

ME 451C
Winter Quarter, 2004-05
Supplementary Notes

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Abstract

This is an erratum on *radical pointer* presented in my March 1 lecture and some important modifications on the homework problem of Week #8.

1 Radical Pointer

It is useful to find out which components of \mathbf{X} qualify to be called *fast* for each of the M fast modes. The concept of *radical pointer* was introduced in [1] in 1993 to serve this purpose. The radical pointer—denoted by $Q_m(i)$ in [1]—for fast mode m is the N diagonal elements of the matrix $\mathbf{a}_m \mathbf{b}^m$:

$$Q_m(i) = \text{the } i\text{-th diagonal element of } \mathbf{a}_m \mathbf{b}^m \quad (1)$$

The sum of all N components of the radical pointer of the m -th mode is unity:

$$\sum_{i=1}^N Q_m(i) = \sum_{i=1}^N a_m^i b_i^m = \mathbf{b}^m \cdot \mathbf{a}_m = 1 \quad (2)$$

Thus, if the radical pointer is evenly distributed, the “averaged” value would be $1/N$. The i -th component of \mathbf{X} is eligible to be called fast for this mode if its radical pointer is significantly larger than $1/N$. In

particular, if the radical pointer of a certain component of \mathbf{X} is near unity, then the classical QSSA approximation is applicable for that component for that mode.

In my March 1 lecture, I defined a radical pointer for the whole fast subspace—instead of for each fast m -th mode. The sum of all elements of such a (fast subspace) radical pointer would be M . I erred when I said this sum was unity.

2 Modified Week #8 homework

In the original Week #8 homework, I omitted the CSP step two refinement. The consequence is that the analytical results we obtained in Eq.(14) of Week #8 Notes would not be recovered directly. To recover it, some additional work needs to be done—and I will talk about it on March 3rd. It turns out that this homework problem points out the importance and usefulness of the CSP step two refinement procedure.

The following modifications will make the homework problem more instructive.

1. For the toy problem ($N = 2$) in §1, use the following as your trial set of fast basis vectors ($M=1$):

$$\mathbf{a}_1 = \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix}, \quad \mathbf{b}^1 = [\beta_1, \beta_2] \quad (3)$$

Pick two random numbers for α_1 and α_2 , find β_1 and β_2 .

2. Do one CSP refinement (step one) for \mathbf{b}^1 —get \mathbf{b}_o^1 —to leading order in ϵ .¹ Do one more CSP refinement (step two) for \mathbf{a}_1 —get \mathbf{a}_1^o to leading order in ϵ . Now use $(\mathbf{a}_1^o, \mathbf{b}_o^1)$ as your chosen pair of fast basis vectors.
3. Find \mathbf{Q}_{fast} .
4. Find \mathbf{Q}_{slow} .
5. Find $\mathbf{Q}_{fast} \cdot (\mathbf{w} + \mathbf{d})$ —use \mathbf{Q}_{fast} from #3, and keep all terms.
6. Find the reduced chemistry model (by neglecting $\mathbf{Q}_{fast} \cdot (\mathbf{w} + \mathbf{d})$ —use \mathbf{Q}_{slow} from #4, and keep all terms

¹Note: Only W_1 explicitly depends on ϵ ; W_2 and W_3 do not.

7. Find $(\mathbf{a}_2, \mathbf{b}^2)$ to accompany the above refined $(\mathbf{a}_1^o, \mathbf{b}_o^1)$ to form a complete basis vector set for our 2-dimensional vector space. (I am not asking for a step two refinement. Just to get the complement of the fast subspace—it is the slow subspace).
8. Find f_∞^1 obtained from the refined set $(\mathbf{a}_1, \mathbf{b}_o^1)$, then compare it to f_∞^1 obtained from the un-refined set $(\mathbf{a}_1, \mathbf{b}^1)$. What happens in the small ϵ limit in the slow evolutionary period (did refinement drop the magnitude of f_∞^1)? Does it make any difference whether you use \mathbf{a}_1 or \mathbf{a}_1^o ? Ignore the diffusion term.

References

- [1] “Using CSP to understand complex chemical kinetics,” *Combust. Sci. and Tech.*, **89**, pp. 375-404, 1993.