Workout Exam April 22, 2010

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1. (a) LN chnulp1:9 Book 2.3.
   In the Newton method the estimate of the next zero of f is the zero of the linear approximation of f at the previous zero.

   (b) LN chnulp1: 14 Book 2.3
   In the secant method the estimate of the next zero of f is the zero, say x_{n+1}, of the line that passes through the last two pairs $(x_n, f(x_n))$, $(x_{n-1}, f(x_{n-1}))$. The algorithm of Newton's method needs both the function and its derivative, the secant method only needs the function. So for the secant method the user only has to program the function.

2. (a) LN chnulp2d:3 Book 10.1-2
   Here

$$\mathbf{g}(\mathbf{x}) = \begin{bmatrix} x - \frac{1}{2}f_1(x,y) + \frac{1}{4}f_2(x,y) \\ y - \frac{1}{4}f_2(x,y) \end{bmatrix}$$

   The Jacobian matrix of g is defined by

$$\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} (g_1)_x & (g_1)_y \\ (g_2)_x & (g_2)_y \end{bmatrix}$$

   Hence

$$\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 1 - \frac{1}{2}(f_1)_x + \frac{1}{4}(f_2)_x & -\frac{1}{2}(f_1)_y + \frac{1}{4}(f_2)_y \\ -\frac{1}{4}(f_2)_x & 1 - \frac{1}{4}(f_2)_y \end{bmatrix}$$

   One can also express the Jacobian of $\mathbf{g}$ in the Jacobian of $\mathbf{f}$. First we write

$$\mathbf{g}(\mathbf{x}) = \mathbf{x} + \begin{bmatrix} -\frac{1}{2} & \frac{1}{4} \\ 0 & -\frac{1}{4} \end{bmatrix} \mathbf{f}(\mathbf{x})$$

   So the Jacobian of $\mathbf{g}$ can be expressed in that of $\mathbf{f}$ by

$$\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} = I + \begin{bmatrix} -\frac{1}{2} & \frac{1}{4} \\ 0 & -\frac{1}{4} \end{bmatrix} \frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}}$$

   The Jacobian of $\mathbf{f}(\mathbf{x})$ is given by

$$\frac{\partial \mathbf{f}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} (f_1)_x & (f_1)_y \\ (f_2)_x & (f_2)_y \end{bmatrix} = \begin{bmatrix} \exp(x) & 1 \\ 2x & 2y \end{bmatrix}$$

   So the Jacobian of $\mathbf{g}$ is

$$\frac{\partial \mathbf{g}(\mathbf{x})}{\partial \mathbf{x}} = \begin{bmatrix} 1 - \frac{1}{2}\exp(x) + \frac{1}{2}x & -\frac{1}{2} + \frac{1}{2}y \\ -\frac{1}{2}x & 1 - \frac{1}{2}y \end{bmatrix}$$

   (b) See LN chnulp2d:3 or 4, Book 10.1-2
   We just have to study the eigenvalues of the Jacobian of $\mathbf{g}$ in the fixed point (0,1):

$$\begin{bmatrix} \frac{1}{2} & 0 \\ 0 & \frac{1}{2} \end{bmatrix}$$

The matrix is already in diagonal form hence the eigenvalues can be read from the diagonal and both a $\frac{1}{2}$. Since these are clearly less than 1 in magnitude the method will converge near the fixed point.
Instead of the eigenvalues one can also look to the norm of the Jacobian (though this gives only a sufficient condition for convergence) which is also $\frac{1}{2}$ here.

3. (a) See LN chinterpFW:1, book 3.1
This is simply a straight line through the points $(0, 1)$ and $(1, \exp(2))$. Hence $p_1(x) = 1 + (\exp(2) - 1)x$. The interpolated value at $x = \frac{1}{2}$ is $p_1(\frac{1}{2}) = \frac{1}{2}(1 + \exp(2))$. One could also use the Lagrange basis functions ($p_1(x) = \frac{x-1}{0-1} f(0) + \frac{x-0}{1-0} f(1)$) or Newton divided differences ($p_1(x) = f(0) + (x-1)f[0, 1]$) to derive the same interpolation formula.

   (b) See LN chinterpFW:2, book 3.1
The error fomula is in this case $f(x) - p_1(x) = x(x-1)\frac{f''(\xi(x))}{2}$. The second derivative of our function is $4\exp(2x)$. So we end up with the error formula $f(x) - p_1(x) = 2x(x-1)\exp(2\xi(x))$ where $\xi(x)$ is a point on the smallest interval containing 0,1 and x. Since in our case $x = 1/2$ we can take for $\xi(x)$ the point where $\exp(2x)$ becomes maximal on the interval [0,1]. Here at 1. So we have

$$|f(\frac{1}{2}) - p_1(\frac{1}{2})| \leq \frac{\exp(2)}{2}$$

The only condition for this error estimate to hold is that the function f must be twice differentiable which is clearly the case.

   (c) See LN chinterpFW:3 The true error is $f(\frac{1}{2}) - p_1(\frac{1}{2}) = e - \frac{1}{2}(1 + \exp(2)) = -(\frac{1}{2}(1 + \exp(2)) - e)$ which is clearly negative. This should be less than what is found as bound. So

$$\frac{1}{2}(1 + \exp(2)) - e \leq \frac{\exp(2)}{2}$$

or $\frac{1}{2} - e \leq 0$ which is clearly the case.
In the formula in (b) there is a point $\xi(\frac{1}{2})$ on [0,1] for which there is equality. We just took the worst case where the exponential is maximal on the interval, which yields an upperbound.

4. (a) The interval [0,1] is split up in 25 equal parts of length 0.04.
(1) LN chintgrFW: 9, book 4.3. Since 25 is odd, one of the intervals runs from 0.48 to 0.52. The "Rechthoek methode" is the midpoint method in the book/LN. So the approximation is the value of the function in the midpoint of the interval times the length of the interval. This yields here $(12(\frac{1}{2})^2)\frac{1}{25} = \frac{3}{25}$
(2) LN chintgrFW: 4, book 4.3. The trapezium rule just takes the average of the function values at the endpoints and multiplies it by the length of the interval. So that results in $\frac{1}{2}12(0.48^2 + 0.52^2)\frac{1}{25} = \frac{1}{2}12[(\frac{1}{2} - \frac{1}{50})^2 + (\frac{1}{2} + \frac{1}{50})]^2\frac{1}{25} = \frac{12}{25}[(\frac{1}{2})^2 + (\frac{1}{50})^2] = \frac{3}{25}[1 + (\frac{1}{25})^2]$

   (b) LN chintgrFW: 15,16,17
The integrand is infinitely times differentiable, hence one can use the Taylor formula to any order. This is needed to derive expressions like the q-factor. For $I(64)$ we have

$$q(64) = \frac{I(32) - I(64)}{I(64) - I(128)} = \frac{7.32\ 10^{-4}}{1.83\ 10^{-4}} = 4.00$$

So there is second order convergence here.

(c) LN chintgrFW: 26, book 4.2 So we know that $I = I(n) + ch^2 + O(h^3)$ and hence $I = I(n/2) + 4ch^2 + O(h^3)$, where c is some constant. We want an approximation that has an higher order than 2. So we have to get rid of the $O(h^2)$ term. Multiply the first by four and subtract the second one and we get

$$3I = 4I(n) - I(n/2) + O(h^3)$$

Hence

$$I = \frac{4I(n) - I(n/2)}{3} + O(h^3)$$

So $\hat{I}(n) = \frac{4I(n)-I(n/2)}{3}$ gives a more accurate approximation of I. Plugging in the numbers I find on my calculator the $\hat{I}(n) = 4$, which is more accurate than $I(128)$.
The extrapolated value is indeed exact here. Observe that the integrand is quadratic and that both the midpoint method and trapezium method are exact for linear functions. However an extrapolated result based on either of the methods will be exact for at least 1 degree higher polynomials, so for quadratic polynomials.

5. (a) LN as in 4c but also chgdvFW:42,43, book 5.8.
Since it is second order we can reuse our formula derived in 4c. The error is $I - I(n)$ and hence it holds

$$I - I(n) = \frac{I(n) - I(n/2)}{3} + O(h^3)$$

Hence $\frac{I(n)-I(n/2)}{3}$ approximates the error. Here that is (0.198991-0.195838)/3=0.001051. Another way of deriving this expression is to eliminate I from the first two expressions in 4c and then to find the expression for the main term of the error ch^2 which leads exactly to the same formula as above.

(b) For a better result we can use our original formula in 4c or just add $I(n)$ to the error which is 0.198991+0.001051=0.200042

(c) The method of Heun is a Runge-Kutta method with two steps. Probably it is easiest remembered by deriving it from the trapezium method as on page 41 of the LN. The method reads

$$w_{n+1} = w_n + \frac{1}{2}h[f(x_n, w_n) + f(x_{n+1}, \hat{w}_{n+1})]$$

where $\hat{w}_{n+1} = w_n + hf(x_n, w_n)$ Here $f(x, y) = -y^2$. Using this $\hat{w}_{n+1} = w_n - hw_n^2$ and

$$w_{n+1} = w_n + \frac{1}{2}h[-w_n^2 - \hat{w}_{n+1}^2] = w_n - \frac{1}{2}h[w_n^2 + (w_n - hw_n^2)^2] = w_n - hw_n^2 + h^2w_n^3 - \frac{1}{2}h^3w_n^5$$

One should check that the second term in the last expression is indeed an approximation of $hf(x_n, w_n)$.

6. (a) LN chla1: 8,9, book 6.5. The LU factorization is performed column by column. We have to sweep zeros below the diagonal in the first two columns of the matrix. L contains the multipliers needed to make the zeros. So for the first column we have to multiply the first row by a half and subtract it from the second row (this action forms a intermediate result). This means that the multiplier for the second row is $\frac{1}{2}$. The first row U remains unchanged. We can write this as

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & \frac{3}{2} & -\frac{1}{2} \\ 0 & 1 & 2 \end{bmatrix}$$

Note that when you multiply these two matrices you get the original matrix. Now we proceed on the 2×2 submatrix in the lower right corner in the right matrix. It is clear that from this matrix we have to multiply the first row by $\frac{2}{3}$ and subtract it from the second row. This is the new multiplier. The result of this subtraction is put in the last row. We get now

$$\begin{bmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ 0 & \frac{2}{3} & 1 \end{bmatrix} \begin{bmatrix} 2 & 1 & 1 \\ 0 & \frac{3}{2} & -\frac{1}{2} \\ 0 & 0 & 2\frac{1}{3} \end{bmatrix}$$

This is the LU factorization of the original matrix.

(b) book 6.3 Row interchanges are performed to constrain the propagation of round off errors. In the first column of the submatrix in the current elimination step, one seeks for the largest element in modulus. The row with the largest element is interchanged with the current first row. As a result of this all multipliers will be less than one in modulus.

7. (a) LN chpdv:1-4 book 11.3, 12.2.
Let $\Delta x = 1/m$. The discretization is performed in two steps, first in space and next in time. The standard discretization for u_{xx} is

$$u_{xx}(x_i, t) \approx \frac{u_{i+1}(t) - 2u_i(t) + u_{i-1}(t)}{\Delta x^2} \quad \text{for } i = 1, ..., m-1$$

where $u_i(t) = u(x_i, t)$. With this approximation we transform the PDE into a system of ordinary differential equations

$$\frac{dv_i}{dt}(t) = \kappa \frac{v_{i+1}(t) - 2v_i(t) + v_{i-1}(t)}{\Delta x^2} \quad \text{for } i = 1, ..., m-1 \tag{1}$$

where $v_i(t)$ approximates $u_i(t)$. The initial condition is $v_i(0) = 100 \sin(\pi i \Delta x)$ and the boundary conditions $v_0(t) = 0$ and $v_m(t) = \sin^2(\pi t)$. This completes the discretization in space. Next we apply the explicit Euler method to this system of equations. Let $w_i^n \approx v_i(n\Delta t)$. Then we write

$$w_i^{n+1} = \kappa \frac{w_{i+1}^n - 2w_i^n + v_{i-1}^n}{\Delta x^2}$$

with initial condition $w_i^0 = 100 \sin(\pi i \Delta x)$ and boundary conditions $w_0^n = 0$, $w_m^n = \sin^2(\pi n \Delta t)$.

(b) LN chpdv: 7-9. book 12.3
The maximum time step is restricted by $\Delta t \leq \frac{2}{\kappa}\Delta x^2$. Here $\Delta t \leq \frac{2}{10^{-3}}(200)^{-2} = \frac{1}{20}$

(c) LN chpdv: 14, book 12.3 If we employ the backward Euler to the system of ODEs (1) we get

$$w_i^{n+1} = \kappa \frac{w_{i+1}^{n+1} - 2w_i^{n+1} + v_{i-1}^{n+1}}{\Delta x^2}$$

with exactly the same initial and boundary conditions as the forward Euler method. The backward Euler method is unconditionally stable for this problem. So there is no restriction on the time step.