Scientific Computing II: Exam Solutions

May 29, 2023

Question 1: The correct answer is 1.65805.
For the given ODE we have $f(t, y) = 10y(t)^2 + t$. Only a single step of Heun's method needs to be computed since we are considering a step size of $h = 0.1$ and are interested in finding the value of y at $t = 0.1$. So we have $K_1 = f(t_0, y_0) = f(0, 0.7) = 10 \times (0.7)^2 + 0 = 4.9$ and $K_2 = f(t_1, y_0 + hK_1) = f(0.1, 0.7 + 0.1 \times 4.9) = 14.267$. Finally, $y_1 = y_0 + \frac{h}{2}(K_1 + K_2) = 0.7 + 0.05(4.9 + 14.267) = 1.65805$.

Question 2: The correct answer is 7.
The given table contains frequencies for each side of the dice. First we compute probabilities by dividing by the sum, here 150:

Side (k)	1	2	3	4	5	6	7	8
Probability (p_k)	21/150	33/150	12/150	25/150	8/150	15/150	26/150	10/150

To apply the inverse transform method (ITM), we compute the cumulative density values $F_k = \sum_{j=1}^{k} p_j$ in the table below:

Side (k)	1	2	3	4	5	6	7	8
CDF (F_k)	21/150	54/150	66/150	91/150	99/150	114/150	140/150	150/150=1

According to ITM for generating from a discrete distribution, the uniform number $u = 0.8012$ corresponds to side 7 because it lies between 114/150 and 140/150.

Question 3: What are the characteristics of a stiff ODE? Correct answers are:

- [x] The solution can have vastly different scales components ✓
- [x] The solution varies quickly ✓
- [x] Implicit methods are beneficial ✓
- [ ] The solution varies slowly
- [ ] The RK4 method can solve it with a relatively large steplength
- [x] It requires a small steplength for stability in explicit methods ✓
- [ ] Explicit methods are beneficial

Question 4: Classification:

	Deterministic Model	Stochastic Method	Deterministic Method	Stochastic Model
Monte Carlo integration		✓		
Explicit Euler (Euler forward)			✓	
$\frac{dS}{dt} = \mu N - \mu S - \beta \frac{I}{N} S$ $\frac{dI}{dt} = \beta \frac{I}{N} S - \mu I - \gamma I$ $\frac{dR}{dt} = \gamma I - \mu R$	✓			
SSA (Gillespies algorithm)		✓		
Mid-point rule for integration			✓	
$\emptyset \xrightarrow{\mu N} S$ $S \xrightarrow{\beta \frac{I}{N} S} I$ $I \xrightarrow{\gamma I} R$				✓

Question 5: The answer is $N = 40000$.
For a given probability (for example 99%) and by increasing the number of samples, i.e. N, the length of the confidence interval (or the size of standard deviation of the mean) is reduced by rate $1/\sqrt{N}$. Thus, we can write

$$\frac{0.2}{0.1} = \frac{\varepsilon_1}{\varepsilon_2} = \frac{\sqrt{N_2}}{\sqrt{N_1}} = \frac{\sqrt{N_2}}{\sqrt{10000}}$$

which gives $N_2 = 4 \times 10000 = 40000$.

Question 6: The answer is 0.00062.

The order of convergence of the RK4 is h^4, thus we can write

$$\frac{\varepsilon_1}{\varepsilon_2} = \left(\frac{h_1}{h_2}\right)^4$$

or

$$\frac{0.05}{\varepsilon_2} = \left(\frac{0.3}{0.1}\right)^4$$

which gives $\varepsilon_2 = 0.05/81 \doteq 0.00062$.

Question 7: Specify the suitable method for each application:

	Explicit method	Implicit method
y'(t)=-(y-cos(t))+sin(t)	✓	
lower complexity per timestep	✓	
Non-stiff equation	✓	
Fast transients		✓
Stiff equation		✓
Stability is critical		✓
y'(t)=-10000(y-cos(t))+sin(t)		✓
Systems with highly different scales		✓

Question 8: Specify the suitable method for each application:

	Stokastisk metod	Deterministisk metod
ODE		✓
Integral 2D		✓
Stochastic process	✓	
Solution is continuous (concentration, velocity, ...)		✓
Solution is discrete (individuals, number of molecules, ...)	✓	
Scenarios in epidemic models with limited number of individuals	✓	
Integral 10D	✓	

Question 9: The probability density function (pdf) is $f(x) = \frac{e^{-x}}{(1+e^{-x})^2}$ for $x \in (-\infty, \infty)$. The cumulative density function (cdf) is given by $F(x) = \frac{1}{1+e^{-x}}$. To apply the inverse transform method we must compute $F^{-1}(x)$. If we set $F(y) = x$ then we have $\frac{1}{1+e^{-y}} = x$ which gives $e^{-y} = \frac{1}{x} - 1$ or

$$y = \ln \frac{x}{1-x} = F^{-1}(x).$$

To generate a random number X from f we generate a uniform random number $U \sim \mathcal{U}(0,1)$ and set

$$X = F^{-1}(U) = \ln \frac{U}{1-U}.$$

To estimate the given integral by Monte Carlo method we can write

$$I = \int_{-\infty}^{\infty} (1+x^2) f(x) dx = \mathbb{E}_f(1+x^2) \approx \frac{1}{N} \sum_{k=1}^{N} (1+X_k^2)$$

where X_k are generated from the logistic density f. A (pseudo) code is given as below:

```
for k = 1:N
  u = rand;
  x(k) = log(u/(1-u));
end
I = sum(1+x.^2)/N;
```

Question 10: Replacing $f(t,y)$ by λy in the given method, we obtain

$$\begin{aligned} y_{k+1} &= y_k + \lambda h z_2 \\ &= y_k + \lambda h\Big(y_k + \frac{1}{2}\lambda h y_k\Big) \\ &= y_k + \lambda h y_k + \frac{1}{2}(\lambda h)^2 y_k \\ &= \Big(1 + \lambda h + (\lambda h)^2/2\Big) y_k \\ &= R(z) y_k \quad (\text{if } z \equiv \lambda h) \end{aligned}$$

where $R(z) = 1 + z + z^2/2$. The absolute stability region is obtained by assuming $|R(z)| \leqslant 1$, or

$$S = \Big\{ z \in \mathbb{C} : |1 + z + z^2/2| \leqslant 1 \Big\}.$$

If z is real, i.e. $z = x + 0i \in \mathbb{R}$, then we can write

$$\begin{aligned} &|1 + x + x^2/2| \leqslant 1 \Longrightarrow -1 \leqslant 1 + x + x^2/2 \leqslant 1 \Longrightarrow -2 \leqslant 2 + 2x + x^2 \leqslant 2 \Longrightarrow \\ &-3 \leqslant 1 + 2x + x^2 \leqslant 1 \Longrightarrow -3 \leqslant (1+x)^2 \leqslant 1 \Longrightarrow 0 \leqslant (1+x)^2 \leqslant 1 \Longrightarrow \\ &|1+x| \leqslant 1 \Longrightarrow -2 \leqslant x \leqslant 0 \end{aligned}$$

In this case, the stability region (interval) is $[-2, 0]$ which mean $-2 \leqslant \lambda h \leqslant 0$ or $0 \leqslant h \leqslant -2/\lambda$. Keep in mind that λ is negative.

Question 11: First we convert the given ODE into a first order system of 4 equations by doing the following change of variables

$$y_1 = \theta_1, \quad y_2 = \theta_1', \quad y_3 = \theta_2, \quad y_4 = \theta_2'.$$

The new system is

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= -\sin(y_1) - \alpha(y_1 - y_3) \\ y_3' &= y_4 \\ y_4' &= -\sin(y_3) + \alpha(y_1 - y_3) \end{aligned}$$

with initial conditions

$$y_1(0) \sim \mathcal{N}(\pi/4, 0.02), \quad y_2(0) = 0, \quad y_3(0) \sim \mathcal{N}(\pi/4, 0.02), \quad y_4(0) = 0.$$

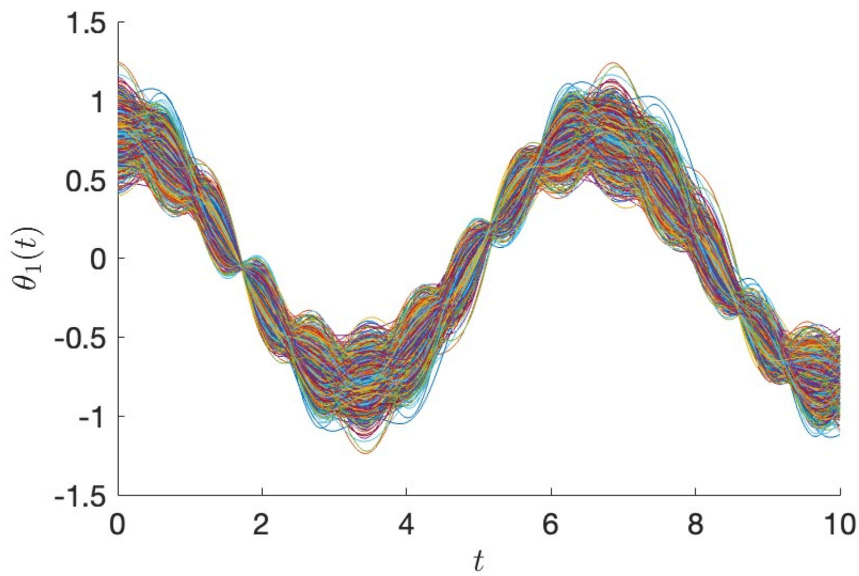
To generate a normal number X with mean μ and variance σ^2, we can generate a standard normal number Z using command `randn` and set $X = \mu + \sigma Z$. Also, to generate a uniform random number α in interval $[10 - \delta, 10 + \delta]$, we can generate a uniform number U in interval $[0, 1]$ using `rand` and set $\alpha = 10 + (2U - 1)\delta$. The code is given below:

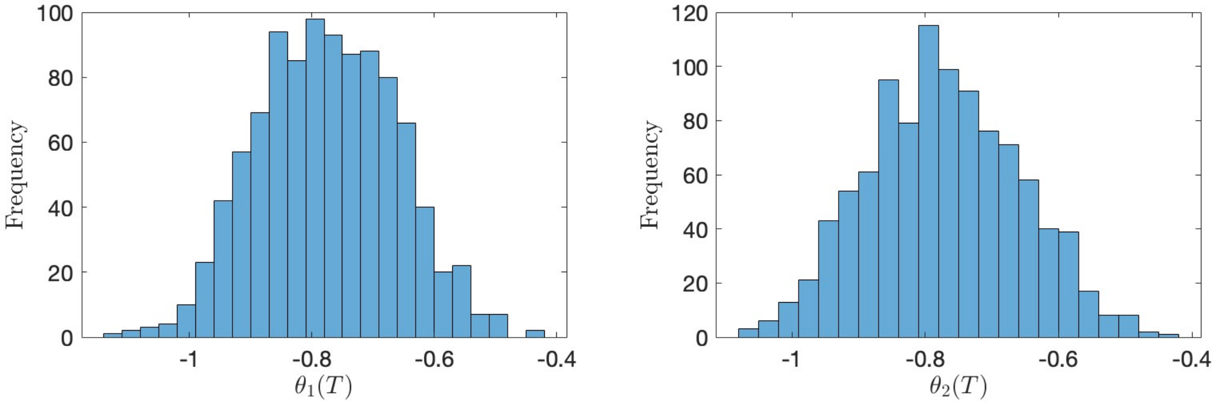
```
clearvars; close all
T = 10;      % final time
N = 1000;
hold on
for k = 1:N
    % initial values for parameters
    y1 = pi/4 + sqrt(0.02)*randn;
    y2 = 0;
    y3 = pi/4 + sqrt(0.02)*randn;
    y4 = 0;
    y0 = [y1 y2 y3 y4];
    del = 0.2;
    alpha = 10 + del*(2*rand-1);

    % here we define the right hand side equations of the system
```

```
    pendulum = @(t,y) [y(2);
                       -sin(y(1))-alpha*(y(1)-y(3));
                       y(4);
                       -sin(y(3))+alpha*(y(1)-y(3))];

    [t,y] = ode45(pendulum,[0 T],y0);

    theta1(k) = y(end,1);  % theta1(T)
    theta2(k) = y(end,3);  % theta2(T)
    % Task 1
    plot(t,y(:,1));
end
% Task 2
figure; histogram(theta1);
figure; histogram(theta2);
% Task 3
mean_theta1 = sum(theta1)/N       % or mean(theta1)
std_theta1 = sqrt(sum((theta1-mean_theta1).^2)/(N-1))
% or std(theta1)
```

We use `ode45` as there is no sign of stiffness in the system. `ode23` is also a suitable alternative. In the event of an observed nonphysical or blown-up solution, we can improve the error options within the ode setting or opt for `ode23t` or `ode15s` instead.

Below you can find the plot of the solutions θ_1 with various random parameters, as well as histograms of the random variables $\theta_1(T)$ and $\theta_2(T)$ for an execution. Please note that this portion is not included in the requested solution since Matlab access was unavailable to you.





100
80
60
40
20
0
Frequency
-1
-0.8
-0.6
-0.4
$\theta_1(T)$
120
100
80
60
40
20
0
Frequency
-1
-0.8
-0.6
-0.4
$\theta_2(T)$