Rochester Institute of Technology, Fall 2022
MATH-411 Numerical Analysis
Midterm – Project 1

Due: Friday September 30, 2022 at 11.59pm EST.
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Remark:

- All assignments are uploaded on MyCourses as pdf.
- For this project your can handwrite or typeset your solution.
- Figure out how to upload your files on MyCourses before the due dates.
- You can discuss ideas on how to tackle the problems on **Piazza** but do not post solutions. Thanks.
- **Important Note:**
  1. This is a group project
  2. You must write your solution in your own words and writing
  3. This project will be submitted and graded individually
  4. Include the name of your group members on the first page of your solution document
  5. Please provide detailed explanations and show all your work clearly.
  6. If any of the problems involves MATLAB, please turn in your code and figures as well.

Chemistry Background:

The problem I am going to describe here comes by way of work done by Professor David Ross. Before getting to the problem, let's discuss some chemistry. Don't worry if you don't absorb all the chemistry, as it will not be necessary for the math that follows. It is good (and interesting), though, to have an idea of where the problem is coming from.

An important class of chemical reaction systems is the class of *ligand-binding* systems. In such reactions, the chemicals involved fall into two categories: *Ligands* and *Binding Molecules*. The basic assumption in modeling these reactions mathematically is that ligands react with binding molecules but not with other ligands, and that binding molecules react only with ligands, not with other binding molecules.

Immuno-Assay Chemistry is one field in which such models are applied.

The Task:

Suppose that there are N ligands and M binding molecules, If X_i is a ligand and Y_j is a binding molecule and Z_{ij} is the complex of the two (meaning the two are bonded), this system is described chemically by the equations

$$X_i + Y_j \xrightarrow{\mathrm{C_{ij}}} Z_{ij}$$

$$Z_{ij} \xrightarrow{\Gamma_{\mathrm{ij}}} X_i + Y_j$$

The first of these equations says that X_i and Y_j combine to form Z_{ij} in a second-order reaction with rate C_{ij}. The second says that Z_{ij} dissociates back into X_i and Y_j in a first-order reaction with rate Γ_{ij}. Here, C_{ij} and Γ_{ij} are constants, called the forward and reverse rate constants.

Let x_i and y_j and z_{ij} be the concentrations of the ligands, the binding molecules, and the complexes. If we were interested in the kinetics of these reactions, we would have to solve the system of differential equations

$$\frac{dx_i}{dt} = -x_i \sum_{j=1}^{M} C_{ij} y_j + \sum_{j=1}^{M} \Gamma_{ij} z_{ij}$$

$$\frac{dy_j}{dt} = -y_j \sum_{i=1}^{N} C_{ij} x_i + \sum_{i=1}^{N} \Gamma_{ij} z_{ij}$$

$$\frac{dz_{ij}}{dt} = C_{ij} x_i y_j - \Gamma_{ij} z_{ij}$$

to see how the concentrations progress in the course of the reactions. We would need initial conditions for these differential equations. For example, if we assumed that at time $t = 0$ the ingredients were mixed together, and that no complexes had yet formed, we would use the initial conditions

$$x_i = \xi_i$$

$$y_j = \eta_j$$

$$z_{ij} = 0$$

where ξ_i and η_j are the total concentrations of ligand i and binding molecule j

However, we are only interested in equilibria. So, we must solve the nonlinear algebraic equations.

$$
\begin{aligned}
0 &= -x_i \sum_{j=1}^{M} C_{ij} y_j + \sum_{j=1}^{M} \Gamma_{ij} z_{ij} \\
0 &= -y_j \sum_{i=1}^{N} C_{ij} x_i + \sum_{i=1}^{N} \Gamma_{ij} z_{ij} \\
0 &= C_{ij} x_i y_j - \Gamma_{ij} z_{ij}
\end{aligned}
$$

$$
\begin{aligned}
x_i + \sum_{j=1}^{M} z_{ij} &= \xi_i \\
y_j + \sum_{i=1}^{N} z_{ij} &= \eta_j
\end{aligned}
$$

We can eliminate z_{ij} easily,

$$
z_{ij} = \frac{C_{ij} x_i y_j}{\Gamma_{ij}}
$$

and substitute this expression into the others to obtain.

$$
\begin{aligned}
x_i \left(1 + \sum_{j=1}^{M} k_{ij} y_j \right) &= \xi_i \\
y_j \left(1 + \sum_{i=1}^{N} k_{ij} x_i \right) &= \eta_j
\end{aligned}
$$

and finally, after solving this last equation for y_j and substituting

$$
x_i \left(1 + \sum_{j=1}^{M} \frac{k_{ij} \eta_j}{1 + \sum_{s=1}^{N} k_{sj} x_s} \right) = \xi_i
$$

where $k_{ij} = \frac{C_{ij}}{\Gamma_{ij}}$, is the equilibrium constant. At this point, there is no further simplification to do by hand, we must simply solve these equations numerically.

References

H. A. Feldman: "Mathematical Theory of Complex Ligand-Binding Systems at Equilibrium", Analytical Biochemistry, **48**, pp. 317-338 (1972)

Friedman, A., Mathematics in Industrial Problems, Part 5 , Springer-Verlag, 1992.

Gerlach, Jurgen, *Accelerated Convergence in Newton's Method* SIAM Review, V.36 #2, http://www.jstor.org/view/00361445/di977121/97p0317h/0