Optimal Progress Variable for Flamelet Manifolds

Hao Wu
Stanford University

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1 Formulation

A collection of laminar non-premixed flames along the S-shape curve can form a 2D manifold $\phi = \phi(z, \Lambda)$,where z is the mixture fraction and $\Lambda$is any choise of flamelet identifying variable which ensures the validity and the smoothness of the mapping. One plausible choice of Λ is the arc-length along the S-shape curve.

1.1 Notations

- $b \in R^p$: the coefficients of the progress variable and p is the number of species
- $\mathbf{X}_z \in R^{n_z \times p}$: p-dimensional thermo-chemical states accociated at mixture fraction z and a series of Λ
- $\mathbf{C} \in R^{N\times p}$: $C_{ij} = \partial \phi_j(i)/\partial\Lambda$ and $N = \sum_z n_z$

1.2 Optimal Progress Variable

We define the optimal progress variable as the solution to

$$\begin{aligned} b^* \quad &= \quad \arg\min_b \left\{ \min_{a_z} \sum_z \|\mathbf{X}_z - \mathbf{1}_{n_z}\mu_z^T - \mathbf{X}_z b {a_z}^T\|_F^2 + \lambda_2\|b\|_2^2 + \lambda_1\|b\|_1 \right\} \\ & \qquad \text{subject to:} \quad \mathbf{C}b > 0,\, a_z^T a_z = 1. \end{aligned}$$

Minimizing $\|\mathbf{X}_z - \mathbf{1}_{n_z}\mu_z^T - \mathbf{X}_z b {a_z}^T\|_F^2$ encourages the unfolding (flattening) of the manifold with respect to the progress varibale of choise. The L_1 regularization of b helps the sparsity such that most of the species will have zero weight in the definition of the progress variable. L_2 regularization is for numerical purposes to prevent potential ill condition of the problem.

The first inequality constrains is guarantees the monotonicity condition such that a bijection between Λ and the progress variable exists. The second constraint is to avoid arbitrary scaling between b and a_z which will nullify the L_1 and L_2 regularization. Additional linear equality or inequality constraints on b can also the incorporated into this formula without any difficulties.

This problem is equivalent to,

$$\min_{a_z,\, b} \sum_z -2b^T \mathbf{X}_z^T \mathbf{X}_z a_z + b^T \mathbf{X}_z^T \mathbf{X}_z b$$
$$\text{subject to:} \quad \mathbf{C}b \geq 0,\ a^T a = 1,\ \|b\|_1 < c_1\,,$$

Note that

$$\begin{aligned}
\hat{a}_z(b) &= \mathbf{X}_z^T \mathbf{X}_z b / \|\mathbf{X}_z^T \mathbf{X}_z b\|_2 \\
\hat{b}(a) &= \arg\max_b \|\mathbf{Y} - (\mathbf{X} - \mathbf{M})b\|_2^2 + \lambda \|b\|_2^2 \\
& \quad\ \text{subject to:} \quad \mathbf{C}b > 0,\ \|b\|_1 < c_1\,.
\end{aligned}$$

$$\mathbf{X} = \begin{pmatrix} \mathbf{X}_{z_1} \\ \mathbf{X}_{z_2} \\ \cdots \\ \mathbf{X}_{z_n} \end{pmatrix} \quad \mathbf{M} = \begin{pmatrix} \mathbf{1}_{z_1} \bar{x}_{z_1} \\ \mathbf{1}_{z_2} \bar{x}_{z_2} \\ \cdots \\ \mathbf{1}_{z_n} \bar{x}_{z_n} \end{pmatrix} \quad \mathbf{Y} = (\mathbf{X} - \mathbf{M}) \begin{pmatrix} a_{z_1} \\ a_{z_2} \\ \cdots \\ a_{z_n} \end{pmatrix}$$

2 Numerical procedure

1. $k = 0$: initialize a_k
2. $k = k + 1$: $\hat{b}_k = \hat{b}(a_{k-1}), \quad \hat{a}_k = \hat{a}(b_k)$
3. Repeat 2 until converge