

Parameter Identification with a Wavelet Collocation Method for ODEs and DAEs

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Abstract

This article describes parameter identification with a wavelet collocation method which minimizes the sum of squares of residuals. In the examples we use the Shannon wavelet and a Daubechies wavelet. The parameter identification is a problem, where an ODE, PDE or DAE is given with unknown parameters. The parameters should be estimated by given measurements. Such problems appear in the chemical reaction kinetics or in n-body problems. If the problem is stiff, we need a boundary value approach. The advantage of the wavelet collocation is that we can use it for different types of problems and even for stiff problems. As an example we use the test problem of H. H. Robertson, which is based on a stiff ODE or DAE and an unstable system from H. G. Bock. In the examples we apply additionally an estimation in two steps, which leads under certain conditions to two quadratic minimization problems. For the assessment of the approximation and of the approximated parameters we use sum of squares of residuals.

Keywords: parameter identification, wavelet collocation, sinc collocation

Introduction

In the wavelet theory a scaling function ϕ is used, which belongs to a MSA (multi scale analysis). From the MSA we know, that we can construct an orthonormal basis of a closed subspace V_j , where V_j belongs to a the sequence of subspaces with the following property:

$$\dots \subset V_{-1} \subset V_0 \subset V_1 \subset \dots \subset L^2(\mathbb{R}),$$

$\{\phi_{j,k}(t)\}_{k \in \mathbb{Z}}$ is an orthonormal basis of V_j with $\phi_{j,k}(t) = 2^{j/2} \phi(2^j t - k)$, where ϕ ist he scaling function of the MSA.

We use the following approximation function

$$y_j(t) := \sum_{k=k_{\min}}^{k_{\max}} c_k \cdot \phi_{j,k}(t) \quad , \text{ with } \phi \in C^l(\mathbb{R}).$$

k_{\max} and k_{\min} depend on the approximation interval $[t_0, t_{\text{end}}]$ (see [35]).

Now we can approximate the solution of an initial value problem $y' = f(y,t)$ and $y(t_0) = y_0$ by minimization of the following function

$$(1) \quad Q(c) = \sum_{i=1}^m \left\| y_j'(t_i) - f(y_j(t_i), t_i) \right\|_2^2 + \left\| y_j(t_0) - y_0 \right\|_2^2 .$$

For $m = |k_{\max} - k_{\min}|$ we get an equivalent problem:

$$y_j'(t_i) = f(y_j(t_i), t_i) \text{ for } i = 1, 2, \dots, m \text{ and } y_j(t_0) = y_0 .$$

Analogous we could treat boundary conditions instead of the initial condition. This method can be even used analogous for PDEs, ODEs of higher order or ODEs, which have the Form $F(y', y, t) = 0$.

If $y' = f(y, t)$ is an ODE system, then we use the approximation function

$$y_j(t) = \left(\sum_{k=k_{\min}}^{k_{\max}} c_{k,1} \phi_{j,k}(t), \sum_{k=k_{\min}}^{k_{\max}} c_{k,2} \phi_{j,k}(t), \dots, \sum_{k=k_{\min}}^{k_{\max}} c_{k,n_f} \phi_{j,k}(t) \right)^T.$$

For the i -th component of the solution y , we use - as usual, the notation y_i . We use for the i -th component of y_j the notation $y_j^{(i)}$, so that it does not lead to a confusion with the approximation y_j out of V_j and it will be always noticed in context whether it is the approximation y_j or it is the i -th component of y .

We use the collocation points t_i , with $t_i = t_0 + i \cdot h$ and

$$(2) \quad h = \frac{t_{\text{end}} - t_0}{m} \quad (m \geq |k_{\max} - k_{\min}|).$$

For the assessment of the approximation we use the value Q_a , with

$$Q_a = \sum_{i=1}^{m_a} \|y_j'(t_i) - f(y_j(t_i), t_i)\|_2^2 + \|y_j(t_0) - y_0\|_2^2,$$

$t_i = t_0 + i \cdot h/a$, $m_a = a \cdot m$ and $a > 1$ is an integer.

If nothing is known about the solution y , many simulations have shown that a usable starting value of m is $m = |k_{\max} - k_{\min}|$. For this choice of m we would have for the case $n = 1$ in c together $m + 1$ coefficients, m collocation points and one initial value. In the case that y has big slopes or big curvatures, we need a bigger m . A too small m leads to a big Q_{\min} or a big Q_a (see (6)).

For the parameter identification we minimize

$$(3) \quad Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=0, \dots, m} \|y_j'(t_i) - f(y_j(t_i), t_i, p)\|_2^2 + \beta \cdot \sum_{i=1, \dots, \tilde{m}} \|\tilde{m}_i - M(y_j(\hat{t}_i))\|_2^2.$$

Boundary conditions or initial conditions can be used as constrains or can be considered in Q .

In the following example we minimize

$$(4) \quad Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=0, \dots, m} \|y_j'(t_i) - f(y_j(t_i), t_i, p)\|_2^2 + \beta \cdot \sum_{i=1, \dots, \tilde{m}} \|\tilde{m}_i - M(y_j(\hat{t}_i))\|_2^2 + \|y_0 - y_j(t_0)\|_2^2$$

with $\alpha = \beta = 1$. The (numerical calculated) minimum value of Q is Q_{\min} .

A method which is a variation of the method above is the minimization in two steps:

In the first step we calculate

$$(5) \quad Q_{0,1}(p, \hat{c}) = \min_c Q_{0,1}(p, c)$$

And in the second step we calculate

$$(6) \quad Q_{1,0}(\hat{p}, \hat{c}) = \min_p Q_{1,0}(p, \hat{c}) \quad .$$

If M and f is linear in p , like in the examples in the reaction kinetics, then we must solve in both steps a quadratic problem. In that case we can apply a parameter identification with a small effort, even more if the problem is stiff.

For the assessment of the approximation we could calculate the following function value:

$$(6) \quad Q_{\alpha,\beta,a}(\hat{p}, \hat{c}) = \alpha \cdot \sum_{i=0, \dots, m_a} \|y_j'(\tau_i) - f(y_j(\tau_i), \tau_i, \hat{p})\|_2^2 + \beta \cdot \sum_{i=1, \dots, m} \|\tilde{m}_i - M(y_j(\hat{t}_i))\|_2^2 + \|y_0 - y_j(t_0)\|_2^2$$

with $\tau_i = t_0 + i \cdot h/a$, $m_a = a \cdot m$ and an integer $a > 1$.

In the case $\alpha = \beta = 1$ we later write in short Q_a (like Q for $Q_{1,1}$).

With the exact solution $Q_{\alpha,0,a}(p, c)$ is equal to zero. If $Q_{\alpha,\beta,a}(\hat{p}, \hat{c}) \gg Q_{\alpha,\beta}(\hat{p}, \hat{c})$, we need more collocation points t_i and if Q_{\min} is relative big, then we need a bigger j . For this criteria we must not calculate a second minimization, if $Q_{\alpha,\beta,a}(\hat{p}, \hat{c})$ is small. For $a \gg 1$ we should use $1/a \cdot Q_{\alpha,\beta,a}(\hat{p}, \hat{c})$ instead of $Q_{\alpha,\beta,a}(\hat{p}, \hat{c})$ for the comparison with $Q_{\alpha,\beta}(\hat{p}, \hat{c})$.

Remarks:

1) By using the Shannon wavelet and if the measurement points \hat{t}_i can be chosen freely (if this is technically possible in a practical problem), then a good choice would be $\hat{t}_{i+1} - \hat{t}_i = \Delta t \leq 2^{-j}$, which follows from Shannon's Theorem. If y is in V_j then we would get $c_k = 2^{-j/2} y(2^{-j} \cdot k)$. That could be used for the choice of starting values for the coefficients c_k in the iteration, if $M(y) = y$.

2) In case of $M(y) = y$ we could apply a discrete wavelet transformation on the measurements, to get an information about the involved frequencies.

Example 1 (ROBER)

1966 H. H. Robertson introduced an example in the reaction kinetics ([33]), which includes a very fast reaction,. This fast reaction is responsible for the stiffness of the system. This example is a test set of the INdAM-Bari Group. E. Hairer ([22]) used the short name ROBER for this example.

The reaction schema is:

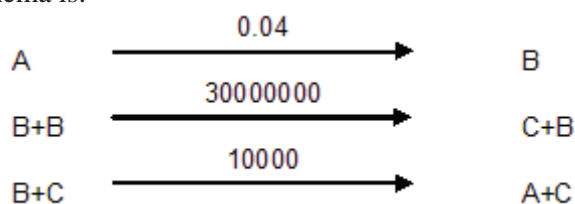


Fig. 1. Reaction schema of ROBER

Here is the resulting ODE:

$y_1' = -p_1 y_1 + p_3 y_2 y_3$
$y_2' = p_1 y_1 - p_3 y_2 y_3 - p_2 y_2^2$
$y_3' = p_2 y_2^2$,

with $p = (0.04, 3 \cdot 10^7, 10^4)^T$. We use the starting vector $y(0) = (1, 0, 0)^T$.

With $p = (0.04, 3 \cdot 10^7, 10^4)^T$ the system cannot be solved with an explicit method. We need an implicit method or boundary value method.

H. H. Robertson 1966:

When the equations represent the behaviour of a system containing a number of fast and slow reactions, a forward integration of these equations becomes difficult.

Now we use **the wavelet collocation method** with the Shannon wavelet. We simulate measurements by using the points $\hat{t}_i = 0.1 \cdot i$, with $i = 1, \dots, 50$, the measurement function $M(y) = y$ and the approximation interval $I = [0, 5]$, that means $t_{\text{end}} = 5$.

We set $j = 1$, $k_{\text{max}} = 25$ and $k_{\text{min}} = -5$ for y_j . k_{min} is not so small, because we start with $t_0 = 0$. The collocation points are

$$t_i = 0.05 \cdot i, \text{ with } i = 1, \dots, 100 ,$$

so $m = 100$.

We make two estimations of p . In the first estimation we estimate as described in two steps. In the first step we estimate c with \hat{c} , by setting in

$$Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=1, \dots, 100} \|y_j'(t_i) - f(y_j(t_i), t_i, p)\|^2 + \beta \cdot \sum_{i=1, \dots, 50} \|\tilde{m}_v - M(y_j(\hat{t}_i))\|^2 + \|y_j(t_0) - y_0\|^2$$

the coefficients $\alpha = 0$ and $\beta = 1$ and calculate

$$Q_{0,1}(p, \hat{c}) = \min_c Q_{0,1}(p, c) .$$

In the second step we estimate p with

$$Q_{1,0}(\hat{p}, \hat{c}) = \min_p Q_{1,0}(p, \hat{c}) .$$

Therefore we only have to solve a system of the normal equation twice, because the problems are quadratic (for an error analysis see [36]).

We got:

$$Q_{0,1}(p, \hat{c}) = \min_c Q_{0,1}(p, c) \approx 4.41611 \cdot 10^{-13}$$

Now we see the curves of $y_1^{(i)} - y_i$, beginning with $i = 1$ (here y is not the exact solution, but the numerical solution of the system with the exact parameter p , by using the Mathematica-function NDSolve):

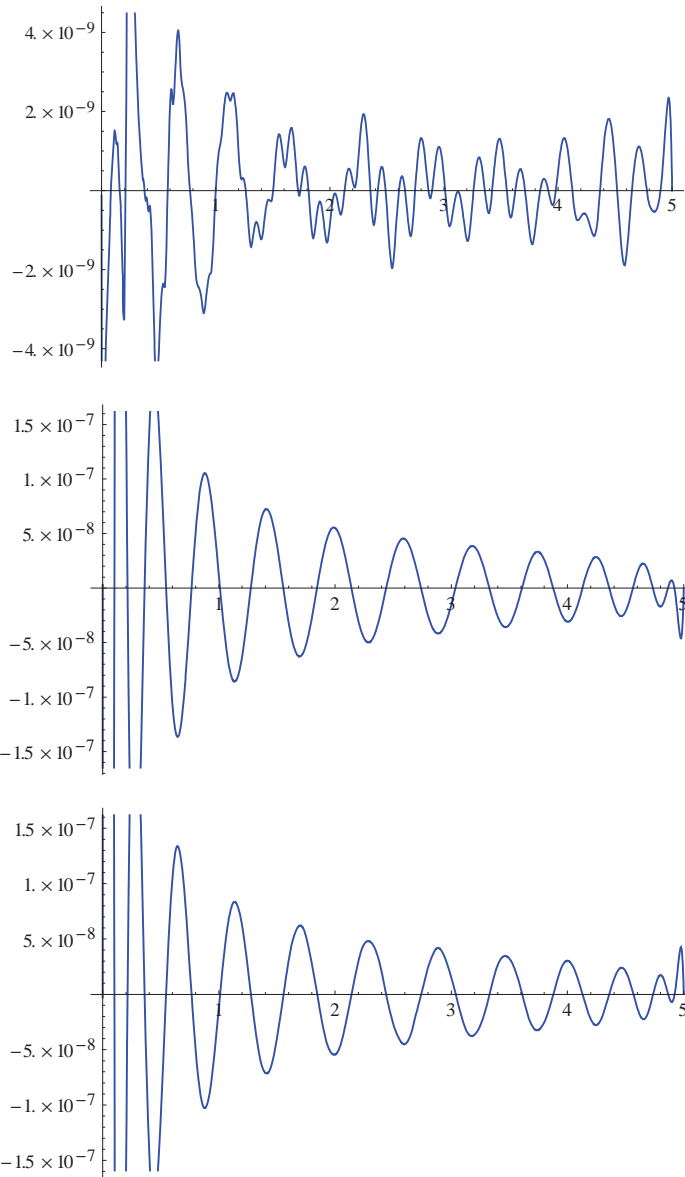


Fig. 3. Curves of $y_1^{(i)} - y_i$

Here are the graphs for $i = 2$ (y_2 in red):

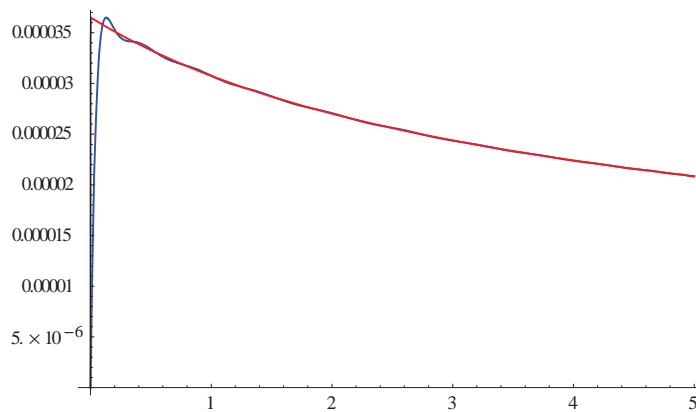


Fig. 4. Curves of $y_1^{(2)}$ and y_2 .

For $y^{(2)}$ and a smaller area:

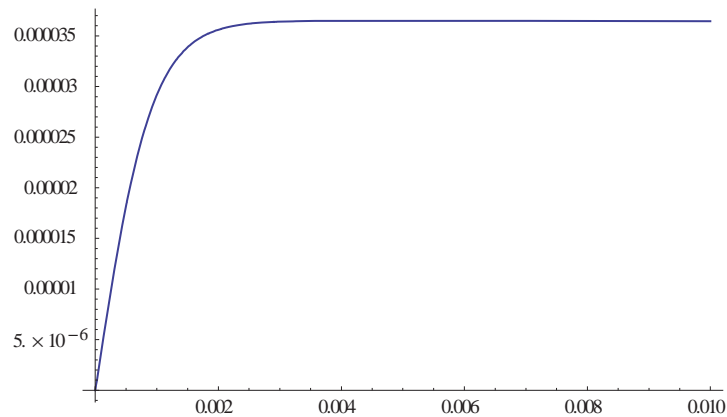


Fig. 5. Curves of $y_1^{(2)}$ at the beginning.

For the iteration the parameter has been rescaled, so instead of the system

$y_1' = -p_1 y_1 + p_3 y_2 y_3$
$y_2' = p_1 y_1 - p_3 y_2 y_3 - p_2 y_2^2$
$y_3' = p_2 y_2^2$,

with $p = (0.04, 3 \cdot 10^7, 10^4)^T$ we use the system

$y_1' = -p_1 y_1 + 10^4 p_3 y_2 y_3$
$y_2' = p_1 y_1 - 10^4 p_3 y_2 y_3 - 10^7 p_2 y_2^2$
$y_3' = 10^7 p_2 y_2^2$,

with $p = (0.04, 3, 1)^T$.

Although in step 1 in the area $[0, 0.1]$ the approximation for $y_1^{(2)}$ was not very good but the estimation of p was not bad:

p_i	\hat{p}_i	$ (\hat{p}_i - p_i)/p_i $
0.04	0.0399575	0.00106353
3	3.01548	0.00516115
1	1.00002	0.0000249715

Table 1.

Using the Daubechies wavelet of order 7 (with $k_{\max} = 19$, $k_{\min} = -5$ und $j = 2$) we get the following approximation in the second step:

p_i	\hat{p}_i	$ (\hat{p}_i - p_i)/p_i $
0.04	0.039746	0.00634911
3	2.98796	0.00401307
1	0.999414	0.000585899

Table 2.

In many simulations with Daubechies wavelets it has been seen that we need a bigger j but less coefficients c_i (in comparison to Shannon wavelets), because of the compact support of the Daubechies wavelets.

Now, we estimate the parameter p together with c and set $\alpha = \beta = 1$ (using the Shannon wavelet. We get:

$$\min_{c,p} Q_{1,1}(p, c) \approx 2.2264 \cdot 10^{-9}$$

For comparison: $Q_2 \approx 3.09351 \cdot 10^{-9}$.

Now we see the curves of $y_1^{(i)} - y_i$ beginning with $i = 1$:

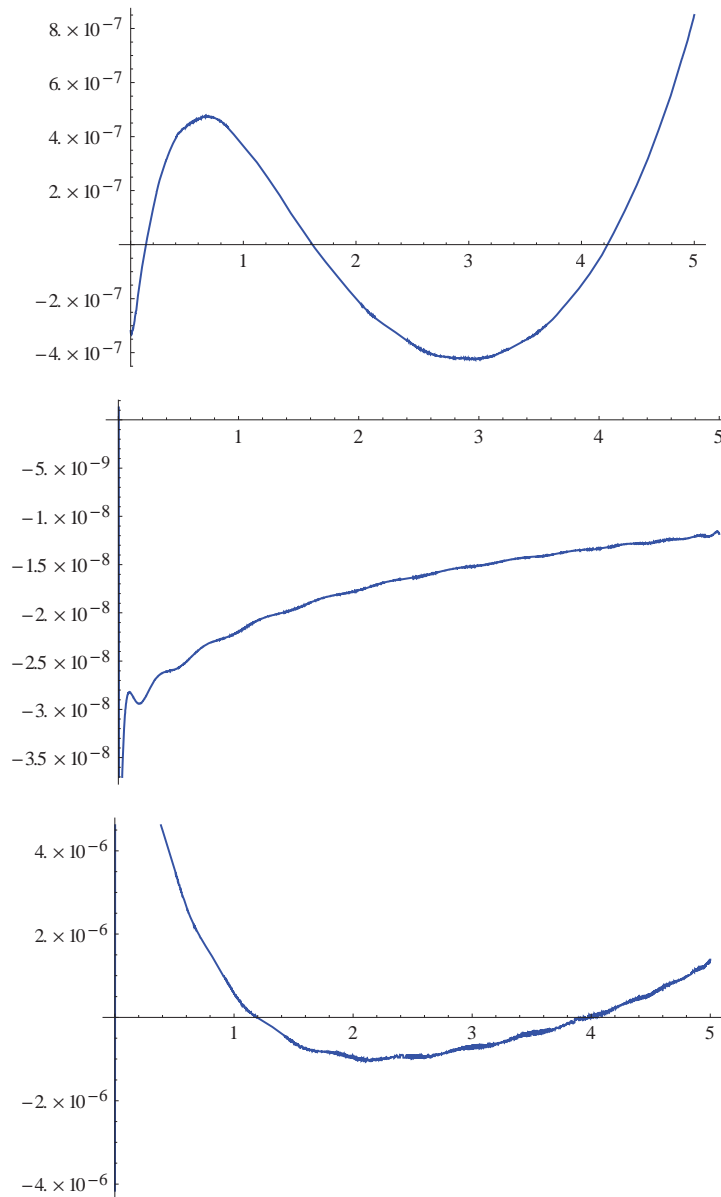


Fig. 6. Curves of $y_1^{(i)} - y_i$.

$y^{(2)}$ was approximated well (in red we see $y^{(2)}$ together with $y_1^{(2)}$):

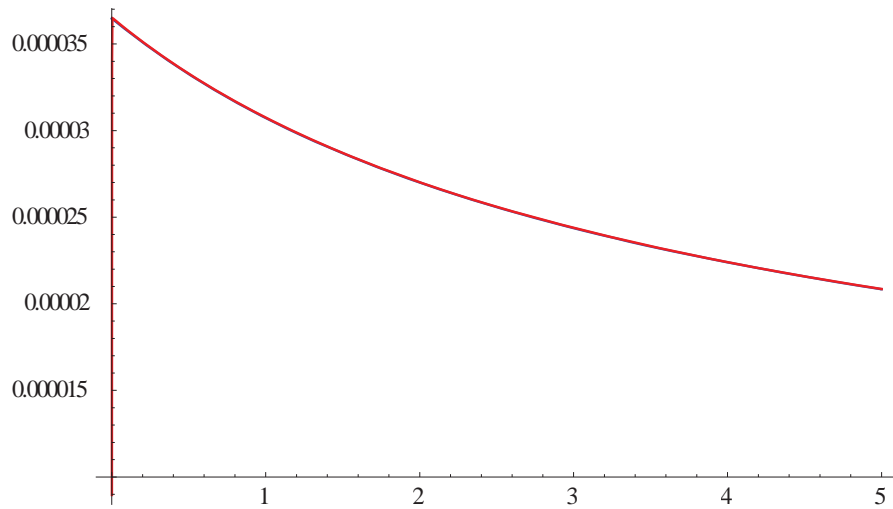


Fig. 7. Curves of $y_1^{(2)}$ and y_2 .

p_i	\hat{p}_i	$ (\hat{p}_i - p_i)/p_i $
0.04	0.0399879	0.000303367
3	3.00382	0.00127247
1	1.00063	0.000627453

Table 3.

For comparison, we do the same estimation with the Daubechies wavelet of order 7 (with $k_{\max} = 19$, $k_{\min} = -5$ und $j = 2$):

p_i	\hat{p}_i	$ (\hat{p}_i - p_i)/p_i $
0.04	0.0399279	0.00180237
3	3.02962	0.00987431
1	1.00349	0.00348764

Table 4.

The method for the approximation and estimation can be applied analogous to a DAE. We can write the System in an equivalent DAE:

$y_1' = -p_1 y_1 + 10^4 p_3 y_2 y_3$
$y_2' = p_1 y_1 - 10^4 p_3 y_2 y_3 - 10^7 p_2 y_2^2$
$1 = y_1 + y_2 + y_3$

with $p = (0.04, 3, 1)^T$ and $y(0) = (1, 0, 0)^T$.

We use the same measurements and minimize

$$Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=1, \dots, 100} \|F(y_j'(t_i), y_j(t_i), t_i)\|_2^2 + \beta \cdot \sum_{i=1, \dots, 50} \|\tilde{m}_v - M(y_j(\hat{t}_i))\|_2^2 + \|y_j(t_0) - y_0\|_2^2$$

with

$$F(y'', y', t_i) = (y_1' + p_1 y_1 - 10^4 p_3 y_2 y_3, y_2' - p_1 y_1 + 10^4 p_3 y_2 y_3 + 10^7 p_2 y_2^2, 1 - y_1 - y_2 - y_3)^T.$$

We use again $\alpha = \beta = 1$ and we get with the Shannon wavelet:

$$\min_{c,p} Q_{1,1}(p,c) \approx 2.22412 \cdot 10^{-9}$$

For comparison: $Q_2 \approx 3.80903 \cdot 10^{-9}$.

Here is the estimation:

p_i	\hat{p}_i	$ (\hat{p}_i - p_i)/p_i $
0.04	0.0399879	0.000303616
3	3.00382	0.00127394
1	1.00063	0.000628092

Table 5.

Now we see the curves of $y_1^{(i)} - y_i^{(i)}$ beginning with $i = 1$:

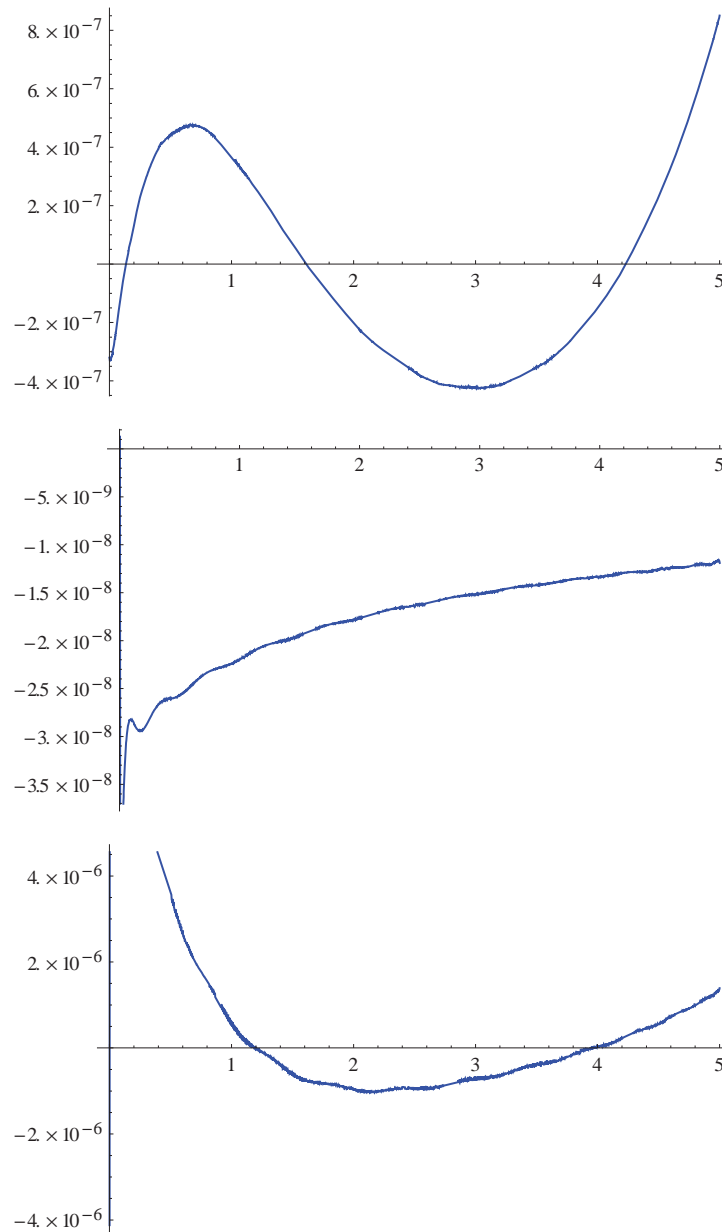


Fig. 8. Curves of $y_1^{(i)} - y_i^{(i)}$.

Here are the curves of the approximation functions $y_1^{(i)}$ beginning with $i = 1$:

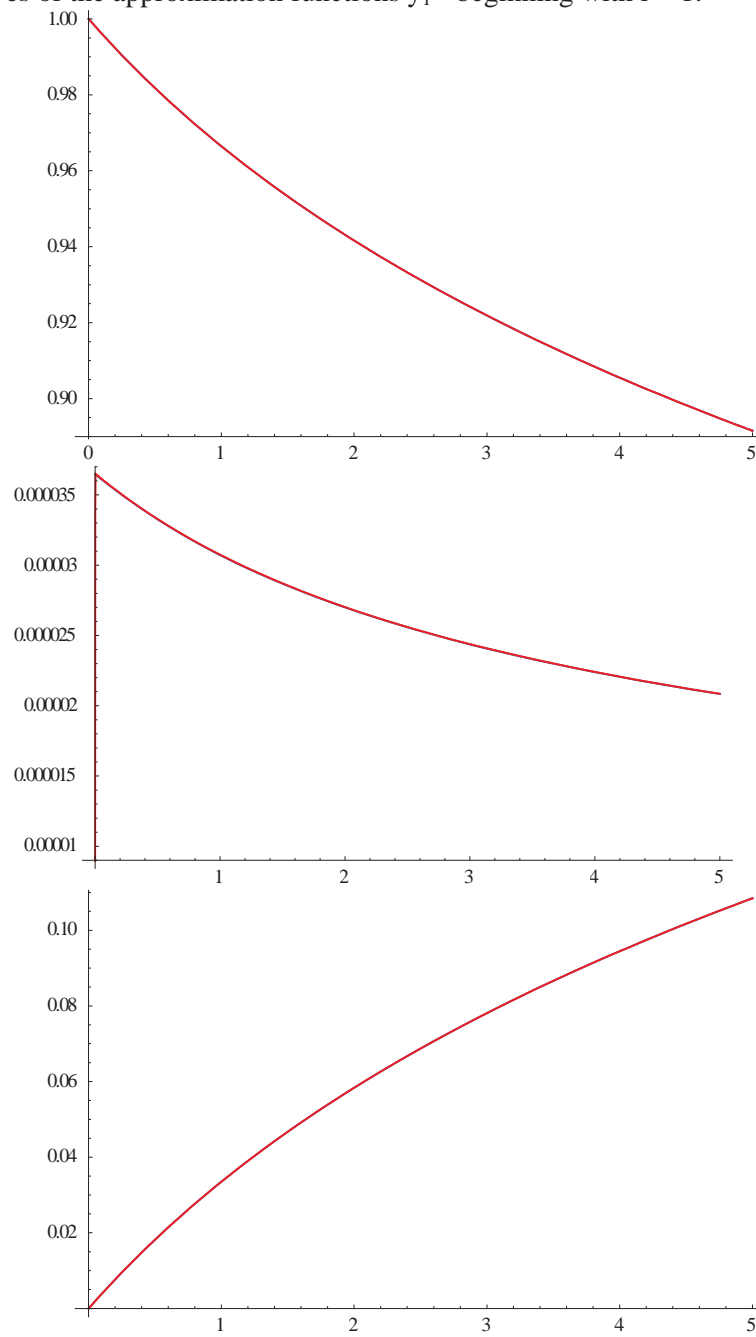


Fig. 9. Curves of $y_1^{(i)}$.

Example 2 (BOCK)

An example of a parameter identification problem with an instable System is from H. G. Bock ([12]). Here we apply the same Method of wavelet collocation.

Here is the problem:

$$\begin{aligned} y_1' &= y_2 \\ y_2' &= \tau^2 \cdot y_1 - (\tau^2 + \theta^2) \cdot \sin(\theta \cdot t), \\ y(0) &= (0, \theta)^T. \end{aligned}$$

The solution is

$$y_1(t) = \sin(\theta \cdot t) \text{ und } y_2(t) = \theta \cdot \cos(\theta \cdot t) .$$

The solution without starting value would be:

$$y_1(t) = c_1 \cdot e^{\tau t} + c_2 \cdot e^{-\tau t} + \sin(\theta \cdot t)$$

and

$$y_2(t) = \tau \cdot c_1 \cdot e^{\tau t} - \tau \cdot c_2 \cdot e^{-\tau t} + \theta \cdot \cos(\theta \cdot t) .$$

When we change the value of θ only slightly, we get for bigger $|\tau|$ a strong change of the solution. For example with $\tau = 100$ and $\theta = 3$ the solution curve of y_1 looks like in the following graph:

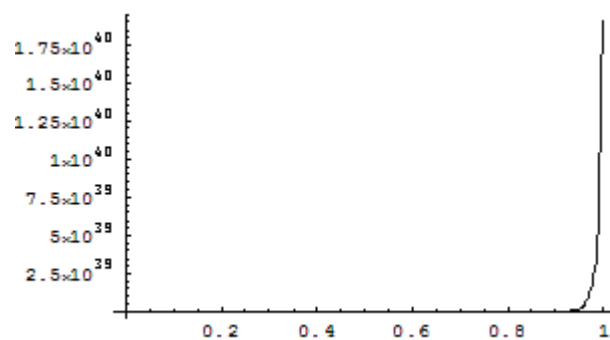


Fig. 10. Curve of y_1 with $\theta = 3$.

For $\theta = \pi$ we now see the curves of the both solutions:

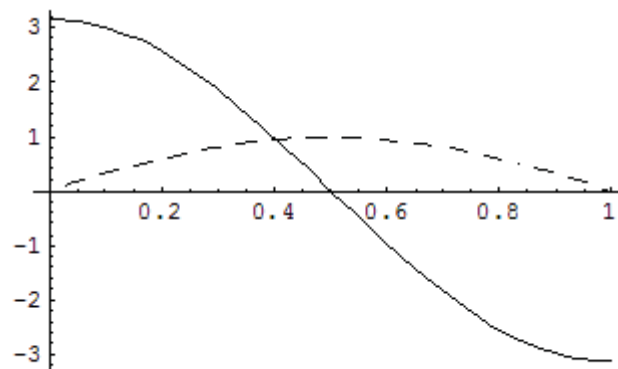


Fig. 11. Curves of y_i with $\theta = \pi$, y_1 is dashed.

Now we come to the estimation of p . We use an approximation function y_j with $j = 1$ and $k_{\max} = -k_{\min} = 15$. We set $\tau = 100$ and θ is the unknown parameter p : $p = \theta$. We simulated measurements with $\theta = \pi$, $M(y) = y$ and the points $\hat{t}_i = 0.1 \cdot i$, with $i = 1, \dots, 9$ ($\hat{m} = 9$).

The approximation interval is $I = [t_0, t_{\text{end}}] = [0, 1]$ and we use the collocation points

$$t_i = 0.05 \cdot i, \text{ with } i = 1, \dots, 20$$

($m = 20$) and set $\alpha = \beta = 1$ and use the constrain $y_j(0) = y(0)$ and the function:

$$Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=0, \dots, m} \|y_j'(t_i) - f(y_j(t_i), t_i, p)\|_2^2 + \beta \cdot \sum_{i=1, \dots, m} \|\tilde{m}_i - M(y_j(\hat{t}_i))\|_2^2$$

The minimal value of Q was: $Q_{\min} \approx 3.02674 \cdot 10^{-23}$

For a comparison: $Q_2 \approx 7.32641 \cdot 10^{-20}$

We've got the estimator $\hat{p} = 3.1415926535896475$ ($|\hat{p} - \pi| \approx 1.45661 \cdot 10^{-13}$).

Here are the curves of $y_1^{(i)} - y_i$ beginning with $i = 1$:

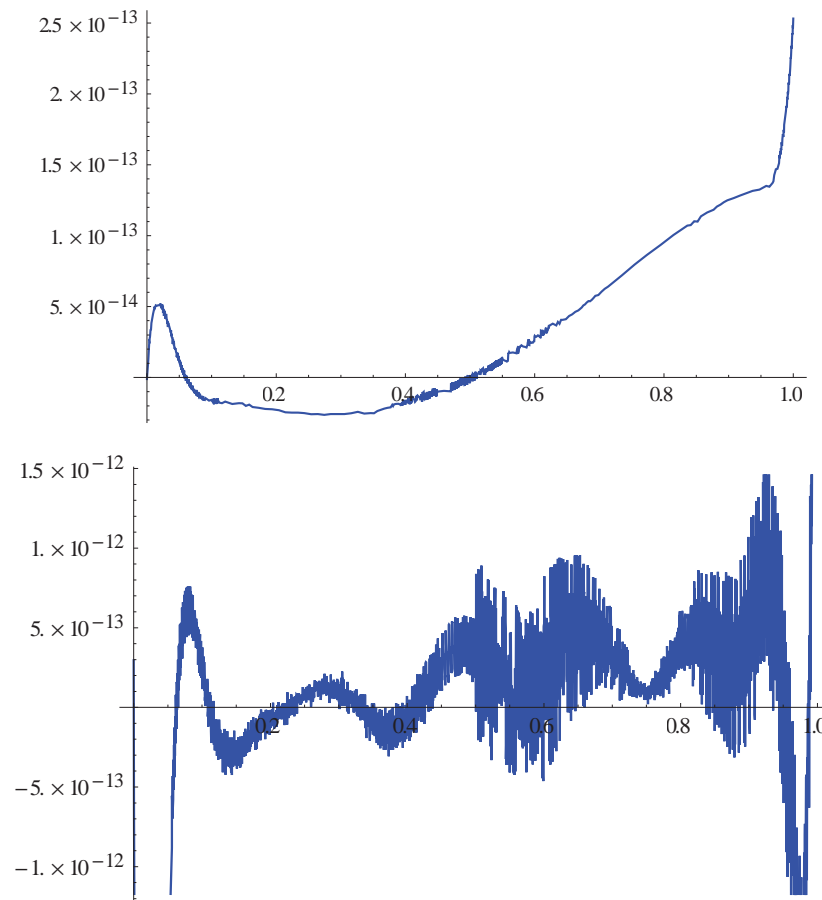


Fig. 12. Curves of $y_1^{(i)} - y_i$.

Now we see that there is a correlation between Q_{\min} and the error of the estimation and between Q_{\min} and the sum of squares of the approximation error.

We estimated the parameter p by minimizing $Q_{\alpha,\beta}$ without constraints with different j and k_{\max} ($j = -1, 0, 1, 2, k_{\max} = 15, 20, 25$). With more iteration steps we could get even smaller Q_{\min} , but we want to show the correlation between Q_{\min} and the errors. With Q_{\min} or better with Q_a we can check if we used a too small j or not enough collocation points.

Because of the term $\sin(\theta \cdot t)$ in the solution with $\theta = \pi$ the parameter j should not be less than zero, if we use the Shannon wavelet. The reason is: With the Shannon theorem we know, that y is in V_j if the support of the Fourier transform Y is a subset of $[-2^j \cdot \pi, 2^j \cdot \pi]$. So for the function $h(t) = \sin(at)$ the parameter a should be in $[-2^j \cdot \pi, 2^j \cdot \pi]$.

Here is a table with the results of the estimation for different j and k_{\max} :

j	k_{\max}	Q_{\min}	\hat{p}	$ \hat{p} - \pi $
-1	15	31.370117	0.8081795	2.333413
-1	20	29.996680	1.1156355	2.025957
-1	25	31.305504	0.8332533	2.308339
0	15	5.12784E-07	3.141578325	1.43284E-05
0	20	2.04753E-07	3.141583363	9.29025E-06
0	25	1.70835E-07	3.141584148	8.50521E-06
1	15	4.19137E-07	3.141584247	8.40653E-06
1	20	3.44747E-07	3.141584891	7.76269E-06
1	25	3.34268E-07	3.141584929	7.72466E-06
2	15	5.42453E-06	3.141540568	5.20854E-05
2	20	7.69676E-06	3.141532863	5.97911E-05
2	25	1.7566E-07	3.141583311	9.34276E-06

Table 6.

We see that Q_{\min} seems to correlate with the error of the estimation. For that reason we apply a linear regression analysis to the points $(-\ln(Q_{\min}), -\ln(|\hat{p} - \pi|))$ which have been calculated with different j and k_{\max} .

Here is the output:

	Estimate	SE	t-Stat	p-Value
1	1.53532	0.246562	6.22691	0.0000979527
x	0.642696	0.0136946	46.9307	$4.65061 \cdot 10^{-13}$

Table 7.

R-Squared = 0.997948

The linear regression fits very well.

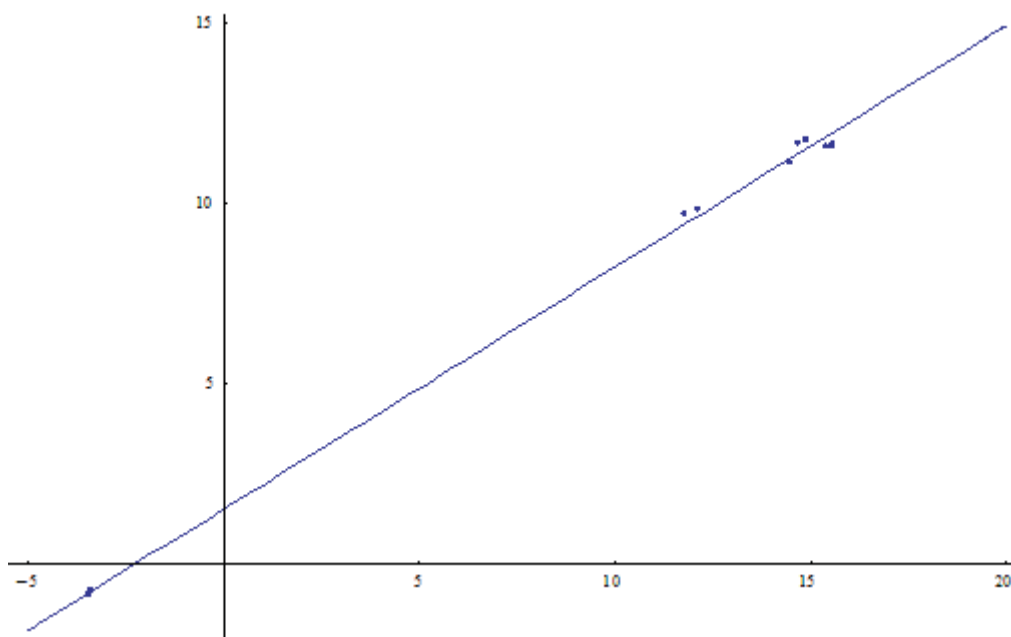


Fig. 13. $\ln(Q_{\min})$ vs. $-\ln(|\hat{p} - \pi|)$ and regression with linear regression line.

Now we see a second correlation between Q_{\min} and the squared error

$$sse = \sum_{i=0}^{100} (y(t_0 + i \cdot h_0) - y_j(t_0 + i \cdot h_0))^2 \quad \text{with } h_0 = (t_{\text{end}} - t_0)/100 = 0.01 ,$$

if we look at the table:

j	k_{\max}	Q_{\min}	sse
-1	15	31.37011658	281.964
-1	20	29.9966803	271.717
-1	25	31.30550382	281.658
0	15	5.12784E-07	1.45331E-06
0	20	2.04753E-07	5.81371E-07
0	25	1.70835E-07	4.86926E-07
1	15	4.19137E-07	1.44924E-06
1	20	3.44747E-07	1.19198E-06
1	25	3.34268E-07	1.15528E-06
2	15	5.42453E-06	2.51805E-05
2	20	7.69676E-06	3.47701E-05
2	25	1.7566E-07	7.96269E-07

Table 8.

We now apply a linear regression analysis on the points $(-\ln(Q_{\min}), -\ln(sse))$ which have been calculated with the different j and k_{\max} .

	Estimate	SE	t-Stat	p-Value
1	-2.02816	0.0706197	-28.7194	$6.1004 \cdot 10^{-11}$
x	1.05317	0.00559448	188.252	$4.39696 \cdot 10^{-19}$

Table 9.

R-Squared =0.999718

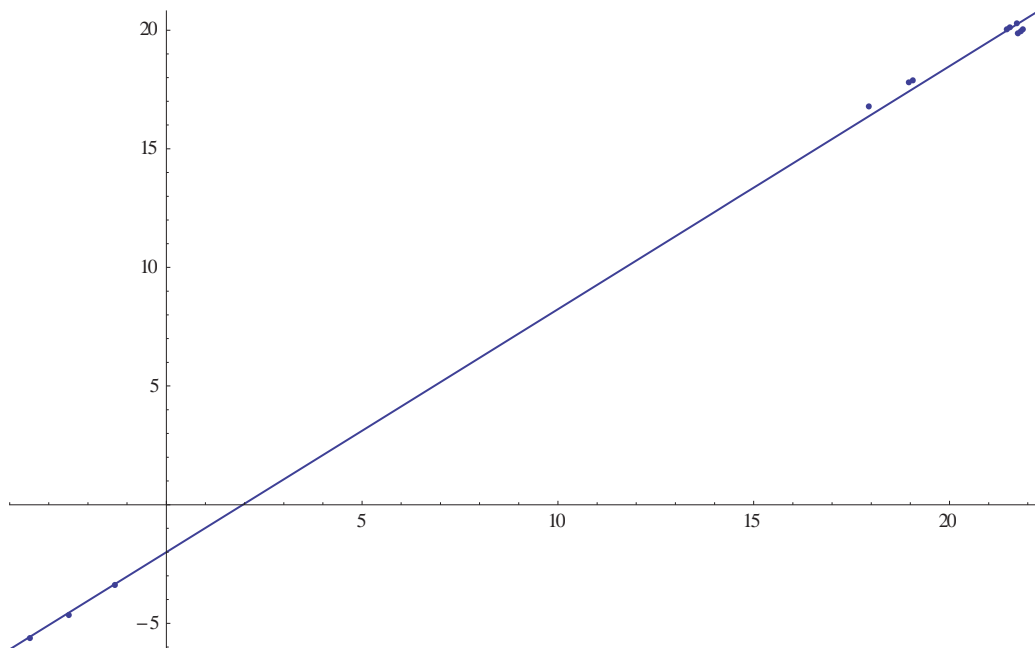


Fig. 14. $-\ln(Q_{\min})$ vs. $-\ln(sse)$ and regression with linear regression line.

At least we estimate the parameter p in two steps, so we must solve only two times a system of the normal equation. We use

$$Q_{\alpha,\beta}(p, c) = \alpha \cdot \sum_{i=1, \dots, 20} \|y_j'(t_i) - f(y_j(t_i), t_i, p)\|^2 + \beta \cdot \sum_{i=1, \dots, 9} \|\tilde{m}_v - M(y_j(\hat{t}_i))\|^2$$

and estimate at first c with $\alpha = 0$ and $\beta = 1$:

$$Q_{0,1}(p, \hat{c}) = \min_c Q_{0,1}(p, c)$$

Then we estimate p :

$$Q_{1,0}(\hat{p}, \hat{c}) = \min_p Q_{1,0}(p, \hat{c})$$

In the first step, we get: $Q_{0,1}(p, \hat{c}) = \min_c Q_{0,1}(p, c) \approx 2.78704 \cdot 10^{-30}$.

Here are the curves of $y_j - y$:

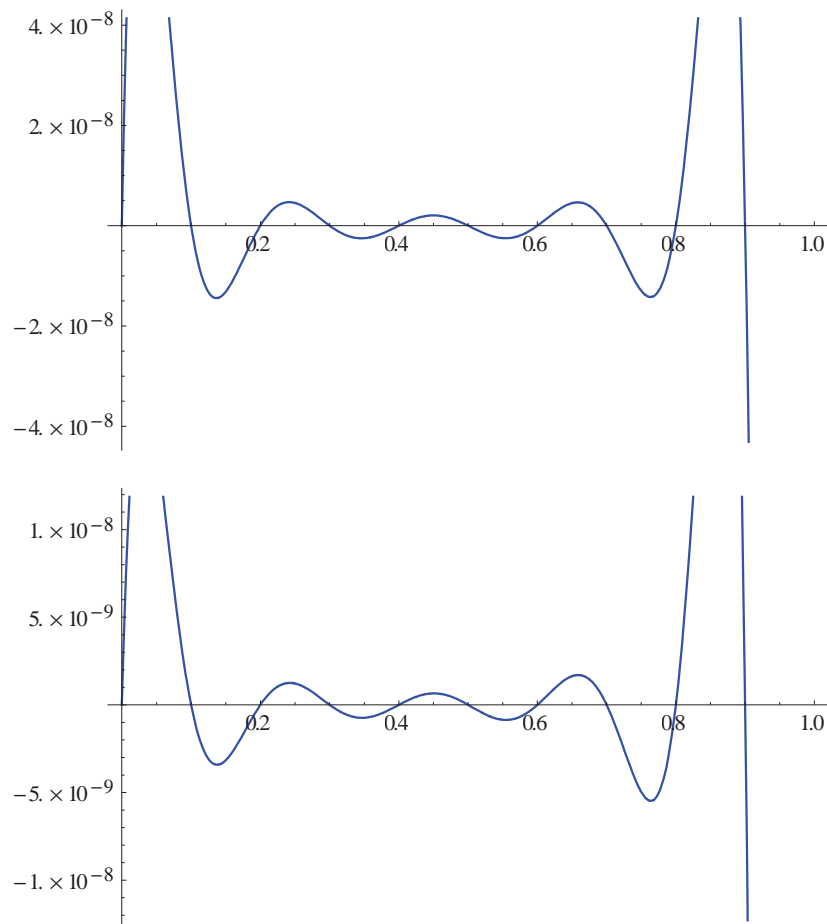


Fig. 15. Curves of $y_j - y$.

In the second step, we estimate p with

$$Q_{1,0}(\hat{p}, \hat{c}) = \min_p Q_{1,0}(p, \hat{c})$$

and we get the following error $|\hat{p} - \pi| \approx 1.79995 \cdot 10^{-6}$.

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