

Parameters estimation in S-systems

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The S-system

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

has been proposed by E. Voit and has been described in [1] as mathematical model of many biochemical and biophysical processes. The parameters estimation of the S-systems is of great importance in the biochemical systems theory.

We consider the simplest version of system (1)

$$\dot{x} = \alpha x^g - \beta x^h, \quad (2)$$

here $\alpha, \beta \in \mathbb{R}, g, h \in [-1, 2]$. From the Best individual fit theorem [2] we get metamodel of (2)

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

Here $p_i(\cdot), t_i(\cdot)$ are some eigenfunctions, $i = \overline{1, k}$. The discrete metamodel of (2) has the form

$$\vec{\delta x} = \alpha \mathbf{P} \vec{\tau}_g - \beta \mathbf{P} \vec{\tau}_h \quad \text{or} \quad \vec{\delta x} = \mathbf{P} \vec{\tau}. \quad (4)$$

Here $\vec{\tau} = \alpha \vec{\tau}_g - \beta \vec{\tau}_h$, \mathbf{P} is a matrix.

Definition 1. The vector $\tau \in \mathbb{R}^k$ is called a parameters vector of the metamodel (4). It contains the information about the parameters of the S-system (2).

We calculate a parameters vector by the formula

$$\vec{\tau} = \mathbf{P}^+ \vec{\delta x} \quad (5)$$

Here \mathbf{P}^+ is pseudoinverse of \mathbf{P} . The parameters vector allows us to estimate the parameters of the S-system (2).

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References

- [1] E.O. Voit, *Computational Analysis of Biochemical Systems. A Practical Guide for Biochemists and Molecular Biologists*. Cambridge University Press, Cambridge, 2000.
- [2] I. Zabrodskii, and A. Ponosov. *The Principal Component Transform of Parametrized Functions*. *Applied Mathematics*, 8, (2017): 453-475.