gMBAM and Applications to Michaelis-Menten Reduction

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1 Modeling

2 Geometry of Modeling

1. **Reparametrization**: transform parameter space P into Euclidean space $\mathbb{R}^n$
2. **Compactification**: compactify Euclidean space as **manifold with boundaries**: $(\mathbb{R}^n, \partial\mathbb{R}^n)$
3. **Embedding**: isomorphically embed $(\mathbb{R}^n, \partial\mathbb{R}^n)$ in prediction space
4. **Homotopy**: predict function f as homotopy morphing $(\mathbb{R}^n, \partial\mathbb{R}^n)$ into $(f(\mathbb{R}^n), \partial f(\mathbb{R}^n))$ that establishes the correspondence between $\partial\mathbb{R}^n$ and $\partial f(\mathbb{R}^n)$
5. **Partition**: $(f(\mathbb{R}^n), \partial f(\mathbb{R}^n))$ induces partition on P as a function of $\dim \partial_i f(\mathbb{R}^n)$
6. **Rule**: follow rule to identify parameter conditions for a specific model reduction: *e.g.*, $\bigcup \partial_i \mathbb{R}^n \leftrightarrow \Sigma_i \cdots$

3 MBAM

3.1 hMBAM

h for heuristic data centric, computationally cheap, etc.

3.2 gMBAM

g for global

4 Michaelis-Menten Reduction

4.1 Model

$$\mathrm{E} + \mathrm{S} \underset{k_r}{\overset{k_f}{\rightleftharpoons}} \mathrm{C} \xrightarrow{k_c} \mathrm{E} + \mathrm{P}$$

$$\frac{dE}{dt} = -k_f ES + (k_r + k_c)C \tag{1}$$
$$\frac{dS}{dt} = -k_f ES + k_r C \tag{2}$$
$$\frac{dC}{dt} = k_f ES - (k_r + k_c)C \tag{3}$$
$$\frac{dP}{dt} = k_c C \tag{4}$$
$$\Longrightarrow E + C = E_0, \quad S + C + P = S_0 \tag{5}$$

$$\frac{dS}{dt} = -k_f S(E_0 - C) + k_r C \tag{6}$$
$$\frac{dC}{dt} = k_f S(E_0 - C) - (k_r + k_c)C \tag{7}$$