Parameters Estimation in S-systems

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The S-systems[1]

$$\dot{x}_i = \alpha_i \prod_{j=1}^{n} x_j^{g_{ij}} - \beta_i \prod_{j=1}^{n} x_j^{h_{ij}}, \quad i = \overline{1, n}. \tag{1}$$

Typical values

- Rate constants $\alpha_i \geq 0$ and $\beta_i \geq 0$.
- Kinetic order parameters g_{ij} and $h_{ij} \in [-1, 2]$.

The one-variable system

$$\begin{aligned} \dot{x} &= \alpha x^g - \beta x^h. \\ x(t_0) &= x_0 \end{aligned} \tag{2}$$

[1] E.O. Voit, *Computational Analysis of Biochemical Systems. A Practical Guide for Biochemists and Molecular Biologists.* Cambridge University Press, Cambridge, 2000.

Metamodel

The metamodel of one-variable s-system

$$\dot{x} = \alpha \sum_{i=1}^{k} p_i(x) t_i(g) - \beta \sum_{i=1}^{k} p_i(x) t_i(h). \tag{3}$$

The discrete metamodel has the form

$$\delta x = \alpha \mathbf{P}_k \tau_g - \beta \mathbf{P}_k \tau_h. \tag{4}$$

or

$$\delta x = \mathbf{P}_k (\alpha \tau_g - \beta \tau_h) = \mathbf{P}_k \tau. \tag{5}$$

Definition

The vector $\tau \in \mathbb{R}^k$ is called a parameter vector of the metamodel. It contain the information about the parameters of the S-system.

Metamodel

$$f(x) = x^{\omega}$$

$$x \in [0.1, 10] - \text{operation domain} : 0.1 = x_1 < x_2 < \dots < x_n = 10,$$

$$\omega \in [-1, 2] : \qquad -1 = \omega_1 < \omega_2 < \dots < \omega_m = 2.$$

$$A = \begin{bmatrix} x_1^{\omega_1} & x_2^{\omega_1} & \dots & x_n^{\omega_1} \\ x_1^{\omega_2} & x_2^{\omega_2} & \dots & x_n^{\omega_2} \\ \dots & \dots & \dots & \dots \\ x_1^{\omega_m} & x_2^{\omega_m} & \dots & x_n^{\omega_m} \end{bmatrix}, \quad \text{– Data matrix}$$

$$A = (US)V^* = TP^* = \sum_{i=1}^{r} t_i p_i^*; \quad A_k = \sum_{i=1}^{k} t_i p_i^*$$

$$f = [f(x_1), f(x_2), \dots, f(x_n)] \approx \sum_{i=1}^{k} t_{il} p_i^* = \tau_{\omega_l} P_k^*.$$

$$\tau_{\omega_l} = [t_{1l}, t_{2l}, \dots, t_{kl}]; \quad P_k = [p_1 \; p_2 \; \dots \; p_k].$$

Metamodel

Let $f(u,\omega) = u^\omega$

Assume that $u \in [a,b],\ a,b \in \mathbb{R}, a > 0,\ \omega \in [0,1]$. Then we obtain the following representations of the kernels γ and δ

$$\gamma(u,v) = \int_0^1 u^\omega v^\omega d\omega = \int_0^1 (uv)^\omega d\omega = \frac{uv-1}{\ln(uv)},$$

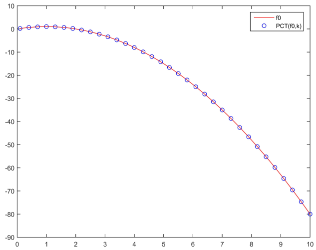
$$\delta(\omega,\xi) = \int_a^b u^\omega u^\xi du = \int_a^b u^{\omega+\xi} du = \frac{b^{\omega+\xi+1} - a^{\omega+\xi+1}}{\omega+\xi+1}$$

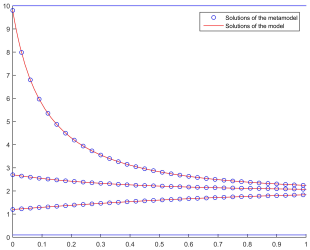
Therefore the normalized eigenfunctions $p_i(u)$ can be obtained from the equation $\int_0^1 \left(\frac{uv-1}{\ln(uv)}\right) p_i(u) du = \sigma_i^2 p_i(u)$

The functions $t_i(\omega) = \int_a^b u^\omega p_i(u) du$ can be found from the equations $\int_0^1 \left(\frac{b^{\omega+\xi+1} - a^{\omega+\xi+1}}{\omega+\xi+1)}\right) t_i(\omega) d\omega = \sigma_i^2 t_i(\omega)$

Example 1

Validation of the discrete metamodel





$$\dot{x} = 2x^1 - x^2, \tag{6}$$

$$x_{0,1} = 1.2, \quad x_{0,2} = 2.7, \quad x_{0,3} = 9.8.$$

$$\dot{x} = \alpha x^g - \beta x^h, \qquad \delta x = \mathbf{P}_k(\alpha \tau_g - \beta \tau_h) = \mathbf{P}_k \tau.$$

$$A = (US)V^* = TP^*$$

Let

$$x^{(1)}, x^{(2)}, ..., x^{(q)}$$

be a given solutions of the S-system at the points $s_1, s_2, ..., s_{m+1}$.

$$\delta x^{(j)}(s_i) = (x^{(j)}(s_{i+1}) - x^{(j)}(s_i))/(s_{i+1} - s_i) \tag{7}$$

Here $\delta x^{(j)} \in \mathbb{R}^m$, $i = \overline{1, m}$, $j = \overline{1, q}$. and obtain the vector

$$\delta x = \begin{pmatrix} \delta x^{(1)} \\ \vdots \\ \delta x^{(q)} \end{pmatrix}, \quad \delta x \in \mathbb{R}^{mq}.$$

The Parameter Estimation method

$$\delta x = \mathbf{P}_k(\alpha\tau_g - \beta\tau_h) = \mathbf{P}_k\tau.$$

$$\mathbf{P}_k^{(1)} = \begin{pmatrix} p_1^{(1)}(x_1) & p_2^{(1)}(x_1) & \dots & p_k^{(1)}(x_1) \\ p_1^{(1)}(x_2) & p_2^{(1)}(x_2) & \dots & p_k^{(1)}(x_2) \\ \dots & \dots & \dots & \dots \\ p_1^{(1)}(x_m) & p_2^{(1)}(x_m) & \dots & p_k^{(1)}(x_m) \end{pmatrix};$$

Here

$$p_i^{(1)}(x_1) = p_i(x_j), x_j \approx x_(s_1),$$
$$p_i^{(2)}(x_1) = p_i(x_j), x_j \approx x_(s_2),$$
$$\dots$$
$$p_i^{(m)}(x_1) = p_i(x_j), x_j \approx x_(s_m).$$

and $i = \overline{1, k}$.

Similarly we create the matrix $\mathbf{P}_k^{(2)}, \dots, \mathbf{P}_k^{(q)}$

The Parameter Estimation method

Finally, we obtain the matrix $\hat{\mathbf{P}}_k = \begin{pmatrix} \mathbf{P}_k^{(1)} \\ \vdots \\ \mathbf{P}_k^{(q)} \end{pmatrix}$

Now we can compute the **parameter vector** τ by the formula

$$\tilde{\tau} = (\hat{\mathbf{P}}_k)^{+}\delta x$$

$$\alpha\tau_i - \beta\tau_j = \tilde{\tau}, i, j = \overline{1, l}$$

We rewrite those equations on the form

$$\begin{pmatrix} \tau_i & \tau_j \end{pmatrix} \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = \tilde{\tau}$$

Then

$$\begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = \begin{pmatrix} \tau_i & \tau_j \end{pmatrix}^{+} \tilde{\tau}$$

The Parameter Estimation method

$$\alpha\tau_i - \beta\tau_j = \tilde{\tau}, i, j = \overline{1, l}$$

$$\begin{pmatrix} \tau_i & \tau_j \end{pmatrix} \begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = \tilde{\tau}$$

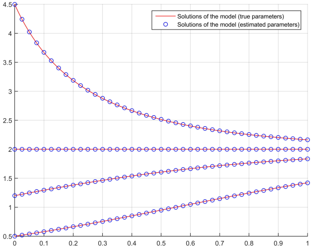
Then

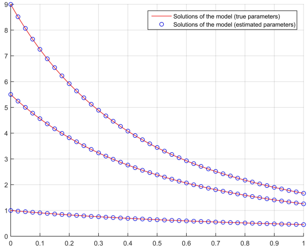
$$\begin{pmatrix} \alpha \\ -\beta \end{pmatrix} = \begin{pmatrix} \tau_i & \tau_j \end{pmatrix}^{+} \tilde{\tau}$$

Every solution gives us the parameter vector τ_{ij}.
We choose nearest to $\tilde{\tau}$ vector (by Euclidean norm) and denote it by $\hat{\tau}$, $\quad \hat{\tau} = \hat{\alpha}\hat{\tau_g} - \hat{\beta}\hat{\tau}_h$.
The vectors $\hat{\tau_g}$ and $\hat{\tau}_h$ give us the $\hat{g}$ and $\hat{g}$.
We found the estimated parameters $\hat{\alpha}$, $\hat{\beta}$, $\hat{g}$ and $\hat{g}$.

Example 2

The Parameter Estimation method





$\dot{x} = 2x^1 - x^2$

True parameters

2 1 1 2

Estimated parameters:

1.9989 0.9993 1.0000 2.0000

$\dot{x} = 4x^1 - 5x^{1.1}$

True parameters

4 5 1 1.1

Estimated parameters:

4.0694 5.0639 1.0000 1.1000

Thank you for your attention!

Děkuji za pozornost!