Another Estimate for A-Posteriori Validation of the Invariant Manifolds

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1 Linear Operator (Revisited)

The troubling estimate comes from the following Lemma:

Lemma 1 (Lemma 4.3 GS paper)**.** *The the linear operator $\mathfrak{L} : X_0 \to X_0$ defined by*

$$\mathfrak{L}(h) = Dh \circ \Lambda_s - Dg[P_N] \cdot h \tag{1}$$

is well defined and boundedly invertible as long as

$$N + 1 > \frac{C_1}{\mu}.$$

Supposing this is so, we have the bound

$$\|\mathfrak{L}^{-1}\|_{\mathcal{X}_0} \leq \frac{1}{(N+1)\mu - C_1}$$

The condition $N + 1 > C_1/\mu$ is essentially requiring us to take the order so high that there can be no possible resonance (as J.B. pointed out). I will call this an *a-priori condition* on the parameterization order, because it is something we have to check in order to begin the error analysis of the manifolds. The a-priori condition seems to be completely independent of the a-posteriori error ϵ_{tol}.

For the revised estimate I will assume that the vector field $g : \mathbb{R}^n \to \mathbb{R}^n$ is polynomial. Recall the setup of the proof of the lemma. We define

$$A(t) = Dg[P_N(e^{\Lambda t}\theta)]$$

$$\bar{p}(\theta, t) = \bar{p}(t) = p(e^{\Lambda t}\theta)$$

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and

$$C(\theta, t) = e^{-\int_0^t A(\theta,s)\ ds}$$

The critical estimate is the estimate of $C(t)$. In the GS paper we obtain an elementary bound of the form

$$\|C(t)\|_{M,\nu} \leq e^{C_1 t}$$

where C_1 is a bound on $Dg[P_N(\theta)]$ over the poly disk of radius ν. This is the estimate we will try to improve.

Suppose that g is an M-th order polynomial. Then the entries of Dg are $M-1$-th order polynomials. Since P_N is an N-th order polynomial, we have that $Dg \circ P_N$ is an $\bar{N} = N(M+1)$-th order polynomial. Then let's write

$$Dg[P_N(\theta)] = \sum_{0 \leq |\alpha| \leq \bar{N}} A_\alpha \theta^\alpha$$

where each coefficient A_α is an $n \times n$ matrix. In fact,

$$A_\alpha^{ij} = \left[\partial_j g_i(z)|_{z=P_N(\theta)}\right]_\alpha$$

where g_i is the i-th component of the vector field and $[\cdot]_\alpha$ is the α-th coefficient of the power series $[\cdot]$. We will use that this is a finite sum.

Using this notation we have that

$$\begin{aligned}
A(t) = -\int_0^t \sum_{0 \leq |\alpha| \leq \bar{N}} A_\alpha (e^{\Lambda s}\theta)^\alpha\ ds = -\int_0^t \sum_{0 \leq |\alpha| \leq \bar{N}} A_\alpha e^{<\Lambda,\alpha>s} \theta^\alpha\ ds \\
= -\int_0^t A_{(0,\dots,0)} + \sum_{1 \leq |\alpha| \leq \bar{N}} A_\alpha e^{<\Lambda,\alpha>s} \theta^\alpha\ ds \\
= -\int_0^t A_{(0,\dots,0)}\ ds - \int_0^t \sum_{1 \leq |\alpha| \leq \bar{N}} A_\alpha e^{<\Lambda,\alpha>s} \theta^\alpha\ ds \\
= -A_0 t - \sum_{1 \leq |\alpha| \leq \bar{N}} A_\alpha \theta^\alpha \int_0^t e^{<\Lambda,\alpha>s}\ ds \\
-A_0 t - \sum_{1 \leq |\alpha| \leq \bar{N}} \frac{A_\alpha}{|<\Lambda,\alpha>|} \left(1 - e^{<\Lambda,\alpha>t}\right) \theta^\alpha.
\end{aligned}$$

Note that the coefficients of Λ have negative real part, hence the reversal of the sign in the $e^{\cdot} - 1$ term and the absolute value in the denominator. Then

$$\begin{aligned}
|C(\theta,t)| \leq |e^{A(\theta,t)}| \\
= |\exp\left(-A_0 t - \sum_{1 \leq |\alpha| \leq \bar{N}} \frac{A_\alpha}{|<\Lambda,\alpha>|} \left(1 - e^{<\Lambda,\alpha>t}\right) \theta^\alpha\right)| \\
\leq e^{|A_0| t} \exp\left(\sum_{1 \leq |\alpha| \leq \bar{N}} \frac{|A_\alpha|}{|<\Lambda,\alpha>|} |\nu|^{|\alpha|}\right)
\end{aligned}$$

as $|1-e^{<\Lambda,\alpha>t}| \leq 1$ uniformly in α and t, due to the fact that Λ have negative real part. If we let C_3 be any number with

$$\exp\left(\sum_{1\leq|\alpha|\leq\bar{N}} \frac{|A_\alpha|}{|<\Lambda,\alpha>|}|\nu|^{|\alpha|}\right) \leq C_3$$

and C_1 be any number with

$$|A_0| \leq C_1$$

then we have

$$|C(\theta,t)| \leq C_3 e^{C_1 t}.$$

Then C_3 is a finite sum of known quantities, and can be computed numerically via interval arithmetic as long as there are no resonances up to order $\bar{N}$. Since we are using interval arithmetic the condition is self checking. To obtain C_1, note that A_0 is the leading coefficient of $Dg[P_N(\theta)]$, i.e.

$$A_0 = Dg[P_N(0)] = Dg(p).$$

Then C_1 is any bound on the differential of g at the equilibria. This is an improvement over the old C_1 which was a global bound on the differential. The cost is the introduction of C_3, which still carries the global information, but which appears in a less troublesome place. To see this, consider the estimate which concludes with Equation (74) in the GS paper. That estimate will now become

$$|\mathfrak{L}^{-1}[p](\theta)| \leq \frac{C_3}{(N+1)\mu - C_1}$$

where C_1 is more tractable than before. For example, in GS

$$A_0 = Dg(1,0,0,0) = \begin{pmatrix} 0 & 1 & 0 & 0 \\ L^2\lambda & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & L^2/\gamma & 0 \end{pmatrix}$$

so that

$$C_1 \leq \max(1, L^2\lambda, L^2/\gamma)$$

Then we will only have to insure that

$$N+1 > \frac{\max(1, L^2\lambda, L^2/\gamma)}{\mu}.$$

Preliminary experimentation with Gray Scott suggests that using the new estimate we can reduce the required order for N by a factor of a little more than 2. I'll start looking at how it effects the Hex system (where we really need improvements) as soon as possible.

Remark 2. *1. This still imposes an a-priori order condition on N. While the a-priori condition is better than before, I had hoped to eliminate it completely. The order condition could be completely eliminated if we could obtain a uniform bound on $C(t)$. Say something like*

$$|C(t)| \leq C_3.$$

Initially I thought I had something for this, but it did not work out.

2. *For Gray Scott the order condition*

$$N + 1 > \frac{\max(1, \lambda L^2, L^2/\gamma)}{\mu},$$

is disturbingly sensitive to L. This is counter-intuitive, as J.P has pointed out many times. We would like to think that as L is increased, the connecting orbit gets closer and closer to the equilibria, so that the problem becomes easier and easier.

Of course the "easiness" does appear in other places, like that we can take scaleEigs smaller and smaller when L is larger. This makes the other constants such as C_3, and ϵ_{tol} easier to control as we can take ρ smaller. But large L makes the a-priori condition for manifold validation worse and worse. Maybe this is because larger L increases the "speed" of the dynamics, making the local manifolds harder to control? It makes sense for the spectral radius of the differential to increase as L increases.

3. *It may be possible to obtain a slightly better estimate as follows. There exists a norm so that*

$$\|e^{-A_0 t}\|_1 \leq e^{-\tau t}$$

where τ is the modulus of the largest negative eigenvalue of $Dg(p)$. In terms of resonance conditions, this would lead to a truly minimal a-priori condition. But it's not clear to me right now how to compare the norm $\| \cdot \|_1$ with the ones we are using.

4. *So maybe some a-priori condition is necessary, as somehow we really do have to guarantee that there are no high order resonances hiding in the definition of h. Maybe this is why we cannot get around some kind of a-priori condition... Even using JPs inductive approach there would surly be some lower bound on the Parameterization order, as you have to take enough coefficients to detect the exponential decay. It's just that with the inductive method we don't know before hand how many is enough. Maybe enough is large enough to rule out any resonance, and we are right back to the same kind or a-priori condition... It's kind of a "small divisors" kind of condition, and maybe the best we can hope to do is minimize it?*

5. *Or... Maybe we could try to compute a bound of the form*

$$|C(t)| \leq C_3 e^{C_1 t}$$

directly, using an approach similar to JPs. And perhaps the two approaches converge to the same answer...