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Computational Physics
Final Exam

1.
$$\begin{bmatrix} 4 & 1 & 2 \\ 2 & 4 & -1 \\ 1 & 1 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 9 \\ -5 \\ -9 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 0.25 & 0.50 \\ 0 & 3.50 & -2 \\ 1 & 1 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.25 \\ -9.5 \\ -9 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 0.25 & 0.50 \\ 0 & 3.50 & -2 \\ 0 & 0.75 & -3.50 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.25 \\ -9.5 \\ -11.25 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 0.25 & 0.50 \\ 0 & 1 & -0.57 \\ 0 & 1 & -4.67 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.25 \\ -2.71 \\ -15 \end{bmatrix}$$

$$\Rightarrow \begin{bmatrix} 1 & 0.25 & 0.50 \\ 0 & 1 & -0.57 \\ 0 & 0 & -4.10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 2.25 \\ -2.71 \\ -12.29 \end{bmatrix}$$

$$\therefore \quad -4.10\, x_3 = -12.29 \quad \text{--- (1)}$$

$$x_2 - 0.57\, x_3 = -2.71 \quad \text{--- (2)}$$

$$x_1 + 0.25\, x_2 + 0.50\, x_3 = 2.25 \quad \text{--- (3)}$$

∴ From - ① :

$x_3 = 2.99 \approx 3$

from - ② :

$x_2 - 0.57(2.99) = -2.71$

$\Rightarrow x_2 = -2.71 + 1.70$

$= -1.01 \approx -1$

from - ③ :

$x_1 + 0.25(-1.01) + 0.50(2.99) = 2.25$

$\Rightarrow x_1 - 0.25 + 1.50 = 2.25$

$\Rightarrow x_1 = 1.00 \approx 1$

$\therefore$ $\boxed{\begin{aligned} x_1 &= 1 \\ x_2 &= -1 \\ \& \; x_3 &= 3 \end{aligned}}$

2. (a) numpy.fft.fft

(b) numpy.linalg.qr

(c) numpy.random.lognormal / numpy.random.random

(d) gsl_odeiv2_step_rk8pd

(e) numpy.linalg.svd

(f) numpy.random.pdf (size = (n, dim))

(g) gsl_odeiv2_control

(h). gsl_monte_plain_integrate

(i) gsl_odeiv2

(j) numpy.linalg.eig / numpy.linalg.eigh

3. $$\begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 & \cdots \\ a_{21} & a_{22} & a_{23} & 0 & 0 & \cdots \\ 0 & a_{32} & a_{33} & a_{34} & 0 & \cdots \\ \vdots & \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & 0 & & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

Now, <u>step 1</u> is :

ⓐ divide R_1 by a_{11} ..

ⓑ Use the pivot row R_1 to get convert $a_{21} = 0$

$$R_2 = R_2 - a_{21} R_1$$

Here, a_{12} and b_1 are only non-zero elements. So, only <u>two</u> steps.

$$a_{22}^{(1)} = a_{22} - a_{21} \cdot a_{12}^{(1)} \quad \text{— ①}$$
$$b_2^{(1)} = b_2 - a_{21} \cdot b_1 \quad \text{— ②}$$

<u>At step 1 :</u>

$$\begin{bmatrix} 1 & a_{12}^{(1)} & 0 & \cdots \\ 0 & a_{22}^{(1)} & a_{23} & \cdots \\ 0 & a_{32} & a_{33} & \cdots \\ \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

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$$\begin{bmatrix} b_1^{(1)} \\ b_2^{(1)} \\ \vdots \\ b_n \end{bmatrix} \begin{matrix} \longrightarrow 2 \text{ divisions} \\ \longrightarrow 2 \text{ additions } + \\ 2 \text{ div / multiplication} \\ \text{steps} \end{matrix}$$

So, in step 1 :

we have 2 addition / substraction + 4 Multiplication / divisions steps.

Similarly, in step 2 :-

ⓐ Divide R_2 by $a_{22}^{(1)}$

ⓑ Use the pivot row R_2 to convert $a_{32} = 0$.

only computation will be for row 3.

At step 2 :-

$$\begin{bmatrix} 1 & a_{12}^{(1)} & 0 & 0 & \cdots \\ 0 & 1 & a_{23}^{(2)} & 0 & \cdots \\ 0 & 0 & a_{33}^{(2)} & a_{34} & \cdots \\ \vdots & \vdots & \vdots & \vdots & \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1^{(1)} \\ b_2^{(2)} \\ b_3^{(2)} \\ \vdots \\ b_n \end{bmatrix}$$

so in step 2 :-

similarly we have, 2 additions/ subtractions + 4 multiplications / divisions steps.

$\therefore$ for total $(n-1)$ rows :-

total computation requirements :

$$= (n-1)\,2 + (n-1)\,4$$
$$= (2n-2) + (4n-4)$$
$$= 6n - 6 = 6(n-1)$$

So, it is an $O(n)$ process.

[proved]

5. ⓐ I will verify which Library takes the least time for the same computation. Because, time saving is very necessary for computational purpose.

ⓑ I will check for which library the experimental result and theoretical prediction are very similar. I mean, the error between these two is the least. Then that library is better than others.

ⓒ I will verify by using which library I have to code the least, because less coding means probability of making mistakes is also less. Then that library package is more complete than others. So, I will choose that.

7. There are four "magic" numbers which are

modulus → m

multiplier → a

increment → c

and seed → X_0

The sequency of random numbers is obtained by :

$$X_{i+1} = (a X_i + c) \bmod m$$

for $i \geq 0$.

The linear congruential generator completely breaks down if the numbers m, a, c are not chosen carefully.

For example, if I take, $m = 10$, $a = 7$, $c = 7$, then $X_0 = 7$ generates; the repeating sequence :

7, 6, 9, 0, 7, 6, 9, 0, ...

But, if we choose :

$a = 1664525$

$c = 1013904223$

$m = 4294967296$

$x = 1$

This gives the sequence of numbers :

1015568748

1586005467

2165703038

3027450565

217083232

⋮

So, the numbers do look random, there is no repeatation.

4. (e) Here we can see that after doing Fourier transform of an uniform deviate we get delta function. So, from this we can interpret that our plot is correct.

6. Arguement :-

$$\frac{dy_1}{dx} = 32 y_1 + 66 y_2 + \frac{2}{3} x + \frac{2}{3} \quad \text{--- (1)}$$

$$\frac{dy_2}{dx} = -66 y_1 - 133 y_2 - \frac{1}{3} x - \frac{1}{3} \quad \text{--- (2)}$$

So, from eqn. - (1) we can see that from the slope of 'y_1' we can say that at first 'y_1' should increase at higher rate, then it will almost saturate. from solution i.e. the graph that nature of the 'y_1'.

from eqn. - (2): we can say that at first 'y_2' will fall at a higher rate and then after some point it will almost saturate. We get almost same nature of 'y_2' from the solution i.e. the graph. So, our solution is correct.