

Introduction

In many situations, two things are known to researchers:

1. experimental data $\{\mathbf{s}_i, \mathbf{P}_i\}_{i=0}^m$ where $\mathbf{s}_i$ are the times data $\mathbf{P}_i \in \mathbb{R}^{d_M}$ are collected, and
2. a dynamical system model of differential equations with model parameters $\{\alpha_i\}_{i=1}^{n_\alpha}$.

In many applications the value of the model parameters which best fit the experimental data are difficult to determine. Many techniques have been developed to determine the parameters in a given system of differential equations that best fit a given data set. We applied least squares fitting method [1] to estimate the parameters for Chua circuit data.

Model: Chua Circuit

$$\begin{aligned}\frac{\partial \mathbf{x}_1}{\partial t} &= \alpha (\mathbf{x}_2 - (1 + m_1)\mathbf{x}_1 + \frac{1}{2}(m_0 - m_1)\mathbf{h}(\mathbf{x}_1)), \\ \frac{\partial \mathbf{x}_2}{\partial t} &= \mathbf{x}_1 - \mathbf{x}_2 + \mathbf{x}_3, \\ \frac{\partial \mathbf{x}_3}{\partial t} &= -\beta \mathbf{x}_2 - \gamma \mathbf{x}_3,\end{aligned}$$

where $\mathbf{h}(\mathbf{x}_1) = |\mathbf{x}_1 + \mathbf{1}| - |\mathbf{x}_1 - \mathbf{1}|$, and parameters are $\alpha, \beta, \gamma, m_0, m_1$. The Chua circuit can be written as a vector equation in terms of parameters $\{\alpha_i\}_{i=1}^4$ where each α_i is a vector of parameters in $\mathbb{R}^3$.

Method: B-spline fit to data

The solution to the dynamical system model is assumed to be a B-spline, defined from a set of $n + 1$ control points $\{\mathbf{b}_i\}_{i=0}^n$ on $t \in [0, 1]$ as

$$\mathbf{u}(t) = \sum_{i=0}^n N_{i,d}(t) \mathbf{b}_i,$$

where $\mathbf{b}_i$ is a vector of dimension $\mathbb{R}^{d_M}$, and the basis functions $N_{i,d}(t)$ are defined recursively as

$$\begin{aligned}N_{i,0}(t) &= \begin{cases} 1 & t_i \leq t \leq t_{i+1} \\ 0 & \text{otherwise} \end{cases} \\ N_{i,j}(t) &= \frac{t - t_i}{t_{i+j} - t_i} N_{i,j-1}(t) + \frac{t_{i+j+1} - t}{t_{i+j+1} - t_{i+1}} N_{i+1,j-1}(t).\end{aligned}$$

We use $d = 3$ so the splines are cubic, although in principle higher order splines could be used.

Least squares is used to minimize the error between the B-spline and the data,

$$E_D(\mathbf{b}) = \sum_{i=0}^m (\mathbf{u}(\tau_i) - \mathbf{P}_i)^2,$$

where time $\mathbf{s}$ has been scaled to $\tau \in [0, 1]$. This results in the equation is solved for $\mathbf{b}$,

$$\mathbf{A}^T \mathbf{A} \mathbf{b} - \mathbf{A}^T \mathbf{P} = \mathbf{0}, \quad (1)$$

where matrix $\mathbf{A}$ has elements $a_{ik} = N_{k,d}(\tau_i)$.

Method: Estimating Model Parameters

The function to minimize to obtain the model parameters is

$$\tilde{E}(\mathbf{b}, \alpha, \hat{\mathbf{u}}) = E_D(\mathbf{b}) + \lambda \hat{E}_M(\mathbf{b}, \alpha, \hat{\mathbf{u}}), \quad (2)$$

where

$$\hat{E}_M(\mathbf{b}, \alpha, \hat{\mathbf{u}}) = \sum_{i=0}^m \left(\sum_{j=0}^n \frac{d}{dt} [N_{j,d}(\tau_i)] \mathbf{b}_j - \sum_{l=1}^{n_\alpha} f_l(\hat{\mathbf{u}}(\tau_i), \tau_i) \alpha_l \right)^2.$$

The parameter $\lambda > 0$ can be chosen to adjust weight between the fit to data $E_D(\mathbf{b})$ and the fit to model $\hat{E}_M(\mathbf{b}, \alpha, \hat{\mathbf{u}})$.

Least squares is used to minimize (2) with respect to $\mathbf{b}$ and α . This results in the equation

$$\begin{pmatrix} \mathbf{A}^T \mathbf{A} + \lambda \mathbf{C}^T \mathbf{C} & -\lambda \mathbf{C}^T \mathbf{F} \\ (\mathbf{C}^T \mathbf{F})^T & -\mathbf{F}^T \mathbf{F} \end{pmatrix} \begin{pmatrix} \mathbf{b} \\ \alpha \end{pmatrix} = \begin{pmatrix} \mathbf{A}^T \mathbf{P} \\ \mathbf{0} \end{pmatrix} \quad (3)$$

where $\mathbf{F}$ has elements $f_k(\hat{\mathbf{u}}(\tau_i))$ and $\mathbf{C}$ has elements $d/dt[N_{k,d}(\tau_i)]$. The model parameters will be found by determining the convergence of the sequence $(\mathbf{b}^{(k)} \alpha^{(k)})^T$, $k = 0, 1, 2, \dots$, in the following manner:

1. Solve (1) for $\mathbf{b} = \mathbf{b}^{(0)}$ and compute $\mathbf{u}^{(0)}$.
2. Use $\mathbf{u}^{(0)}$ to create $f_k(\hat{\mathbf{u}}^{(0)}(\tau_i))$, then solve (3) for $(\mathbf{b}^{(1)} \alpha^{(1)})^T$.
3. Iterate until the sequence $(\mathbf{b}^{(k)} \alpha^{(k)})^T$ converges.

Gaussian noise was added to the data to simulate experimental error. We create hundreds of different data sets with a Gaussian distribution error, then average the model parameter estimates to get final results.

We used two different matrix form to estimate the parameters.

• **Method 1: Matrix without Rearrangement**

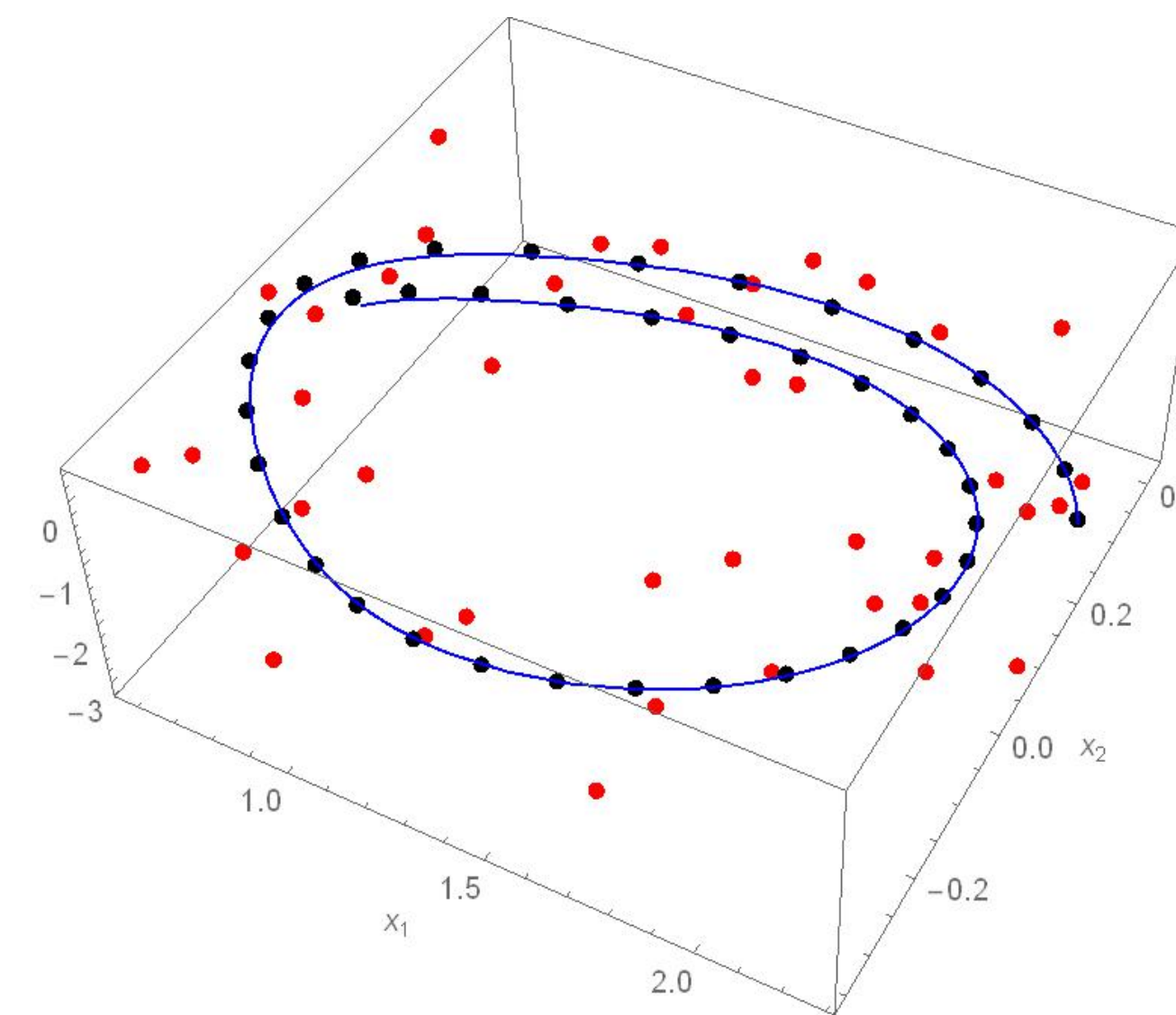
We have matrix with 12 different parameters (4x3) by variable $\mathbf{x}_1$, $\mathbf{x}_2$, $\mathbf{x}_3$, and $\mathbf{h}(\mathbf{x}_1)$ and the three dimension of system.

• **Method 2: Matrix with Rearrangement**

Since we aware some parameter are 0 and 1, eliminating the known parameters will provide some reduction of time. We rearranged matrix to (1x4) and (1x2) to only calculate 6 parameters.

Results

The fit generated by estimated parameters with noise $\sigma = 0.1$ for one data set.



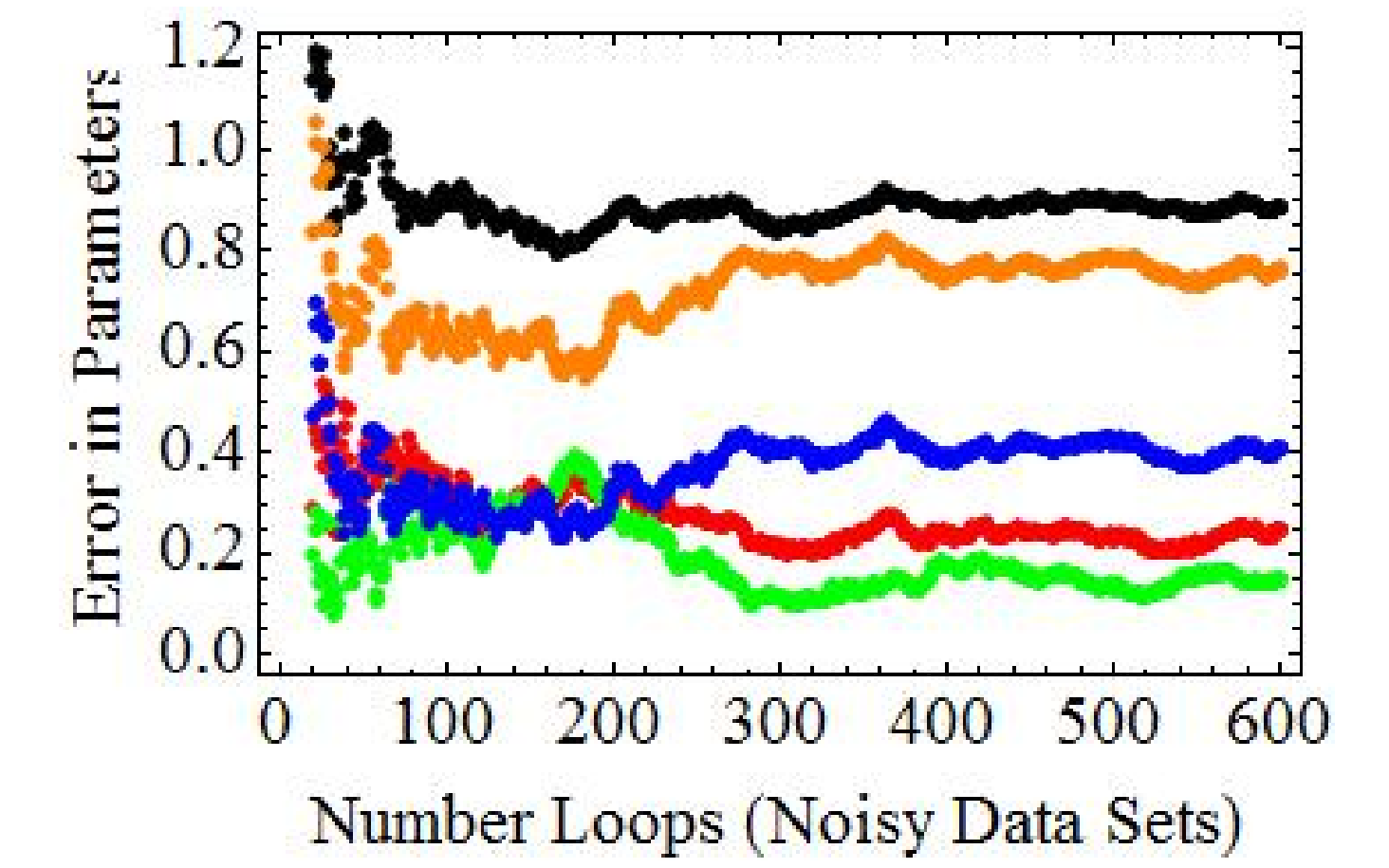
The red dot represents the data with the noise, the black dot represents data without noise, the blue dot represents control points $\mathbf{b}$, and blue line represents fitted B-spline.

Results

We used $\alpha = 15.6$, $\beta = 28$, $\gamma = 0.1$, $m_0 = -8/7$, $m_1 = -5/7$ for our analysis, and we generate using several different λ values and noise to estimate the parameter. Here is the parameter error in Chua circuit when $d = 3$, $m = 30$, $n = m - d - 1 = 26$.

		parameter for Chua-Circuit					
		α	β	γ	m_1	m_0	time
λ	original	15.6	28	0.1	-0.714286	-1.14286	
	0	14.921	28.3988	0.201465	-0.71662	-1.15069	1.2s
	0.001	15.378	28.007	0.10157	-0.173602	-1.14579	1 2s
	0.01	15.4273	28.0143	0.10402	-0.71357	-1.14522	1 2s
	0.1	15.5614	28.0143	0.1054	-0.71443	-1.14333	2 3s
	1	15.6242	-27.9927	0.0970	-0.714781	-1.14231	2 3s

Table represents the different λ value to determine the parameter error of estimation of the Chua circuit. Method without rearrangement usually took more than 10 to 30 seconds per iteration, and method with rearrangement, the calculation time has been decreased significantly.



The color of the graph shows different lambda values [Black=0.001 Red=0.01 Green=0.1 Blue=1 Orange=2].

Conclusions

1. The method studied is powerful since it does not require initial estimates of model parameters.
2. The rearrangement method does not affect the accuracy of the results, but had a significant decrease in computational time.
3. The weighting factor of $\lambda = 0$ surprisingly still obtained a reasonable result. We believe more investigation of $\lambda = 0$ could improve the running time, and possibly make the method useful to initialize other methods (such as Newton's method, which requires an initialization).

References

- [1] D. Brewer, M. Barenco, R. Callard, M. Hubank and J. Stark, *Fitting ordinary differential equations to short time course data*, Phil. Trans. R. Soc. A, 366 (2008), pp. 519–544.
- [2] P. Massopust, *Interpolation and Approximation with Splines and Fractals*, Oxford University Press, New York, (2010).
- [3] U. Parlitz *Lyapunov exponents from chua's circuit*, Journal of Circuits, 1993 (1993).