ME 451C
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Notes on Homework #7

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Abstract

I hope you find these commentaries on Homework for week #7 useful.

1 Problem # 1

We are interested in this linear ODE:

$$\frac{D\mathbf{X}}{Dt} = \mathbf{L}\mathbf{X} \tag{1}$$

where $\mathbf{X}$ is a 5-dimensional column vector.

This was the $\mathbf{L}$ matrix I gave:

$$\mathbf{L} = \begin{bmatrix} -560600 & -560000 & -39200 & -599200 & 40000 \\ -219600 & -220001 & 19600 & -200399 & -20000 \\ -340200 & -340000 & -59800 & -399800 & 60000 \\ -219600 & -220000 & 19600 & -200400 & -20000 \\ 340200 & 340000 & 59800 & 399800 & -60000 \end{bmatrix} \tag{2}$$

I inadvertently entered it with some slight typos—which made the third row to be precisely the negative of the fifth row. But we will deal with it as it stood, and talk about it later.

The eigenvalues are easily found. They are (with Mathematica): $-10^6, -10^5, -10^3, -1, 0$; all except the last mode are decaying modes.[1] The eigenvectors of $\mathbf{L}$ tells us that the following transformation will diagonalize the $\mathbf{L}$ matrix:

$$\mathbf{Y} = \mathbf{Q} \cdot \mathbf{X} \tag{3}$$

where

$$\mathbf{Q} = \begin{bmatrix} -1 & -1 & 0 & -1 & 0 \\ 1 & 1 & -1 & 0 & 1 \\ -1 & 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 & 1 \end{bmatrix} \tag{4}$$

Each of the 5 components of $\mathbf{Y}$ has its private time scale (the reciprocal of its eigenvalue—magnitude of the real part). Written out in long hand (and ordered in descending magnitudes of the eigenvalues), we have:

$$\begin{aligned} Y_1 &= -X_1 - X_2 - X_4, & (5)\\ Y_2 &= X_1 + X_2 - X_3 + X_5, & (6)\\ Y_3 &= -X_1 + X_3 + X_4, & (7)\\ Y_4 &= -X_2 + X_4, & (8)\\ Y_5 &= X_3 + X_5, & (9) \end{aligned}$$

So if you are interested in the milli-second time range, mode # 3 with eignevalue -10^3 is the dominant active mode. Both modes #1 and # 2 are dead (regardless of initial conditions) because of their much bigger negative eigenvalues:

$$\begin{aligned} 0 &\approx -X_1 - X_2 - X_4, & (10)\\ 0 &\approx X_1 + X_2 - X_3 + X_5. & (11) \end{aligned}$$

These two algebraic equations are called *equations of state*.

In addition, mode #4 and mode #5 are much too slow and their (approximate) amplitudes in the milli-second time interval are determined by their initial conditions:

$$\begin{aligned} -X_2 + X_4 &\approx -X_2(0) + X_4(0), & (12)\\ X_3 + X_5 &\approx X_3(0) + X_5(0), & (13) \end{aligned}$$

[1] I had wanted a the smallest eigenvalue $O(0.01)$, and my typo ruined it. The lower right corner entry should have been 340200.1. The smallest eigenvalue would then be +0.04.

These two algebraic equations provide two *conserved scalars*.[2]

The above four algebraic equations can be used to eliminate any four of the unknowns in favor of a chosen (last) one, and the governing ODE for that chosen unknown is easily derived.

If one had developed the original ODE (and the **L** matrix) for a real life problem, it would be important to realize (and to point out) that the prediction of this mathematical model in the time interval of tens and hundred seconds range is suspect—the answers can be affected by slight uncertainties of the matrix elements. This was my original point of giving this homework problem (and asking for a plot of your numerical solutions in this time range).

2 Problem # 2

I promised to do this problem in class, but did not get around to it.

The ODEs are:

$$\frac{DX_1}{Dt} = \frac{X_2^2 - X_1}{\epsilon} + (1 - X_1), \tag{14}$$

$$\frac{DX_2}{Dt} = -\frac{X_2^2 - X_1}{\epsilon} - \gamma X_2. \tag{15}$$

I inserted a γ here, where it may be any differentiable function of X_1 or X_2, or a constant. In the original problem as assigned, I had chosen $\gamma = 1$.

When ϵ is small (and positive), we obviously have one fast reaction (which decays). It is not clear whether the QSSA is applicable, and if so, whether X_1 or X_2 should have the honor.

Adding the two equations, we have:

$$\frac{D}{Dt}(X_1 + X_2) = 1 - (X_1 + \gamma X_2). \tag{16}$$

This ODE is exact, independent of the value of ϵ.

I unfortunately gave the initial condition such that $X_1 + X_2$ was initially unity, and $\gamma = 1$. Hence, the exact solution for this specific problem as posed is $X_1 + X_2 = 1$ for all t. But it is clear that if $\gamma \neq 1$, this is a single ODE for two dependent variables. We shall proceed assuming γ to be a general parameter (but not excluding the

[2] Slow modes do not always provide conserved scalars. See later.

possibility that it could be 1.0) and that the initial condition is some arbitrary numbers.

In the small ϵ limit, we expect in the slow evolutionary period the following to be valid:

$$X_1 = X_2^2 + O(\epsilon). \tag{17}$$

Hence, the simplified ODE for the slow period is:

$$\frac{DX_2}{Dt} = \frac{1 - (X_2^2 + \gamma X_2)}{1 + 2X_2} + O(\epsilon) \tag{18}$$

The initial condition for this ODE can be obtained by observing that in the brief transient period $t = O(\epsilon)$, $X_1 + X_2$ is approximately a "conserved scalar," while at the tail end of the transient period, Eq.(17) should hold. Together, they can determined the initial condition analytically without numerical integration.

2.1 Does slow modes always provide approximate conserved scalars to the fast modes?

It should be emphasized that the initial conditions for the ODEs in the slow period is not always so easily (and analytically) derived. In particular, across the brief initial transient period, there may *not* be any conserved scalars (coming from the slow modes being very slow in comparison). If so, then the initial condition must be computed numerically. For example, if these are the ODEs to be dealt with

$$\frac{DX_1}{Dt} = \frac{X_2^2 - X_1}{\epsilon} + (1 - X_1), \tag{19}$$

$$\frac{DX_2}{Dt} = -\Gamma(X_1, X_2)\frac{X_2^2 - X_1}{\epsilon} - X_2. \tag{20}$$

where $\Gamma(X_1, X_2)$ is some arbitrary differentiable (positive) function of its arguments, then there may be no approximate conserved scalars.[3] For such cases, one must resort to numerical computations to march across the brief fast transient to determine the initial conditions.

[3] It can be shown that a conserved scalar exists for this problem if $\Gamma(X_1, X_2)$ is "variables separable".