B1 Numerical Algorithms

Computational Class - MT 2023

Wes Armour 30th October 2023



a. Derive the five point central difference formula:

$$f_n' \approx \frac{f_{n-2} - 8f_{n-1} + 8f_{n+1} - f_{n+2}}{12h}$$

b. Demonstrate that the error is $O(h^4)$



a) and to obtain the five point formula taylor sizes expend: $f(x \pm \delta x) = f(x) \pm \delta x \frac{df(x)}{dx} + \frac{\delta x^2}{d^2f(x)} \pm \frac{\delta x^3}{3!} \frac{d^3f(x)}{dx^3} + \frac{\delta x^4}{4!} \frac{d^3f(x)}{dx^3}$ $f(x \pm 2\delta x) = f(x) \pm 2\delta x \frac{df(x)}{dx} + \frac{4\delta x^2}{3!} \frac{d^3f(x)}{dx^3} + \frac{8\delta x^3}{3!} \frac{d^3f(x)}{dx^3} + \frac{16\delta x^4}{4!} \frac{d^3f(x)}{dx^3}$ $dx = \frac{1}{2!} \frac{dx^2}{dx^3} + \frac{8\delta x^3}{3!} \frac{d^3f(x)}{dx^3} + \frac{16\delta x^4}{4!} \frac{d^3f(x)}{dx^3}$



Next note
$$f(x+5x) - f(x-5x) = 25x d(x) + 25x^3 d'(x) + 25x^3 d'(x) + 25x^3 d'(x)$$

$$\int (3x+25x) - f(x-25x) = 4 \int 3x \frac{d^{2}f(x)}{dx} + \frac{16 \int 3x^{2}}{3!} \frac{d^{2}f(x)}{dx^{2}} + \frac{32}{3!} \int \frac{5}{3!} \frac{1}{3!} \frac{1}{$$





10 eliminate
$$O(5x^3)$$
.

8 x $O - O = 8f(x-8x) - 8f(x-8x) - f(x+25x) - f(x-25x) + O(1)$

= $166x df(x) - 45x df(x) + O(1) = 12dx df(x) + O(1)$

doc the

$$\frac{df(x)}{dx} = \frac{f(x-25x) - 8f(x-5x) - 8f(x-5x) - f(x-25x) + 0(69)}{25x}$$

as regarred



a. Using MATLAB, write a code to implement left point rectangular dissection and integrate the following function between x=-4 and x=4

$$f(x) = \frac{1}{2\pi\sigma^2} exp(-(x^2)/2\sigma^2)$$



```
close all;
clear all;
clc;
% Integration range
start point = -4.0;
end point = 4.0;
% The exact analytic result
exact = 1;
% The gaussian function
xg = [start point:.01:end point];
yg = normpdf(xg, 0, 1);
% Number of steps to use
steps=10;
% Calculate our step size
h=(end point-start point)/steps;
% Create a vector that steps through our range
k=start point:h:end point;
```

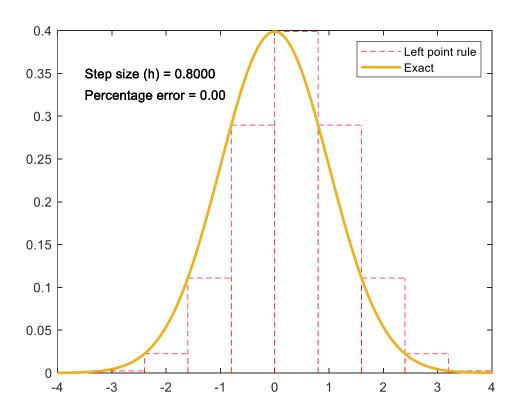


```
% Set the sum that will hold our result to zero
int lpr=0.0;
% Calculate the value of the function at each left point
y point = \exp(-((k).^2)/2)/sqrt(2*pi);
% Create a vector that holds the area of each strip
lpr=y point.*h;
% Sum up all of the areas
int lpr = sum(lpr, 'all')
% Calcluate the error between the exact analytic result and our
left point
% rule approximation
error = (abs(int lpr - exact)/exact).*100;
% Open a figure to plot to
figure;
```



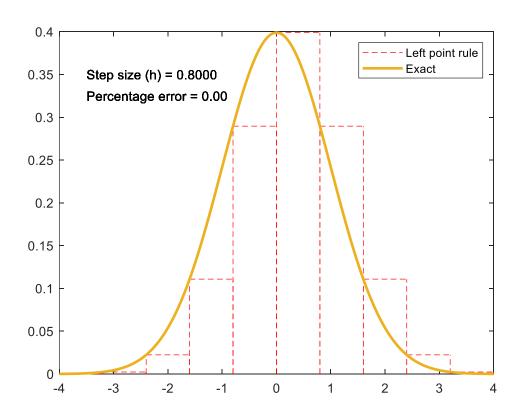
```
% Create a fancy plot!
% Plot the rectangles
for i=1:1:steps
    lp=(i-1)*h+start point;
    rp=(i)*h+start point;
    pt=plot([lp rp], [y point(i) y point(i)], '--r');
    hold on
    plot([rp rp], [0 y point(i)], '--r');
    hold on
    plot([lp lp], [0 y point(i)], '--r');
    hold on
    txt = ['Step size (h) = 'num2str(h, '%4.4f')];
    text(-3.5, 0.35, txt);
    txt = ['Percentage error = ' num2str(error,'%4.2f')];
    text(-3.5, 0.325, txt);
end
% Plot the actual function
hold on
pe=plot(xg, yg, '-', 'LineWidth', 2);
legend([pt pe],'Left point rule','Exact');
hold off
drawnow
```







b. Estimate the error in your result. What do you notice?

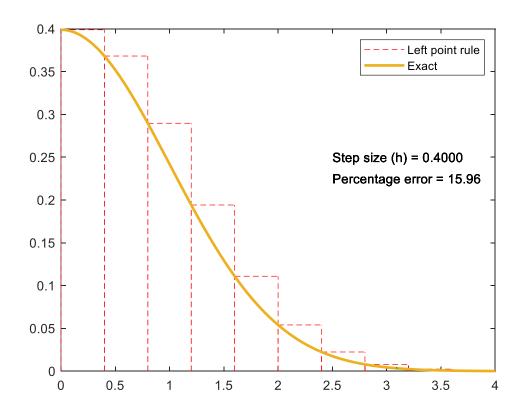




c. Perform a) and b) above for the range x=0 and x=4.



```
% The exact analytic result
exact = 0.5;
% Integration range
start point = 0.0;
end point = 4.0;
 txt = ['Step size (h) = 'num2str(h,'%4.4f')];
 text(2.5,0.25,txt);
 txt = ['Percentage error = ' num2str(error,'%4.2f')];
 text(2.5,0.225,txt);
```





a. Using MATLAB, implement the midpoint rule to integrate the following function between x=-4 and x=4

$$f(x) = \frac{1}{2\pi\sigma^2} exp(-(x^2)/2\sigma^2)$$



```
close all;
clear all:
clc;
% Integration range
start point = -4.0;
end point = 4.0;
% The exact analytic result
exact = 1.0;
% The gaussian function
xg = [start point:.01:end point];
yg = normpdf(xg, 0, 1);
% Number of steps to use
steps=10;
% Calculate our step size
h=(end point-start point)/steps;
% Create a vector that steps through our range
k=start point:h:end point;
```

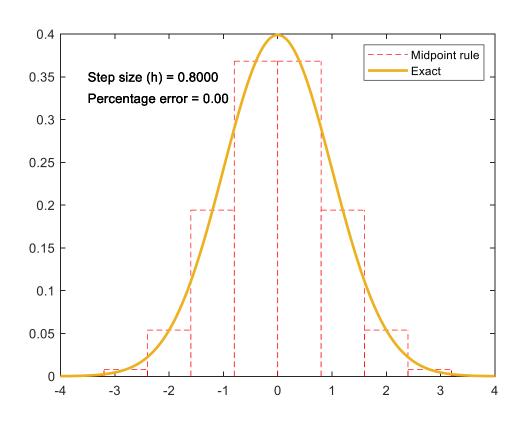


```
% Set the sum that will hold our result to zero
int mpr=0.0;
% Calculate the value of the function at each midpoint
y point = \exp(-((k+0.5*h).^2)/2)/sqrt(2*pi);
% Create a vector that holds the area of each strip
mpr=y point.*h;
% Sum up all of the areas
int mpr = sum(mpr, 'all')
% Calcluate the error between the exact analytic result and our
midpoint
% rule approximation
error = (abs(int mpr - exact)/exact).*100;
% Open a figure to plot to
figure;
```



```
% Create a fancy plot!
% Plot the rectangles
for i=1:1:steps
    lp=(i-1)*h+start point;
    rp=(i)*h+start point;
    pt=plot([lp rp], [y point(i) y point(i)], '--r');
    hold on
    plot([rp rp], [0 y point(i)], '--r');
    hold on
    plot([lp lp], [0 y point(i)], '--r');
    hold on
    txt = ['Step size (h) = 'num2str(h, '%4.4f')];
    text(-3.5, 0.35, txt);
    txt = ['Percentage error = ' num2str(error,'%4.2f')];
    text(-3.5, 0.325, txt);
end
% Plot the actual function
hold on
pe=plot(xg, yg, '-', 'LineWidth', 2);
legend([pt pe],'Midpoint rule','Exact');
hold off
drawnow
```



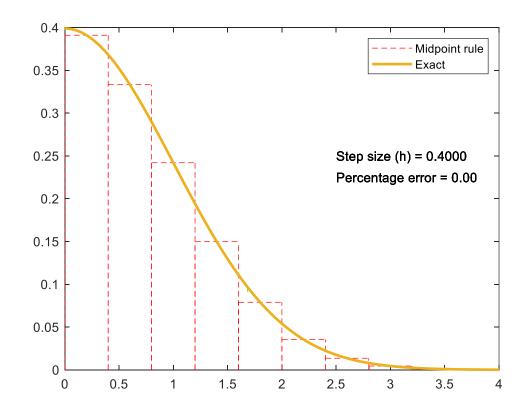




Bonus Question! – how about the range:

$$x = 0$$
 and $x = 4$

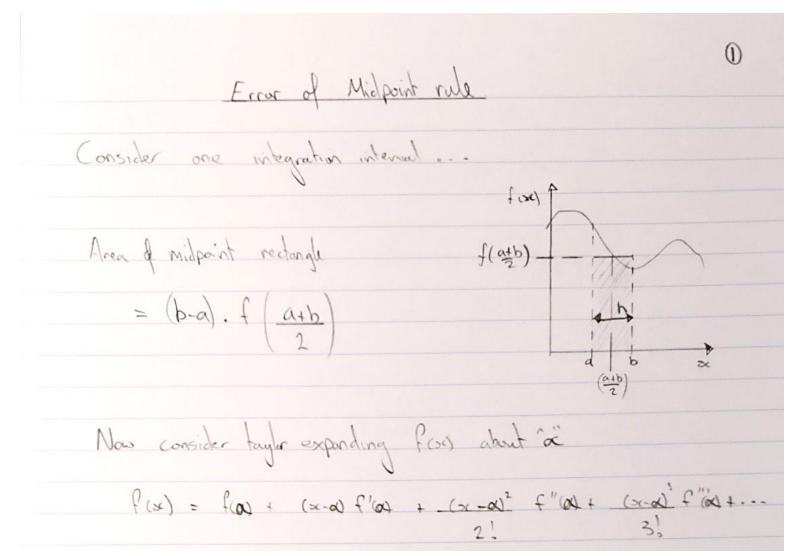




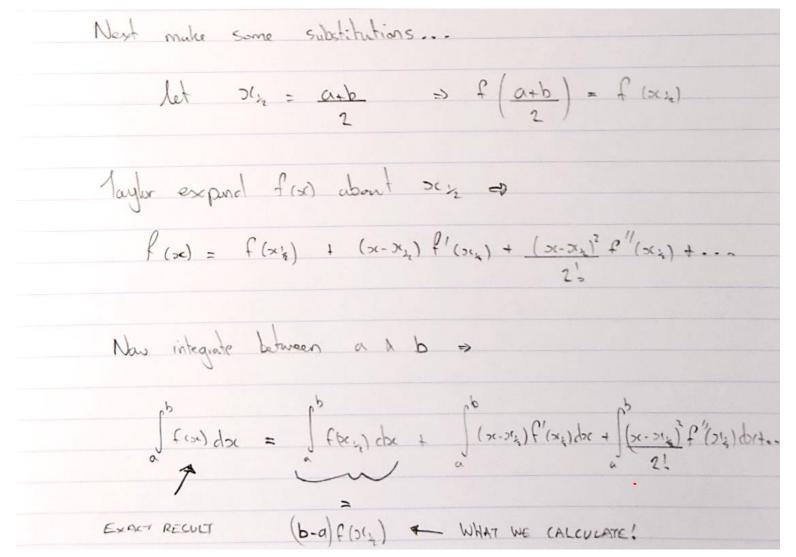


b. Derive the error of the midpoint rule.

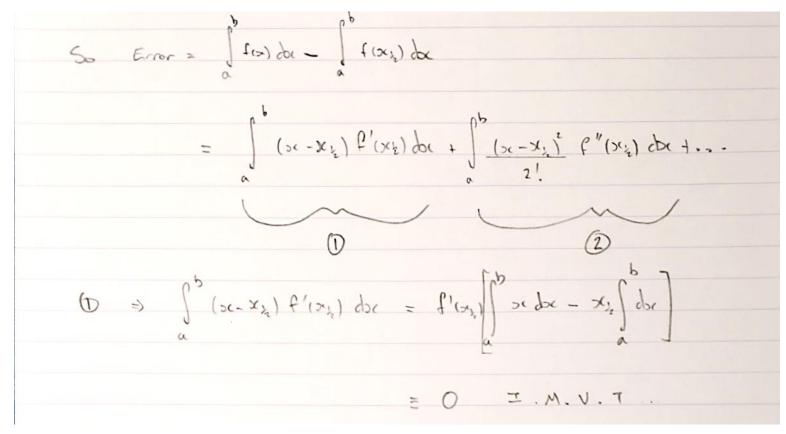




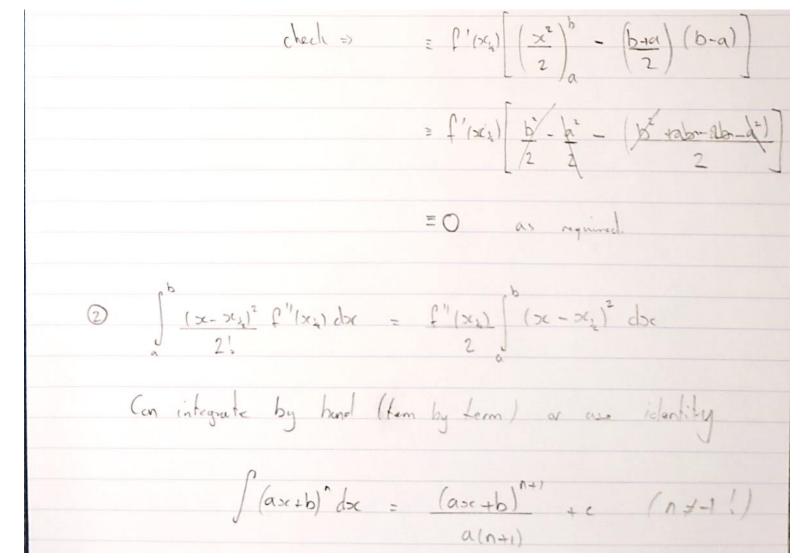






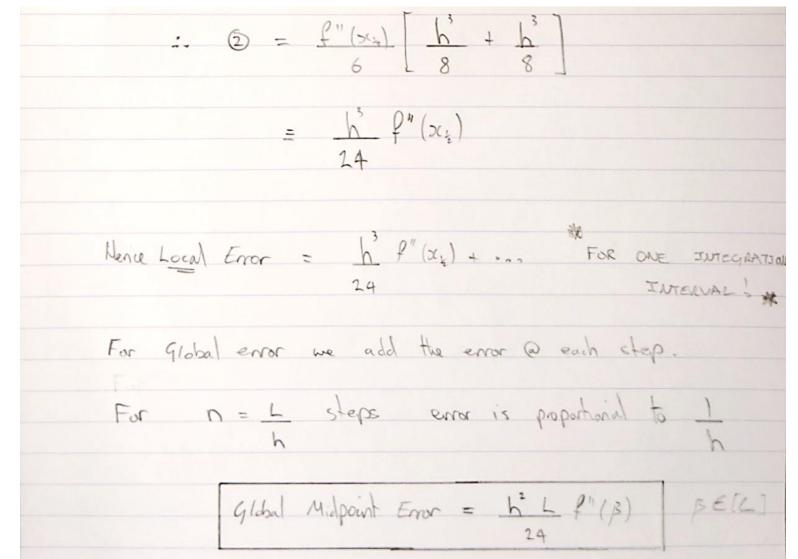














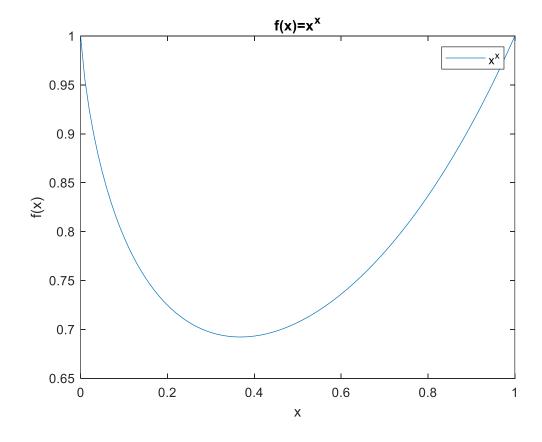
a. Use Richardson's method and the forward difference to gain an accurate estimate for the derivative of

$$f(x) = x^x$$

At x = 0.3679



```
clear all;
close all;
clc;
% We want to estimate dy/dx at x=0.3679
start point=0.3679;
end point=1.0;
% To use Richardson extrapolation we need
% several values of step size
step=0.1;
max step=0.5;
min step=0.2;
% The actual function and derivative
x = 0:0.01:end point;
y = (x.^x);
dydx = (x.^x).^*(log(x)+1);
dydx exact=0;
% Plot of f(x)
figure;
plot(x,y,'-');
legend('x^x');
xlabel('x'), ylabel('f(x)');
title('f(x)=x^x');
```

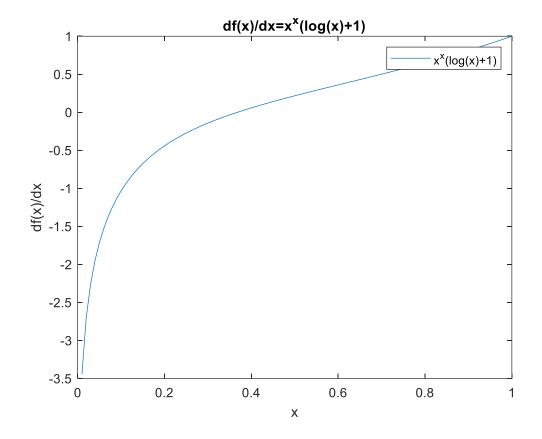




```
% Plot of f'(x)
figure;
plot(x,dydx,'-');
legend('x^x(log(x)+1)');
xlabel('x'),ylabel('df(x)/dx');
title('df(x)/dx=x^x(log(x)+1)');

% Arrays to hold different step size values
% and forward difference values at those points.
forward_difference_size = [];
h_size = [];

% Open a figure to plot to
figure;
```





```
% Next step through the step sizes
for h=max step:-step:min step
    % Values of x and x+h
   x=start point;
   x plus h=x+h;
    % Forward difference approximation
    forward difference = ((x plus h^x plus h) - (x^x))/h;
    % Store this step size and value of forward difference
    forward difference size = [ forward difference size...
         forward difference ];
    h size = [ h size h];
    % Clear the figure
    clf;
    % Plot the actual function and the forward difference
    subplot(3,1,1);
    fplot(@(x) (x.^x), [0,1], 'b');
   xlabel('x'), ylabel('y');
    hold on;
   y=(x^x);
    y h=(x plus h^x plus h);
    plot([x,x plus h],[y,y h],'-o');
    legend('f(x)=x^x)');
    axis([0 1 0.6 1]);
```



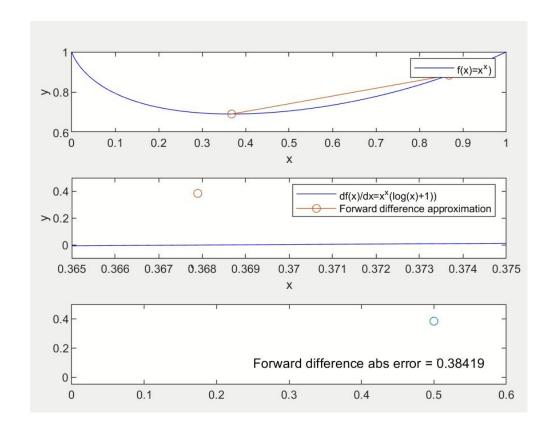
```
% Plot the actual df(x)/dx against the forward difference
% approximation at the x point of interest x=1/e
subplot(3,1,2);
fplot(@(x) (x.^x).^*(\log(x)+1), [0,1], 'b');
xlabel('x'), ylabel('y');
hold on;
plot(x, forward difference, '-o');
legend('df(x)/dx=x^x(\log(x)+1))','Forward difference...
      approximation');
axis([0.365 \ 0.375 \ -0.1 \ 0.5]);
% Plot the forward difference against step size
subplot(3,1,3);
plot(h size, forward difference size, '-o');
axis([0.0 max step+0.1 -0.05 0.5]);
txt = ['Forward difference abs error = '...
    num2str(abs(dydx exact - forward difference))'.'];
text(0.25, 0.10, txt);
pause (0.75);
drawnow;
```

end



```
% Fit a polynomial (straight line for O(h) error in our algorithm
P = polyfit(h_size, forward_difference_size,1);
% Plot the extrapolation based on the above fit x=[0:0.001:h_size(1)];
yfit = P(1).*x+P(2);
P(2)
hold on;
plot(x,yfit,'r-.');
% Calculate the Richardson extrapolation error and print r_error=abs(dydx_exact - P(2));
txt = ['Richardson extrapolation abs error = 'num2str(r_error)'.'];
text(0.025,0.415,txt);
drawnow;
```







b. Derive the analytic derivative of the function, use this to find the minima of the function.



$$Q(4, b) \frac{d}{dbc} = \frac{1}{2} \ln x^{2c}$$
but
$$\ln (a^{b}) = \frac{1}{2} \ln (a)$$

$$\frac{d}{dx}$$
 $\frac{d}{dx}$



but
$$\frac{d}{dx} = \frac{2x}{x} + \frac{1}{x} \ln x$$

$$\frac{d}{dx} = \frac{2x}{x} \left(\ln x + 1 \right).$$



a. Write a predictor-corrector code to solve the following ODE

$$y'' = \frac{d^2y}{dx^2} = -y$$



```
clear all;
close all;
clc;

% Start and end points.
x_start=0.0;
x_end=11.0;

% The analytic solution to compare numerical results
xx=[x_start:0.001:x_end]';
fn=cos(xx);

% Open a figure to plot to
figure;
```



```
% Loop over a different number of steps to see how
% step size influences solution
for numSteps=2:1:100;
    % clear the figure
    clf;
    % Calculate step size
    h=(x end-x start)/numSteps;
    % The x range for our step size
   x=[x start:h:x end]';
    % Size vectors for Euler and PC methods.
    y=x;
    dydx=x;
    y pc=x;
    dydx pc=x;
    % Initial values (as in lecture).
   y(1) = 1;
    dydx=0;
    y pc(1)=1;
    dydx pc=0;
```

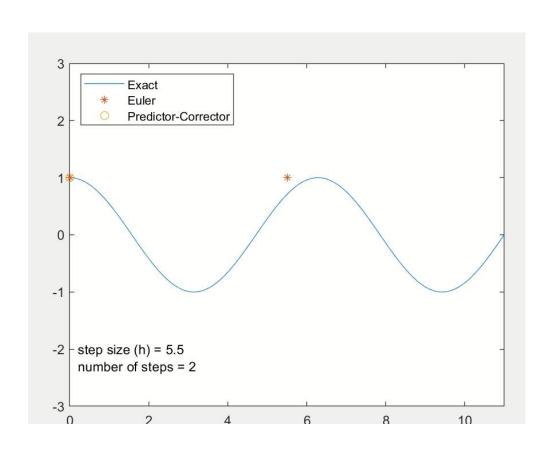


```
% Perform Euler
for i=1:(length(x)-1)
    y(i+1) = y(i) + h*dydx(i);
    dydx(i+1) = dydx(i) - h*y(i);
end
% Perform PC
for i=1:(length(x)-1)
    ypred=y pc(i)+h*dydx pc(i);
    dydxpred=dydx pc(i)-h*y pc(i);
    y pc(i+1)=y pc(i)+(h/2.0)*(dydx pc(i)+dydxpred);
    dydx pc(i+1) = dydx pc(i) - (h/2.0)*(y pc(i) + ypred);
end
% Plot Euler and PC results for this step
plot(xx,fn);
hold on
plot(x, y, '*');
hold on
plot(x,y pc, 'o');
```



```
% Axis, legend, step size adn number of steps
legend('Exact', 'Euler', 'Predictor-Corrector', 'Location', 'northwest');
axis([x_start x_end -3 3]);
txt = ['step size (h) = ' num2str(h)'.'];
text(0.2,-2.0,txt);
txt = ['number of steps = ' num2str(numSteps)'.'];
text(0.2,-2.3,txt);
drawnow;
if mod(numSteps,20)==0
% pause(5);
end
end
```







b. Given the boundary values y(0) = 1 and y(11) = 0, find the value of y'(0) using the shooting method. Verify your answer.



```
clear all;
close all;
clc;
% Start and end points
x start=0.0;
x end=11.0;
% The analytic solution to compare numerical results
xx=[x start:0.001:x end]';
fn=cos(xx);
% Let's work with a fixed number of steps, 40 is good.
numSteps=40;
% Calculate our step size
h=(x end-x start)/numSteps;
% The x points for us to evaluate at
x=[x start:h:x end]';
```

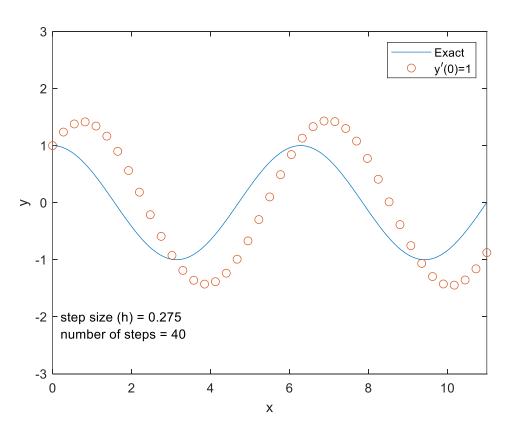


```
% Now we make two guesses dy(0)/dx = 1 and -1
% First Guess...
% Size our vectors
y1 pc=x;
dydx1 pc=x;
% Initial Value y(0)=1
y1 pc(1)=1;
% Initial guess dy(0)/dx = 1
dydx1 pc=1;
% Now perform predictor corrector
for i=1: (length(x)-1)
   ypred=y1 pc(i)+h*dydx1 pc(i);
   dydxpred=dydx1 pc(i)-h*y1 pc(i);
   y1 pc(i+1)=y1 pc(i)+(h/2.0)*(dydx1 pc(i)+dydxpred);
   dydx1 pc(i+1)=dydx1 pc(i)-(h/2.0)*(y1_pc(i)+ypred);
end
```



```
% Plot our results for the first guess
figure;
plot(xx,fn);
hold on
plot(x,y1_pc,'o');
hold on

legend('Exact','y^{\prime}(0)=1');
xlabel('x');
ylabel('y');
axis([x_start x_end -3 3]);
txt = ['step size (h) = ' num2str(h)'.'];
text(0.2,-2.0,txt);
txt = ['number of steps = ' num2str(numSteps)'.'];
text(0.2,-2.3,txt);
```



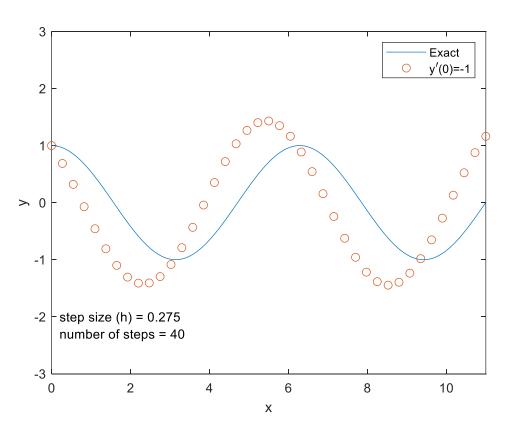


```
% Second Guess...
% Size our vectors
y2 pc=x;
dydx2 pc=x;
% Initial Value y(0)=1
y2 pc(1)=1;
% Next guess dy(0)/dx = -1
dydx2 pc=-1;
% Now perform predictor corrector
for i=1: (length(x)-1)
    ypred=y2 pc(i)+h*dydx2 pc(i);
    dydxpred=dydx2 pc(i)-h*y2 pc(i);
    y2 pc(i+1)=y2 pc(i)+(h/2.0)*(dydx2 pc(i)+dydxpred);
    dydx2 pc(i+1) = dydx2 pc(i) - (h/2.0) * (y2 pc(i) + ypred);
end
```



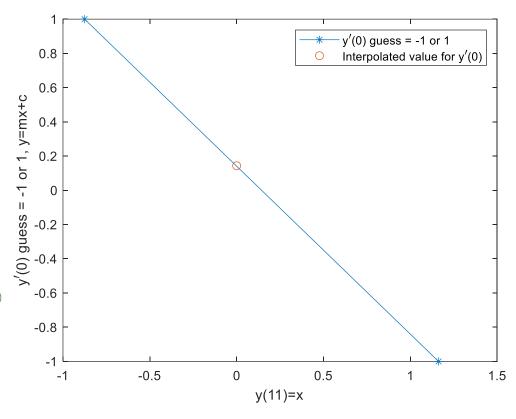
```
% Plot our results for the second guess
figure;
plot(xx,fn);
hold on
plot(x,y2_pc,'o');
hold on

legend('Exact','y^{\prime}(0)=-1');
xlabel('x');
ylabel('y');
axis([x_start x_end -3 3]);
txt = ['step size (h) = ' num2str(h)'.'];
text(0.2,-2.0,txt);
txt = ['number of steps = ' num2str(numSteps)'.'];
text(0.2,-2.3,txt);
```



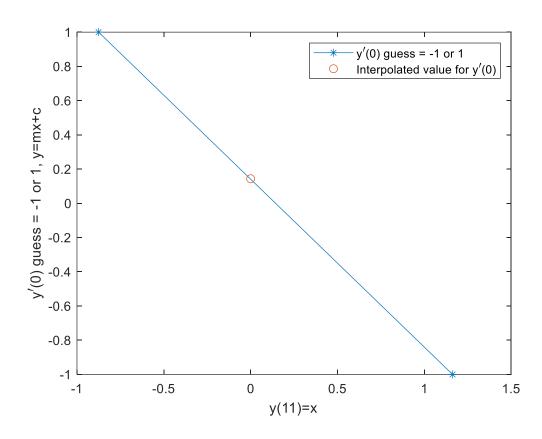


```
% Use our two quesses to interpolate a value for dy(0)/dx
% ??? HOW ???
% 1. I know that y(11)=0 for the correct value of dy(0)/dx
        -> It's one of my boundary conditions.
% 2. I know when dy(0)/dx = 1, y(11) = a
% 3. I know when dy(0)/dx = -1, y(11) = b
% 4. Now, "plot" y(11) values vs dy(0)/dx values,
        draw a straight line between them.
% 5. We know y(11)=0 for the correct value of dy(0)/dx
        -> Read off the "correct" value of dy(0)/dx, where y(11) = 0
% Create the plot
figure;
plot([ y1 pc(i+1) y2 pc(i+1)],[dydx1 pc(1) dydx2 pc(1)],'-*');
xlabel('y(11)=y=mx+c');
ylabel('y^{\text{prime}}(0) guess = {-1 or 1}');
hold on
```



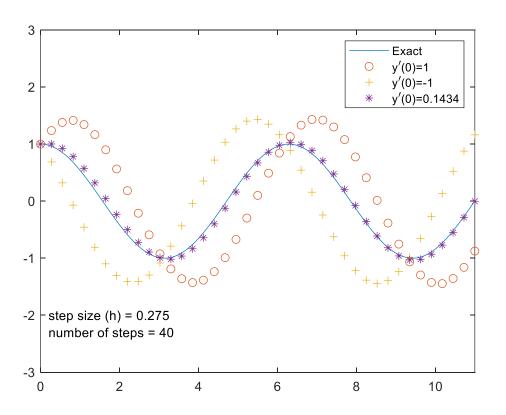


```
% Find "correct" value of dy(0)/dx, where y(11) = 0
grad=(y1 pc(i+1) - y2 pc(i+1))/(dydx1 pc(1)-dydx2 pc(1));
const=y1 pc(i+1)-dydx1 pc(1)*grad;
% Plot the result
plot([0],[const],'o');
legend('y^{\text{prime}}(0) guess = {-1 or 1}','Interpolated value for
y^{\prime}(0)');
% Use the "correct/estimate" value of dy(0)/dx and perform PC
again...
ye pc=x;
dydxe pc=x;
ye pc(1)=1;
dydxe pc=const;
for i=1: (length(x)-1)
    ypred=ye pc(i)+h*dydxe pc(i);
    ydpred=dydxe pc(i)-h*ye pc(i);
    ye pc(i+1) = ye pc(i) + (h/2.0) * (dydxe pc(i) + ydpred);
    dydxe pc(i+1) = dydxe pc(i) - (h/2.0) * (ye pc(i) + ypred);
end
```





```
% Finally plot all three solutions to compare
figure;
plot(xx, fn);
hold on
plot(x,y1 pc,'o');
hold on
plot(x, y2 pc, '+');
hold on
plot(x, ye pc, '*');
legend('Exact','y^{\prime}(0)=1','y^{\prime}(0)=-
1', 'y^{\gamma} \prime\ (0) =0.1434');
axis([x start x end -3 3]);
txt = ['step size (h) = 'num2str(h)'.'];
text(0.2, -2.0, txt);
txt = ['number of steps = ' num2str(numSteps)'.'];
text(0.2, -2.3, txt);
drawnow;
```





a. Solve the following PDE over the range x=0 to x=20, y=0 to y=100, with T=67.5 applied to one of the boundaries (for example T(1:xdim,1) = 67.5) and all other boundary points held at zero.

$$\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} = 0$$



```
% Clearing variables in memory and Matlab command screen
clear all;
close all;
clc;
% Dimensions of the simulation grid in x (xdim) and y (ydim)
directions
xdim=20; ydim=100;
% Error cutoff
cutoff=0.001;
% Initializing previous (T prev) and present (T now) temp
matrices
T \text{ now } = zeros(xdim, ydim);
T prev = zeros(xdim, ydim);
% Constant temperature of 67.5C applied to one boundary
T \text{ now}(1:xdim,1) = 67.5;
% Open a figure to plot to
figure;
% Set the iteration counter to one
t=1;
```



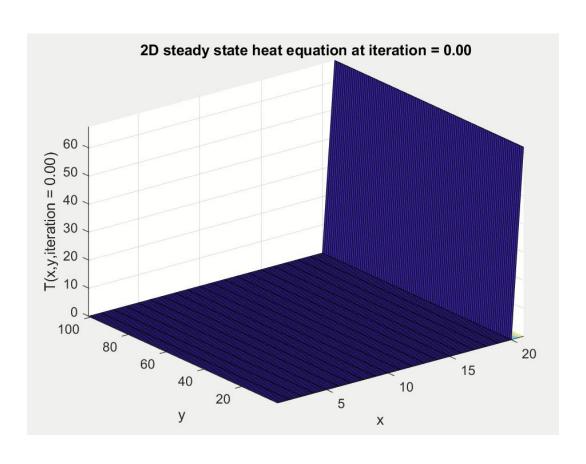
```
% Set a starting value for the error > cutoff;
error=2*cutoff;
% Keep iterating until the error between the current solution
% and last solution is below a predefined cutoff value
while error > cutoff
    % Solve for this time step, using the last time steps values
    % over our solution space (mesh).
    for i=2:1:xdim-1
        for j=2:1:ydim-1
            T now(i,j)=(T prev(i+1,j)+T prev(i-1,j)+T prev(i,j+1)+T prev(i,j-1))/4.0;
        end
    end
    % Calculate the difference between this time step and the last
    error=max(max(abs(T now-T prev)))
    % Now make this time step the last time step.
    T prev=T now;
```



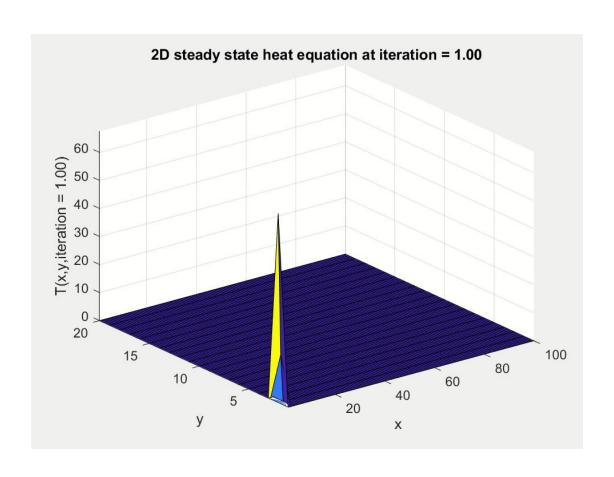
```
% Plot the current time step results
surfc(T_now);
title(sprintf('2D steady state heat equation at iteration = %1.2f',t),'Fontsize',11);
xlabel('x','Fontsize',11); ylabel('y','Fontsize',11);
zlabel(sprintf('T(x,y,iteration = %1.2f)',t),'Fontsize',11);
drawnow;

% Update the iteration counter and go again
t=t+1;
end
```







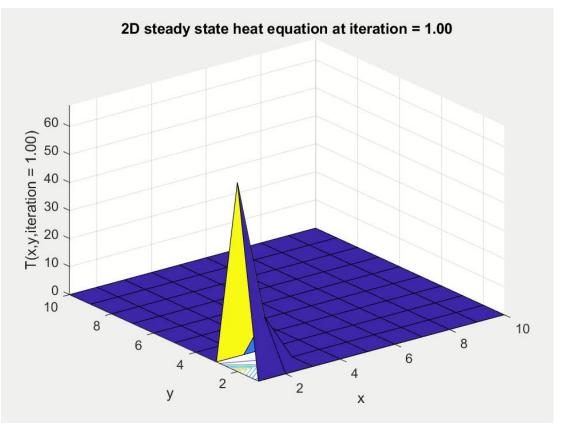




- b. Suggest how you might reach a quicker numerical solution.
- c. Implement your idea in MATLAB.

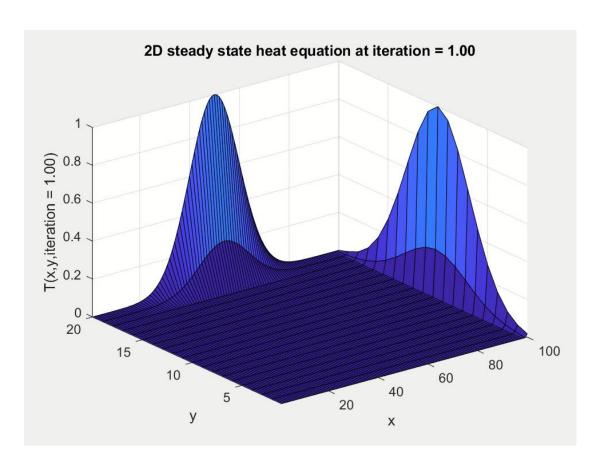


% Dimensions of the simulation grid in x (xdim) and y (ydim) directions xdim=10; ydim=10;





```
% Constant temperature of 67.5C applied to one boundary
T \text{ prev}(2,1) = 67.5;
T \text{ now}(2,1) = 67.5;
% A simulation less ordinary
i=1:1:xdim; %x-co-ordinates for boundary
T now(i, ydim) = \exp((-1.*((xdim/2-i).*(xdim/2-i)))./(1.0.*xdim));
j=1:1:ydim; %x-co-ordinates for boundary
T now(xdim, j) = exp((-1.*((ydim/2-j).*(ydim/2-j)))./(2.0.*ydim));
T prev=T now;
% Open a figure to plot to
figure;
```



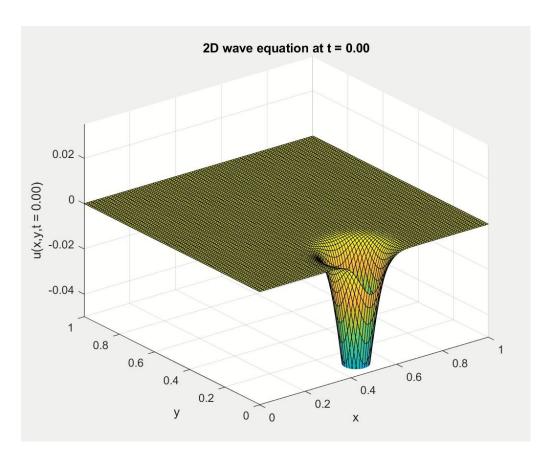


Closing remarks

Hopefully you have enjoyed this course on numerical algorithms and you now have a good grounding in some of the techniques used in numerical methods.

<u>Please</u>, <u>please</u> do leave feedback, positive, or negative, constructive criticism and typo's.

Your feedback helps me improve the course for next year, just as last years students helped me improve the course for you.





That's all Folks!

