ECE 6350

Brief Review of Numerical Methods

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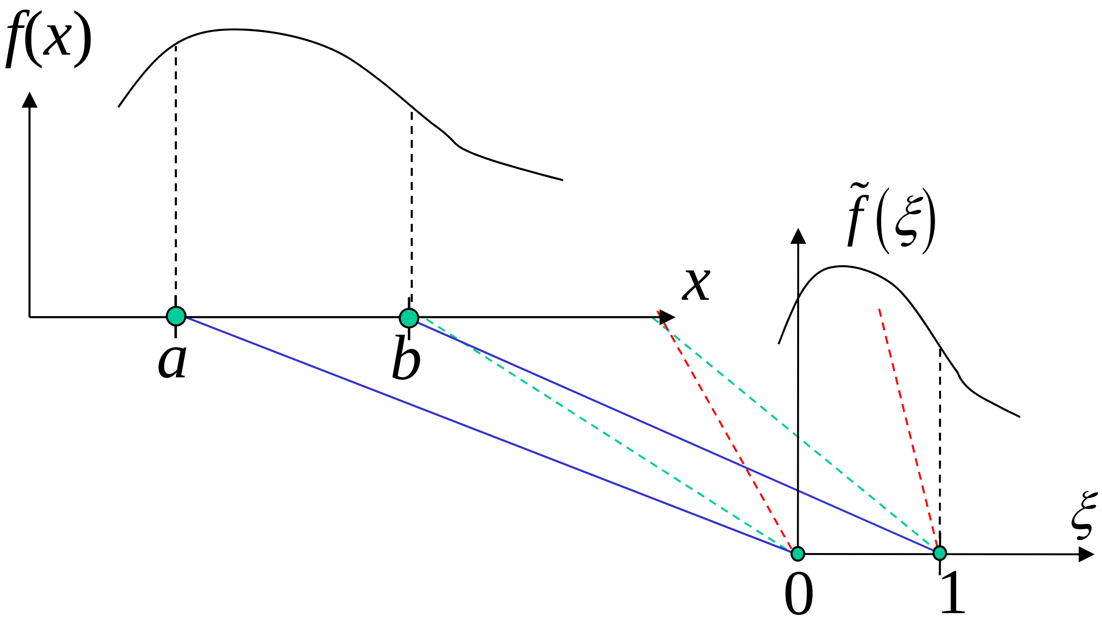
http://www.egr.uh.edu/courses/ece/ece6350/

Some Numerical Considerations

- Interpolation
- Numerical Integration
- Singular Integrals
- “Large” and “small” numbers
- Loss of accuracy resulting from small differences of large numbers

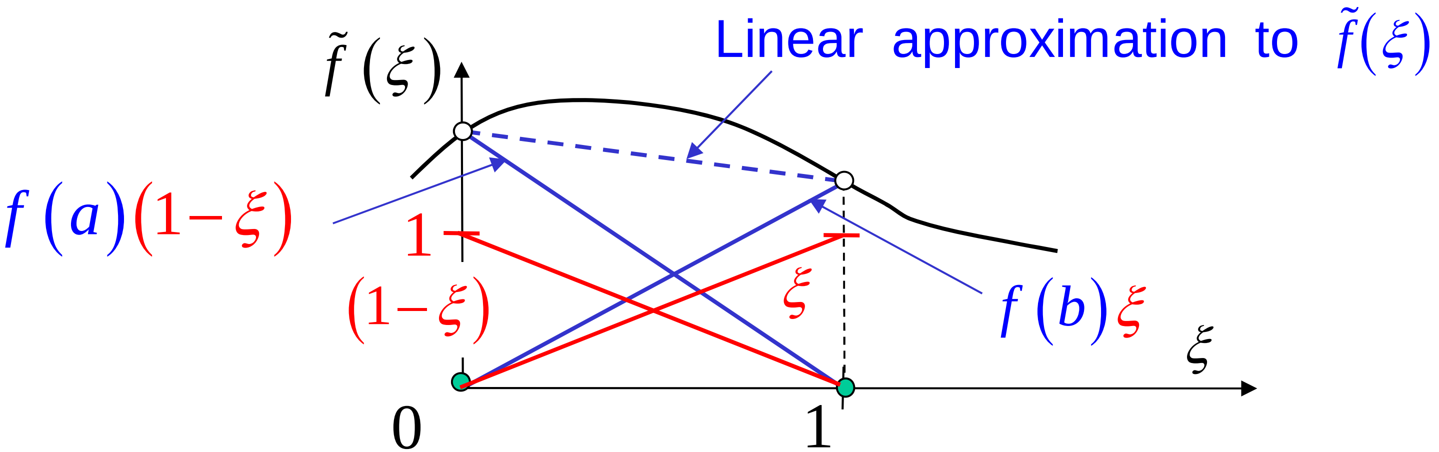
Interpolation



- A function $f(x)$ on any inverval $x \in (a,b)$ can always be mapped to the unit interval $\xi \in (0,1)$ via the interval-normalizing transformation $\xi = \dfrac{x-a}{b-a}$:

$$f(x) = f\left(x(\xi)\right) = f\left[a + (b-a)\xi\right] \equiv \tilde{f}(\xi)$$

Linear Interpolation



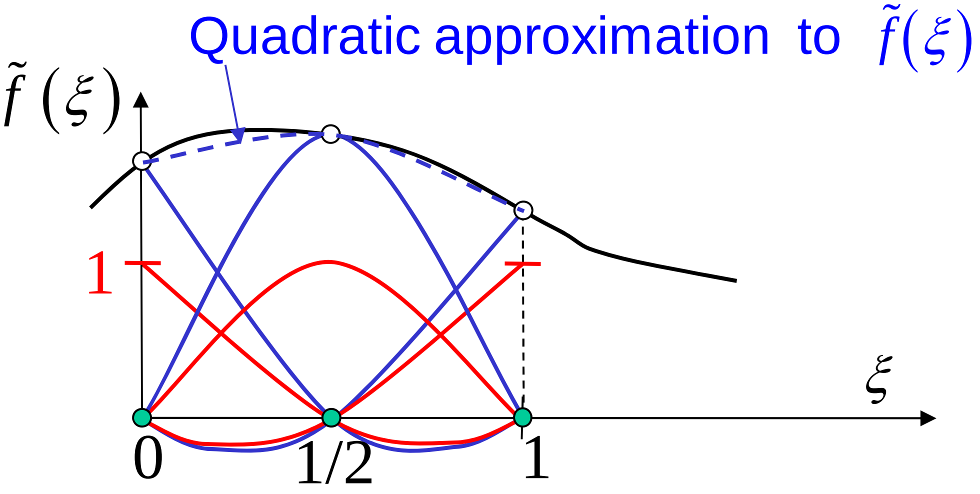
$$\tilde{f}(\xi) \approx \tilde{f}(0)(1-\xi) + \tilde{f}(1)\xi = f(a)(1-\xi) + f(b)\xi$$

Function samples

Interpolation functions

$$= f(a)\frac{b-x}{b-a} + f(b)\frac{x-a}{b-a}$$

Quadratic Interpolation



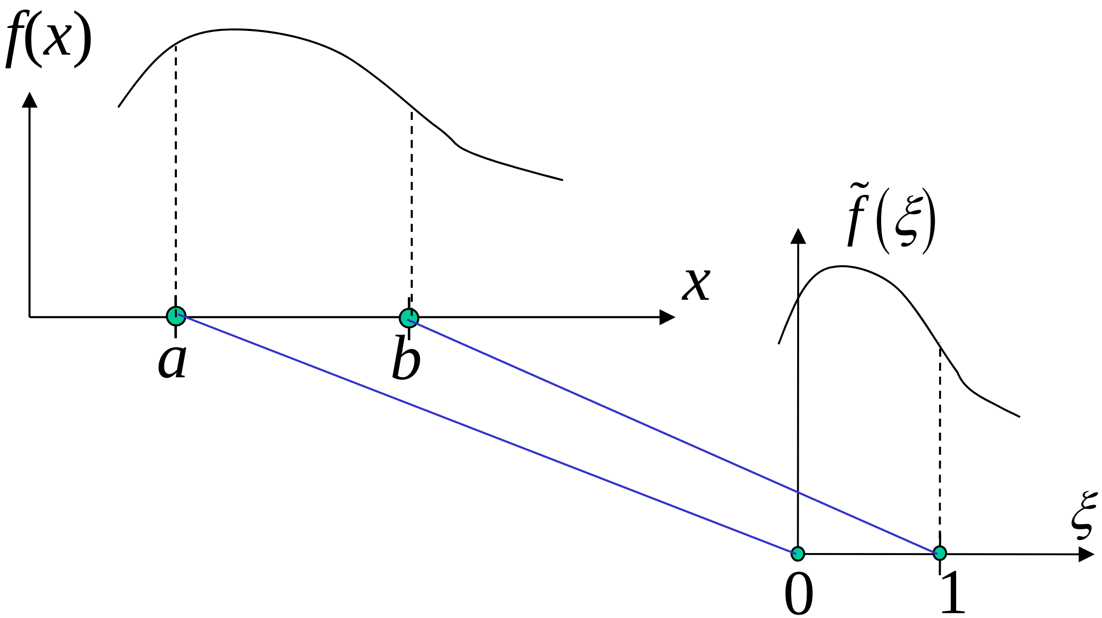
$$\tilde{f}(\xi) \approx \tilde{f}(0)\, 2(\xi - 1)(\xi - \tfrac{1}{2}) + \tilde{f}(\tfrac{1}{2})\, 4\xi(1 - \xi) + \tilde{f}(1)\, 2\xi(\xi - \tfrac{1}{2})$$

Function samples

Interpolation functions

- Each interpolation function is *unity* at its associated interpolation point and *vanishes* at all others

Numerical Integration



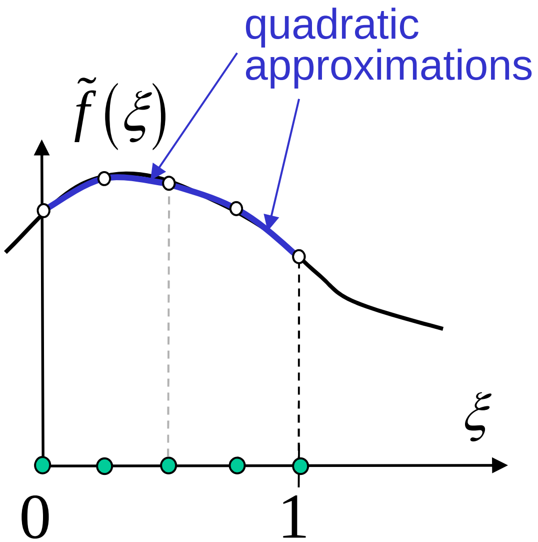
- Integrals $\int_a^b f(x)\,dx$ over any interval (a,b) can always be mapped to the unit interval (0,1) via the transformation $\xi = \dfrac{x-a}{b-a}$:

$$\int_a^b f(x)\,dx = (b-a)\int_0^1 \underbrace{f\left(a+\xi(b-a)\right)}_{\tilde{f}(\xi)} d\xi$$

$$= (b-a)\int_0^1 \tilde{f}(\xi)\,d\xi \approx (b-a)\sum_{k=1}^{K} w_k\,\tilde{f}\left(\xi^{(k)}\right)$$

Numerical Integration, cont'd

$$\int_0^1 \tilde{f}(\xi)\,d\xi \approx \sum_{k=1}^{K} \underbrace{w_k}_{\text{weights}} \tilde{f}\Big(\underbrace{\xi^{(k)}}_{\text{sample points}}\Big)$$



- **Simpson's rule (*K* points):**
  - **- weights and sample points:**

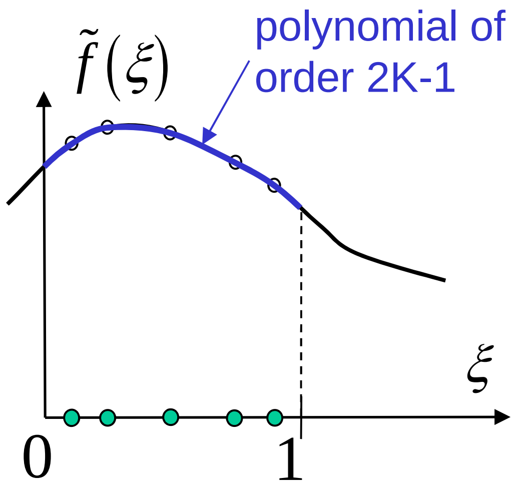
$$w_k = \frac{1}{K-1} \times \left\{ \frac{1}{3}, \frac{4}{3}, \frac{2}{3}, \frac{4}{3}, \frac{2}{3}, \cdots, \frac{4}{3}, \frac{1}{3} \right\}, \quad \left(\text{Note: } \sum_{k=1}^{K} w_k = 1 \right)$$

$$\xi^{(k)} = \left\{ 0, \; \frac{1}{K-1}, \; \frac{2}{K-1}, \; \cdots, \; \frac{K-2}{K-1}, 1 \right\}, \quad K \text{ odd}$$

- error: $\dfrac{K-1}{180} f^{(4)}(x^*) \left(\dfrac{b-a}{K-1} \right)^5, \quad x^* \in (a,b)$

Numerical Integration, cont'd

$$\int_0^1 \tilde{f}(\xi)\,d\xi \approx \sum_{k=1}^{K} w_k \tilde{f}\left(\xi^{(k)}\right)$$



- Gauss-Legendre quadrature:

Find $w_k, \xi^{(k)},\ k = 1, 2, \cdots, K$ such that

$$\int_0^1 \xi^m d\xi = \frac{1}{m+1} = \sum_{k=1}^{K} w_k \left(\xi^{(k)}\right)^m, \quad m = 0, 1, \cdots, 2K-1$$

Note there are *K* points, 2*K* parameters (wghts and sample pts), and 2*K* power series terms in ξ !

- sample points are unequally spaced
- weights and sample points are usually irrational
- convergence w.r.t. *K* is very good for smooth functions
- error:

$$\left(\frac{b-a}{2}\right)^{2K+1} \frac{f^{(2K)}(x^*)}{C_K}, \quad C_K = \frac{(2K+1)\left[(2K)!\right]^3}{2^{2K+1}(K!)^4}, \quad x^* \in (a,b)$$

Numerical Integration, cont'd

- Gaussian quadrature:

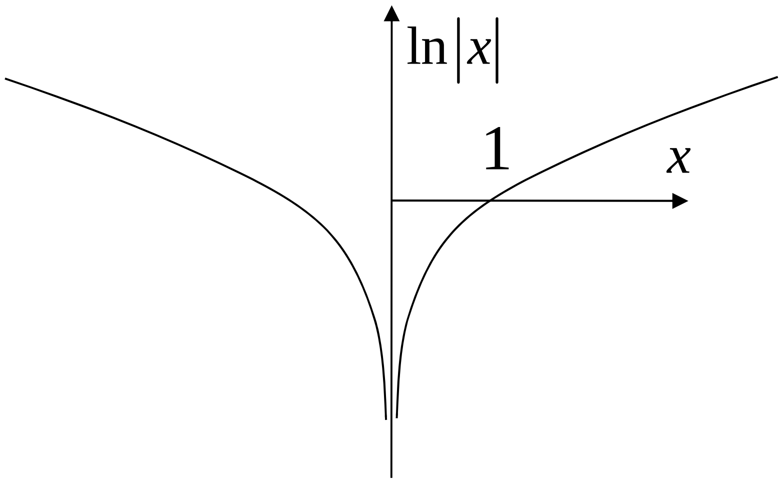
$$\int_0^1 \tilde{f}(\xi)\,d\xi \approx \sum_{k=1}^{K} w_k\,\tilde{f}\left(\xi^{(k)}\right)$$

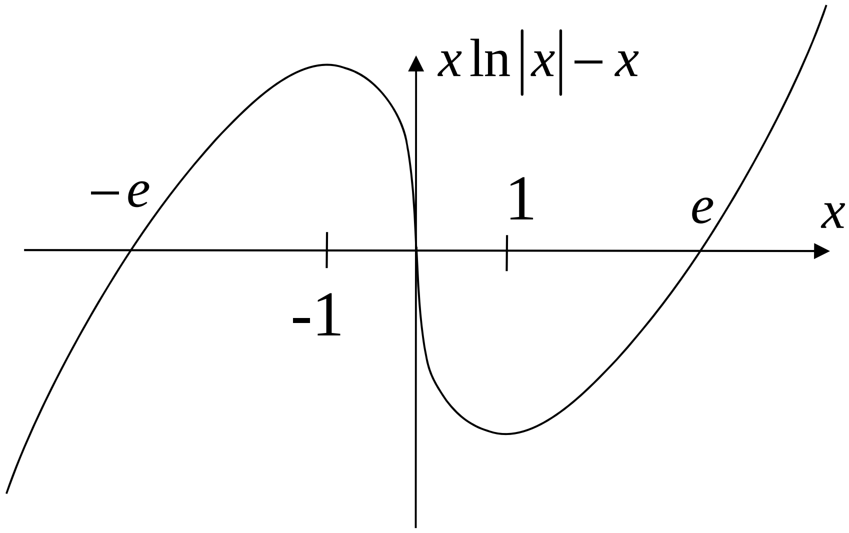
$$\left(\text{Note: } \sum_{k=1}^{K} w_k = 1\right)$$

Table 3 Sample points and weighting coefficients for K-point Gauss-Legendre quadrature.

Sample Points, $\xi_1^{(k)}$	Weights, w_k
K=1:	
0.500000000000000	1.000000000000000
K=2:	
0.211324865405187	0.500000000000000
0.788675134594813	0.500000000000000
K=4:	
0.069431844202974	0.173927422568727
0.330009478207572	0.326072577431273
0.669990521792428	0.326072577431273
0.930568155797027	0.173927422568727

Singular Integrals

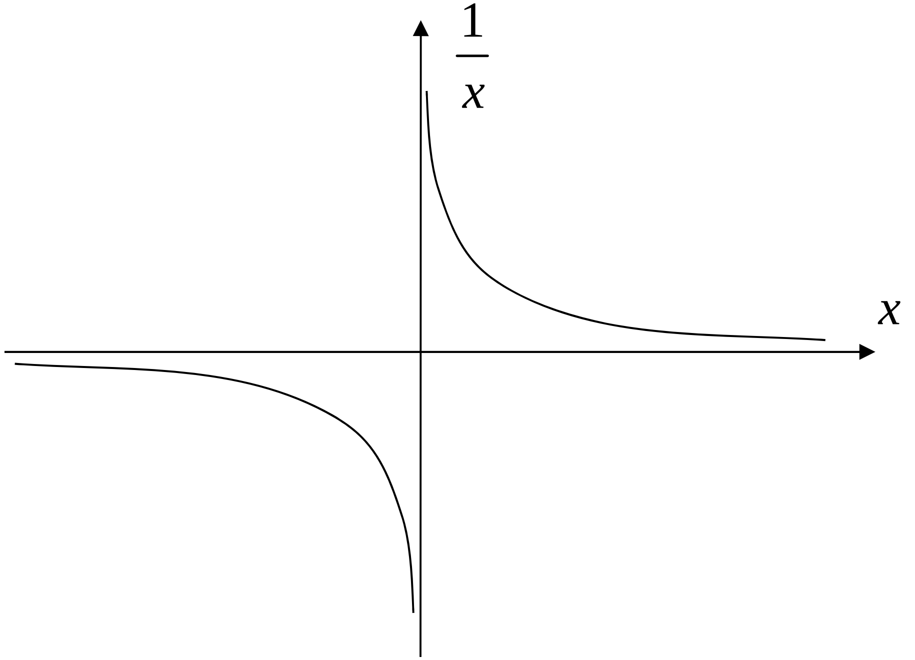




- Logarithmic singularities are examples of *integrable* singularities:

$$\int_0^1 \ln|x|\,dx = \left(x\ln|x|-x\right)\Big|_{x=0}^{1} = -1 \quad \text{since } \lim_{x\to 0} x\ln|x| = 0$$

Singular Integrals, cont'd



- $1/x$ singularities are examples of singularities integrable only in the *principal value* (PV) sense.
- Principal value integrals must not start or end at the singularity, but must *pass through* to permit cancellation of infinities

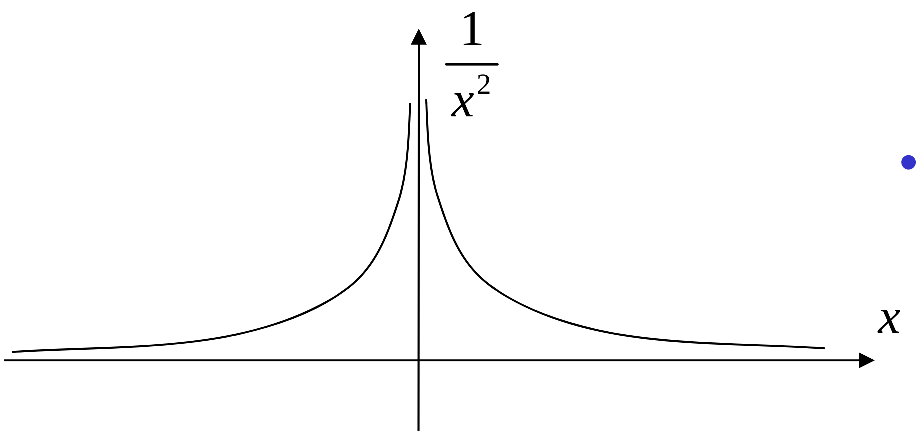
$$\int_0^1 \frac{1}{x}\,dx = \ln|x|\,\Big|_{x=0}^{1} = \infty \quad \text{since} \quad \lim_{x\to 0} \ln|x| = -\infty,$$

$$\text{but} \qquad \mathrm{PV}\int_{-1}^{2} \frac{1}{x}\,dx = \lim_{\varepsilon\to 0}\left(\int_{-1}^{-\varepsilon} + \int_{\varepsilon}^{2}\right)\frac{1}{x}\,dx = \lim_{\varepsilon\to 0}\left[\ln|x|\,\Big|_{x=-1}^{-\varepsilon} + \ln|x|\,\Big|_{x=\varepsilon}^{2}\right]$$

$$= \lim_{\varepsilon\to 0}\left[\cancel{\ln\varepsilon} + \ln 2 - \cancel{\ln\varepsilon}\right] = \ln 2$$

Infinite contributions cancel!

Singular Integrals, cont'd



- Singularities like $1/x^2$ are *non-integrable*:

$$\int_0^1 \frac{1}{x^2}\,dx = \left.\frac{-1}{x}\right|_{x=0}^{1} = \infty \quad \text{since} \quad \lim_{x\to 0}\frac{1}{x} = \infty$$

and infinite contributions from intervals on

both sides of $x = 0$ will add, not cancel!

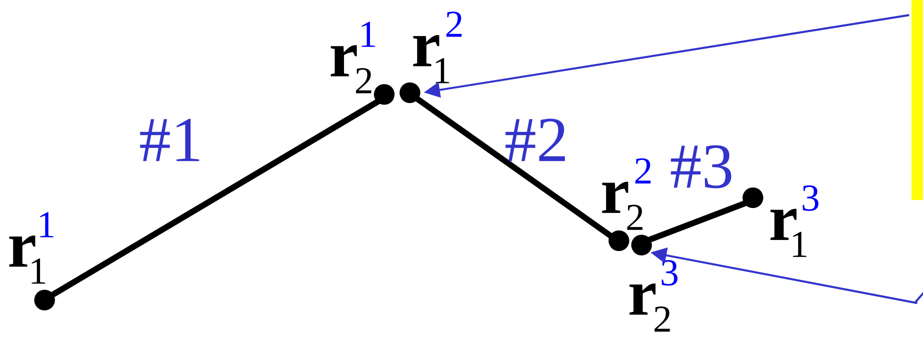
$$\left(\text{But note that } \frac{\operatorname{sgn}(x)}{x^2} = \begin{cases} \frac{1}{x^2}, & x > 0 \\ -\frac{1}{x^2}, & x < 0 \end{cases} \quad \textit{does} \text{ have a PV integral} \right)$$

Singular Integrals, cont'd

Summary:

- $\ln |x|$ is integrable at $x=0$
- $1/x^{\alpha}$ is integrable at $x=0$ for $\alpha<1$
- $1/x^{\alpha}$ is non-integrable at $x=0$ for $\alpha=1$, or $\alpha>1$
- $f(x)\mathrm{sgn}(x)/|x|^{\alpha}$ has a PV integral if $f(x)$ is continuous at $x=0$, for $\alpha<2$
- Above results translate to singularities at a point $x=a$ via the transformation $x \to x-a$

How Big is "Big"?   How Small is "Small"?



if line segment endpoints are sufficiently close, consider them connected

- Suppose, e.g., we want to set $\mathbf{r}_2^1 = \mathbf{r}_1^2$, etc. if the distance between line segments is "small." I.e., if it seems the segments should really be "connected."
- Naïve approach: Set $\mathbf{r}_2^1 = \mathbf{r}_1^2$ if $\left|\mathbf{r}_2^1 - \mathbf{r}_1^2\right| < \varepsilon$
- ε $=10^{-5}$? 10^{-3} ? 10^{-1} ? 10^{2} ? 10^{6} ?
- Better approach: Set $\mathbf{r}_2^1 = \mathbf{r}_1^2$ if $\dfrac{\left|\mathbf{r}_2^1 - \mathbf{r}_1^2\right|}{\min\left|\mathbf{r}_2^n - \mathbf{r}_1^n\right|} << 1$

$$\Rightarrow \left|\mathbf{r}_2^1 - \mathbf{r}_1^2\right| < \varepsilon \min\left|\mathbf{r}_2^n - \mathbf{r}_1^n\right|$$

All Tests for "Smallness" or "Largeness" Should Be *Relative* Tests

- In the example, we assume we'll have a connection if segment endpoints are close ---*relative* to, say, the length of the smallest segment. Therefore we should test if

$$\frac{\textit{distance between two segment endpoints}}{\textit{smallest segment length}} < \varepsilon$$

or, equivalently,

$$\textit{distance between two segment endpoints} < \varepsilon \times \underbrace{\textit{smallest segment length}}_{\text{some typical, lower bound measure of LHS quantities}}$$

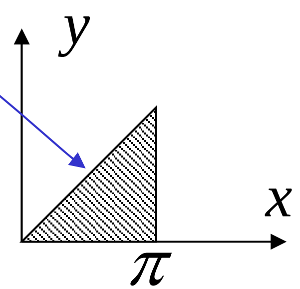
never

$$\cancel{\textit{distance between two segment endpoints} < \varepsilon}$$

Small Differences of Large Numbers

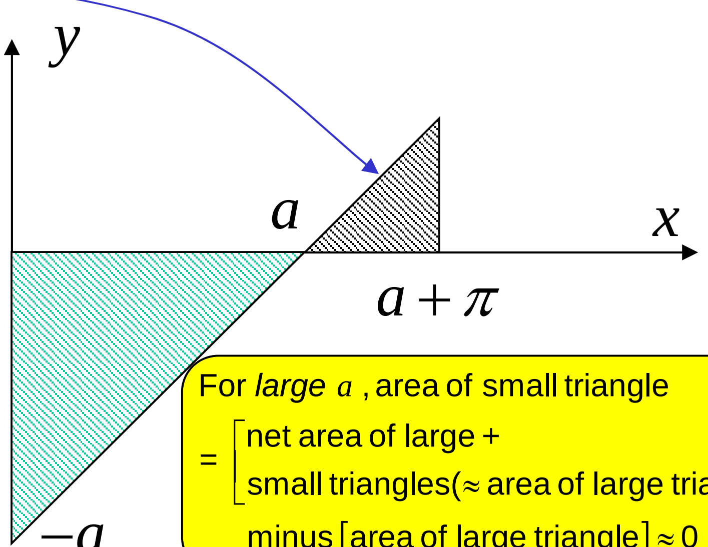
- **Consider the following simple integral:**

$$\int_0^{\pi} \overbrace{x}\, dx = \left.\frac{x^2}{2}\right|_{x=0}^{\pi} = \frac{\pi^2}{2}$$



- **Now shift the integrand, limits, and evaluate:**

$$\int_a^{a+\pi} \overbrace{(x-a)}\, dx = \left.\left(\frac{x^2}{2} - ax\right)\right|_{x=a}^{a+\pi} = \frac{\pi^2}{2}$$



For *large* a, area of small triangle

$= \left[\begin{array}{l}\text{net area of large +} \\ \text{small triangles}(\approx \text{area of large triangle})\end{array}\right]$

minus [area of large triangle] ≈ 0

Small Differences of Large Numbers, cont'd

$$\int_a^{a+\pi} (x-a)\,dx = \left(\frac{x^2}{2} - ax\right)\Bigg|_{x=a}^{a+\pi} = \frac{\pi^2}{2} = 4.93480220054467\ldots$$

•Results for varying values of a

a	upper limit	lower limit	**difference**
1.0	4.434802200544670	-0.50	4.934802200544670
10.0	-45.065197799455300	-50.00	4.934802200544670
100.0	-4995.065197799460000	-5000.00	4.934802200544250
1000.0	-499995.065197799000000	-500000.00	4.934802200528790
10000.0	-49999995.065197800000000	-50000000.00	4.934802196919910
100000.0	-4999999995.065200000000000	-5000000000.00	4.934802055358880
1000000.0	-499999999995.065000000000000	-500000000000.00	4.934814453125000
10000000.0	-49999999999995.100000000000000	-50000000000000.00	4.937500000000000
100000000.0	-4999999999999990.000000000000000	-5000000000000000.00	0.000000000000000
1000000000.0	-500000000000000000.000000000000000	-500000000000000000.00	0.000000000000000
10000000000.0	-50000000000000000000.000000000000000	-50000000000000000000.00	0.000000000000000

Lost significant digits

Ques : What happens if the limit π is replaced by an integer? If a is irrational?

With Numerical Integration, the Error Grows Only Half as Fast

$$\int_a^{a+\pi} (x-a)\,dx = \left(\frac{x^2}{2} - ax\right)\Bigg|_{x=a}^{a+\pi} = \frac{\pi^2}{2} = 4.93480220054467\ldots$$

- **Results for varying values of *a*, but integral is evaluated by Gauss quadrature**
- **Sensitivity is less since integrand is *linear*--- i.e., we are not *squaring* any already large quantities**
- **Observation: Sometimes a numerically obtained result is more accurate than an "exact" one!**

	Two Point
a	**Gauss Quadrature**
1.0	4.93480220054467
10.0	4.93480220054467
100.0	4.93480220054469
1000.0	4.93480220054465
10000.0	4.93480220054572
100000.0	4.93480220052857
1000000.0	4.93480220052857
10000000.0	4.93480220016284
100000000.0	4.93480219431117
1000000000.0	4.93480210068441
10000000000.0	4.93480022814947

With Some Rational Numbers, *No* Error Appears---until Catastrophic Failure Occurs

$$\int_a^{a+1} (x-a)\,dx = \left(\frac{x^2}{2} - ax \right) \Bigg|_{x=a}^{a+1} = \frac{1}{2} \quad \left(= \; 0.100000000\ldots \; \text{ in binary} \right)$$

- **Results for varying values of *a***

a	upper limit	lower limit	difference
1.000	0.000	-0.500	0.500
10.000	-49.500	-50.000	0.500
100.000	-4999.500	-5000.000	0.500
1000.000	-499999.500	-500000.000	0.500
10000.000	-49999999.500	-50000000.000	0.500
100000.000	-4999999999.500	-5000000000.000	0.500
1000000.000	-499999999999.500	-500000000000.000	0.500
10000000.000	-49999999999999.500	-50000000000000.000	0.500
100000000.000	-5000000000000000.000	-5000000000000000.000	0.000
1000000000.000	-500000000000000000.000	-500000000000000000.000	0.000
10000000000.000	-50000000000000000000.000	-50000000000000000000.000	0.000
100000000000.000	-5000000000000000000000.000	-5000000000000000000000.000	0.000