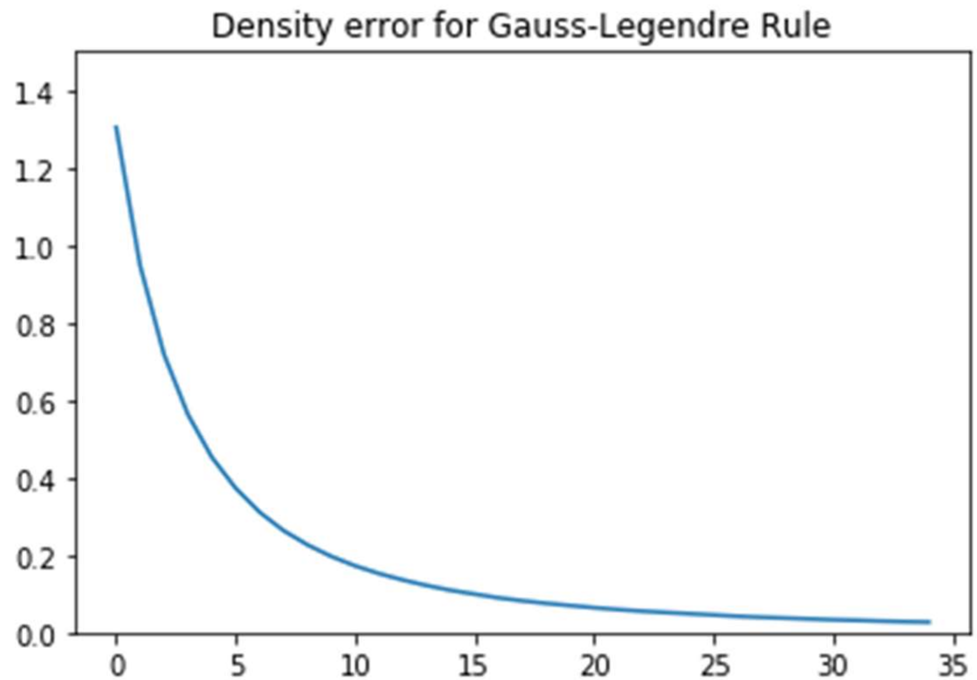
Where

$$g(x) = e^x$$

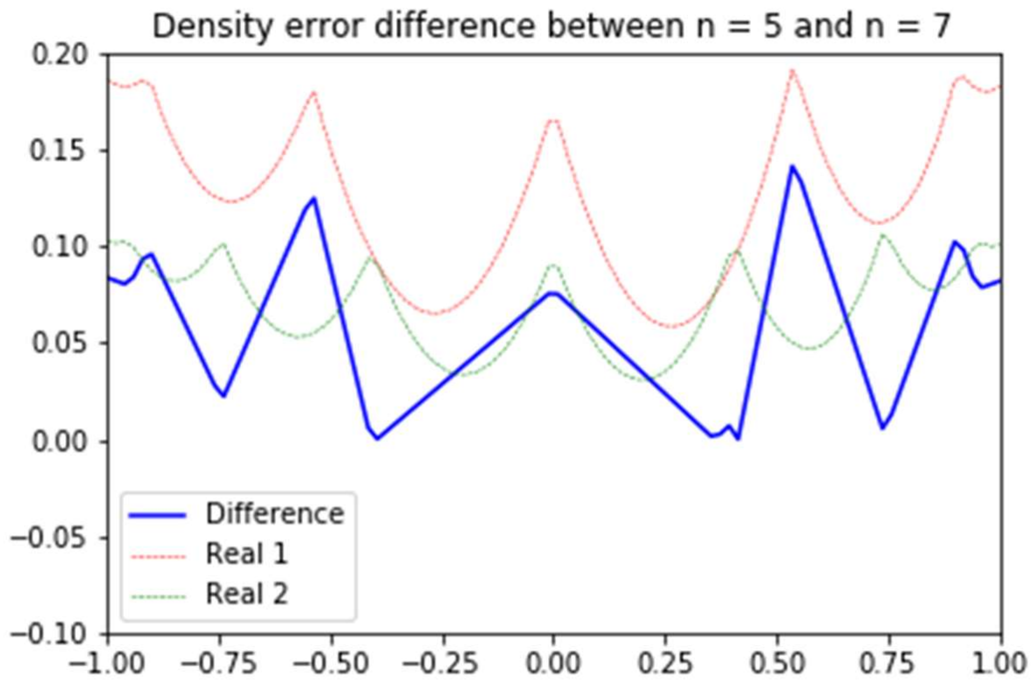
We can compute the solution as

$$\varphi(x) = \frac{1}{2}xe^x + c_1e^x + c_2e^{-x}$$

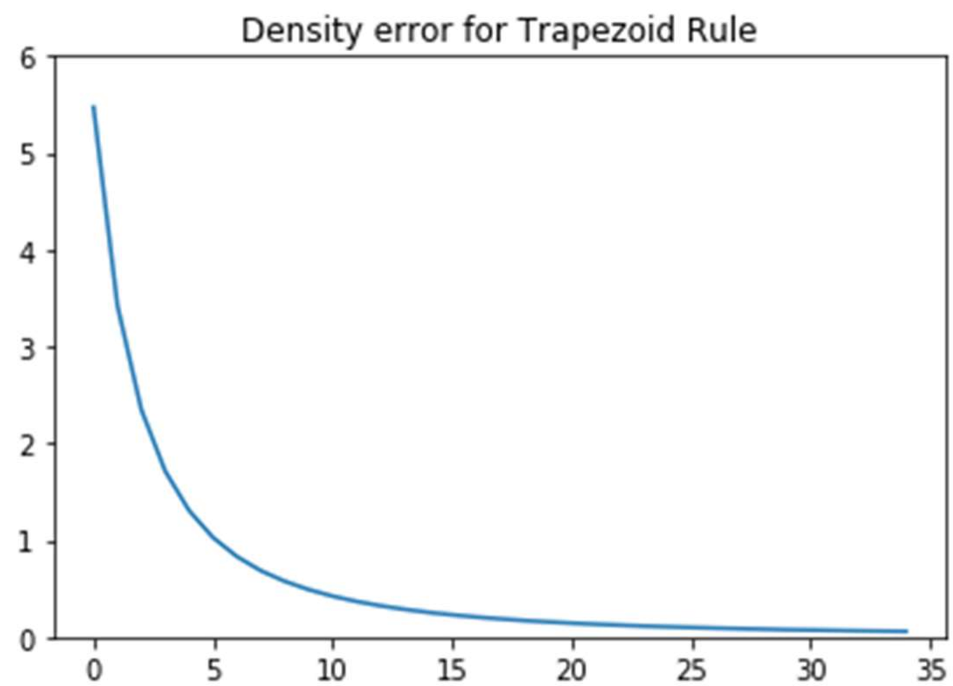
Ex 1 Density Error: Gauss-Legendre



Ex 1: Gauss-Legendre Differences



Ex 1 Density Error: Trapezoid Rule



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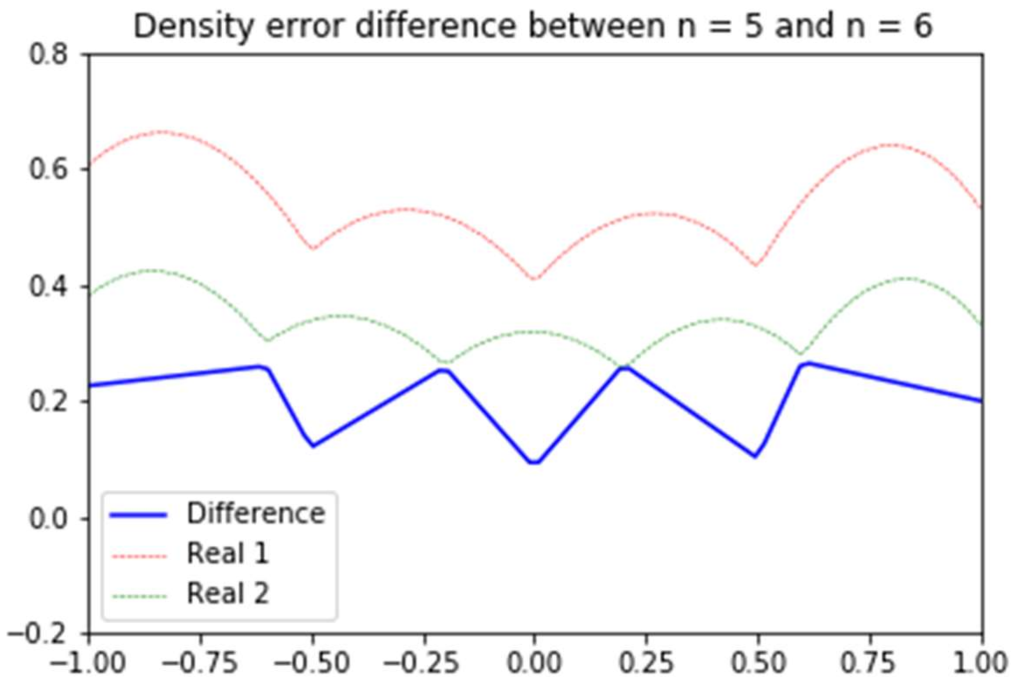

Nyström Local Estimates

Not so good =(

Can we do better?

Nyström Local Estimates

Consider the constant

$$C = \frac{1+||(I-A)^{-1}A_n||}{1-||(I-A)^{-1}(A-A_n)A_n||}$$

Nyström Local Estimates

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Remove the norms (abuse notation)

$$C = \frac{I+(I-A)^{-1}A_n}{I-(I-A)^{-1}(A-A_n)A_n}$$

Nyström Local Estimates

Consider the constant

$$C = \frac{1+||(I-A)^{-1}A_n||}{1-||(I-A)^{-1}(A-A_n)A_n||}$$

Remove the norms (abuse notation)

$$C = \frac{I+(I-A)^{-1}A_n}{I-(I-A)^{-1}(A-A_n)A_n}$$

Let

$$B_n = I + (I-A)^{-1}A_n$$
$$S_n = (I-A)^{-1}(A-A_n)A_n$$

Nyström Local Estimates

Our equation becomes

$$C = \frac{B_n}{I - S_n}$$

It turns out $C = I - A_n$

Nyström Local Estimates

Our equation becomes

$$C = \frac{B_n}{I - S_n}$$

It turns out $C = I - A_n$

Shuffling around

$$B_n(I - A_n) = I - S_n$$

From collective compactness, we have

$$||S_n|| \to 0 \quad n \to \infty$$

Nyström Local Estimates

$$B_n(I - A_n) = I - S_n$$

Stare at this real hard and consider $n \to \infty$

Nyström Local Estimates

$$B_n(I - A_n) = I - S_n$$

Stare at this real hard and consider $n \to \infty$

2 things happen

$$B_n \to (I - A_n)^{-1}$$

Nyström Local Estimates

$$B_n(I - A_n) = I - S_n$$

Stare at this real hard and consider $n \to \infty$

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$$B_n \to (I - A_n)^{-1}$$
$$A_n \to A$$

Nyström Local Estimates

$$B_n(I - A_n) = I - S_n$$

Stare at this real hard and consider $n \to \infty$

2 things happen

$$B_n \to (I - A_n)^{-1}$$

$$A_n \to A$$

↓

$$B_n \to (I - A)^{-1}$$

Nyström Local Estimates

Maybe take a look at

$$B_n = I + (I - A)^{-1} A_n$$

Nyström Local Estimates

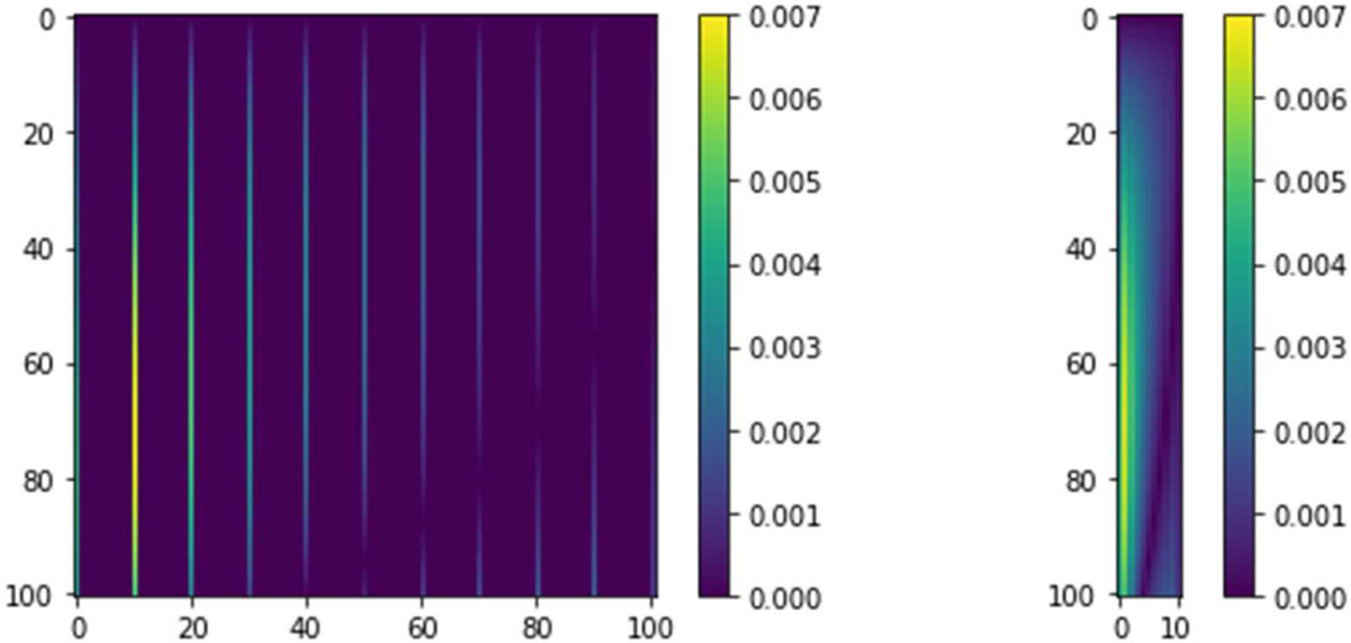
Let's assume we have infinite computational power and compute directly

$$B_n = I + (I - A)^{-1} A_n$$

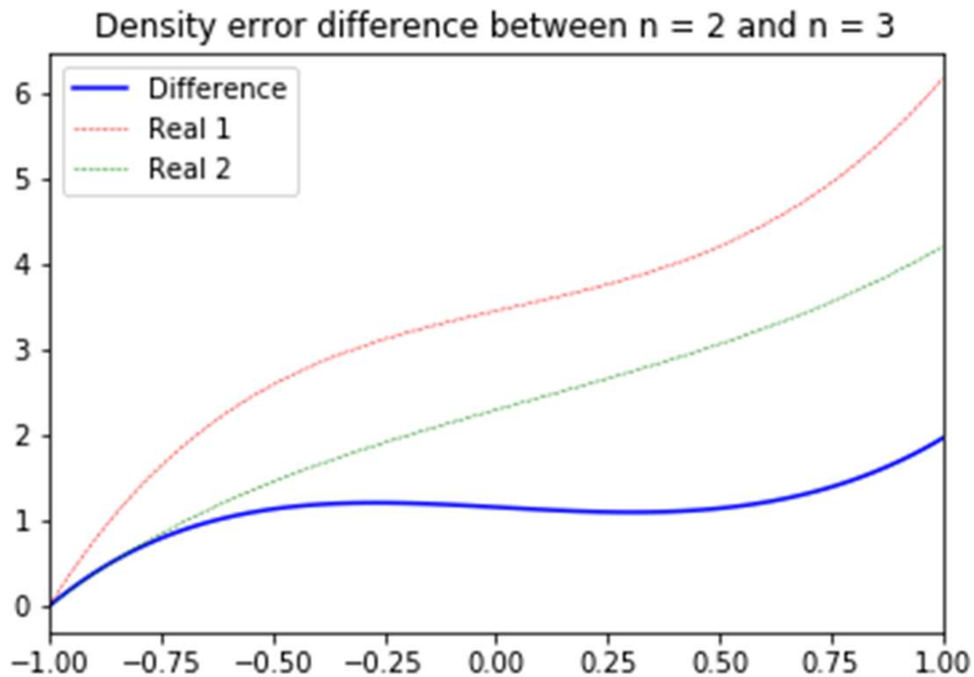
Look at

$$(I - A_n)^{-1} - B_n$$

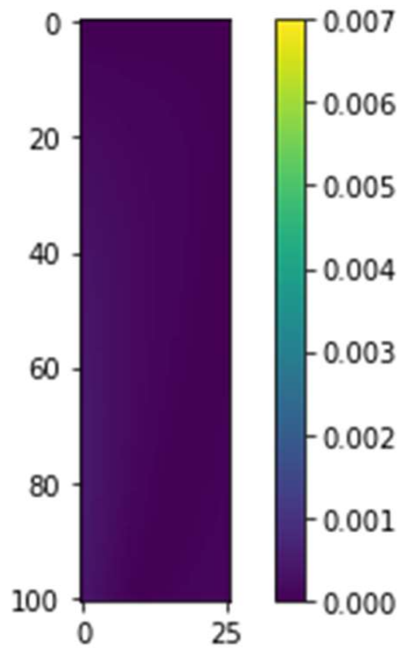
Ex 1: Trapezoid, n = 11



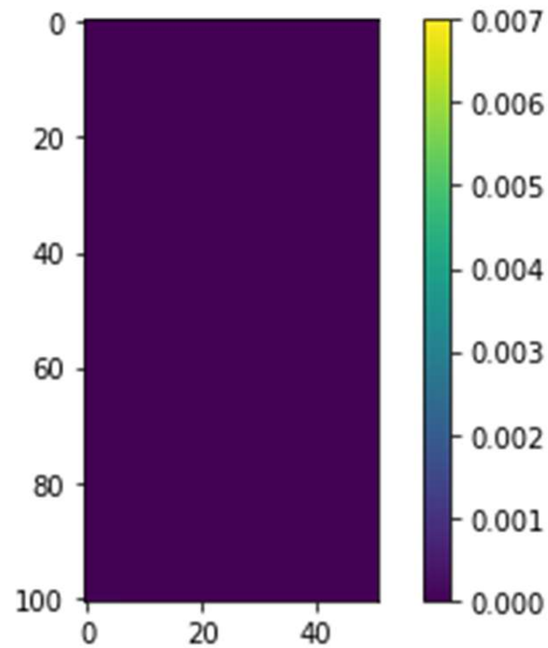
Ex 1: Recall Trapezoid Rule Error



Just to check it works



n=26



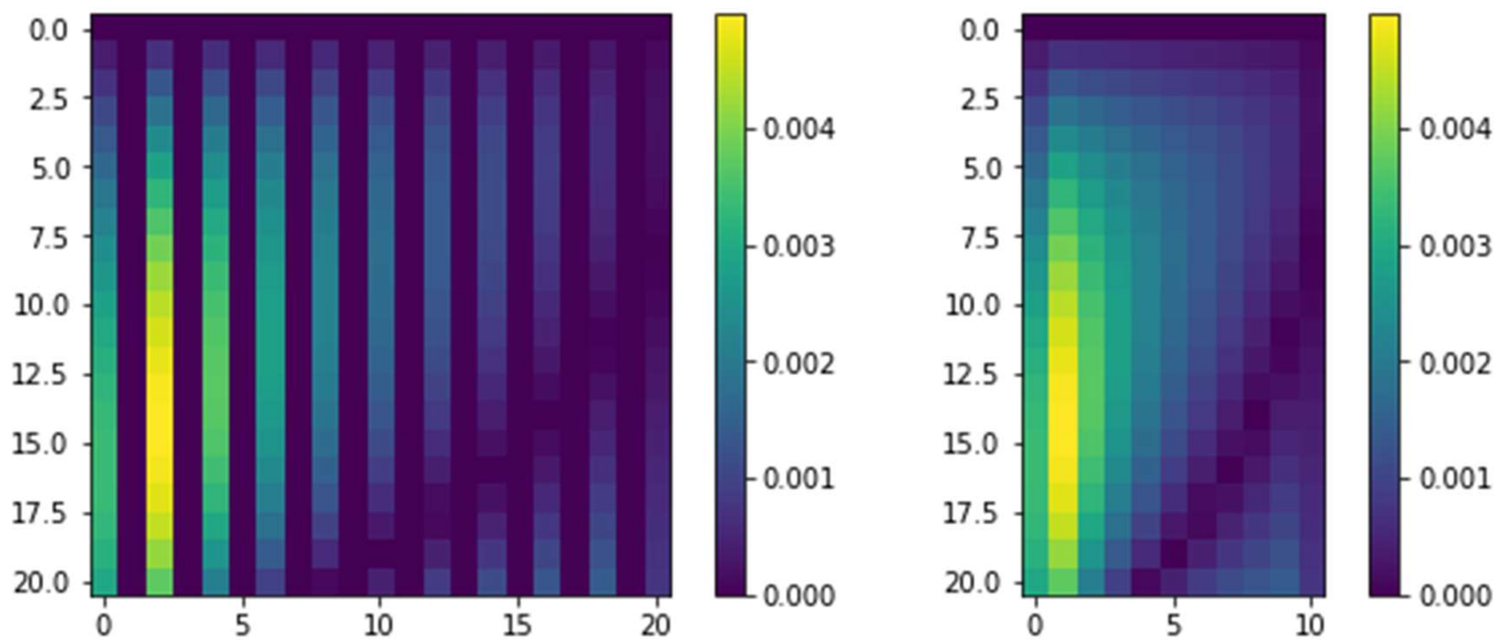
n=51

How can we estimate this?

This is expensive!

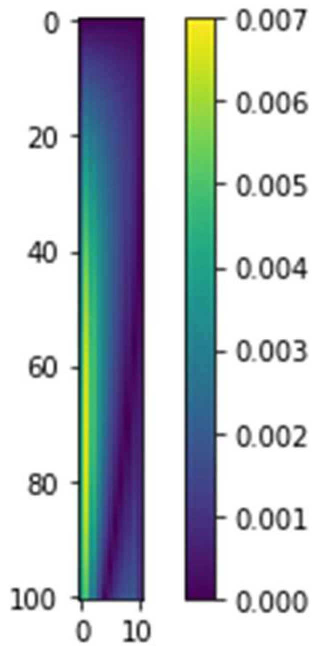
Maybe $B_n - B_m$?

Ex 1: Estimator

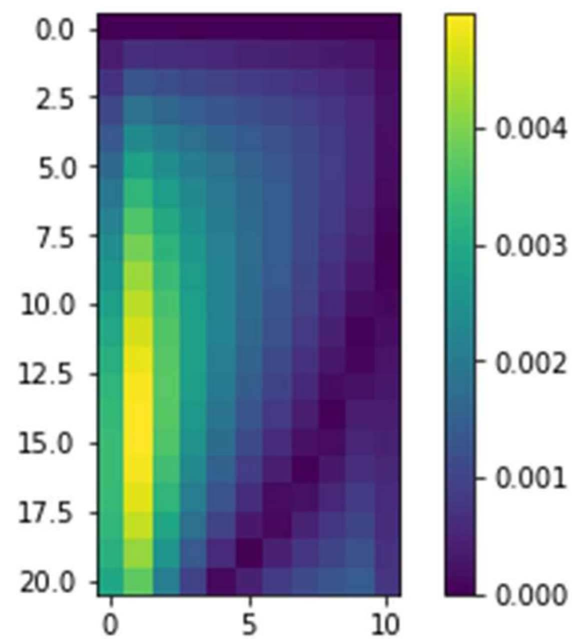


n = 11 vs n = 21

Ex 1: Estimator Comparison

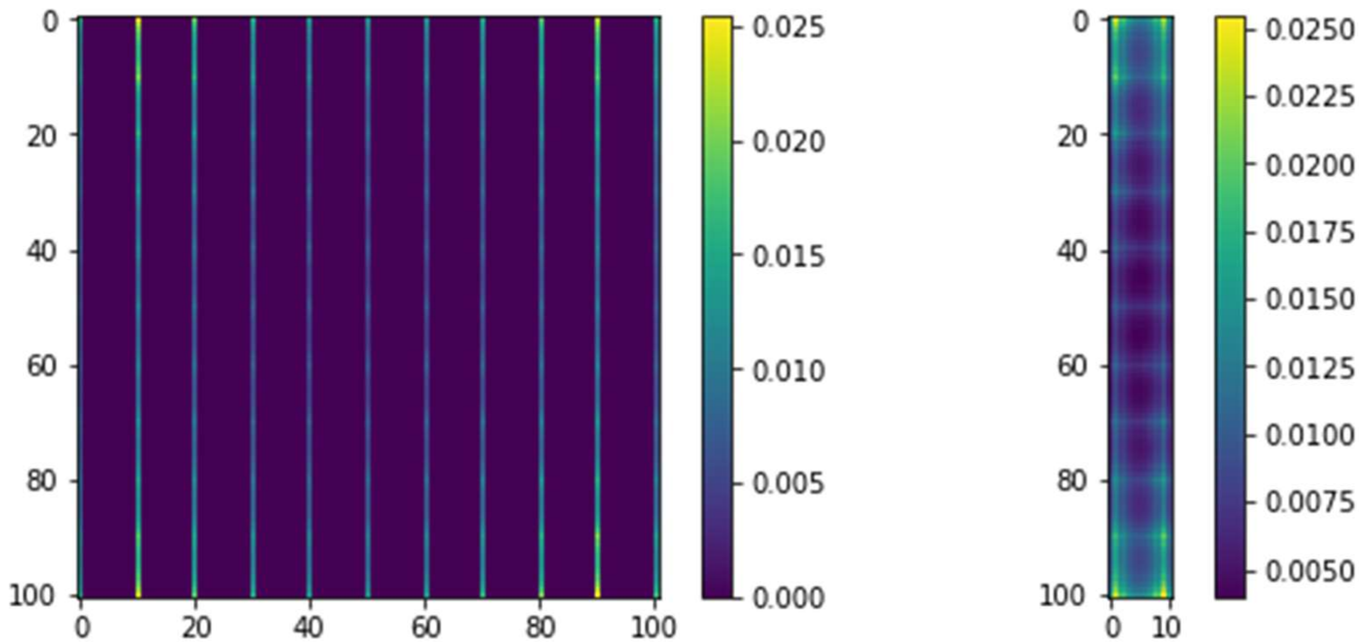


Real



Estimator

Ex 2: Trapezoid, n = 11



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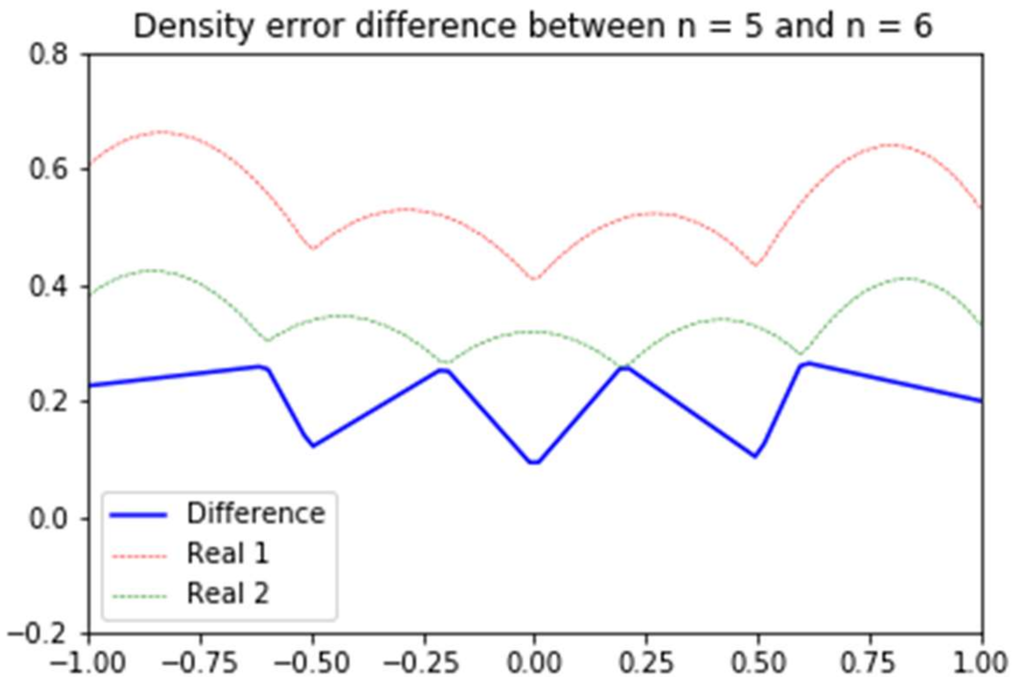
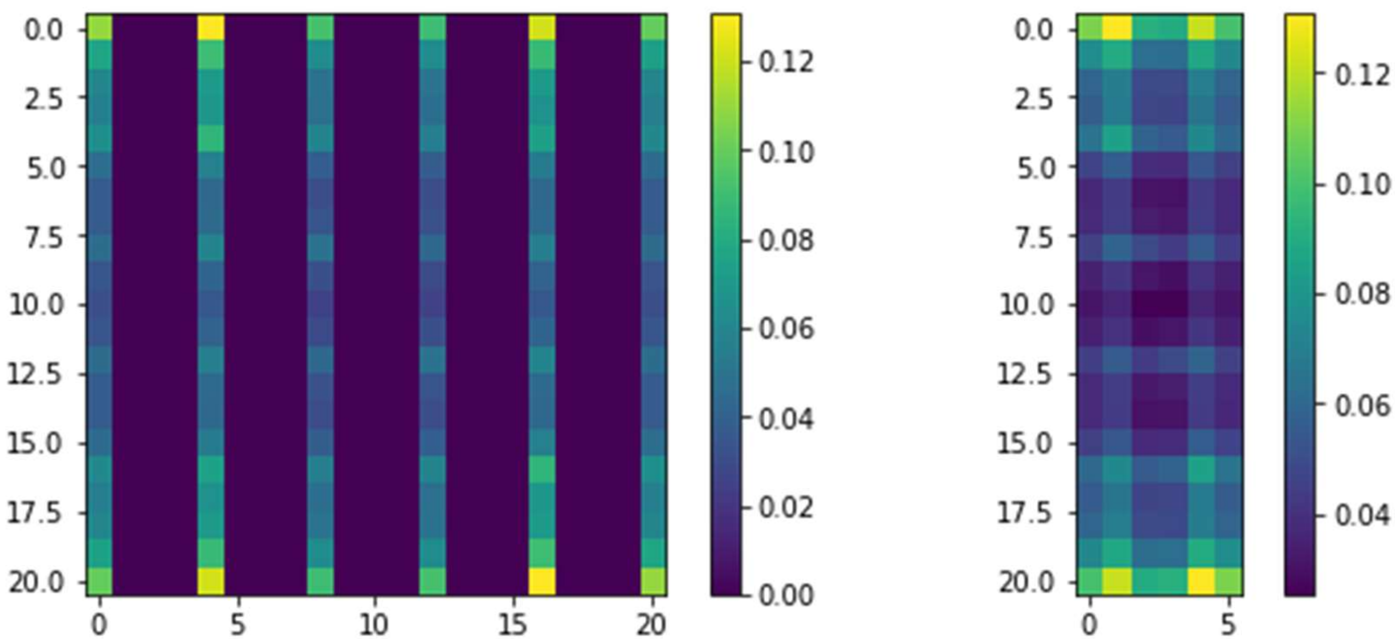


Ex 2: Estimator



n = 11 vs n = 21

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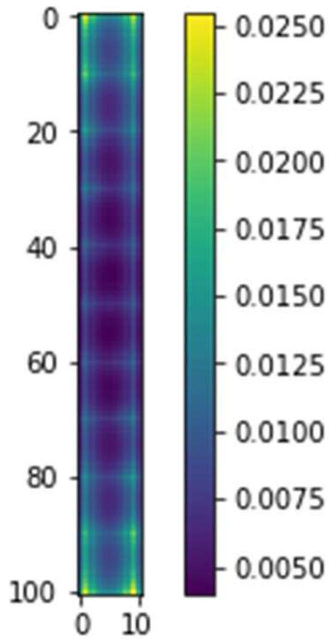
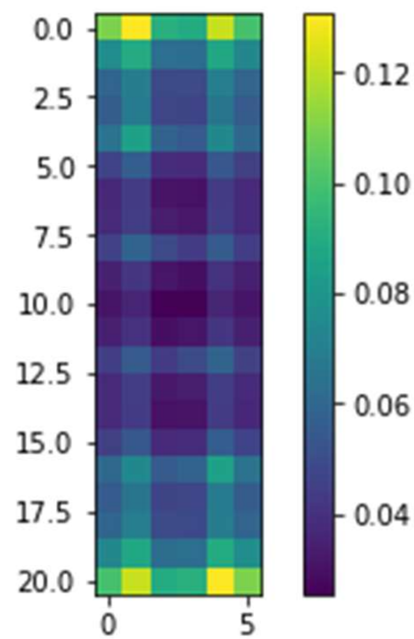


Real



Estimator

Some Thoughts

(done verbally)

=)