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Error estimates for Lie transformations

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Abstract

Lie transformations are commonly used to simplify dynamical systems through asymptotic changes of variables in such a way that the main qualitative features of the original system are preserved. For instance, by means of the analysis of the transformed system one can obtain explicit expressions of periodic orbits or invariant tori of the original one. These transformations are not convergent, in general; nevertheless it is possible to calculate upper bounds of the error of the truncation. What we propose here is an easy but effective way to make an estimation of this error. The central idea is to compose the inverse and direct transformations. In order to illustrate our procedure, some examples of applications to dissipative, as well as Hamiltonian systems, are shown.

Keywords: error estimates, Lie transformations, perturbed dynamical systems
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1 Motivation and Scope

Lie transformations [2, 5] are commonly used to simplify dynamical systems, as they provide asymptotic changes of variables such that the main qualitative features of the original system are preserved. For instance, by means of the analysis of the transformed system one can obtain explicit expressions of periodic orbits or invariant tori of the original one.

In reference [8] we present a method to calculate invariant manifolds of dynamical systems which are defined through an m–dimensional vector field. The technique is based on the calculation of formal symmetries and generalized normal forms associated to this vector field making use of Lie transformations for ordinary differential equations. Once a symmetry is determined up to a certain order, a reduction map allows us to determine the corresponding orbit space and construct in it the equation in normal form, which is the so–called reduced system (of dimension $s < m$). Then, a non–degenerate p–dimensional invariant set of the reduced system (i.e. a critical point, closed trajectory or nD–invariant torus) is transformed, asymptotically, into a $(p+m-s)$–dimensional invariant set of the departure equation.

These transformations are not convergent, but they diverge in general. Nevertheless, in practice one truncates the transformation at a given order. The first terms of the resulting reduced system can provide a very useful information of the original system. If one has a procedure to control the error of the transformation when truncating at a certain order, one can determine the validity of the transformation. In this sense it is possible to calculate upper bounds of the error of the truncation. There are several methods in the literature [3, 4], although they give estimates and upper bounds for a quite narrow class of perturbed differential equations.

Lie transformations provide explicit expressions of the asymptotic changes of variables which allow to pass to the reduce system. Moreover they give also explicit expressions to go back to the original system. What we propose here is an easy but effective way to make an estimation of the error. The central idea of our proposal is to compose the inverse and direct Lie transformations. In order to illustrate the results of this procedure we will estimate the error of a transformation of the type presented in [8] applied to some examples of dissipative, as well as Hamiltonian systems.

The structure of the Paper is as follows. In Section 2 we recall the method used to calculate generalized normal forms [8] giving the Lie transformations involved in it. Section 3 contains the central result: the method to estimate the error. We finish with the examples, which appear in Section 4.

2 Generalized Normal Forms

Let us consider the vector field

$$\frac{d\,\mathbf{x}}{d\,t} = \mathbf{F}(\mathbf{x};\varepsilon;\mathbf{c}) = \sum_{i=0}^{L} \frac{\varepsilon^i}{i!}\mathbf{F}_i(\mathbf{x};\mathbf{c}), \tag{1}$$

where ε and $\mathbf{c}$ are parameters and $\mathbf{x},\mathbf{y} \in \mathbf{R}^m$. We intend to perform an asymptotic change of variables $\mathbf{x} \to \mathbf{y}$ so as to transform (1) into the vector field

$$\frac{d\,\mathbf{y}}{d\,t} = \mathbf{G}(\mathbf{y};\varepsilon;\mathbf{c}) = \sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\mathbf{G}_i(\mathbf{y};\mathbf{c}) + \mathcal{O}\left(\varepsilon^{M+1}\right), \tag{2}$$

in such a way that $\mathbf{G}_0 \equiv \mathbf{F}_0$ and $M \geq L$. In Section 3 we will give a rigorous estimate of the error committed after truncating this transformation at order M. The calculation of (2) is based on the following Theorem [8]:

Theorem 2.1 *Let $M \geq 1$ and $\{\mathcal{P}_i\}_{i=0}^M$, $\{\mathcal{Q}_i\}_{i=1}^M$, $\{\mathcal{R}_i\}_{i=1}^M$ be sequences of vector spaces of analytic functions in $\mathbf{x} \in \mathbf{R}^m$ defined on a common domain $\Omega \subseteq \mathbf{R}^m$ and let $\mathbf{T} \equiv \mathbf{T}(\mathbf{x})$ be a smooth vector field in some $\{\mathcal{P}_i\}_{i=0}^M$ satisfying:*

i) $\mathcal{Q}_i \subseteq \mathcal{P}_i$, $i = 1, \ldots, M$;

ii) $\mathbf{F}_i \in \mathcal{P}_i$, $i = 0, 1, \ldots, M$;

iii) $[\,\mathcal{P}_i\,,\,\mathcal{R}_j\,] \subseteq \mathcal{P}_{i+j}$, $i + j = 1, \ldots, M$;

iv) for any $\mathbf{D} \in \mathcal{P}_i$, $i = 1, \ldots, M$, *there are* $\mathbf{E} \in \mathcal{Q}_i$ *and* $\mathbf{K} \in \mathcal{R}_i$ *such that:*

$$\mathbf{E} = \mathbf{D} + [\,\mathbf{F}_0\,,\,\mathbf{K}\,] \quad \textit{and} \quad [\,\mathbf{E}\,,\,\mathbf{T}\,] = \mathbf{0}.$$

Under such conditions there is a vector field

$$\mathbf{W}(\mathbf{x};\varepsilon) = \sum_{i=0}^{M-1} \frac{\varepsilon^i}{i!}\,\mathbf{W}_{i+1}(\mathbf{x}),$$

with $\mathbf{W}_i \in \mathcal{R}_i$, $i = 1, \ldots, M$, *such that the change of variables* $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$ *is the general solution of the initial value problem:*

$$\frac{d\,\mathbf{x}}{d\,\varepsilon} \;=\; \frac{\partial \mathbf{W}}{\partial \mathbf{x}}(\mathbf{x};\varepsilon), \quad \mathbf{x}(0) \;=\; \mathbf{y},$$

and transforms the convergent vector field

$$\mathbf{F}(\mathbf{x};\varepsilon) = \sum_{i=0}^{L} \frac{\varepsilon^i}{i!}\,\mathbf{F}_i(\mathbf{x}),$$

into the convergent vector field

$$\mathbf{G}(\mathbf{y};\varepsilon) = \sum_{i=0}^{M} \frac{\varepsilon^i}{i!}\,\mathbf{G}_i(\mathbf{y}) + \mathcal{O}(\varepsilon^{M+1}), \tag{3}$$

with $\mathbf{G}_i \in \mathcal{Q}_i$ *and* $[\,\mathbf{G}_i\,,\,\mathbf{T}\,] = \mathbf{0}$, $i = 1, \ldots, M$. *Besides, if* $[\,\mathbf{F}_0\,,\,\mathbf{T}\,] = \mathbf{0}$ *then* $\mathbf{T} \equiv \mathbf{T}(\mathbf{y})$ *is a formal symmetry of* $\mathbf{G}$.

The notation $[\,\cdot\,,\,\cdot\,]$ represents the Lie bracket of two vector fields, that is, if $\partial\mathbf{A}/\partial\mathbf{y}$ and $\partial\mathbf{A}/\partial\mathbf{y}$ are square Jacobian matrices associated to the vector fields $\mathbf{A}$ and $\mathbf{B}$ respectively, one has

$$[\,\mathbf{A}\,,\,\mathbf{B}\,] \;=\; \frac{\partial \mathbf{B}}{\partial \mathbf{y}}\,\mathbf{A} - \frac{\partial \mathbf{A}}{\partial \mathbf{y}}\,\mathbf{B}.$$

The construction of (3) is made step by step. In each order $i = 1, \ldots, M$ we have to calculate $\mathbf{G}_i$ and another vector field $\mathbf{W}_i$, which corresponds to the i–th term of the so–called generating function of the transformation $\mathbf{W}$. For this purpose one has to solve the homology equation

$$[\,\mathbf{F}_0\,,\,\mathbf{W}_i\,] + \mathbf{G}_i \;=\; \widetilde{\mathbf{F}}_i,$$

where $\widetilde{\mathbf{F}}_i$ denotes the vector fields computed in the previous steps. We look for $\mathbf{G}_i$ such that $[\,\mathbf{G}_i\,,\,\mathbf{T}\,] = \mathbf{0}$. For that, we split $\widetilde{\mathbf{F}}_i = \widetilde{\mathbf{F}}_i^{\#} + \widetilde{\mathbf{F}}_i^{\&}$, where $[\,\widetilde{\mathbf{F}}_i^{\#}\,,\,\mathbf{T}\,] = \mathbf{0}$. Then, we identify $\mathbf{G}_i = \widetilde{\mathbf{F}}_i^{\#}$ and $\widetilde{\mathbf{F}}_i^{\&} = \widetilde{\mathbf{F}}_i - \widetilde{\mathbf{F}}_i^{\#}$. The vector field $\mathbf{W}_i$ is a solution of the system of partial differential equations $[\,\mathbf{F}_0\,,\,\mathbf{W}_i\,] = \widetilde{\mathbf{F}}_i^{\&}$.

Once we have calculated the generating function $\mathbf{W}$, we use it to build the direct and inverse changes of variables. The transformation $\mathbf{x} = \mathbf{X}(\mathbf{y};\varepsilon)$ relates the "old" variables $\mathbf{x}$ with the "new" ones $\mathbf{y}$ and is a near–identity change of variables. Explicitly, the direct change is given by

$$\mathbf{x} \;=\; \mathbf{y} + \sum_{i=1}^{M} \frac{\varepsilon^i}{i!}\,\mathbf{y}_0^{(i)}, \tag{4}$$

where $\mathbf{y}_i^{(0)} \equiv \mathbf{0}$ for $i \geq 1$, $\mathbf{y}_0^{(0)} \equiv \mathbf{y}$ and

$$\mathbf{y}_i^{(j)} \;=\; \mathbf{y}_{i+1}^{(j-1)} + \sum_{k=0}^{i} \binom{i}{k} \,(\,\mathbf{y}_k^{(j-1)}\,,\,\mathbf{W}_{i+1-k}\,).$$

The notation (,) means the operator $(\,\mathbf{g}_1\,,\,\mathbf{g}_2\,) = (\partial \mathbf{g}_1/\partial \mathbf{y})\,\mathbf{g}_2$.

Similar formulae can be used to obtain the inverse transformation: $\mathbf{y} = \mathbf{Y}(\mathbf{x};\varepsilon)$, which relates the "new" variables $\mathbf{y}$ with the "old" ones $\mathbf{x}$:

$$\mathbf{y} \;=\; \mathbf{x} + \sum_{i=1}^{M} \frac{\varepsilon^i}{i!}\,\mathbf{x}_0^{(i)}, \tag{5}$$

where $\mathbf{x}_0^{(i)} \equiv \mathbf{0}$ for $i \geq 1$, $\mathbf{x}_0^{(0)} \equiv \mathbf{x}$ and

$$\mathbf{x}_i^{(j)} \;=\; \mathbf{x}_{i-1}^{(j+1)} + \sum_{k=0}^{i-1} \binom{i-1}{k} \,(\,\mathbf{x}_{i-k-1}^{(j)}\,,\,\mathbf{W}_{k+1}\,).$$

With these two transformations it is possible to pass from the original system to the reduced one and viceversa.

3 Estimation of the Error

In order to obtain the error estimation of the Lie transformations constructed in the previous section we can either compose the direct change of variables given by (4) with its inverse change (5) or vice versa. By doing so we get a vector field which depend on the original variables (if we have started the composition with the direct change) or on the transformed variables (if we have composed the inverse change with the direct one). The vector field resulting out of the composition is also a function of the small parameter ε. Moreover, as the changes we construct are asymptotics, the composition is also an asymptotic expression in terms of ε which is built from the explicit formula of the changes.

Given a vector field $\mathbf{S}(\mathbf{x};\varepsilon)$ depending on the $\mathbf{x}$ variables, we transform it by applying a Lie transformation, up to order M. In this way we can express $\mathbf{S}$ as a function of the variables $\mathbf{y}$ using the direct change (4): $\mathbf{S}(\mathbf{x};\varepsilon) = \mathbf{S}(\mathbf{X}(\mathbf{y};\varepsilon);\varepsilon)$. Now, we can reverse the transformation in order to recover the original vector field $\mathbf{S}$ as a function of the "old" coordinates $\mathbf{x}$. For that, we apply the inverse change of variables (5): $\mathbf{S}^*(\mathbf{x};\varepsilon) = \mathbf{S}(\mathbf{X}(\mathbf{Y}(\mathbf{x};\varepsilon);\varepsilon);\varepsilon)$. If the transformation were exact, $\mathbf{S}^*(\mathbf{x};\varepsilon) \equiv \mathbf{S}(\mathbf{x};\varepsilon)$, but unfortunately it is not the usual case. Nevertheless, we know that $\mathbf{S}^* - \mathbf{S}$ has size ε^{M+1}.

Now, if we take $\mathbf{S}$ as the identity map, we arrive at an estimation of the global error $E(\mathbf{x};\varepsilon)$, yielding

$$E(\mathbf{x};\varepsilon) \;=\; \|\mathbf{X}(\mathbf{Y}(\mathbf{x};\varepsilon);\varepsilon) - \mathbf{x}\| = \mathcal{O}(\varepsilon^{M+1}),$$

on a time–scale $1/\varepsilon$, i.e. for $t \in [0, C/\varepsilon]$ and a certain $C > 0$, see for instance [1], as is predicted by the standard time–estimate provided by the near–identity transformations and averaging theory, see for instance [1]. From the construction of the Lie transformation the error will is an expression such that its main term is factored by ε^{M+1}, that is,

$$E(\mathbf{x};\varepsilon) \;=\; \varepsilon^{M+1}\, E_{M+1}(\mathbf{x};\varepsilon) + \mathcal{O}(\varepsilon^{M+2}).$$

Once the expression for $E_{M+1}(\mathbf{x};\varepsilon)$ is calculated we still need to determine also a range of validity for $\mathbf{x}$ such that E_{M+1} remains of order ε^{M+1}. As this cannot be ensured a priori, one needs to make the corresponding composition of changes for each particular situation, as we show in next section.

4 Applications

In this section we show the results given by the procedure explained in Section 3 to estimate the global error committed in three Lie transformations.

4.1 A stiff system in the plane

We consider the following two–dimensional problem:

$$\frac{d\,x_1}{d\,t} \;=\; -2\,x_1 + x_2 + \varepsilon\,(-2\,x_1^2 + x_2^2), \quad \frac{d\,x_2}{d\,t} \;=\; 998\,x_1 - 999\,x_2 + \varepsilon\,(x_1^2 + x_1\,x_2 + x_2^2),$$

with $x_1(0) = 1/2$, $x_2(0) = 3/5$ and $\varepsilon = 10^{-4}$. This system has been studied in reference [6]. There Theorem 2.1 is used to transform the initial differential equation into another one–dimensional system. (Note that since the equations are autonomous, a one–dimensional differential equation is integrable at least by quadratures.) Here we outline the transformation and give an estimation of the error. For details, see [6].

In order to apply Theorem 2.1 so as to reduce the initial system to an equivalent one, but with dimension one, we choose $\mathbf{T}(\mathbf{x}) = T\,\mathbf{x}$, where $T = \operatorname{diag}\{-1000, -1\}$. The

resulting system is:
$$\frac{d\,\mathbf{z}}{d\,t} = T\,\mathbf{z} + \varepsilon\,(z_1^{999/1000}\,z_2, 0)^t,$$
where $\mathbf{z} = (z_1, z_2)^t$ are the "new" variables.

The generator $\mathbf{W}(\mathbf{z}) = (W_1(\mathbf{z}), W_2(\mathbf{z}))^t$ of the Lie transformation is the following:
$$\begin{aligned} W_1(\mathbf{z}) &= -\tfrac{498001}{500}\,z_1^2 - 2000\,z_1\,z_2 - \tfrac{1}{998}\,z_2^2 + \tfrac{1}{1000}\,,z_1^{999/1000}\,z_2\log z_1,\\ W_2(\mathbf{z}) &= -\tfrac{995007}{1999}\,z_1^2 - \tfrac{2991}{1000}\,z_1\,z_2 - 3\,z_2^2. \end{aligned}$$
With this we can calculate the direct change of variables (4):
$$\begin{aligned} x_1 &= z_1 - \varepsilon\left(\tfrac{498001}{500}\,z_1^2 + 2000\,z_1\,z_2 + \tfrac{1}{998}\,z_2^2 - \tfrac{999}{1000}\,z_1^{999/1000}\,z_2\log z_1\right),\\ x_2 &= z_2 - \varepsilon\left(\tfrac{995007}{1999}\,z_1^2 + \tfrac{2991}{1000}\,z_1\,z_2 + 3\,z_2^2\right), \end{aligned}$$
as well as the inverse (5) one:
$$\begin{aligned} z_1 &= x_1 + \varepsilon\left(\tfrac{498001}{500}\,x_1^2 + 2000\,x_1\,x_2 + \tfrac{1}{998}\,x_2^2 - \tfrac{999}{1000}\,x_1^{999/1000}\,x_2\log x_1\right),\\ z_2 &= x_2 + \varepsilon\left(\tfrac{995007}{1999}\,x_1^2 + \tfrac{2991}{1000}\,x_1\,x_2 + 3\,x_2^2\right). \end{aligned}$$
If we take $\varepsilon = 10^{-4}$ and $\mathbf{z}$ satisfies that $\max\{|z_1|, |z_2|\} \le 1$, we have that $E(\mathbf{z}) \le 1.79177\times 10^{-8}$, which is an error of the order ε^2, as it should be, because the Lie transformation has been carried out up to first order.

4.2 Lorenz equation

Now we consider the Lorenz system which represents a three–dimensional differential equation. It is used to model the convection in the atmosphere of the Earth. In the context of generalized normal forms this problem has been studied in [6] and [7]. Here we make an outline of the methodology and the results, but we do not show the details or the calculations. For that aspect the reader is addressed to references [6, 7].

The equations of the system are the following:
$$\frac{d\,x_1}{d\,t} = 10\,(x_2 - x_1), \quad \frac{d\,x_2}{d\,t} = 28\,x_1 - x_2 - x_1\,x_3, \quad \frac{d\,x_3}{d\,t} = x_1\,x_2 - \frac{8}{3}\,x_3.$$
We intend to reduce the system in one dimension by means of the application of Theorem 2.1. For that, first of all we diagonalise the linear part and introduce a small parameter ε as follows: $\mathbf{x} = (x_1, x_2, x_3)^t \to \varepsilon\,\mathbf{y} = \varepsilon\,(y_1, y_2, y_3)^t$. Then, we choose $\mathbf{T} = T\,\mathbf{y}$ with $T = \operatorname{diag}\{1, \sqrt{2}, 0\}$. At this moment we apply Theorem 2.1 arriving at the following (two–dimensional) reduced system:
$$\begin{aligned} \frac{d\,z_1}{d\,t} &= -\tfrac{8}{3}\,z_1 + \varepsilon\,\tfrac{(-9+\sqrt{1201})}{56}\,z_3^2 - \varepsilon^3\,\tfrac{238268911748107+3427671328157\,\sqrt{1201}}{3389702400\left(32622739+543621\,\sqrt{1201}\right)}\,z_3^4,\\ \frac{d\,z_2}{d\,t} &= -\tfrac{11+\sqrt{1201}}{2}\,z_2 + \varepsilon^2\,\tfrac{3\left(1893759619-24165531\,\sqrt{1201}\right)}{10117320080\left(25+3\,\sqrt{1201}\right)}\,z_3^3,\\ \frac{d\,z_3}{d\,t} &= \tfrac{-11+\sqrt{1201}}{2}\,z_3 + \varepsilon^2\,\tfrac{15\left(1201-1689\,\sqrt{1201}\right)}{134512\left(25+3\,\sqrt{1201}\right)}\,z_3^3, \end{aligned}$$

where $\mathbf{z} = (z_1, z_2, z_3)^t$ are the "new" coordinates coming out from the Lie transformation. This asymptotic change of variables has been carried out up to third order. Now, if we choose $\varepsilon = 10^{-2}$ and $\|\mathbf{x}\| \le 0.1$, then the global error is $E(\mathbf{x}) \le 1.33969 \times 10^{-7}$, which is valid on a time–scale $t \approx 100$.

4.3 Rydberg atom

Finally we have chosen a problem from Physics. This is the Hydrogen atom in crossed electric and magnetic fields. In [9] we studied the transition state in reaction dynamics and particularized the results for this example. For achieving that, we calculated the normal form associated to the system. This is the reduction to the central manifold. Here we estimate the global error of this transformation. The details of the computation of the normal form and the subsequent determination of the normally hyperbolic invariant manifold, together with its stable and unstable manifolds, can be found in [9].

The problem is formulated as the following 3DOF Hamiltonian system:

$$\mathcal{H} \;=\; \tfrac{1}{2}\,(\hat{P}_1^2 + \hat{P}_2^2 + \hat{P}_3^2) - \tfrac{1}{\mathcal{R}} + \tfrac{1}{2}\,(\hat{x}_1\hat{P}_2 - \hat{x}_2\hat{P}_1) + \tfrac{1}{8}\,(\hat{x}_1^2 + \hat{x}_2^2) - \varepsilon\,\hat{x}_1 - \varepsilon^{1/2},$$

where $\mathcal{R} = ((\hat{x}_1 - x_s)^2 + \hat{x}_2^2 + \hat{x}_3^2)^{1/2}$ and $x_s = -\varepsilon^{-1/2}$, with ε a small parameter.

First of all we expand $\mathcal{H}$ in Taylor series up to polynomials of degree 8 in the form:

$$\mathcal{H}' = \mathcal{H} + 2\varepsilon^{\frac{1}{2}} = \sum_{n=2}^{8} \mathcal{H}_n,$$

where each $\mathcal{H}_n$ is a homogeneous polynomial in $(\hat{\mathbf{x}}, \hat{\mathbf{P}})$ of degree $n+2$. The normal form has been calculated up to order 6 in ε with the goal of determining the normally hyperbolic invariant manifolds of the origin.

We have estimated the global error of the transformation taking $\|(\hat{\mathbf{x}}, \hat{\mathbf{P}})\| \le 10^{-2}$ — which is enough for our computation concerning transition state theory — and $\varepsilon = 0.58$. In the table below we show the error when the transformation is carried out from order 1 to order 6:

order 1	$7.51681572767062 \times 10^{-7}$
order 2	$7.440374042482777 \times 10^{-9}$
order 3	$1.3601828348825097 \times 10^{-10}$
order 4	$2.2895973941086116 \times 10^{-12}$
order 5	$3.813254946932333 \times 10^{-14}$
order 6	$5.676373185504885 \times 10^{-16}$

Let us note that for the 6th order, each term of the composed series has around 13000 monomials, this is the reason why we omit the expressions here.

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