1TD352

Exam Jan. 2024

Exam and solutions by:

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Question 1 (Concept)

1 **1TD352_Concept_1**

Classify methods and models.
*** In order to get 2 points, you need to provide at least 6 correct answers out of the total 7. Otherwise, you will receive 0 points (no intermediate points).**

	Deterministic model	Stochastic model	Deterministic method	Stochastic method
Power method			✓	
QR-iteration			✓	
SSA (Gillespies algorithm)				✓
F and R real-valued $\frac{dF}{dt} = \beta F R - \gamma F$ $\frac{dR}{dt} = \alpha R - \beta F R$	✓			
Least squares problem $\min_{\boldsymbol{x}} \lVert A\boldsymbol{x} - \boldsymbol{b} \rVert_2$	✓			
Monte Carlo algorithm				✓
F and R integer-valued $R \xrightarrow{\alpha} 2R$ $R + F \xrightarrow{\beta} 2F$ $F \xrightarrow{\gamma} \emptyset$		✓		

Rätt. 2 av 2 poäng. Försök igen

Question 2 (Concept)

2 **1TD352_Concept_2**

Select the correct alternative.
*** In order to get 2 points, you need to provide at least 6 correct answers out of the total 7. Otherwise, you will receive 0 points (no intermediate points).**

(a) The SVD *is not* used to compute the [norm infinity] ✔ (norm 2, pseudo-inverse, low rank approximation, norm infinity) of a matrix.

(b) Orthogonal matrices when applied to a vector, [only rotate it] ✔ (only rotate it, change its Euclidean norm (norm 2), either stretch or shrink it).

(c) The Schur decomposition of a symmetric matrix is identical with its [eigen-decomposition] ✔ (SVD, LU decomposition, QR factorization, eigen-decomposition).

(d) Given a uniform random number, the [inverse transform method] ✔ (basis Monte Carlo method, inverse transform method, Gillespies algorithm) can be used to generate a random number from an arbitrary distribution f.

(e) The Brownian motion $X(t)$ is [normally] ✔ (uniformly, exponentially, normally) distributed with

variance [t] ✔ (t, 0, 1)

(f) A stochastic process is called a [Markov] ✔ (non-Markovian, continuous time, Markov, discrete time) process, if one can make predictions for the future of the process based solely on it's present state.

Rätt. 2 av 2 poäng. Försök igen

Question 3 (Algorithm)

The ansatz is $y = a_0 + a_1 x + a_2 x^2 \Rightarrow A a \approx y$

$$\underbrace{\begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \end{bmatrix}}_{A} \underbrace{\begin{bmatrix} a_0 \\ a_1 \\ a_2 \end{bmatrix}}_{a} \approx \underbrace{\begin{bmatrix} -1 \\ 2 \\ 1 \\ -3 \end{bmatrix}}_{y}$$

A is 4×3 and all 3 singular values are positive so A is full-rank.

The least squares solution using SVD is

$$a = A^+ y = V \Sigma_1^{-1} U_1^T y$$

$$= \begin{bmatrix} -0.3 & 0.68 & 0.67 \\ -0.42 & -0.72 & 0.55 \\ -0.86 & 0.11 & -0.50 \end{bmatrix} \begin{bmatrix} \frac{1}{4.90} & 0 & 0 \\ 0 & \frac{1}{1.69} & 0 \\ 0 & 0 & \frac{1}{1.08} \end{bmatrix} \begin{bmatrix} -0.15 & -0.06 & -0.32 & -0.93 \\ 0.90 & 0.40 & 0.04 & -0.19 \\ -0.35 & 0.62 & 0.67 & -0.21 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ 1 \\ -3 \end{bmatrix}$$

$V \quad \Sigma_1^{-1} \quad U_1^T$

$$\doteq \begin{bmatrix} 1.84 \\ 1.04 \\ -1.74 \end{bmatrix} \Longrightarrow a_2 = -1.74$$

$$\text{residual} = \| U_2^T y \|_2 = \left\| \begin{bmatrix} -0.22 & 0.67 & -0.67 & 0.22 \end{bmatrix} \begin{bmatrix} -1 \\ 2 \\ 1 \\ -3 \end{bmatrix} \right\|_2 = 0.23$$

Question 4 (Algorithm)

$$\int_0^\infty (x^2-3x)e^{-0.5x}\,dx = \int_0^\infty \underbrace{2(x^2-3x)}_{g(x)}\,\underbrace{0.5e^{-0.5x}}_{f(x)}\,dx$$

random points are generated from f. The MC solution is

$$\frac{1}{N}\sum_{k=1}^{N} g(x_k) = \frac{1}{6}\sum_{k=1}^{6} 2(x_k^2-3x_k) \doteq 4.252$$

Question 5 (Analysis)

Using the central limit theorem we have

$$|e| \le 1.96\frac{s}{\sqrt{N}} \quad \text{at 95\% probality}$$

where s is the sample standard deviation. For this example $N=600$ and $s=38$ which gives

$$|e| \le 1.96\frac{38}{\sqrt{600}} \doteq 3.0$$

Since the order of convergence is $c.\frac{1}{\sqrt{N}}$, to decrease the error by a factor of 3 the number of realizations must be increased by a factor of $3^2=9$. The solution is $9 \times 600 = 5400$

Question 6 (Analysis)

Part (a): Eigenvalues of A are identical with eigenvaluse of $\tilde{T}$. Real eigenvalues of $\tilde{T}$ are single on-diagonals and imaginary eigenvalues are those of the 2x2 diagonal matrix.

$$\tilde{T} = \begin{bmatrix} \boxed{4.0} & 1.0 & -1.3 & 2.0 \\ 0 & 2.0 & 1.0 & 3.1 \\ 0 & -.5 & 1.0 & 2.5 \\ 0 & 0 & 0 & \boxed{0.5} \end{bmatrix}$$

A simple computation shows that eigenvalues of $\begin{bmatrix} 2.0 & 1.0 \\ -.5 & 1.0 \end{bmatrix}$ are $1.5 \pm 0.5j$, thus we have

$$\lambda_1 = 4, \quad \lambda_2 = 1.5 + 0.5j, \quad \lambda_3 = 1.5 - 0.5j, \quad \lambda_4 = 0.5$$

Part (b): $\text{rank}(A) = \text{number of non-zero } \sigma_k = 3$

$$\text{Cond}_2(A) = \frac{\max \sigma_k}{\min \text{ positive } \sigma_k} = \frac{3.0}{0.2} = 15$$

$$\|A - A_2\|_2 = \sigma_3 = 0.2$$

Question 7 (higher grade)

Since the values (amounts of drug in body) are rapidly decreasing from 1000 mg to 31 mg and is supposed to be vanished as soon, the best model to fit these data is the exponential model

$$\boxed{y = \alpha e^{\beta t}}$$

where t is time (hours) and y is the amount of drug.

We can linearize it by taking logarithm from both sides:

$$\ln(y) = \ln(\alpha e^{\beta t}) \Rightarrow \ln y = \ln \alpha + \ln e^{\beta t}$$

$$\Rightarrow \underbrace{\ln y}_{\tilde{y}} = \underbrace{\ln \alpha}_{\tilde{\alpha}} + \underbrace{\beta t}_{\beta t}$$

$$\tilde{y} = \tilde{\alpha} + \beta t \rightarrow \text{the linear model}$$

Time values remain the same but we use logarithm values of y:

t	0	5	10	15	20	25	30
$\tilde{y} = \ln y$	6.91	6.31	5.76	5.19	4.44	4.03	3.43

- First approach for stabilization (shifting and scaling):

To stabilize the algorithm for normal equations replace t_k's by $\dfrac{t_k - \bar{t}}{\sigma}$ where $\bar{t}$ is mean and

σ is standard deviation of time values:

$\bar{t} = 15, \quad \sigma \doteq 10.80$

The new table is

$\frac{t-\bar{t}}{\sigma}$	-1.39	-0.93	-0.46	0	0.46	0.93	1.39
$\tilde{y}$	6.91	6.31	5.76	5.19	4.44	4.03	3.43

with new ansatz $\tilde{y} = \tilde{\alpha} + \beta\left(\frac{t-\bar{t}}{\sigma}\right)$. Writting it back to the exponential model, we get

$$\boxed{y = \alpha e^{\beta\left(\frac{t-\bar{t}}{\sigma}\right)}}$$

We solve the LS problem $\|Ax-b\|_2 \to \min$ using normal equation $\boxed{A^T A x = A^T b}$ where $b = \tilde{y}$ and

$$x = \begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} \quad \text{and} \quad A = \begin{bmatrix} 1 & \frac{t_1-\bar{t}}{\sigma} \\ 1 & \frac{t_2-\bar{t}}{\sigma} \\ \vdots & \vdots \\ 1 & \frac{t_7-\bar{t}}{\sigma} \end{bmatrix} = \begin{bmatrix} 1 & -1.39 \\ 1 & -0.93 \\ \vdots & \vdots \\ 1 & 1.39 \end{bmatrix}$$

The normal equation is

$$\begin{bmatrix} 7.00 & 0.00 \\ 0.00 & 6.02 \end{bmatrix} \begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} = \begin{bmatrix} 36.70 \\ -7.56 \end{bmatrix}$$

Solve this with python to get $\begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} \doteq \begin{bmatrix} 5.15 \\ -1.26 \end{bmatrix}$

$$\tilde{\alpha} = 5.15 \Longrightarrow \alpha = e^{\tilde{\alpha}} = 172.43$$

$$\Rightarrow y(t) = \alpha e^{\beta\left(\frac{t-\bar{t}}{\sigma}\right)} = 172.43\, e^{-1.26\left(\frac{t-15}{10.80}\right)}$$

The amount of drug in body after 40 hr is estimated as:

$$y(40) = 172.43\, e^{-1.26\left(\frac{40-15}{10.80}\right)} \doteq 9.33 \text{ mg}$$

Note: at each step we rounded numbers to 2 decimal places. If you run the whole algorithm in double precision the final solution will be $y(40) \doteq 9.4054$

- 2nd approach for stabilization: (QR factorization)

The matrix A for the primary table, and its reduced QR factors:

$$A = \begin{bmatrix} 1 & 0 \\ 1 & 5 \\ 1 & 10 \\ 1 & 15 \\ 1 & 20 \\ 1 & 25 \\ 1 & 30 \end{bmatrix} \doteq \underbrace{\begin{bmatrix} -0.38 & -0.57 \\ -0.38 & -0.38 \\ -0.38 & -0.19 \\ -0.38 & 0.0 \\ -0.38 & 0.19 \\ -0.38 & 0.38 \\ -0.38 & 0.57 \end{bmatrix}}_{Q_1} \underbrace{\begin{bmatrix} -2.65 & -39.69 \\ 0.0 & 26.46 \end{bmatrix}}_{R_1}$$

The LS solution is obtained by solving

$$R_1 \begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} = Q_1^T \tilde{y}$$

$$\Rightarrow \begin{bmatrix} -2.65 & -39.69 \\ 0.0 & 26.46 \end{bmatrix} \begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} = \begin{bmatrix} -13.71 \\ -3.10 \end{bmatrix} \Rightarrow \begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} \doteq \begin{bmatrix} 6.93 \\ -0.12 \end{bmatrix}$$

$$\Rightarrow \alpha = e^{\tilde{\alpha}} = e^{6.93} \doteq 1022.49$$

$$\Rightarrow \boxed{y(t) = \alpha e^{\beta t} \doteq 1022.49\, e^{-0.12t}}$$

$$y(40) = 1022.49\, e^{-0.12 \times 40} \doteq 8.42 \text{ mg}$$

The difference between this and normal equation solutions comes from roundoff errors of using 2 decimal digits.

— 3rd approach for stabilization (SVD):

The SVD factors of A (reduced form) are:

$$U_1 = \begin{bmatrix} 0.0 & .068 \\ 0.11 & 0.52 \\ 0.21 & 0.37 \\ 0.31 & 0.21 \\ 0.42 & 0.05 \\ 0.52 & -0.11 \\ 0.63 & -0.26 \end{bmatrix}, \quad \Sigma_1 = \begin{bmatrix} 47.75 & 0 \\ 0 & 1.47 \end{bmatrix}, \quad V = \begin{bmatrix} 0.05 & 1.0 \\ 1.0 & -0.05 \end{bmatrix}$$

The LS solution is $\begin{bmatrix} \tilde{\alpha} \\ \beta \end{bmatrix} = A^{+}\tilde{y} = V\Sigma^{-1}U_1^T\tilde{y}$

We compute $\tilde{\alpha}$ and β and then set $\alpha = e^{\tilde{\alpha}}$ and continue as the same as the QR approach.

For exam it is enough to write one of the stabilization approaches.

Question 8 (higher grade)

Assume that $y = [S, E, C, P]$. We have 3 reactions and 4 states.

reactions	propensity functions	state-change vectors
1. $S + E \xrightarrow{c_1} C$	$\Rightarrow w_1 = c_1 S E = c_1 y_1 y_2$,	$v_1 = [-1, -1, 1, 0]$
2. $C \xrightarrow{c_2} S + E$	$\Rightarrow w_2 = c_2 C = c_2 y_3$,	$v_2 = [1, 1, -1, 0]$
3. $C \xrightarrow{c_3} P + E$	$\Rightarrow w_3 = c_3 C = c_3 y_3$,	$v_3 = [0, 1, -1, 1]$

At $t=0.1$ we have $y(t)=[300, 200, 100, 50]$. With the given constant rates we have

$$\begin{cases} w_1 = c_1 y_1 y_2 = 0.002 \times 300 \times 200 = 120 \ \text{mol/sec.} \\ w_2 = c_2 y_3 = 0.1 \times 100 = 10 \ \text{mol/sec.} \\ w_3 = c_3 y_3 = 0.75 \times 100 = 75 \ \text{mol/sec.} \end{cases}$$

$$a = w_1 + w_2 + w_3 = 205 \ \text{mol/sec.}$$

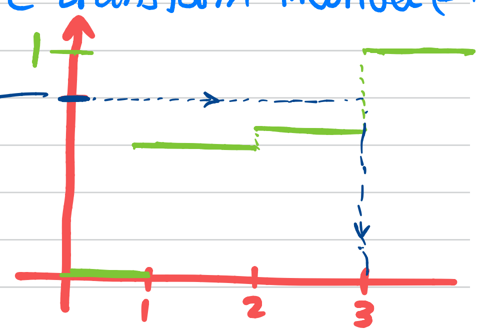
The probability of each reaction is $p_j = \dfrac{w_j}{a}$, $j=1,2,3$

j	1	2	3
p_j	0.585	0.049	0.366

In Gillespie's algorithm we sample from this distribution to determine the next reaction. We use the inverse transform method (ITM)

The cdf is obtianed as

$u=0.83$



j	1	2	3
F_j	0.585	0.634	1.000

and the uniform random number is given $u = 0.83$

Since $0.634 < 0.83 < 1.000$, the ITM samples the 3rd reaction.

To obtain the steplength τ, we must sample from the exponential distribtion $f(x) = \lambda e^{-\lambda x}$, for $\lambda = a = 205$

Again using ITM we have $\tau = F^{-1}(u) = \dfrac{1}{\lambda} \ln \dfrac{1}{1-u}$

$$\Longrightarrow \quad \tau = \frac{1}{\lambda}\ln\frac{1}{1-u} = \frac{1}{205}\ln\frac{1}{1-0.64} = 0.005 \text{ sec.}$$

Therefore, the next time level is

$$\boxed{t+\tau = 0.1 + 0.005 = 0.105}$$

At this time level the 3rd reaction occurs. the state-change vector V_3 obtained as $V_3 = [\underset{S}{0}, \underset{E}{+1}, \underset{C}{-1}, \underset{P}{+1}]$

thus $y(t+\tau) = y(t) + V_3 = [300, 200, 100, 50] + [0, +1, -1, +1]$
$= [300, 201, 99, 51]$

$S(t+\tau) = 300$ mol
$E(t+\tau) = 201$ mol
$C(t+\tau) = 99$ mol
$P(t+\tau) = 51$ mol

Question 9 (higher grade)

First of all we obtain the model of data from the inverse transform method. If $u \sim U(0,1)$ then $x = F^{-1}(u)$ has distribution f (Weibull distribution): $F(x) = 1 - e^{-(x/\lambda)^k}$. A straightforward calculation shows that

$$F^{-1}(u) = \lambda\left[\ln\frac{1}{1-u}\right]^{1/k}$$

Thus the model for date is

$$\boxed{x = \lambda\left[\ln\frac{1}{1-u}\right]^{1/k}}$$

Apply logarithm on both sides to get

$$\underbrace{\ln x}_{\tilde{x}} = \underbrace{\ln \lambda}_{\tilde{\lambda}} + \underbrace{\frac{1}{k}}_{\tilde{k}}\underbrace{\left(\ln\ln\frac{1}{1-u}\right)}_{\tilde{u}}$$

The linear model is $\boxed{\tilde{x} = \tilde{\lambda} + \tilde{k}\tilde{u}}$

Form normal equation on data $(\tilde{u}_k, \tilde{x}_k)$; $k=1,2,\cdots,6$:

$$A = \begin{bmatrix} 1 & \tilde{u}_1 \\ 1 & \tilde{u}_2 \\ \vdots & \vdots \\ 1 & \tilde{u}_6 \end{bmatrix}, \quad c = \begin{bmatrix} \tilde{\lambda} \\ \tilde{k} \end{bmatrix}, \quad b = \begin{bmatrix} \tilde{x}_1 \\ \tilde{x}_2 \\ \vdots \\ \tilde{x}_6 \end{bmatrix}$$

$$A^T A c = A^T b \Rightarrow \begin{bmatrix} 6.000 & -2.183 \\ -2.183 & 3.022 \end{bmatrix}\begin{bmatrix} \tilde{\lambda} \\ \tilde{k} \end{bmatrix} = \begin{bmatrix} -0.142 \\ 4.502 \end{bmatrix}$$

solve with python to get $\tilde{\lambda} = 0.703$, $\tilde{k} = 1.997$

$$\Rightarrow k = \frac{1}{\tilde{k}} \doteq 0.501, \quad \lambda = e^{\tilde{\lambda}} = e^{0.703} \doteq 2.020$$

Note:
You can also avoid the inverse function and directly work with F:

$$x = F^{-1}(u) \Rightarrow u = F(x) \Rightarrow$$

$$u = 1 - e^{-(x/\lambda)^k} \Rightarrow 1-u = e^{-(x/\lambda)^k} \Rightarrow \ln(1-u) = -\left(\frac{x}{\lambda}\right)^k$$

$$\Rightarrow \ln\frac{1}{1-u} = \left(\frac{x}{\lambda}\right)^k \Rightarrow \ln\ln\frac{1}{1-u} = k\ln\frac{x}{\lambda} = k(\ln x - \ln\lambda)$$

$$\Rightarrow \underbrace{\ln x}_{\tilde{x}} = \underbrace{\ln\lambda}_{\tilde{\lambda}} + \underbrace{\frac{1}{k}}_{\tilde{k}}\Big[\underbrace{\ln\ln\frac{1}{1-u}}_{\tilde{u}}\Big)$$

Now continue as before ...