

Homework #1: Linear Algebra

Problem 1. (30 points)

1. Develop a MATLAB¹ function to perform Gaussian elimination (without pivoting) on the system

$$\mathbf{Ax} = \mathbf{b},$$

where \mathbf{A} is a $N \times N$ matrix for which the only non-zero elements are $A_{i(i+j)} = a_j$ with $|j| \leq M \leq N$. Here, $A_{i(i+j)}$ denotes the i^{th} row and $(i+j)^{\text{th}}$ column of \mathbf{A} , a_j is the value stored on the j^{th} diagonal of \mathbf{A} , and \mathbf{b} is a full $N \times 1$ vector. Note that \mathbf{A} is a particular type of banded matrix: a Toeplitz matrix with bandwidth M .

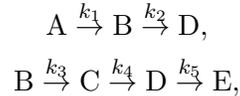
Your function should take as input, the values of N and M as well as a vector \mathbf{a} storing the values on the diagonals: a_j , $j = -M, -(M-1), \dots, M-1, M$ and \mathbf{b} . Use a single $N \times 2M+1$ array to represent the matrix \mathbf{A} as it is transformed by the elimination procedure. The idea of this problem is to have you code the detailed algorithm yourself; for this part, do *not* use any built-in MATLAB functions for matrix factorization. To show your function works, apply it to the linear system described in part 2 with $M = 3$ and check the result.

2. Apply your function to solve a linear system of equations with $a_j = -1/4, -1/4, 1, -1/4, -1/4$ for $j = -M, -1, 0, 1, M$ and zero otherwise for various values of $M \in (2, 100)$. Set $N = M^2$. In all cases, let $\mathbf{b} = \mathbf{1}$ (which is a vector whose components are each equal to 1). Record the solution time for your Gaussian elimination algorithm developed in previous part using the `tic` and `toc` commands in MATLAB. Additionally, construct the same banded matrix explicitly as a sparse matrix using the MATLAB command `spdiags` and as a full matrix. Solve the same system of equations with the sparse and full matrices using the MATLAB “\” command. Record the solution time with each matrix for various values of $M \in (2, 100)$. Plot all the solution times and discuss the results.
3. Discretization of partial differential equations converts them into equations involving sparse, banded matrices such as \mathbf{A} . In this case, the quantity $1/M$ is a proxy for spatial resolution of the discretization. Often, large values of M are preferred since these enhance the resolution of the numerical solution and minimize numerical errors. For each solution method systematically try values of M larger than 100 until the method fails to execute. Use these numerical experiments to estimate the value of M at which each method fails. Use your timing results to estimate how the CPU time required scales with M for large values of M . Discuss your results.
4. Use the built-in MATLAB function “`pcg`” to construct an approximate solution to the system of equations with relative error 10^{-8} . Note, we will discuss such iterative methods in class in another week. Use the sparse matrix representation of \mathbf{A} and the same \mathbf{b} . Record and plot the solution time for various values of $M \in (2, 100)$. Compare this with the solution times of your other methods. Approximate solvers such as “`pcg`” utilize the product of the matrix \mathbf{A} with different vectors to iteratively refine an approximation for the solution of the system of linear equations. If this method required no additional storage beyond the sparse representation of

\mathbf{A} and the vector \mathbf{b} , estimate the value of M at which the storage requirements exceed your computer's available memory. Extrapolate from the solution times you recorded to estimate how long it would require to solve a system of equations that large.

Problem 2. (20 points)

Feel free to use all the features of MATLAB for this problem. Consider the chemical reaction network:



where each reaction is irreversible and elementary. The dynamics of this network in a batch reactor at constant volume and temperature are described by the system of differential equations:

$$\frac{d\mathbf{c}}{dt}(t) = \mathbf{S}\mathbf{r}(t), \quad \forall t, \quad (1)$$

$$\mathbf{r}(t) = \mathbf{K}\mathbf{c}(t), \quad \forall t, \quad (2)$$

$$\mathbf{c}(0) = \mathbf{c}_0, \quad (3)$$

where:

$$\mathbf{c}(t) = \begin{bmatrix} c_A(t) \\ c_B(t) \\ c_C(t) \\ c_D(t) \\ c_E(t) \end{bmatrix} \in \mathbb{R}^5$$

is the vector of species concentrations at time t ,

$$\mathbf{r}(t) = \begin{bmatrix} r_1(t) \\ r_2(t) \\ r_3(t) \\ r_4(t) \\ r_5(t) \end{bmatrix} \in \mathbb{R}^5$$

is the vector of reaction rates or *fluxes* at time t , $\mathbf{S} \in \mathbb{R}^{5 \times 5}$ is the stoichiometry matrix for the reaction network, $\mathbf{K} \in \mathbb{R}^{5 \times 5}$ is the matrix defining the fluxes in terms of the concentrations and $\mathbf{c}_0 \in \mathbb{R}^5$ is the vector of initial concentrations.

1. Program the matrices \mathbf{S} and \mathbf{K} in MATLAB and display them (you will need to declare the reaction rates k_1, \dots, k_5 as symbolic variables using MATLAB's Symbolic Math Toolbox).
2. What are the ranks of \mathbf{S} and \mathbf{K} ? Is either one rank deficient?
3. What does the irreversibility of the reactions tell you about the possible fluxes at any time?
4. Characterize the null spaces of \mathbf{S} and \mathbf{K} in terms of a dimension and a basis.
5. What does your analysis tell you about the possible fluxes at steady state?
6. What does your analysis tell you about the possible concentrations at steady state?
7. Characterize the left null space of \mathbf{S} in terms of a dimension and a basis.

8. Multiply Eqn. (1) from the left by an arbitrary nontrivial left null vector. What does this tell you about the time evolution of certain weighted sums of the concentrations? Given your characterization of the left null space of \mathbf{S} , can you provide a physical interpretation for this particular reaction network?
9. Does this give you new information about the possible concentrations at steady state?
10. Characterize the left null space of \mathbf{K} in terms of a dimension and a basis. What does this tell you about the time evolution of the fluxes? Can you provide a physical interpretation for this particular reaction network?
11. Characterize the column spaces of \mathbf{S} and \mathbf{K} in terms of a dimension and a basis. Use these results to characterize the column space of \mathbf{SK} .
12. The solution of the differential equations can be written as the equivalent integral equations:

$$\mathbf{c}(\tau) = \mathbf{c}_0 + \int_0^\tau \mathbf{SK}\mathbf{c}(t) dt.$$

Use your analysis to characterize a set within which all solutions of the differential equations must lie.

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