

ME 451C  
Winter Quarter, 2004-05  
Notes on Homework #8

Harvey Lam  
lam@princeton.edu

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**Abstract**

I hope you find these commentaries on Homework for week #8 useful.

## 1 The original toy problem

The original ODE system is:

$$\frac{DX_1}{Dt} = W_1 + W_2, \quad (1)$$

$$\frac{DX_2}{Dt} = -2W_1 + W_3, \quad (2)$$

$$W_1 = \frac{X_2^2 - X_1}{\epsilon}, \quad W_2 = W_2(X_1, X_2), \quad W_3 = W_3(X_1, X_2). \quad (3)$$

We are interested in the time interval of  $t = O(1)$  in the limit of asymptotically small  $\epsilon > 0$ . It is assumed that  $X_1, X_2$  are  $O(1)$  in this limit. The goal is to find a simplified model to this toy problem valid after a very brief initial transient.

We have already done the paper and pencil version of singular perturbation of this toy problem. The idea of this homework is to do it by CSP, computational singular perturbation. The basic advantage of CSP is that it can handle problems with a big  $N$ , and it needs no

“intelligent” normalization of (independent or dependent) variables, or explicit identification of a small parameter to do asymptotics on. Everything can be done by a computer program.

## 2 The Jacobian

The Jacobian of the right side of the ODEs with respect to  $(X_1, X_2)$  is denoted by  $\mathbf{J}$ :

$$\mathbf{J} = \begin{bmatrix} -\frac{1}{\epsilon} + \frac{\partial W_2}{\partial X_1} & \frac{2X_2}{\epsilon} + \frac{\partial W_2}{\partial X_2} \\ 2\frac{1}{\epsilon} + \frac{\partial W_2}{\partial X_1} & -2\frac{2X_2}{\epsilon} + \frac{\partial W_3}{\partial X_2} \end{bmatrix} \quad (4)$$

It is easy to show that one of the eigenvalues is  $O(1/\epsilon)$  and the other one is  $O(1)$ . If you don't have a toy problem (with an  $\epsilon$ ), then getting the eigenvalues numerically will provide you with the needed information.

## 3 Trial basis vectors

To get started, we pick the following as our trial fast basis vectors:

$$\mathbf{a}_1 = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix}, \quad \mathbf{b}^1 = \begin{bmatrix} \beta^1 & \beta^2 \end{bmatrix} \quad (5)$$

where  $\alpha_1$  and  $\alpha_2$  are two random numbers of order unity. Hence orthonormality says:

$$\beta^1 \alpha_1 + \beta^2 \alpha_2 = 1. \quad (6)$$

Without loss of generality, we can arbitrarily leave  $\beta^1$  to be free, which says  $\beta^2 = (1 - \beta^1 \alpha_1)/\alpha_2$ . Since our chosen set of trial fast basis vector is constant. So  $D\mathbf{b}^1/Dt$  is zero.

### 3.1 CSP step one

So our (unrefined)  $\Lambda_1^1$  is readily computed:

$$\Lambda_1^1 = -\frac{(\alpha_1 - 2\alpha_2 X_2)(\beta^1 - 2\beta^2)}{\epsilon} + O(1) \quad (7)$$

The inverse (reciprocal) is the fast time scale  $\tau_1^1$ :

$$\tau_1^1 = -\frac{\epsilon}{(\alpha_1 - 2\alpha_2 X_2)(\beta^1 - 2\beta^2)} + O(\epsilon^2) \quad (8)$$

The refined  $\mathbf{b}_o^1$  is—in the asymptotically small  $\epsilon$  limit:

$$\mathbf{b}_o^1 = \tau_1^1 \mathbf{b}^1 \cdot \mathbf{J} = \frac{1}{\alpha_1 - 2\alpha_2 X_2} [1, -2X_2]. \quad (9)$$

If we don't have a toy problem and we don't know what  $\epsilon$  is, we will do the refinement numerically using dimensional numbers in the calculations. Whatever  $\mathbf{b}_o^1$  comes out is OK to be used (provided the existence of an eigenvalue gap is verified). Note that

$$\mathbf{b}_o^1 \cdot \mathbf{a}_1 = 1 \quad (10)$$

is automatically satisfied. We shall use this refined  $\mathbf{b}_o^1$  to proceed to step two refinement.

### 3.2 CSP step two

We proceed with CSP step two with  $\mathbf{a}_1$  and  $\mathbf{b}_o^1$  as our trial set of fast basis vectors. Note that  $\mathbf{a}_1$  is a constant vector. So  $D\mathbf{a}_1/Dt$  is zero.

The refined  $\mathbf{a}_1^o$  is given by CSP step two procedure by:

$$\mathbf{a}_1^o = \mathbf{J} \cdot \mathbf{a}_1 \tau_{o1}^1 \quad (11)$$

where  $\tau_{o1}^1$  is the inverse (reciprocal) of  $\Lambda_{o1}^1$  computed using  $\mathbf{a}_1$  and  $\mathbf{b}_o^1$ . Note that  $\mathbf{b}_o^1$  is now NOT a constant vector. However, we can take  $D/Dt$  of Eq.(10) and use it to conclude that  $D\mathbf{b}_o^1/Dt \cdot \mathbf{a}_1 = 0$  and caused no troubles. Straightforward algebra will yield, to leading order in  $\epsilon$ , the following refined  $\mathbf{a}_1^o$ :

$$\mathbf{a}_1^o = \frac{\alpha_1 - 2\alpha_2 X_2}{1 + 4X_2} \begin{bmatrix} 1 \\ -2 \end{bmatrix} + O(\epsilon) \quad (12)$$

Note that  $\mathbf{b}_o^1 \cdot \mathbf{a}_1^o = 1$ . Remember,  $\alpha_1$  and  $\alpha_2$  are random numbers.

You may also notice that, except for a scaling factor, the refined  $\mathbf{a}_1^o$  is the same as the original *stoichiometric vector* for reaction # 1. And if you stop and think about it, this is entirely reasonable.

## 4 The step one-two refined set of fast basis vectors

We notice that the  $(\alpha_1 - 2\alpha_2 X_2)$  factor is irrelevant. So, to keep things clean and neat, the following are now chosen as our refined

(orthonormal) fast basis vectors:

$$\mathbf{a}_1^o = \frac{1}{1+4X_2} \begin{bmatrix} 1 \\ -2 \end{bmatrix}, \quad \mathbf{b}_o^1 = \begin{bmatrix} 1 & -2X_2 \end{bmatrix} \quad (13)$$

## 5 The fast subspace projector

The fast subspace ( $M = 1$ ) projector is:

$$\mathbf{Q}_{fast} = \mathbf{a}_1^o \mathbf{b}_o^1 = \frac{1}{1+4X_2} \begin{bmatrix} 1 & -2X_2 \\ -2 & +4X_2 \end{bmatrix} \quad (14)$$

## 6 The slow subspace projector

The fast subspace ( $M = 1$ ) projector is:

$$\mathbf{Q}_{slow} = \mathbf{a}_1^o \mathbf{b}_o^1 = \frac{1}{1+4X_2} \begin{bmatrix} 4X_2 & 2X_2 \\ 2 & 1 \end{bmatrix} \quad (15)$$

## 7 The rapid initial transient

In the initial rapid transient, the slow subspace is essentially irrelevant.

$$\frac{D}{Dt} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \overbrace{\frac{1}{1+4X_2} \begin{bmatrix} 1 & -2X_2 \\ -2 & 4X_2 \end{bmatrix}}^{\mathbf{Q}_{fast}} \cdot \overbrace{\begin{bmatrix} W_1 + W_2 \\ -2W_1 + W_3 \end{bmatrix}}^{\text{orig. right hand side}}. \quad (16)$$

Multiplying the right hand side out, we have:

$$\frac{D}{Dt} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 1 \\ -2 \end{bmatrix} \left( W_1 + \frac{W_2 - 2X_2 W_3}{1+4X_2} \right). \quad (17)$$

Remember,  $W_1$  is  $(X_2^2 - X_1)/\epsilon$ . Note that by inspection  $2X_1 + X_2$  is approximately a constant in the initial transient. CSP does not pick this up. It relies on the computer to do what it does best here. Note: tiny integration steps  $O(\epsilon)$  are needed to get the correct structure of this initial transient.

## 8 Reduced chemistry model in the slow subspace

The right hand side of the original ODE is approximated by its projection in the slow subspace after the fast mode dies.

$$\frac{D}{Dt} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \overbrace{\frac{1}{1+4X_2} \begin{bmatrix} 4X_2 & 2X_2 \\ 2 & 1 \end{bmatrix}}^{\mathbf{Q}_{slow}} \cdot \overbrace{\begin{bmatrix} W_1 + W_2 \\ -2W_1 + W_3 \end{bmatrix}}^{\text{orig. right hand side}}. \quad (18)$$

Multiplying the right hand side out, we have:

$$\frac{D}{Dt} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} 2X_2 \\ 1 \end{bmatrix} \left( \frac{2W_2 + W_3}{1+4X_2} \right). \quad (19)$$

And remember,  $W_2$  and  $W_3$  may contain diffusion terms.

## 9 What if we did not do step two

If we did not do step two, the ODEs for the rapid initial transient would be, instead of Eq.(17), the following:

$$\frac{D}{Dt} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} = \begin{bmatrix} \alpha_1 \\ \alpha_2 \end{bmatrix} \left( W_1 + \frac{W_2 - 2X_2W_3}{1+4X_2} \right) \quad (20)$$

The curly bracket is the inner product of  $\mathbf{b}_o^1$  with the right hand side of the original ODE, does not change. At the tail end of the rapid initial transient, we would expect everything to quiet down, yielding:

$$W_1 \rightarrow -\frac{W_2 - 2X_2W_3}{1+4X_2}. \quad (21)$$

In the ODE derived for the slow subspace,  $W_1$  will make its appearance, instead of not showing its face at all in Eq.(19). This term in general would make trouble for numerical computations. But if Eq.(21) is used to eliminate  $W_1$ , then everything is fine again.

So, the bottomline is: CSP step two should be done at least once (or occasionally). Its job is not to lower the error when the fast modes are neglected (that is the job of step one). Its job is to cleanse the slow subspace of any fast mode mixing.

## 10 Comments

It is worth noting that the CSP algorithm does not take advantage of the dormant modes being dormant or the zero eigenvalue modes (which usually have the meaning of something is conserved). In addition, it does not reduce the number of dependent variables as would be done under the pencil and pencil version of singular perturbation (*e.g.* it does not say approximate  $X_1$  by  $X_2^2$  anywhere, and work on  $X_2$  only).

Theoretically, of course, when reduce chemistry modelling is valid, the number of dependent variables can indeed be reduced. From the computational point of view, the smaller the number of dependent variables that needs to be tracked, the better. Generally speaking, the amount of computations involved in using CSP is substantially more than the amount needed by a good stiff ODE solver. So, the main application of CSP is a diagnostic one: it can be used to study unfamiliar and massively complicated reaction systems to find out who is doing what to whom and when. Such studies can provide guidance in making progress on writing practical codes and developing theories.

It is fair to say that the coupling between reduced chemistry and diffusion is still not fully appreciated by the research community at this moment in 2005.