Exercise 3

Introduction

Let's consider the following two-population model that simulates the evolution of two types of yeasts competing for the same substrate, with their volumes denoted by $C(t)$ and $K(t)$, respectively:

$$\begin{cases} \dot{C(t)} = 0.2586C(t) - 0.0203C^2(t) - k_1 C(t)K(t) \\ \dot{K(t)} = 0.0574K(t) - 0.0098K^2(t) - k_2 C(t)K(t) \end{cases}$$

with initial conditions $C(0) = 0.04184$ and $K(0) = 0.6315$. Experimental volume measurements for the indicated times are collected in the attached file `yeasts.dat`. We aim to determine experimentally the values of the parameters $k1 \in [0.05, 0.06]$ and $k2 \in [0.004, 0.005]$ in order to minimize the discrepancy between the experimental data and the model.
In other words, we want to find:

$$(k_1, k_2)^* = \arg\min_{k_1,k_2} \sum_{j=1}^{N} \| d_j - y_j\,(k_1, k_2) \|^2$$

where d_j is the experimental data at time t_j, and y_j represents the simulated quantities.
Both d and y will be considered as vectors containing pairs of volumes for a certain time.
Subsequently, we will numerically integrate the differential problem using a numerical technique and, finally, discuss the obtained results.

Analysis

Reorganization of experimental data The experimental data in `yeasts.dat` is in the form of two vectors $VolC$ and $VolK$, which represent the experimental values of $C(t)$ and $K(t)$ at different times, given by the vector t_{esp}. We have:

t_{esp} (s)	$VolC$	$VolK$
0	0.3750	0.2900
1.5000	0.9200	0.3700
9.0000	3.0800	0.6300
10.0000	3.9900	0.9800
18.0000	4.6900	1.4700
23.0000	6.1500	1.4600
25.5000	9.9100	1.1100
27.0000	9.4700	1.2250
38.0000	10.5700	1.1000
42.0000	7.2700	1.7100
45.5000	9.8800	0.9600
47.0000	8.3000	1.8400
18.0000	5.7800	1.2200

As we can observe, for $t_{exp} = 18$, we have two different experimental measurements. In order for our optimization process to take both measured values into account, we will consider the average value of $VolC$ and $VolK$ at time $t_{exp} = 18$. Hence, from now on the experimental dataset that we will consider is shown in the following table:

t_{esp} (s)	$VolC$	$VolK$
0	0.3750	0.2900
1.5000	0.9200	0.3700
9.0000	3.0800	0.6300
10.0000	3.9900	0.9800
18.0000	5.2350	1.3450
23.0000	6.1500	1.4600
25.5000	9.9100	1.1100
27.0000	9.4700	1.2250
38.0000	10.5700	1.1000
42.0000	7.2700	1.7100
45.5000	9.8800	0.9600
47.0000	8.3000	1.8400

Optimization Approach and Code Description We will use the MATLAB scrip `minimizing` to compute $(k_1, k_2)^*$.
The optimization approach used in the code is a brute-force search over a predefined grid of k_1 and k_2 values. The grid is defined by the vectors k_{11} and k_{22}, which are generated using a step size of 0.0001 and 0.00001, respectively. The code iterates over all combinations of k_1 and k_2 values, simulates the ODE system using the ode45 MATLAB solver, and computes the squared deviation between the simulated values and the experimental data. If the current deviation is smaller than the previously recorded minimum, the indexes of the vectors k_{11} and k_{22} and the value of the current deviation are stored.
After the computation, we obtain:

$$(k_1, k_2)^* = (0.05, 0.005)$$

Hence, our best-fitted differential model is:

$$\begin{cases} \dot{C}(t) = 0.2586C(t) - 0.0203C^2(t) - 0.05C(t)K(t) \\ \dot{K}(t) = 0.0574K(t) - 0.0098K^2(t) - 0.005C(t)K(t) \end{cases}$$

Finally, the code generates two plots, one for $C(t)$ and one for $K(t)$, which show the simulated values as a function of time for the optimal values $k_1 = 0.05$ and $k_2 = 0.005$.

Results The solutions $C(t)$ and $K(t)$ of the differential system (for $(k_1, k_2)^* = (0.05, 0.005)$), and the experimental values $VolC$ and $VolK$ for times t_{esp} are shown below. A table summarizing the obtained results is also presented.

t_{esp} (s)	$C(t)$	$K(t)$	$VolC$	$VolK$
0	0.0418	0.6315	0.3750	0.2900
1.5000	0.0580	0.6814	0.9200	0.3700
9.0000	0.2727	0.9812	3.0800	0.6300
10.0000	0.3305	1.0275	3.9900	0.9800
18.0000	1.2904	1.4349	5.2350	1.3450
23.0000	2.4407	1.6914	6.1500	1.4600
25.5000	3.1126	1.8067	9.9100	1.1100
27.0000	3.5147	1.8696	9.4700	1.2250
38.0000	5.5084	2.1796	10.5700	1.1000
42.0000	5.7583	2.2456	7.2700	1.7100
45.5000	5.8481	2.2940	9.8800	0.9600
47.0000	5.8613	2.3131	8.3000	1.8400

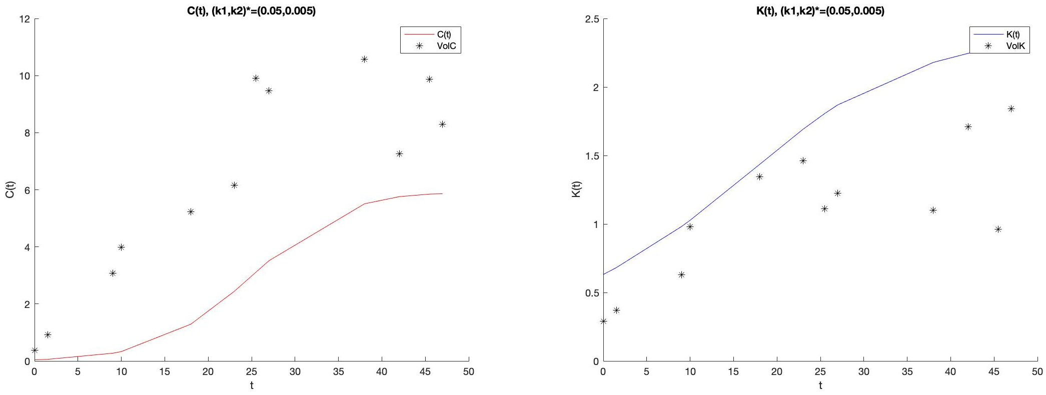

Figure 7: Comparison between experimental data ($VolC$ and $VolK$) and model results ($C(t)$ and $K(t)$).

Conclusion Based on the results reported above, we can conclude that, despite optimizing the values of k_1 and k_2, the proposed differential model does not provide a good representation of the experimental values. In fact, the squared deviation between the experimental values and the differential solutions is $\sum_{j=1}^{N} \|d_j - y_j(k_1, k_2)\|^2 = 130.1159$, which is a rather high value. A similar outcome was somewhat predictable: it is sufficient to observe how the initial values of the differential model differ substantially from the experimental ones. Moreover, the experimental values do not follow a monotonic trend (i.e., increasing or decreasing), unlike the model solutions. This heterogeneity underlies the highlighted discrepancies.