

TESTING THE METHOD OF MULTIPLE SCALES AND THE AVERAGING PRINCIPLE FOR MODEL PARAMETER ESTIMATION OF QUASIPERIODIC TWO TIME-SCALE MODELS

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Abstract: Some dynamical systems are characterized by more than one time-scale, e.g. two well separated time-scales are typical for quasiperiodic systems. The aim of this paper is to show how singular perturbation methods based on the slow-fast decomposition can serve for an enhanced parameter estimation when the slowly changing features are rigorously treated. Although the ultimate goal is to reduce the standard error for the estimated parameters, here we test two methods for numerical approximations of the solution of associated forward problem: (i) the multiple time-scales method, and (ii) the method of averaging. On a case study, being an under-damped harmonic oscillator containing two state variables and two parameters, the method of averaging gives well (theoretically predicted) results, while the use of multiple time-scales method is not suitable for our purposes.

Keywords: dynamical system, singular perturbation, averaging, parameter estimation, slow-fast decomposition, damped oscillations

MSC: 92C45, 34A34, 65F60, 65K10

1. Introduction

In this study, we present a development and testing of suitable methods for the numerical simulation of the forward problem associated with the inverse problem of model parameter estimation. The key feature of a process under study is that two well separated time-scales are present, which is typical for quasiperiodic systems, i.e. there is a periodic behavior in a fast time-scale and some other phenomenon, evolving in much slower time-scale, to be identified.

Although the ultimate goal is to quantify and reduce the standard error (confidence interval) for the model parameter estimates, an accurate and fast numerical

approximation of the forward problem associated with the inverse problem is wanted. Here, we test two methods: (i) the multiple time-scales method, and (ii) the method of averaging. In summary, we highlight how singular perturbation methods serve the corresponding problem of model parameter estimation. On a (linear) model of an under-damped harmonic oscillator containing two state variables and two parameters, we demonstrate both the known pitfalls of the multiple time-scales method and the feasibility of the averaging method (the first order averaging) employed for a numerical simulation of the associated forward problem.

2. Preliminaries

2.1. State variables, model parameters, and governing equations

As follows, we present an ODE system in general (linearized) form describing the first order dynamics of a process depending on model parameters p_1, \dots, p_m and evolving in continuous time. A general form of a linear first order ODE system describing the dynamics of state variable vector $x \in \mathbb{R}^n$ is

$$\frac{dx(t;p)}{dt} = A(p)x(t;p) \quad (1)$$

with the square matrix $A(p)$ of order n . Vector $p \in \mathbb{R}^m$ contains all model parameters defining the system under study. Finally, there are the initial conditions $x_0 = x(t_0; p)$ which can be taken as system inputs.

Although our motivation for studying first order dynamical systems (1) dwells on a prospect to study inverse problems of parameter estimation arising from pharmacokinetics models, here, as a case study, we shall consider the governing dynamic equations for a weakly damped linear (harmonic) oscillator. In branch of mechanics, a mechanical oscillator under the influence of a linear restoring force and friction is described (using the Newton second law) by the ODE

$$m \ddot{y} = -k y - b \dot{y} + m g, \quad (2)$$

where y is the vertical position of the center of mass (the positive direction is upside down), $m > 0$ is the mass, $k > 0$ is the spring force constant, and $b > 0$ measures the strength of the damping. Setting the origin of y -axis at the equilibrium (i.e. at the position $y = 0$ the force of gravity is acting on the mass equalized by an adequate spring force), the governing equation of the system becomes

$$\ddot{y} + 2\delta \dot{y} + \omega_0^2 y = 0, \quad (3)$$

where $\delta \equiv \frac{b}{2m}$ and $\omega_0 \equiv \sqrt{k/m}$ are a usual damping constant and an undamped oscillation frequency, respectively [cf., Equation (8) for $\delta = 0$ below].

We shall refer to the preceding equation (3) as the damped harmonic oscillator

equation. Let the initial conditions be¹

$$y(0) = 1, \quad \dot{y}(0) = 0. \quad (4)$$

Further, inspired by [6], let us introduce the following transformation of state variables

$$x_1 = y, \quad x_2 = \frac{\dot{y}}{\omega_0}, \quad (5)$$

then the single ODE of the second order (3) can be described in the form of (1), where the state variables vector is

$$x(t) = \begin{pmatrix} x_1(t) \\ x_2(t) \end{pmatrix},$$

the corresponding form of matrix A is

$$A(p) = \begin{pmatrix} 0 & \omega_0 \\ -\omega_0 & -2\delta \end{pmatrix} = \omega_0 \begin{pmatrix} 0 & 1 \\ -1 & -2\frac{\delta}{\omega_0} \end{pmatrix}, \quad (6)$$

and the initial conditions are

$$x(0) = \begin{pmatrix} x_1(0) \\ x_2(0) \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (7)$$

2.2. Exact solution of the system (3)-(4)

Assuming that $\delta < \omega_0$ and setting $\omega := \sqrt{\omega_0^2 - \delta^2}$, the exact solution of system (3) with initial conditions (4) is given by

$$y_{\text{ex}}(t) = e^{-\delta t} \left(\cos \omega t + \frac{\delta}{\omega} \sin \omega t \right). \quad (8)$$

Remark 2.1. *If we define a scalar dimensionless quantity $\varepsilon := \frac{\delta}{\omega_0} \ll 1$, then $\omega = \omega_0 \sqrt{1 - \varepsilon^2}$. Furthermore, employing a usual scaling of time t , i.e. $t_{\text{scaled}} := \omega_0 t$, then the exact solution (8) has the form*

$$y_{\text{ex}}(t_{\text{scaled}}) = e^{-\varepsilon t_{\text{scaled}}} \left(\cos \sqrt{1 - \varepsilon^2} t_{\text{scaled}} + \frac{\varepsilon}{\sqrt{1 - \varepsilon^2}} \sin \sqrt{1 - \varepsilon^2} t_{\text{scaled}} \right). \quad (9)$$

As follows, the above single parameter form (9) is used and the scaled time is (in seek of simplicity) expressed as t , which in fact is fulfilled for the value $\omega_0 = 1$. Moreover, given the transformation of state variables (5), it holds $x_2 = \frac{dx_1}{dt_{\text{scaled}}}$.

Remark 2.2. *Let us underline that the expression (9) is employed in Section 4.3 for the quantification of errors corresponding to different numerical approximation methods.*

The numerical values of two (only) model parameters used in equations (3)–(9) within some other related quantities are summarized in Table 1.

¹This is done without loss of generality because the y coordinate can be scaled or normalized by the maximum value of $y(t)$, i.e. $y(0)$ value. Another usual setting of initial conditions for Equation (3) is $y(0) = 0$, $\dot{y}(0) = 1$.

Parameter	Formula	Value	Meaning
ω_0	$\sqrt{k/m}$	1.0 [s ⁻¹]	undamped oscillation frequency
δ	$\frac{b}{2m}$	10 ⁻³ [s ⁻¹]	damping constant
ε	$\frac{\delta}{\omega_0}$	10 ⁻³ [-]	dimensionless damping constant

Table 1: Description and values of model parameters used in (3)–(9).

3. Perturbation theory and the averaging principle

Some dynamical systems can be represented by differential equations that are a small perturbation of an integrable problem.² Therefore, methods that allow to approximate the solutions of a perturbed problem, like $\dot{x} = f(t, x; \varepsilon)$, where $0 < \varepsilon \ll 1$, starting from the solutions of the unperturbed one (for $\varepsilon = 0$), are forming the perturbation theory, see e.g. [1, 2]. Instead of providing a detailed theoretical description of the singular perturbation (SP) techniques and their variants, for a class of systems defined by (1) we mention only two of them: (i) the method of multiple scales (MMS),³ and (ii) the first order averaging.

3.1. Failure of the naive implementation of the MMS technique

Consider a first order expansion of a solution vector x , i.e. $x(t, \varepsilon) = x^{(0)}(t) + \varepsilon x^{(1)}(t) + O(\varepsilon^2)$. Then (1) reads

$$\frac{d}{dt} (x^{(0)}(t) + \varepsilon x^{(1)}(t)) = A(\varepsilon) (x^{(0)}(t) + \varepsilon x^{(1)}(t)).$$

For our weakly damped oscillator (1), with matrix A as (6), and after applying the scaling for both state variables and time, we have

$$\frac{dx(t)}{dt} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} x(t) + \begin{pmatrix} 0 & 0 \\ 0 & -2\varepsilon \end{pmatrix} x(t) \quad (10)$$

with initial conditions (4), i.e.

$$x^{(0)}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad x^{(1)}(0) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Then we find for the leading order problem that

$$\frac{dx^{(0)}(t)}{dt} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} x^{(0)}(t) \quad (11)$$

²We say that a system of ODEs is integrable if its solutions can be expressed by analytic formulas up to inversions (by the implicit function theorem) or quadratures; we call the system non-integrable if this is not possible.

³Because of the inconvenience of method of multiple scales for numerical solution of a class of pharmacokinetic models, the setting of *solvability conditions* in frame of MMS is omitted here, for more details see Remark 3.2.

with a solution

$$x^{(0)}(t) = \begin{pmatrix} \cos t \\ -\sin t \end{pmatrix}.$$

At next order (for ε^1), we find that

$$\frac{dx^{(1)}(t)}{dt} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} x^{(1)}(t) + \begin{pmatrix} 0 & 0 \\ 0 & -2 \end{pmatrix} x^{(0)}(t), \quad (12)$$

which is in fact the ODE for a resonantly forced oscillator, and the solution for the first component is

$$x_1^{(1)}(t) = \sin t - t \cos t.$$

Therefore, a two-term (first order) approximate solution for the component x_1 is

$$x_1(t) = x_1^{(0)}(t) + \varepsilon x_1^{(1)}(t) = \cos t + \varepsilon \sin t - \varepsilon t \cos t = (1 - \varepsilon t) \cos t + \varepsilon \sin t. \quad (13)$$

Remark 3.1. *The above example clearly shows the failure when the naive implementation of the regular expansion is employed. On the result (13) it can be observed that the weakly damping system undergoes small changes of the amplitude of the oscillation (as $(1 - \varepsilon t)$) which cannot be longer negligible on a time scale $\varepsilon^{-1} \sim 1000$, i.e. when the so-called secular terms invalidate the expansion, see Fig. 1.*

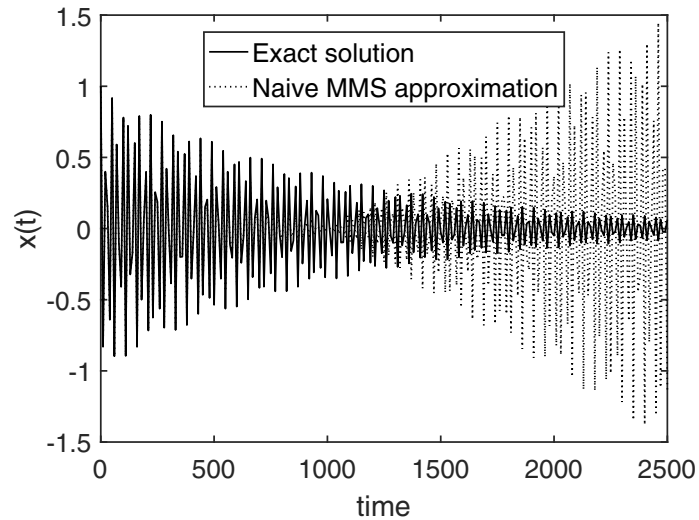


Figure 1: Comparison of the exact solution (9) (solid black curve) with the naive MMS approximation (13) (dotted curve).

Remark 3.2. *The correct employment of the MMS techniques resides in the use of what are known as solvability conditions in the formal derivation. It can be seen as a trick to avoid secular terms, and actually it is. Here, we reject this method because it poses big problem for the numerical implementation of the method.*

Remark 3.3. *There is some similarity of MMS to the Poincaré-Lindstedt method which provides a way to construct asymptotic approximations of periodic solutions. Nevertheless, the Poincaré-Lindstedt method cannot be used to obtain solutions that evolve aperiodically on a slow time-scale. Thus, the method of multiple scales, and mainly its WKB variant (WKB method requires the state variable x to be 2π -periodic function of the “fast” time variable θ , see e.g. [2] and references within), is a more general approach.*

3.2. Averaging principle

The averaging principle consists in solving averaged equations, obtained by an integral average of the original equations (which can be put into a periodic standard form) over some angular variables; then we consider the solutions of the averaged equations as representative of the solutions of the original equations for a long time span (of the order $1/\varepsilon$). A review of the classical results on averaging methods in perturbation theory can be found in [2, 6]. Further, in sake of completeness, we announce (without proofs) two theorems dealing with approximation error estimation (published in [4]) and we present the approximate solution to (3)–(4) using the first order averaging (see Section 4.1).

Theorem 3.4. *Consider a system of ODEs for $x(t) \in \mathbb{R}^n$ which can be written in the standard form*

$$\dot{x} = \varepsilon f(x, t; \varepsilon). \quad (14)$$

Here, $f: \mathbb{R}^n \times \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}^n$ is a smooth function, 2π -periodic in “fast” variable t :

$$f(x, t + 2\pi, \varepsilon) = f(x, t, \varepsilon).$$

For $R > 0$ let $B_R(x_0) = \{x(t) \in \mathbb{R}^n; |x - x_0| < R\}$ and $M = \sup_{x \in B_R(x_0), t \in \mathbb{T}} |f(x, t)|$. Then there is a unique solution of the IVP,

$$x: (-T/\varepsilon, T/\varepsilon) \rightarrow B_R(x_0) \subset \mathbb{R}^n$$

that exists for $|t| < T/\varepsilon$, where $T = \frac{R}{M}$.

Theorem 3.5 (Krylov-Bogoliubov-Mitropolski). *With the same notation as in the previous theorem: There exists a unique solution*

$$\bar{x}: (-T/\varepsilon, T/\varepsilon) \rightarrow B_R(x_0) \subset \mathbb{R}^n$$

of the averaged equation

$$\dot{\bar{x}} = \varepsilon \bar{f}(\bar{x}), \quad \bar{x}(0) = x_0, \quad (15)$$

where $\bar{f}(x) = \frac{1}{2\pi} \int_{\mathbb{T}} f(x, t) dt$. Moreover, there exist constants $\varepsilon_0 > 0$ and $C > 0$ such that for all $0 \leq \varepsilon \leq \varepsilon_0$

$$|x(t) - \bar{x}(t)| \leq C\varepsilon \quad \text{for} \quad |t| \leq T/\varepsilon. \quad (16)$$

4. Numerical example

On the ODE system (3)–(4) we now perform some numerical experiments. As mentioned, the MMS method produces naive numerical results, and thus we use the averaging principle and compare it with the backward Euler method. First, we introduce approximate solutions for both approaches.

4.1. Approximate solution to (3)–(4) using the first order averaging

Consider the ODE system (3)–(4) in the following form:

$$\ddot{y} + y = -2\varepsilon \dot{y}, \quad y(0) = 1, \quad \dot{y}(0) = 0.$$

Using the transformation

$$y = r \sin(t - \phi), \quad \dot{y} = r \cos(t - \phi), \quad (17)$$

the new variables r, ϕ satisfy the system

$$\dot{r} = \varepsilon \cos(t - \phi)(-2r \cos(t - \phi)) \equiv \varepsilon f_r(t),$$

$$\dot{\phi} = \varepsilon \frac{1}{r} \sin(t - \phi)(-2r \cos(t - \phi)) \equiv \varepsilon f_\phi(t).$$

Applying the averaging principle to the above equations leads to solving the system

$$\dot{\bar{r}} = \varepsilon \bar{f}_r, \quad \dot{\bar{\phi}} = \varepsilon \bar{f}_\phi, \quad (18)$$

where

$$\bar{f}_r = \frac{1}{2\pi} \int_0^{2\pi} f_r(t) dt, \quad \bar{f}_\phi = \frac{1}{2\pi} \int_0^{2\pi} f_\phi(t) dt. \quad (19)$$

Remark 4.1. Clearly it holds $\bar{f}_r = -r$ and $\bar{f}_\phi = 0$ but unlike our simple case study, the integrals of functions f_r, f_ϕ in (19) cannot be usually computed easily. For this purpose we compute it numerically using the trapezoidal rule at points $0 = t_0, t_1, \dots, t_n = 2\pi$.

Let F_r, F_ϕ be the values of integrals of functions f_r, f_ϕ computed numerically, i.e.

$$F_r \approx \int_0^{2\pi} \cos^2(t) dt, \quad F_\phi \approx \int_0^{2\pi} \sin(t) \cos(t) dt.$$

Then

$$\bar{f}_r = -\frac{r}{\pi} F_r, \quad \bar{f}_\phi = -\frac{1}{\pi} F_\phi$$

and substituting into (18), the system of equations which approximates (3)–(4) is

$$\dot{\bar{r}} = -\varepsilon \frac{F_r}{\pi} \bar{r}, \quad \dot{\bar{\phi}} = -\varepsilon \frac{F_\phi}{\pi}.$$

The solution is

$$\bar{r} = C_r \exp\left(-\varepsilon \frac{F_r}{\pi} t\right), \quad \bar{\phi} = -\varepsilon \frac{F_\phi}{\pi} t + C_\phi,$$

where C_r and C_ϕ are some constants. Substituting into (17), the approximate averaging solution is then

$$y(t) = \bar{r} \sin(t - \bar{\phi}) = C_r \exp\left(-\varepsilon \frac{F_r}{\pi} t\right) \sin\left(t + \varepsilon \frac{F_\phi}{\pi} t - C_\phi\right),$$

$$\dot{y}(t) = \bar{r} \cos(t - \bar{\phi}) = C_r \exp\left(-\varepsilon \frac{F_r}{\pi} t\right) \cos\left(t + \varepsilon \frac{F_\phi}{\pi} t - C_\phi\right).$$

The constants C_r and C_ϕ will be obtained from initial conditions:

$$y(0) = C_r \sin(-C_\phi) = 1, \quad \dot{y}(0) = C_r \cos(-C_\phi) = 0,$$

which implies

$$\cos(-C_\phi) = 0 \quad \Rightarrow \quad C_\phi = \frac{3}{2}\pi \quad \text{and} \quad C_r = 1.$$

Finally, the approximate solution using the first order averaging has the form

$$y_{\text{av}}(t) = \exp\left(-\varepsilon \frac{F_r}{\pi} t\right) \sin\left(t + \varepsilon \frac{F_\phi}{\pi} t - \frac{3}{2}\pi\right)$$

$$= \exp\left(-\varepsilon \frac{F_r}{\pi} t\right) \cos\left(\left(1 + \varepsilon \frac{F_\phi}{\pi}\right)t\right). \quad (20)$$

4.2. Approximate solution to (3)–(4) using the backward Euler method

Transformation

$$x_1 = y, \quad x_2 = \dot{y}$$

leads to a system

$$\dot{x} = Ax, \quad x = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad A = \begin{pmatrix} 0 & 1 \\ -1 & -2\varepsilon \end{pmatrix},$$

cf. (6), with initial conditions (7). The implicit backward Euler method leads to solving a linear system

$$(I - \Delta t A)x(t + \Delta t) = x(t).$$

The numerical solution to (3)–(4) is the first component, i.e.

$$y_{\text{be}}(t_j) = x_1(t_j), \quad j = 0, \dots, m, \quad t_j = j \Delta t, \quad t_m = T. \quad (21)$$

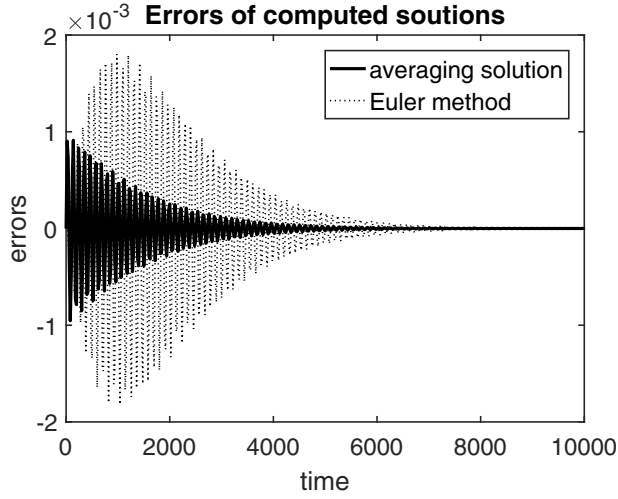


Figure 2: Errors of averaging solution and the backward Euler method from the exact solution, $t \in [0, 10\,000]$.

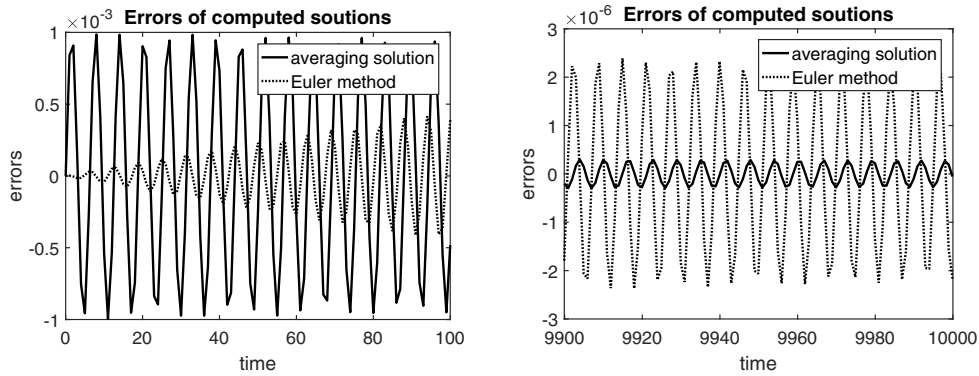


Figure 3: Zoom of errors. Left: $t \in [0, 100]$, Right: $t \in [9\,900, 10\,000]$.

4.3. Comparison of solution errors

Consider problem (3)–(4) and take the exact solution (9), the approximate averaging solution (20), and the solution obtained using the backward Euler method (21). Define the errors of computed solutions from the exact solution as follows:

$$\text{error}_{\text{av}}(t_j) = y_{\text{ex}}(t_j) - y_{\text{av}}(t_j), \quad \text{error}_{\text{be}}(t_j) = y_{\text{ex}}(t_j) - y_{\text{be}}(t_j), \quad (22)$$

where $t_j = j\Delta t$, $j = 0, \dots, m$, $t_m = T$ (final time). For our numerical computations we consider the values

$$\varepsilon = 1.0\text{E-}3 \text{ (see Table 1), } \Delta t = 1.0\text{E-}5, \quad T = 10\,000.$$

Figure 2 shows the errors (22) of averaging solution and the backward Euler method from the exact solution for $t \in [0, 10\,000]$. Figures 3 show zooms. On the left there are errors for the initial time interval $t \in [0, 100]$, while on the right there are errors for the final time interval $t \in [9\,900, 10\,000]$.

The results show that the solution obtained using the averaging principle is really of order $C\varepsilon$ as stated in Theorem 3.5 (here for $\varepsilon = 10^{-3}$ we have $C \approx 1$) and the error envelope is decreasing from the beginning. On the other hand, the error envelope of the Euler method grows at the beginning until the time t reaches the value $1/\varepsilon$, i.e. $t \approx 1000$. This maximum value is even for a relatively small step $\Delta t = 10^{-5}$ twice the maximum value of averaging envelope ($C \approx 2$). For $t > 1/\varepsilon$ the error envelope of the Euler method finally tends to zero. Thus, the averaging principle outperforms the Euler method.

5. Conclusion

We showed the behavior of the **Method of Multiple (time)Scales** (MMS) and mainly the **Averaging method** to approximate the solutions of perturbation problems. The Naïve implementation of MMS generates wrong results due to presence of secular terms which cannot be avoided when using a numerical approach. On the other hand, the averaging method gives satisfactory results, the error is of order $C\varepsilon$ (as predicted by the KBM theorem), and the results are better than those using the Euler method.

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