CS 3200
Introduction to Scientific Computing

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Topic: Adaptive Methods

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
- Examples are linear interpolation and quadrature
- In both cases the error estimate depends on?

Motivation

- When implementing methods we would like them to automatically control the error
- Examples are linear interpolation and quadrature
- In both cases the error estimate depends on?
- The step size and the second derivative of the function $\Delta x^2 \ and \ f"(\zeta)$

Estimating Linear Interpolation Error

$$f(x+h) = f(x) + h\frac{df}{dx} + \frac{h^2}{2}\frac{d^2 f}{dx^2} + \frac{h^3}{6}\frac{d^3 f}{dx^3} + O(h^4)$$

$$f(x-h) = f(x) - h\frac{df}{dx} + \frac{h^2}{2}\frac{d^2 f}{dx^2} - \frac{h^3}{6}\frac{d^3 f}{dx^3} + O(h^4)$$

Adding these equations and subtracting 2*f*(*x*) gives

$$f(x+h) + f(x-h) - 2f(x) = h^2\frac{d^2 f}{dx^2} + O(h^4)$$

$$\frac{d^2 f}{dx^2} = \frac{f(x+h) + f(x-h) - 2f(x)}{h^2} + O(h^2)$$

Error of Linear Polynomial Interpolation

For a linear interpolating polynomial, the error on each interval is given by the second derivative of the unknown function

$$E_i = (x - x_i)(x - x_{i+1}) \frac{f^{"}(\xi)}{6}$$

$$E_i \le h^2 \frac{f^{"}(\xi)}{6}$$

ξ is located in some interval containing the unknown and the data: $[x_i, x_{i+1}]$

For Example Interpolation

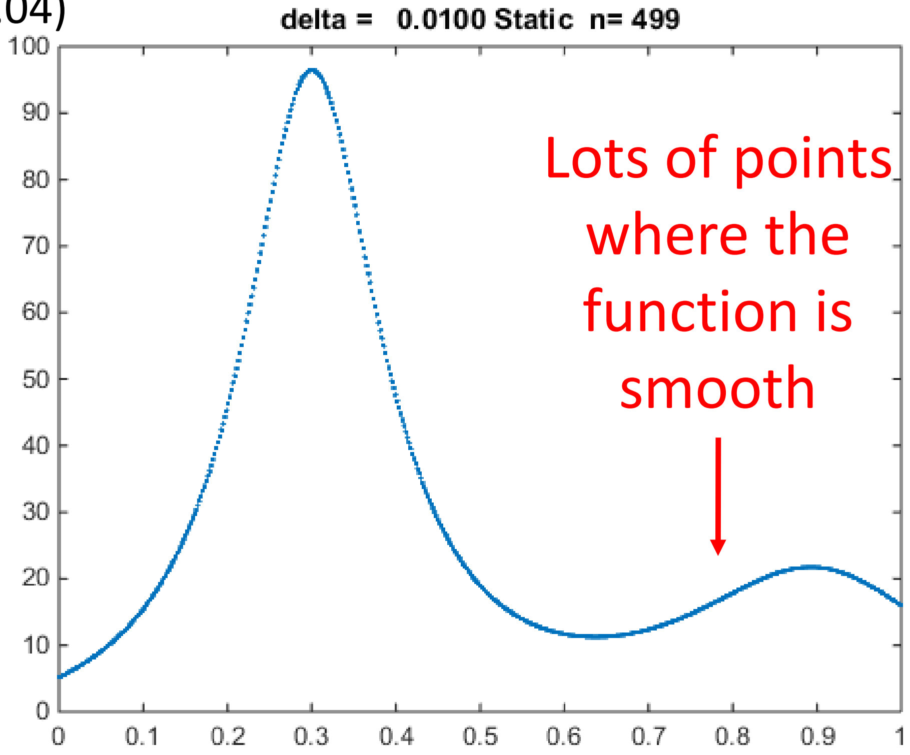
- Error over an interval at any point bounded by* maximum second derivative x maximum stepsize $M_2 \frac{h_{\max}^2}{6}$
- If we require this error in each interval to be less than a user specified error *tol* then number of points *n* defined by

$$h_{\max}^2 \le \frac{6tol}{M_2}, h_{\max} = \frac{(b-a)}{(n-1)}$$

$$n \ge 1 + (b-a)\sqrt{M_2 / 6}$$

Fixed linear Interpolation Applied to Matlab humps function

```
%   humps(x) = 1/((x-.3)^2 + .01)  +  1/((x-.9)^2+.04)
 close all
% Second derivative estimate based
% on divided differences
 z = linspace(0,1,101);
 humpvals = humps(z);
 M2 = max(abs(diff(humpvals,2)/(.01)^2));
 delta = 0.01
 figure
 [x,y] = pwLStatic('humps',M2,0,1,delta);
 plot(x,y,'.');
 title(sprintf('delta = %8.4f Static  n= %2.0f',delta,length(x)))
```

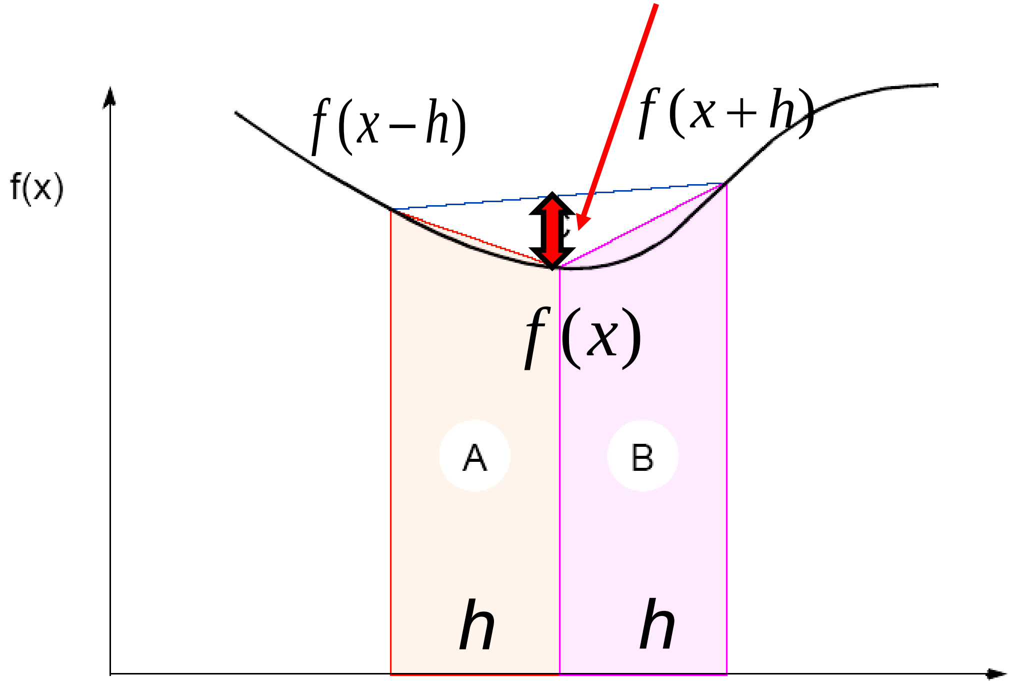


Adaptive Interpolation

Solution adapts to shape of curve. Use two approximations

$$Error = \left(\frac{f(x+h) + f(x-h)}{2} - f(x)\right)$$

$$\approx \frac{h^2}{2}\frac{d^2 f}{dx^2}$$



Implementation MATLAB pwLAdapt

An interval if accepted if $Error = (\frac{f(x+h) + f(x-h)}{2} - f(x)) < tol$

Or if *h*< *hmin* *where tol is a user-defined tolerance*

Intervals are recursively defined until the test is passed or the minimum step hmin reached

This is implemented in the Matlab file pwLAdapt.m

Please see the Canvas webpage

pwLAdapt(xL,fL,xR,fR,delta,hmin)

```
if (xR-xL) <= hmin
    % Subinterval is acceptable form mesh
  else
    mid  = (xL+xR)/2;
    fmid = f(mid);
    if (abs(((fL+fR)/2) - fmid) <= delta )
      % Subinterval accepted form mesh
    else
      % Produce left and right partitions, then synthesize.
      [xLeft,yLeft]   = pwLAdapt(xL,fL,mid,fmid,delta,hmin);
      [xRight,yRight] = pwLAdapt(mid,fmid,xR,fR,delta,hmin);
%       form mesh
      end
  end
```

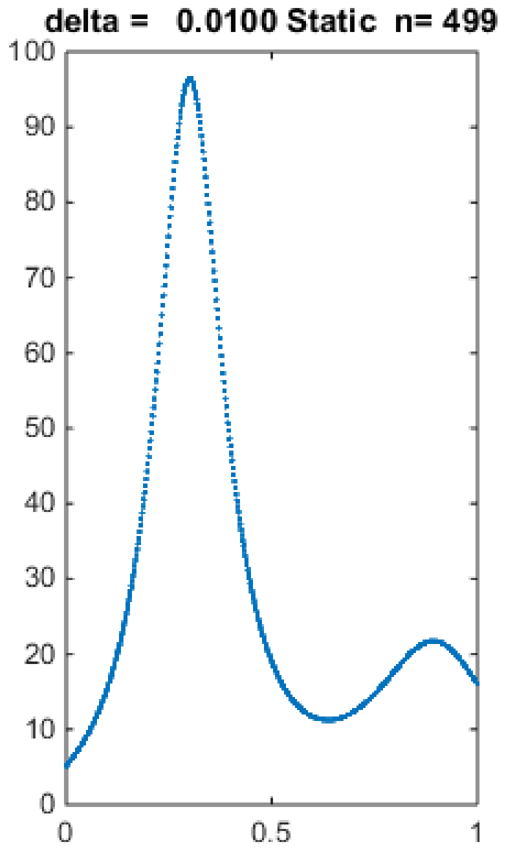
Note there is no mesh formation here just the logic, see full code for the rest

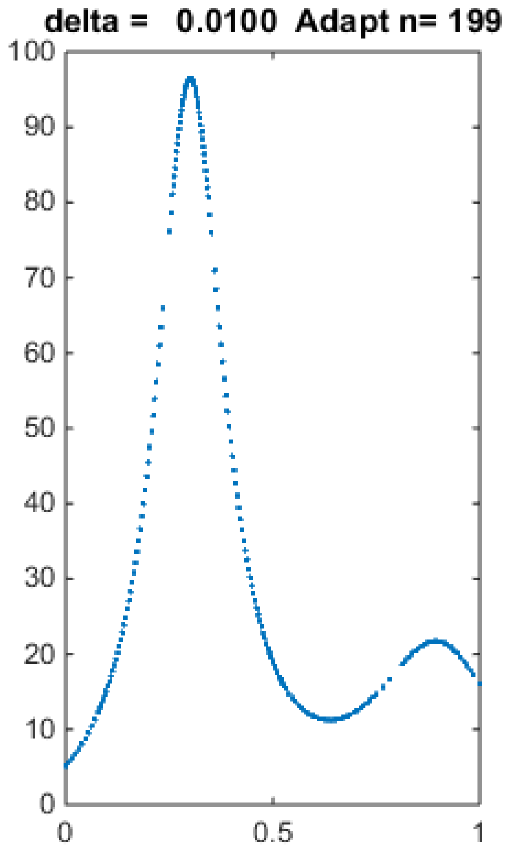
Recursive calls

```
% Script File: ShowPWL2    Compares pwLStatic and pwLAdapt on [0,1] using the function
%   humps(x) = 1/((x-.3)^2 + .01)  +  1/((x-.9)^2+.04)
  close all
z = linspace(0,1,101);
  humpvals = humps(z);
  M2 = max(abs(diff(humpvals,2)/(.01)^2));
  delta = 0.01
    figure
    [x,y] = pwLStatic('humps',M2,0,1,delta);
    subplot(1,2,1)
    plot(x,y,'.');
    title(sprintf('delta = %8.4f Static  n= %2.0f',delta,length(x)))
    [x,y] = pwLAdapt('humps',0,humps(0),1,humps(1),delta,.001);
    subplot(1,2,2)
    plot(x,y,'.');
    title(sprintf('delta = %8.4f  Adapt n= %2.0f',delta,length(x)))
```

Comparison of Adaptive vs Static

The adaptive approach uses only half the points





Richardson Extrapolation – an easy way to estimate the error

Let $I(trap, h)$ be the approximate value of the integral with the Trapezoidal rule and step h. Let $Iexact$ be the exact value.

Then $$Error(h) = Iexact - I(trap, h) \approx \frac{-h^2}{12} f''(\zeta_1)$$

and $$Error(\frac{h}{2}) = Iexact - I(trap, \frac{h}{2}) \approx \frac{-h^2/4}{12} f''(\zeta_1)$$

We don't know these but we know these

Extrapolation – an easy way to estimate the error

Subtract the bottom equation from the top one

$$Iexact - I(trap, h) \approx \frac{(-h^2)}{12} f''(\zeta_1)$$

- -

$$Iexact - I(trap, \frac{h}{2}) \approx \frac{1}{4}\frac{(-h^2)}{12} f''(\zeta_1)$$

$=$ $=$

$$-I(trap, h) + I(trap, \frac{h}{2}) \approx \frac{3}{4}\frac{(-h^2)}{12} f''(\zeta_1)$$

Extrapolation – an easy way to estimate the error

Hence

$$\frac{3}{4}\frac{(-h^2)}{12} f''(\zeta_1) \approx -I(trap,h) + I(trap,\frac{h}{2})$$

or

$$\frac{4}{3}(-I(trap,h) + I(trap,\frac{h}{2})) \approx \frac{(-h^2)}{12} f''(\zeta_1)$$

or

$$Error(h) \approx \frac{4}{3}(-I(trap,h) + I(trap,\frac{h}{2}))$$

Extrapolation – an easy way to estimate the error

As

$$Error(h) \approx \frac{4}{3}(-I(trap,h) + I(trap,\frac{h}{2}))$$

and

$$Error(\frac{h}{2}) \approx \frac{1}{4} Error(h)$$

then

$$Error(\frac{h}{2}) = \frac{1}{3}(-I(trap,h) + I(trap,\frac{h}{2}))$$

Extrapolation – an easy way to estimate the error

As

$$Error(h) \approx \frac{4}{3}(-I(trap,h) + I(trap,\frac{h}{2}))$$

and

$$Error(\frac{h}{2}) \approx \frac{1}{4} Error(h)$$

then

$$Error(\frac{h}{2}) = \frac{1}{3}(-I(trap,h) + I(trap,\frac{h}{2}))$$

In other words by repeating the calculation twice with steps h and h/2 and comparing the answers on the basis of the theory results Wen can estimate the error in either result

Extrapolation – Simpson's rule on one interval

Let $I(Simp,h)$ be the approximate value of the integral on one interval with Simpsons rule and step h.

Let $Iexact$ be the exact value.

Then $$Iexact - I(Simp,h) \approx \frac{-h^5}{2880} f^{(iv)}(\zeta_1)$$

and $$Iexact - I(Simp,\frac{h}{2}) \approx \frac{-h^5/32}{2880} f^{(iv)}(\zeta_1)$$

Extrapolation – Simpson's rule on one interval

Subtracting $Iexact - I(Simp, \frac{h}{2})$ from $Iexact - I(Simp, h)$

shows that the difference between the numerical solutions

gives an estimate of the error

$$I(Simp, \frac{h}{2}) - I(Simp, h) \approx \frac{-h^5}{2880} f^{(iv)}(\zeta_1)(1 - \frac{1}{32})$$

multiplying rhs by $\frac{32}{31}$ estimates the error in $I(Simp, h)$ and

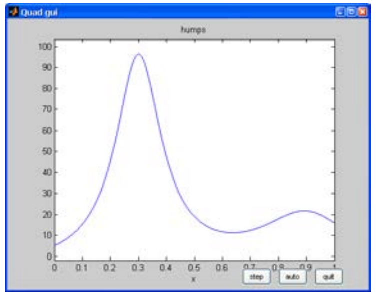
multiplying by $\frac{1}{31}$ estimates the error in $I(Simp, \frac{h}{2})$

Matlab QUADTX

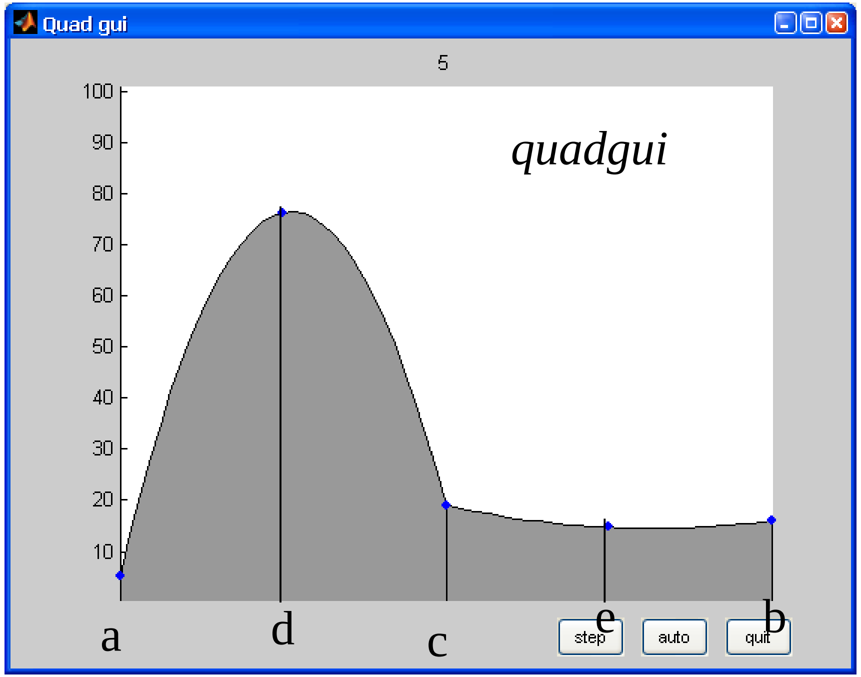
- Uses Simpson’s Rule recursively until the error on each interval is less than *tol* which is user supplied
- A decision to subdivide each interval is made when the error estimated is > *tol*
- Please see the code for an example of this recursive approach

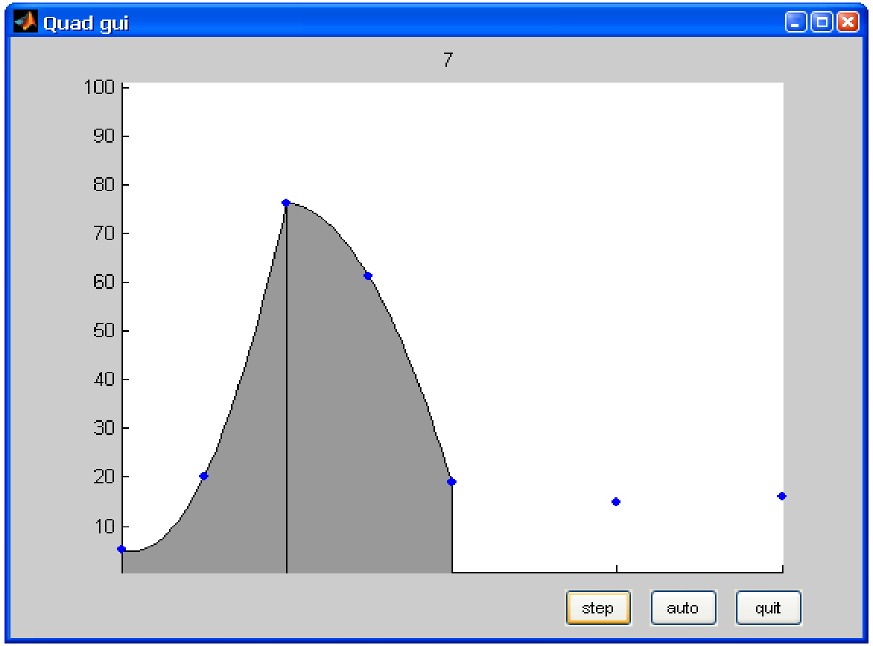
Example of Quadtx in use with the humps example

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



Plot of the function




Quad gui
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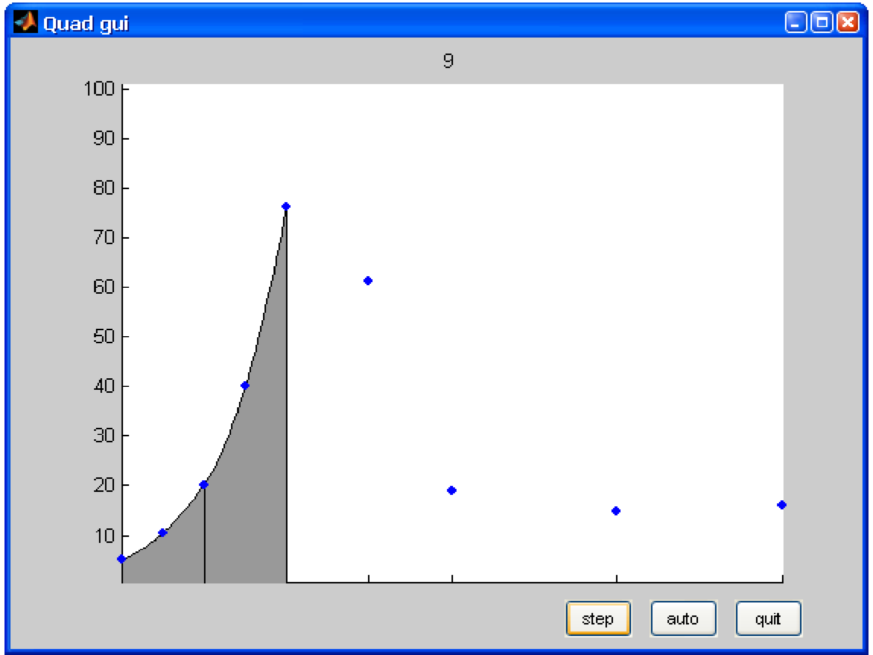
Iterations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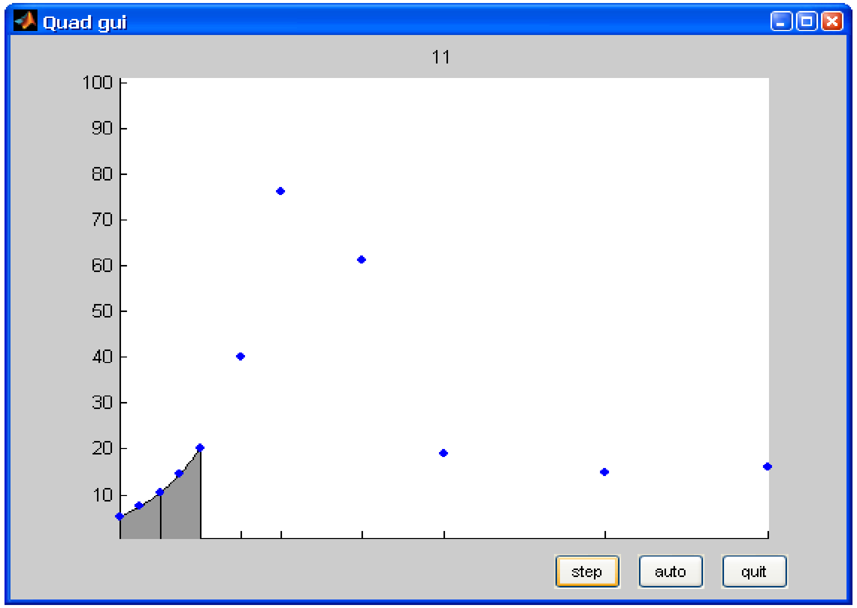
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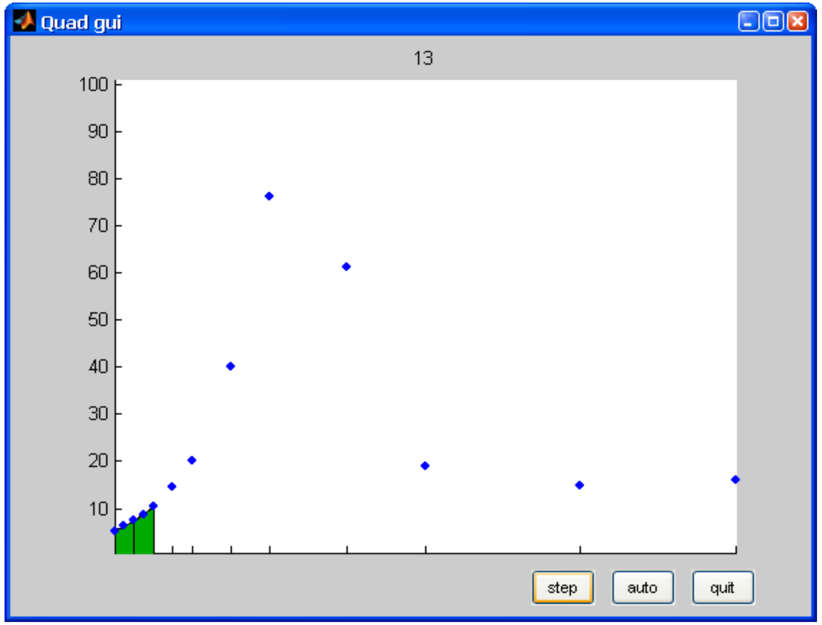
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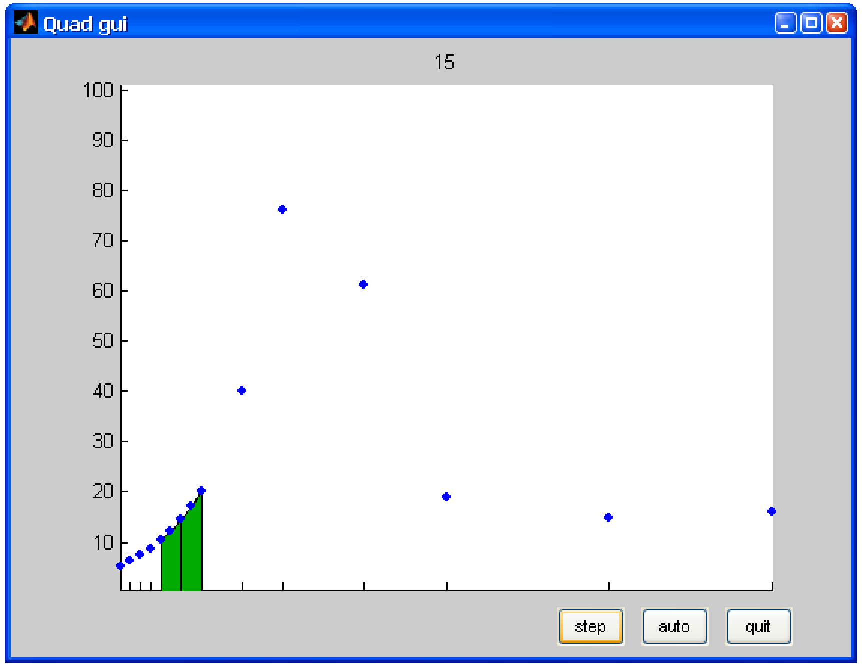
Iterations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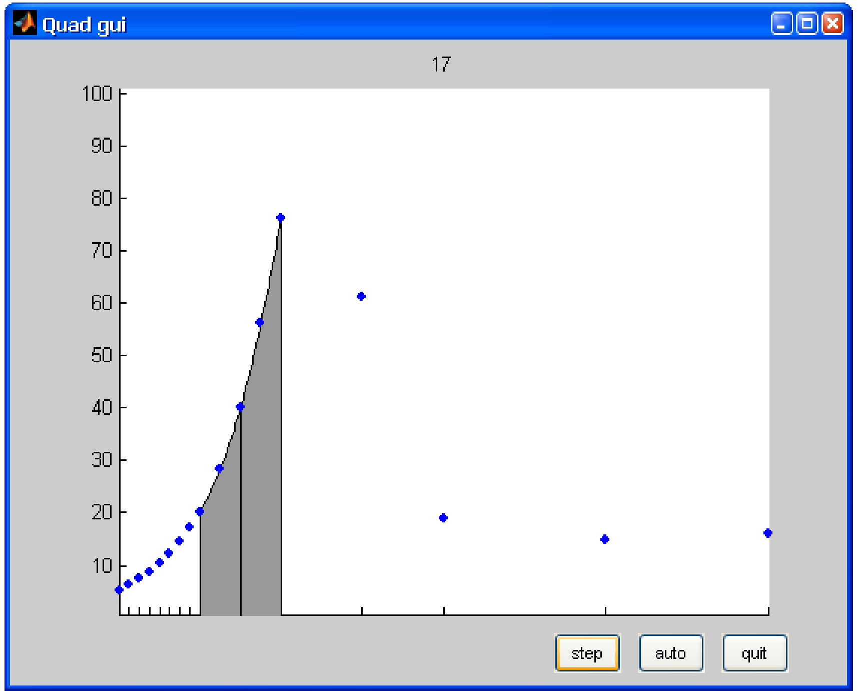
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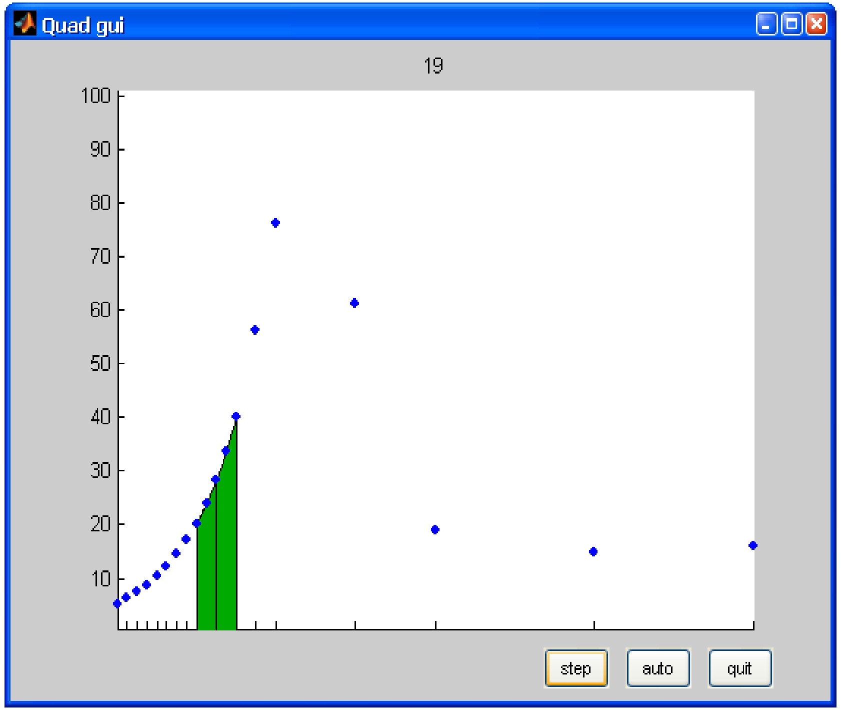
Iterations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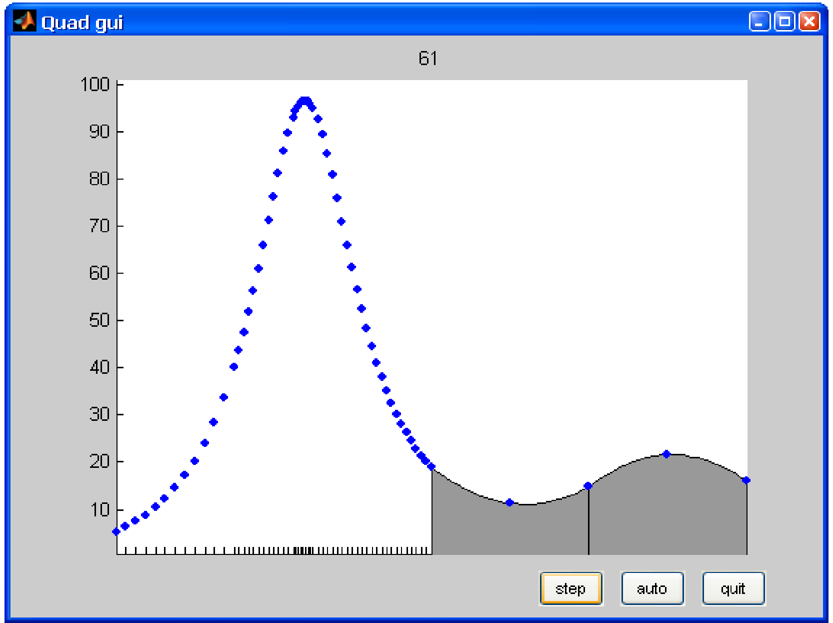
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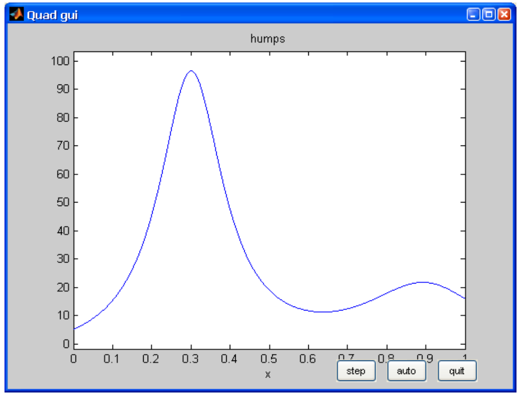
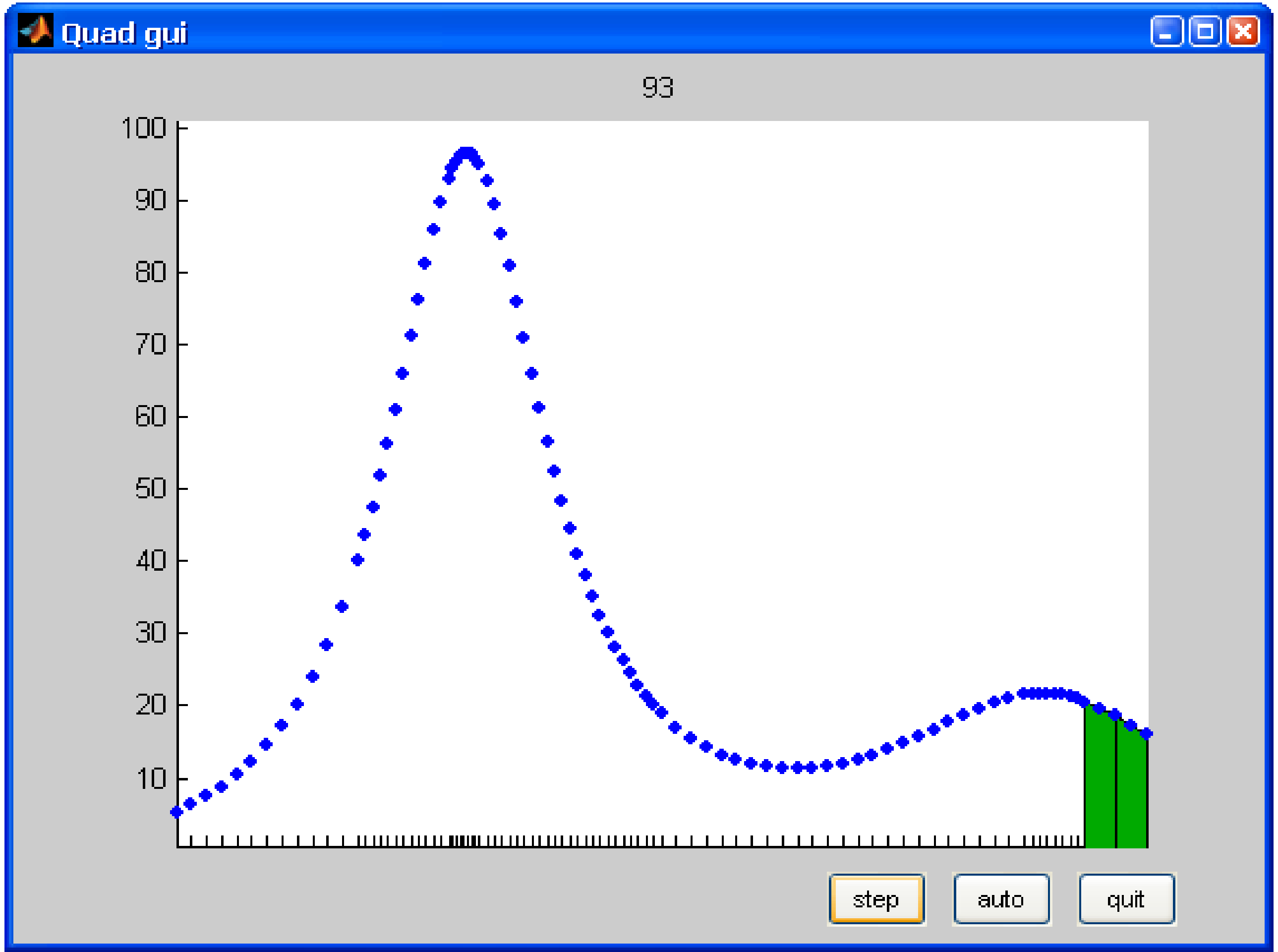
Iterations

Last Step



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

Use of adaptive methods

- Many similar examples in interpolation, quadrature and solution of differential equations
- More challenging to implement and run especially in parallel as we do not know where the work will be in advance.
- Current state of the art is that these kind of methods run on the very largest computers e.g. the Uintah code developed here.