THE UNIVERSITY OF UTAH

SCHOOL OF COMPUTING

CS 3200
Introduction to Scientific Computing

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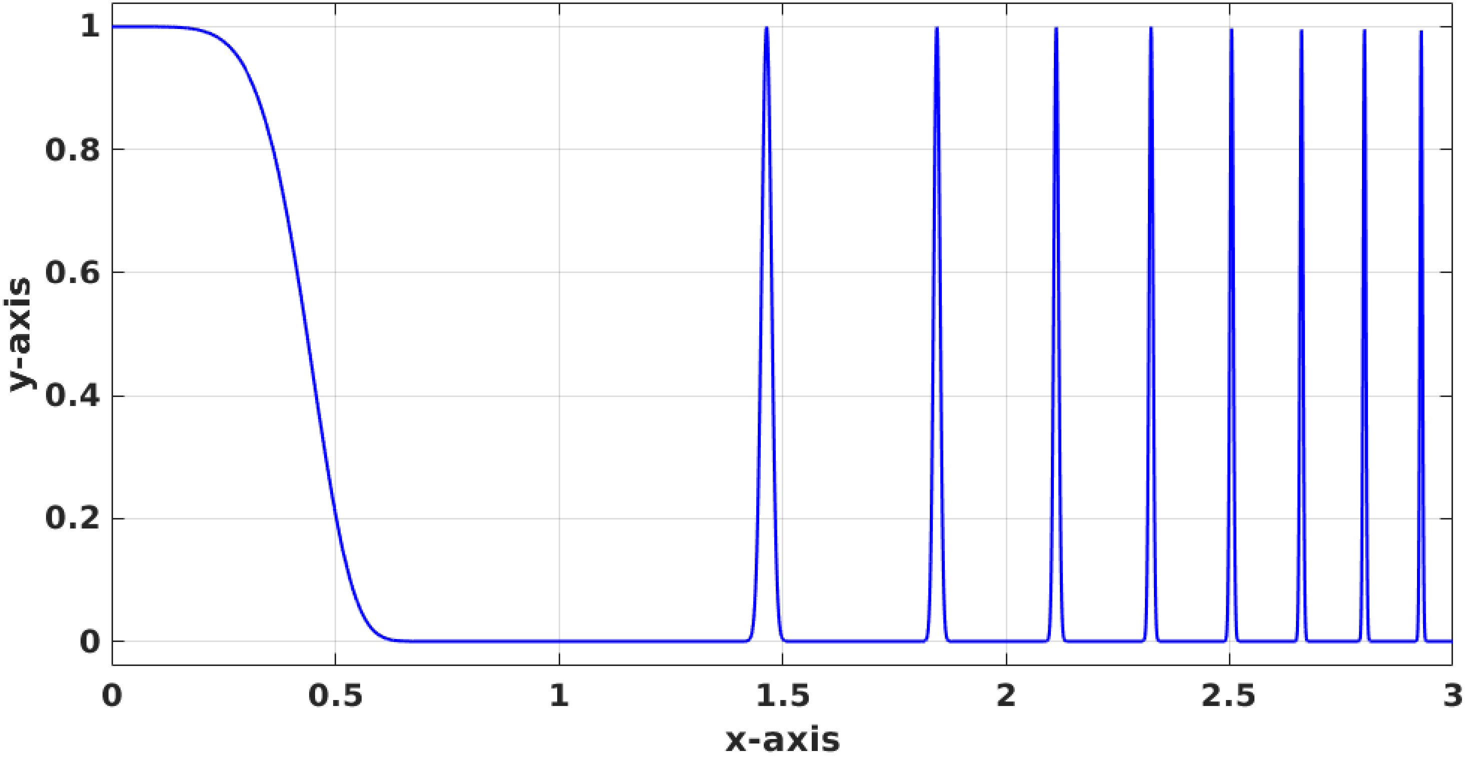
Topic: Adaptive Methods

Using a fixed mesh for Quadrature may not be efficient

E.G. Consider $f(x) = \cos(x^3)^{200}$

Error of 1e-6 needs 19,200 intervals to address peaks



Motivation

- Not only do we want to compute the correct solution but we would like do so efficiently
- When implementing methods we would like them to automatically control the error
- A good examples is quadrature
- What does the error estimate depends on?

Motivation

- When implementing methods we would like them to automatically control the error
- A good example is quadrature
- the error estimate depends on?
- The step size and the some derivative of the function $\Delta x^4 \; and \; f''''(\zeta)$

Simpson's Rule (continued)

Composite Simpson's Rule:

Theorem

If $f(x) \in C^4[a,b]$, then it has 4 continuous drivatives.

For such a function then the composite Simpson's Rule satisfies

$$\int_a^b f(x)dx - I_s \leq \frac{(b-a)}{90} \mathrm{h}^4 \left\| \frac{d^4 f}{dx^4} \right\|_\infty ,$$

where $\left\| \frac{d^4 f}{dx^4} \right\|_\infty = \max_{a \leq x \leq b} \left| \frac{d^4 f}{dx^4} \right|$

I_S Is the value produced by Simpson's Rule

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Extrapolation – Simpson's rule

Let $I(Simp, h)$ be the approximate value of the integral
on the interval [a,b]with
Simpsons rule and step h. Let $Iexact$ be the exact value.

Then $Iexact - I(Simp, h) \approx \dfrac{-(b-a)h^4}{90} f^{(iv)}(\zeta_1)$

and $Iexact - I(Simp, \dfrac{h}{2}) \approx \dfrac{-(b-a)h^4/16}{90} f^{(iv)}(\zeta_1)$

Romberg Extrapolation – Simpson's rule

subtracting shows that the difference between the numerical solutions gives and estimate of the error

$$I(Simp,\frac{h}{2})-I(Simp,h)\approx\frac{-(b-a)h^4}{90}f^{(iv)}(\zeta_1)(1-\frac{1}{16})$$

multiplying rhs by $\frac{16}{15}$ estimates the error in $I(Simp,h)$

and by $\frac{1}{15}$ the error in $I(Simp,\frac{h}{2})$

Romberg Extrapolation – Simpson's rule with improved accuracy

Once we know the estimate of the error we can add it to the solution to get an even more accurate solution

solutions gives and estimate of the error

$$I - I(Simp, \frac{h}{2}) = \frac{1}{15}(I(Simp, \frac{h}{2}) - I(Simp, h)) \approx \frac{-(b-a)h^4}{90 \times 16} f^{(iv)}(\zeta_1) + O(h^6)$$

Hence

$$I - \underbrace{(I(Simp, \frac{h}{2}) + \frac{1}{15}(I(Simp, \frac{h}{2}) - I(Simp, h))}_{\text{Even more accurate estimate}} \approx O(h^6)$$

Even more accurate estimate with error

Example

$$\int_0^1 e^x dx \qquad \text{Exact value } = (e^1 - 1)$$

K	level	fixed Simpson	Romberg Simpson	Error
1	4	1.71831884192175	1.71831884192175	3.701e-05
2	8	1.71828415469990	1.71828184221844	1.376e-08
3	16	1.71828197405189	1.71828182867536	2.163e-10
4	32	1.71828183756177	1.71828182846243	3.385e-12
5	64	1.71828182902802	1.71828182845910	5.240e-14

Matlab QUADTX

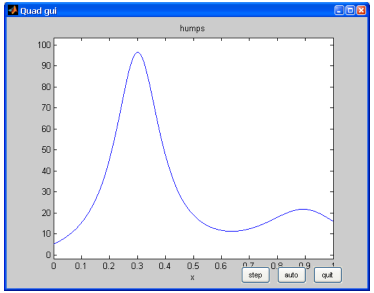
- Uses Simpson's Rule recursively until the error on each interval is less than *tol* which is user supplied
- A decision to subdivide each interval is made when the error estimated is > *tol*
- An alternative approach (and mathematically better) is to control the error so that
  - The estimated error on interval [c,d] is less than tol (d-c)/(b-a) . This way the sum of all errors < tol

```matlab
function [Q,fcount] = quadtx(F,a,b,tol,varargin)
% Default tolerance
if nargin < 4 | isempty(tol)
   tol = 1.e-6;
end

% Initialization
c = (a + b)/2;
fa = feval(F,a,varargin{:});
fc = feval(F,c,varargin{:});
fb = feval(F,b,varargin{:});

% Recursive call
[Q,k] = quadtxstep(F, a, b, tol, fa, fc, fb, varargin{:});
fcount = k + 3;
```

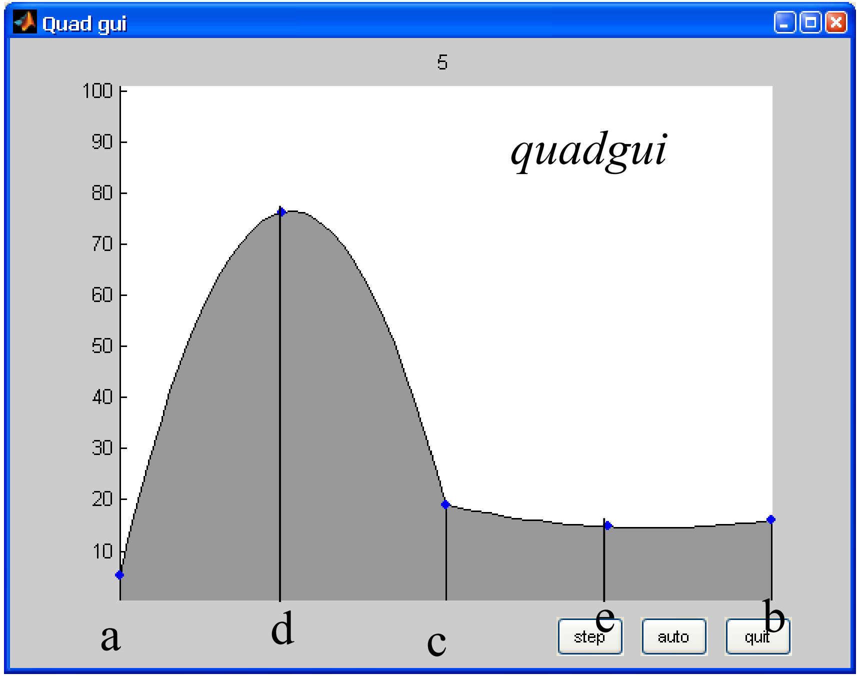
```
• function [Q,fcount] = quadtxstep(F,a,b,tol,fa,fc,fb,varargin)
• h = b - a;
• c = (a + b)/2;
• fd = feval(F,(a+c)/2,varargin{:});
• fe = feval(F,(c+b)/2,varargin{:});
• Q1 = h/6 * (fa + 4*fc + fb);
• Q2 = h/12 * (fa + 4*fd + 2*fc + 4*fe + fb);
• if abs(Q2 - Q1) <= tol
•    Q  = Q2 + (Q2 - Q1)/15;
•    fcount = 2;
• else
•    [Qa,ka] = quadtxstep(F, a, c, tol, fa, fd, fc, varargin{:});
•    [Qb,kb] = quadtxstep(F, c, b, tol, fc, fe, fb, varargin{:});
•    Q  = Qa + Qb;
•    fcount = ka + kb + 2;
• end
```

Example of Quadtx in use with the humps example

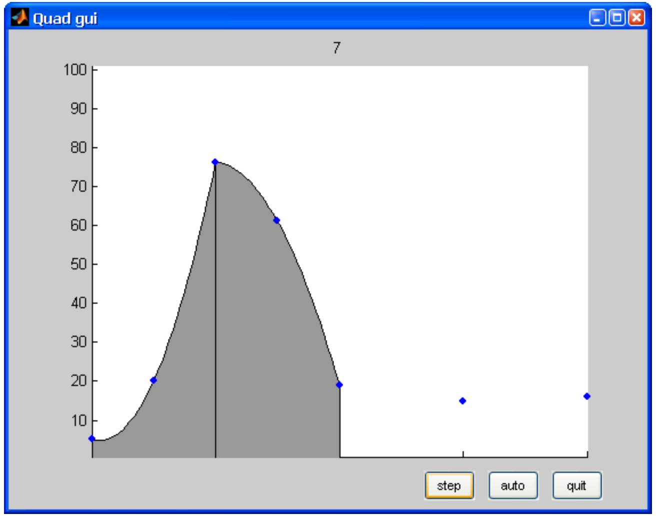
The first evaluation when a = 0 and b = 1 using Extrapolated Simpson's Rule.



Actual plot of the function



Steps


Quad gui
7
100
90
80
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40
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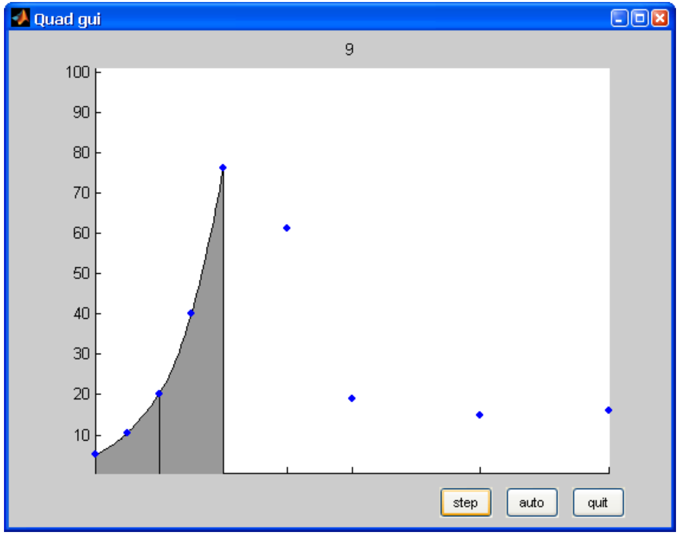
20
10
step
auto
quit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9
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step
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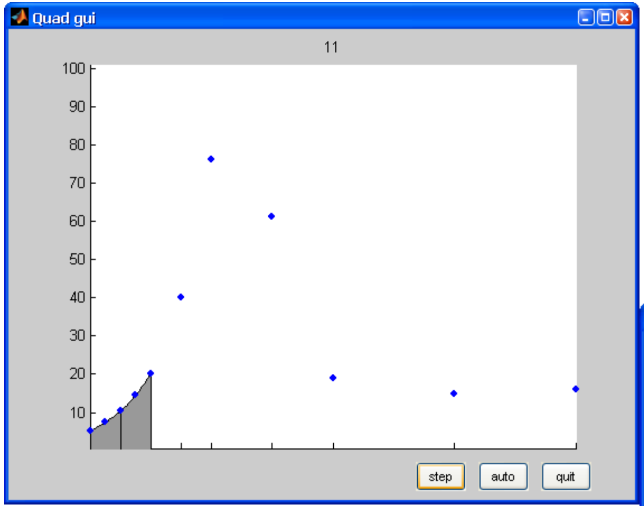
quit

Steps


Quad gui
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step
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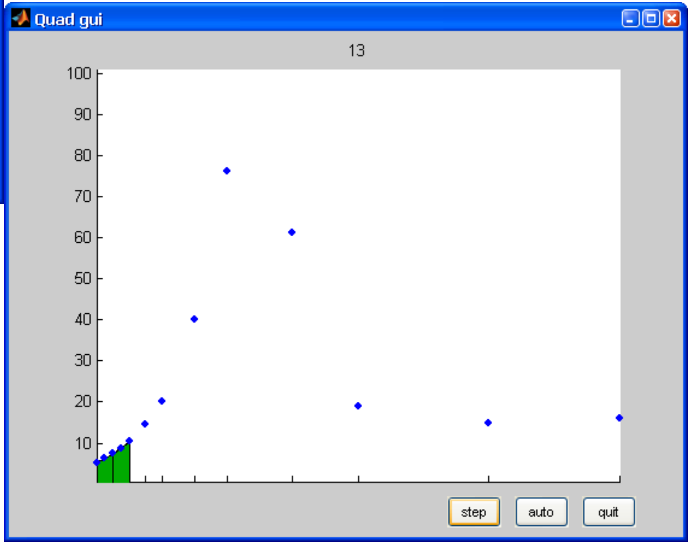
Quad gui
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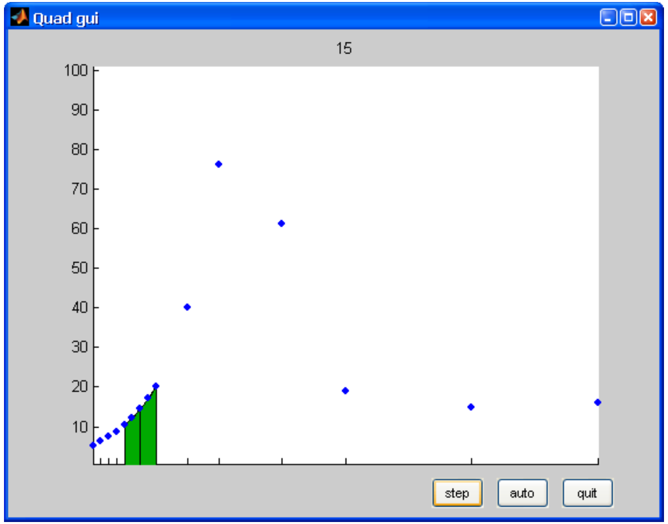
step
auto
quit

Steps



Quad gui
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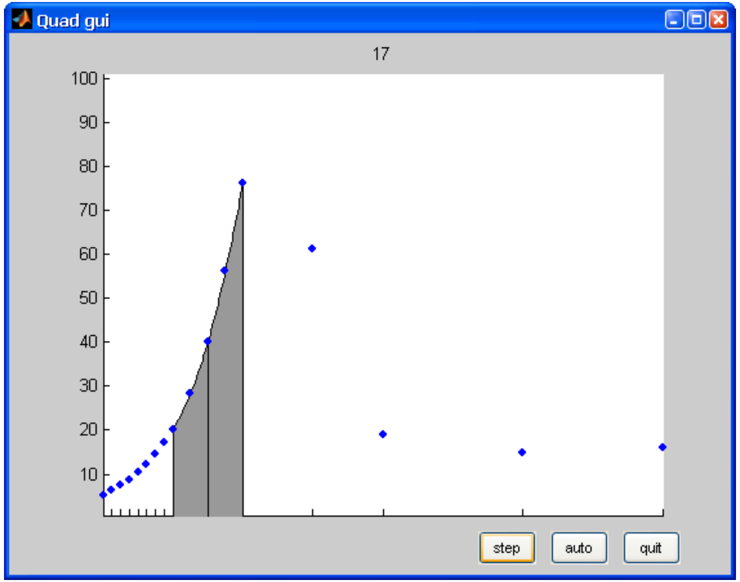
step
auto
quit



Quad gui
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step
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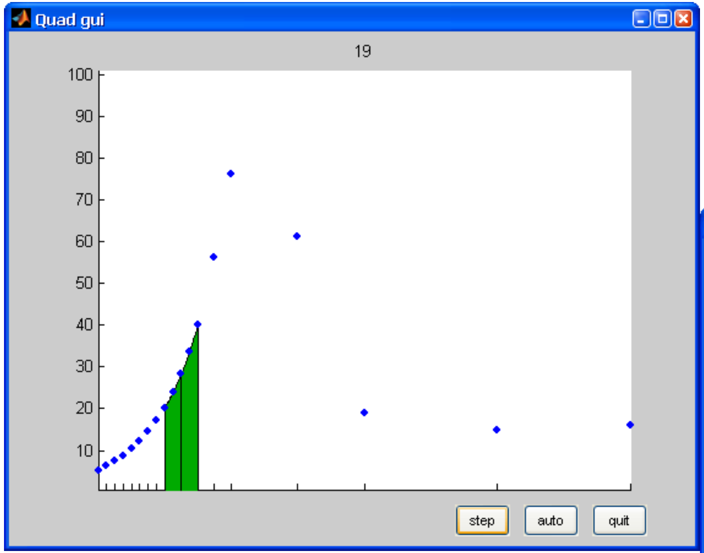
quit

Steps


Quad gui
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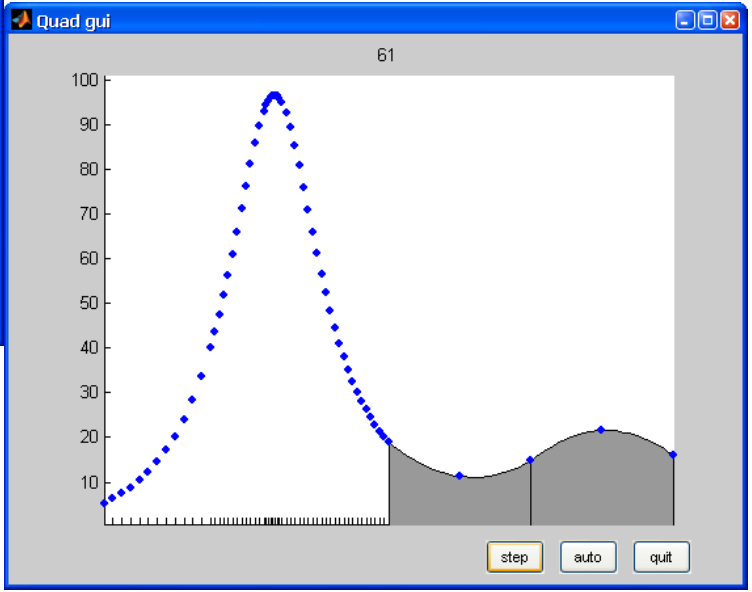
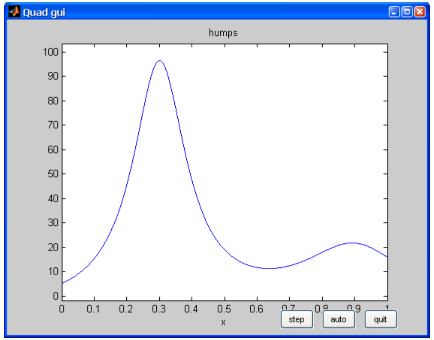
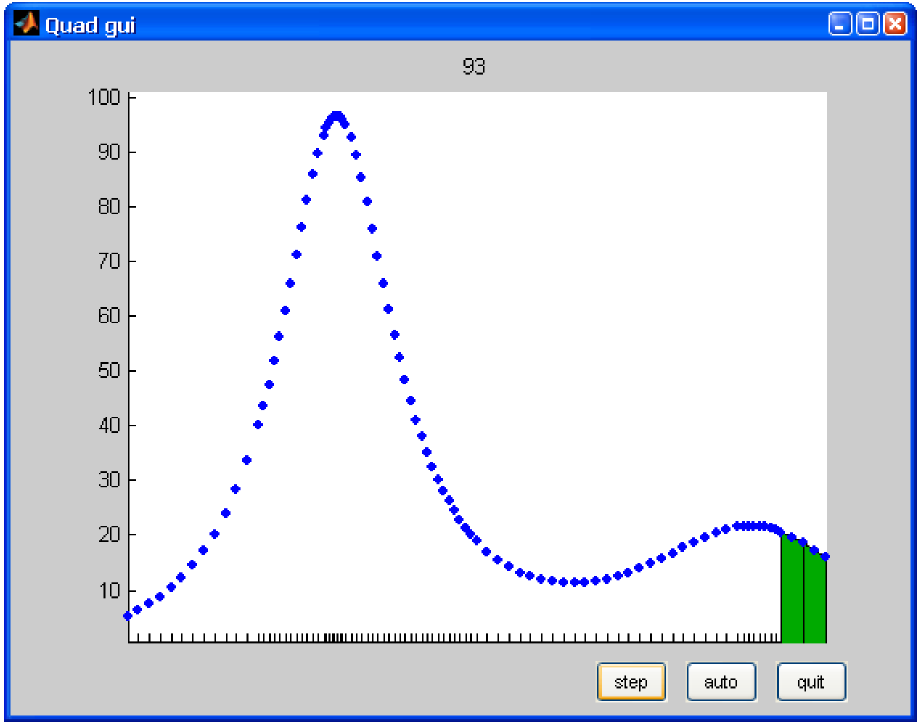

Quad gui
61
100
90
80
70
60
50
40
30
20
10
step
auto
quit

Last Step



Actual plot of the function



Driving code for Humps Example

```
fprintf('  tol            Q                    fcount     err       ratio \n')
for  k = 1:12
    tol = 10^(-k);
    Qexact=29.85832539549867;
    [Q,fcount] = quadtx(@humps,0,1,tol);
    err=Q-Qexact;
    ratio = err/tol;
    fprintf('%8.0e %21.14f %7d %13.3e %9.3f \n',tol,Q,fcount,err,ratio)
end
```

Results for Humps Example

tol	Q	fcount	err	ratio
1e-01	29.83328444174864	25	-2.504e-02	-0.250
1e-02	29.85791444629948	41	-4.109e-04	-0.041
1e-03	29.85834299237637	69	1.760e-05	0.018
1e-04	29.85832444437543	93	-9.511e-07	-0.010
1e-05	29.85832551548643	149	1.200e-07	0.012
1e-06	29.85832540194041	265	6.442e-09	0.006
1e-07	29.85832539499819	369	-5.005e-10	-0.005
1e-08	29.85832539552631	605	2.764e-11	0.003
1e-09	29.85832539549604	1061	-2.636e-12	-0.003
1e-10	29.85832539549890	1469	2.309e-13	0.002
1e-11	29.85832539549867	2429	-3.553e-15	-0.000
1e-12	29.85832539549867	4245	3.553e-15	0.004

Example of Adaptive Simpson Integration

$$\int_0^1 e^{3x}\,dx$$

k	n	Is Simpson	Ir Romberg	Error in Romberg
1	4	1.71831884192175		
2	8	1.71828415469990	1.71828184221844	1.376e-08
3	16	1.71828197405189	1.71828182867536	2.163e-10
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Simpson's rule error is $O(h^4)$ but Romberg based on Simpson is $O(h^6)$

As n is doubled and h = 1/n the error goes down by 2^6= 64

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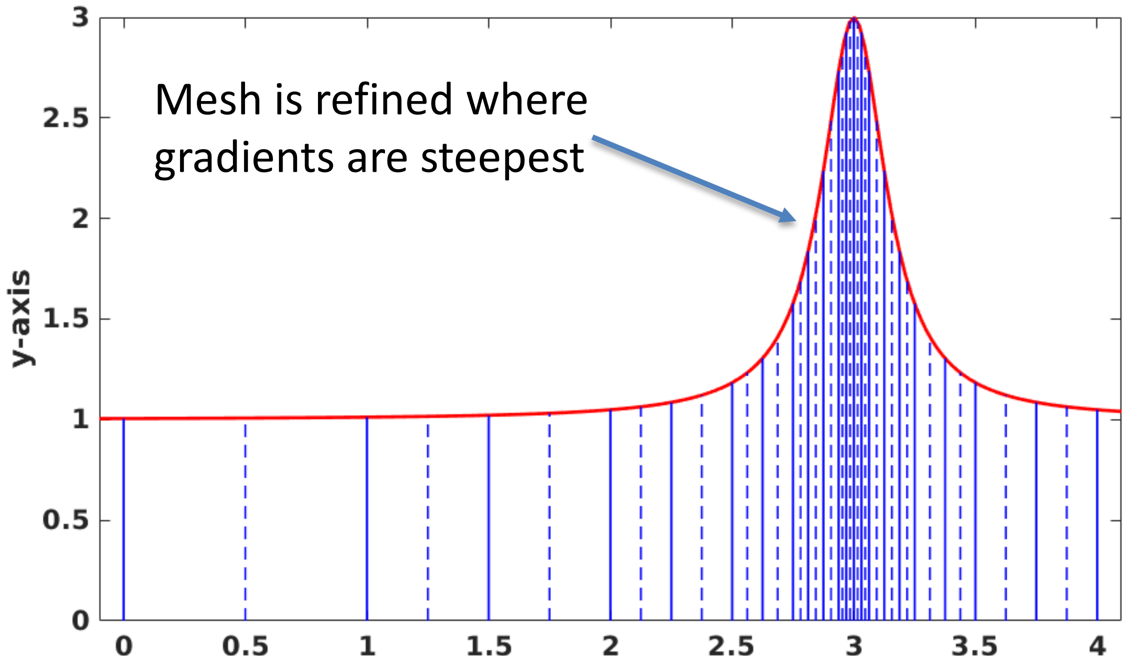
Example Lorentzian Function Integral

$$\int_0^4 1+\frac{1}{\pi}\frac{\omega}{(x-x_0)^2+\omega^2}dx, \quad x_0=3 \text{ and } \omega=1/3$$

Using and adaptive Simpson's rule to achieve an accuracy of 1.0e-6



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Use of adaptive methods

- Many similar examples in interpolation, quadrature and solution of differential equations