Computational Modelling in Chemistry
SIMLAB Homework

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Deadline: 00:00 on November 19, 2025

Homework 1

Generate samples according to the given distributions and correlation coefficients. The sample size must be 10,000, and please use the Latin Hypercube sampling method. The report must include:

- 3 figures on the probability density function (*pdf*) of the original distribution of the variables (one figure for each variable) and information about their characteristics: mean, standard deviation.
- After the sample generation, you have to present three figures (one figure for each variable) about the empirical distribution of the parameters (histograms) and comment on the comparison of the original distributions and the empirical ones.
- You have to present the original correlation table and the raw correlation table of the empirical sample. Comment on the differences/similarities.
- Finally, you have to present three scatterplots (X–Y, Y–Z, and X–Z) and you have to comment on the effect of the correlation.

Name	**Neptun ID**	**Variables (factors)**			**Correlation**
		X	**Y**	**Z**	
Balázs Krisztina	JJS8IN	N(0,2)	U(−3,2)	N(2,4)	Corr(X,Z) = 0.5
Burlacu Péter Dániel	UV0XM9	U(0,4)	N(1,1)	N(−1,2)	Corr(Y,Z) = −0.2
Fábián Lizett	JMHILE	N(0,3)	N(0,3)	U(−2,2)	Corr(X,Y) = 0.6
Galanics Kitti Csenge	CE6COC	N(1,4)	N(−1,1)	U(0,2)	Corr(X,Y) = −0.6
Gargya Noémi Éva	JJDXN7	U(0,3)	N(−1,2)	N(0,3)	Corr(Y,Z) = 0.7
Nagy Eszter	RU4P0X	N(−2,2)	U(0,4)	N(0,3)	Corr(X,Z) = −0.7
Palik Dezső István	BGG35F	U(0,3)	N(0,3)	N(−1,2)	Corr(Y,Z) = −0.3
Rácsai Balázs	WM82LC	U(0,4)	N(2,4)	N(2,3)	Corr(Y,Z) = 0.8
Radócz Roland	G73MSE	N(−2,1)	N(1,2)	U(−3,0)	Corr(X,Y) = 0.9
Riznychenko Tetiana	YOJWT5	N(0,3)	N(−1,2)	U(0,3)	Corr(X,Y) = −0.5
Sajósi Benedek	PRVEB8	N(0,2)	U(−1,4)	N(1,4)	Corr(X,Z) = −0.8
Terbák Enikő Krisztina	D4GW6X	U(−1,3)	N(2,4)	N(−3,1)	Corr(Y,Z) = 0.95
Voigt Inga Maria	IML2PL	N(−1,1)	U(−5,−2)	N(3,3)	Corr(X,Y) = −0.95

Homework 2

A chemical reaction has the following kinetic parameters:
A = … cm³ mol⁻¹ s⁻¹,
E/R = … K,
uncertainty factor f = …,
$\sigma(E)$ = … kJ / mol,
R = 8.314 J / mol⁻¹ K⁻¹ and has no uncertainty.

Assume that

$$\sigma(\ln A) = \frac{f \ln 10}{3},$$

and that both $\ln(A)$ and E/R are normally distributed (truncated at $\pm 3\sigma$).

This reaction is important for an isothermal plug-flow reactor experiment where the nominal temperature is T = … K and its uncertainty is $\sigma(T)$ = … K. The temperature is also normally distributed (truncated at $\pm 3\sigma$). $\ln(A)$, E / R, and T are uncorrelated random variables.

Based on the text above and the following table, create your personalized task description:

Name	Neptun ID	Reaction	A / cm³ mol⁻¹ s⁻¹	(E/R) / K	f	$\sigma(E)$ / kJ mol⁻¹	T / K	$\sigma(T)$ / K
Balázs Krisztina	JJS8IN	H + NO = OH + N	2.16×10^{14}	24910	0.30	10	620	30
Burlacu Péter Dániel	UV0XM9	O + HO_2 = OH + O_2	1.62×10^{13}	−224	0.50	12	640	20
Fábián Lizett	JMHILE	O + N_2 = NO + N	1.80×10^{14}	38400	0.15	5	660	15
Galanics Kitti Csenge	CE6COC	O + N_2O = NO + NO	9.00×10^{13}	13930	0.40	9	680	25
Gargya Noémi Éva	JJDXN7	O + N_2O = N_2 + N_2	3.66×10^{12}	8020	0.50	14	700	30
Nagy Eszter	RU4P0X	H + HO_2 = 2 OH	4.44×10^{14}	700	0.15	4	720	20
Palik Dezső István	BGG35F	H + H_2O_2 = H_2 + HO_2	1.68×10^{12}	1890	0.50	11	740	15
Rácsai Balázs	WM82LC	H + NO_2 = OH + NO	2.52×10^{14}	340	0.30	6	760	24
Radócz Roland	G73MSE	H + CO_2 = OH + CO	2.76×10^{14}	13915	0.20	3	780	26
Riznychenko Tetiana	YOJWT5	OH + CN = O + HCN	6.00×10^{13}	1000	0.60	7	800	28
Sajósi Benedek	PRVEB8	NH_2 + OH = H + H_2NO	6.38×10^{13}	9273	1.00	9	820	19
Terbák Enikő Krisztina	D4GW6X	N + NH_2 = H_2 + N_2	2.45×10^{13}	0	2.00	5	840	21
Voigt Inga Maria	IML2PL	NH_2 + O_2 = H_2NO + O	3.00×10^{13}	14996	0.90	10	860	20

Tasks

1. Calculate the values of $\sigma(\ln A)$ and $\sigma(E/R)$.
2. Using the SimLab program (left panel), generate 100 random parameter vectors ($\ln A$, E/R, T) with the Latin Hypercube Sampling method, according to the specified probability density functions of each parameter.
3. Create a scatter plot with:
   - x-axis: $\ln A$
   - y-axis: E/R
   - The data pairs should be displayed as points.
4. Using the SimLab program (middle panel), calculate the corresponding $\ln k$ values for each parameter vector (see the Arrhenius equation in logarithmic form), and the corresponding $1/T$ values.
5. Create another scatter plot with:
   - x-axis: $1000/T$
   - y-axis: $\ln k$
   - The data pairs should be displayed as points.
6. Using the SimLab program (right panel), determine:
   - The histogram of the random variable $\ln k$
   - The expected value and standard deviation of $\ln k$
   - The Pearson correlation coefficient (PEAR) between the data pairs ($\ln k$, $1/T$)
7. Present the results in a Word file that includes:
   - A detailed description of the computational steps
   - The calculated quantities
   - All generated figures
8. Suggest improvements: How could this assignment be reformulated to make it easier to understand for next year's students? Write your suggestions.

Note: It is not mandatory to use the SIMLAB program for the task. You can also write your own code to perform the calculations.