Fast numerical algorithms to compute invariant tori in Hamiltonian Systems

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Outline

1. Introduction: importance of invariant tori
2. Set up and invariance equations
3. Whiskered tori

Invariant torus

- Invariant torus of dimension ℓ = quasi-periodic solution with ℓ independent frequencies (primary and secondary, maximal and whiskered).
- Importance. Together with their connections organize the long term behavior of the system (celestial mechanics, chemistry, ...)
- Goal Develop numerical algorithms following the theoretical results of KAM Theorem without Action-Angle variables ([LGJV05],[FLS08]) and implement them numerically.

[LGJV05] R. de la Llave, A. González, A. Jorba and J. Villanueva. KAM theory without action-angle variables, *Nonlinearity*,18(2):855–895,2005.
[FLS09] E. Fontich, R. de la Llave and Y. Sire. Construction of invariant whiskered tori by a parameterization method. I. Maps and flows in finite dimensions. *J. Differential Equations*,246(8):3136–3213, 2009.
[HLS11] G. Huguet, R. de la Llave and Y. Sire. Computation of whiskered invariant tori and their associated manifolds: New fast algorithms. Accepted to *Discrete Contin. Dyn. Syst. – Ser. A*, 2011. Preprint at `arXiv:1004.5231`

The invariance equation

- Consider a map F exact symplectic defined on $(U \subset \mathbb{R}^d) \times \mathbb{T}^d$.
- Assume that $\omega \in \mathbb{R}^\ell$ is fixed and Diophantine, i.e. for some $\nu, \tau > 0$,

$$|\omega \cdot k - n|^{-1} \leq \nu |k|^\tau \, \forall \, k \in \mathbb{Z}^\ell - \{0\}, \; n \in \mathbb{Z}$$

- We seek for an embedding $K : \mathbb{T}^\ell \to \mathbb{R}^d \times \mathbb{T}^d$ that satisfies the invariance equation

$$F \circ K - K \circ T_\omega = 0$$

  where $T_\omega(\theta) = \theta + \omega$.
- The dynamics of F restricted on the invariant torus (range of K) is conjugated to a rigid rotation of frequency ω.

Whiskered tori

- The tangent space $T_{K(\theta)}\mathcal{M}$, where $\mathcal{M} = \mathbb{R}^{2d-\ell} \times \mathbb{T}^\ell$, has an invariant analytic splitting:

$$T_{K(\theta)}\mathcal{M} = \mathcal{E}^c_{K(\theta)} \oplus \mathcal{E}^s_{K(\theta)} \oplus \mathcal{E}^u_{K(\theta)} \tag{1}$$

such that, there exist $0 < \mu_1, \mu_2 < 1$, $\mu_3 > 1$ satisfying $\mu_1\mu_3 < 1$, $\mu_2\mu_3 < 1$ and $C > 0$ such that for all $n \geq 1$ and $\theta \in \mathbb{T}^\ell$

$$v \in \mathcal{E}^s_{K(\theta)} \Longleftrightarrow |(DF \circ K \circ T_\omega^{n-1}(\theta) \times \cdots \times DF \circ K(\theta))v| \leq C\mu_1^n |v|$$

$$v \in \mathcal{E}^u_{K(\theta)} \Longleftrightarrow |(DF^{-1} \circ K \circ T_\omega^{-(n-1)}(\theta) \times \cdots \times DF^{-1} \circ K(\theta))v| \leq C\mu_2^n |v|$$

$$v \in \mathcal{E}^c_{K(\theta)} \Longleftrightarrow |(DF \circ K \circ T_\omega^{n-1}(\theta) \times \cdots \times DF \circ K(\theta))v| \leq C\mu_3^n |v|$$

$$|(DF^{-1} \circ K \circ T_\omega^{-(n-1)}(\theta) \times \cdots \times DF^{-1} \circ K(\theta))v| \leq C\mu_3^n |v|$$

- Associate to this splitting the projections $\Pi^c_{K(\theta)}$, $\Pi^s_{K(\theta)}$ and $\Pi^u_{K(\theta)}$ over the invariant spaces $\mathcal{E}^c_{K(\theta)}$, $\mathcal{E}^s_{K(\theta)}$ and $\mathcal{E}^u_{K(\theta)}$, respectively, which are analytic with respect to θ.

- Consider the linearized equation for the Newton method

$$(DF \circ K)\Delta - \Delta \circ T_\omega = -E$$

- The linearized equation for the Newton method splits in three:

$$DF(K(\theta))\Delta^{c,s,u}(\theta) - \Delta^{c,s,u} \circ T_\omega(\theta) = -E^{c,s,u}(\theta) \qquad (2)$$

where $\Delta^{s,c,u}(\theta) = \Pi^{s,c,u}_{K(\theta)}\Delta(\theta)$ and $E^{s,c,u}(\theta) = \Pi^{s,c,u}_{K(\theta)}E(\theta)$

- We solve Δ^c using the automatic reducibility.
- For the hyperbolic spaces, we compute $\Delta^{s,u}$ iteratively:

$$\Delta^s(\theta) = \widetilde{E}^s \circ T_{-\omega}(\theta) + \sum_{k=1}^{\infty}(DF \circ K \circ T_{-\omega}(\theta) \cdots DF \circ K \circ T_{-k\omega}(\theta))(\widetilde{E}^s \circ T_{-(k+1)\omega}(\theta$$

$$\Delta^u(\theta) = -\sum_{k=0}^{\infty}(DF^{-1} \circ K(\theta) \cdots DF^{-1} \circ K \circ T_{k\omega}(\theta))(\widetilde{E}^u \circ T_{k\omega}(\theta))$$

- The contraction of the cocycles guarantees the uniform convergence of these series.

Algorithm for the whiskered invariant tori

Algorithm

Consider given F, ω, K_0 and an approximate solution K (resp. K, λ), perform the following operations:

A) *Compute the invariant splittings and the projections associated to the cocycle $Z(\theta) = DF \circ K(\theta)$ and ω.*

B) *Project the linearized equation to the hyperbolic space and obtain $\Delta^{s,u}$.*

C) *Project the linearized equation on the center subspace and use the Algorithm to obtain Δ^c and δ.*

D) *Set $K + \Delta^s + \Delta^u + \Delta^c \to K$ and $\lambda + \delta \to \lambda$*

Newton method for the projections

Algorithm (Computation of the projections by a Newton method)

Consider given F, K, ω and an approximate solution (Π^s, Π^{cu}). Perform the following calculations:

1. *Compute* $Z(\theta) = DF \circ K(\theta)$
2. (2.1) *Compute* $E^{cu}(\theta) = \Pi^{cu}(\theta + \omega) Z(\theta) \Pi^s(\theta)$
   (2.2) *Compute* $E^s(\theta) = \Pi^s(\theta + \omega) Z(\theta) \Pi^{cu}(\theta)$
3. (3.1) *Compute* $N_s(\theta) = \Pi^s(\theta + \omega) Z(\theta) \Pi^s(\theta)$
   (3.2) *Compute* $N_{cu}(\theta) = \Pi^{cu}(\theta + \omega) Z(\theta) \Pi^{cu}(\theta)$
4. (4.1) *Solve for* Δ^s_s *satisfying*

$$N_s(\theta)\Delta^s_s(\theta) - \Delta^s_s(\theta + \omega) N_{cu}(\theta) = E^s(\theta)$$

   (4.2) *Solve for* Δ^s_{cu} *satisfying*

$$N_{cu}(\theta)\Delta^s_{cu}(\theta) - \Delta^s_{cu}(\theta + \omega) N_s(\theta) = -E^{cu}(\theta)$$

Newton method for the projections

Algorithm

5. (5.1) *Compute* $\widetilde{\Pi}^s(\theta) = \Pi^s(\theta) + \Delta^s_s(\theta) + \Delta^s_{cu}(\theta)$.
   (5.2) *Compute the SVD decomposition of* $\widetilde{\Pi}^s(\theta)$: $\widetilde{\Pi}^s(\theta) = U(\theta)\Sigma(\theta)V^\top(\theta)$.
   (5.3) *Set the values in* $\Sigma(\theta)$ *equal to the closer integer (which will be either 0 or 1).*
   (5.4) *Recompute* $\bar{\Pi}^s(\theta) = U(\theta)\Sigma(\theta)V^\top(\theta)$.
6. *Set* $\bar{\Pi}^s \to \Pi^s$ *and* $\mathrm{Id} - \bar{\Pi}^s \to \Pi^{cu}$ *and iterate the procedure.*

Solutions of iterative cohomolgy equations

Algorithm (Solution of difference equations with non constant coefficient)

Given $A(\theta)$, $B(\theta)$ *such that* $\|A^{-1}(\theta)\| \cdot \|B(\theta)\| \leq \kappa < 1$, *and* $\eta(\theta)$ *perform the following operations:*

1. *Compute* $\Delta(\theta) = A^{-1}(\theta)\eta(\theta)$
2. *Compute*
   (2.1) $\tilde{\Delta}(\theta) = A^{-1}(\theta)\Delta(\theta+\omega)B(\theta) + \Delta(\theta)$
   (2.2) $\tilde{A}^{-1}(\theta) = A^{-1}(\theta)A^{-1}(\theta+\omega)$
   (2.3) $\tilde{B}(\theta) = B(\theta+\omega)B(\theta)$
3. *Set* $\tilde{\Delta} \to \Delta$
   $\tilde{A} \to A$
   $\tilde{B} \to B$
   $2\omega \to \omega$
4. *Iterate points* $2-3$

Algorithm (Solution of difference equations with non constant coeff ($1D$))

Given $A(\theta)$, $B(\theta)$ and $\eta(\theta)$. Perform the following instructions:

1. (1.1) *Compute* $L(\theta) = \log(A(\theta)) - \log(B(\theta))$
   (1.2) *Compute* $\overline{L} = \int_{\mathbb{T}^\ell} L$
2. *Solve for* L_C *satisfying*

$$L_C(\theta) - L_C \circ T_\omega(\theta) = L(\theta) - \overline{L}$$

   as well as having zero average.

3. (3.1) *Compute* $C(\theta) = \exp(L_C(\theta))$
   (3.2) *Compute* $\nu = \exp(\overline{L})$
4. *Compute* $\tilde{\eta}(\theta) = C(\theta + \omega)B^{-1}(\theta)\eta(\theta)$
5. *Solve for* W *satisfying*

$$\nu W(\theta) - W(\theta + \omega) = \tilde{\eta}(\theta)$$

6. *Set* $\Delta(\theta) = C^{-1}(\theta)W(\theta)$

Fast iteration of the cocycles

Given a function $M : \mathbb{T}^\ell \to GL(d, \mathbb{R})$ and a vector $\omega \in \mathbb{R}^\ell$, we consider the cocycle over the rotation T_ω associated to the matrix M. This is the function $\mathcal{M} : \mathbb{Z} \times \mathbb{T}^\ell \to GL(d, \mathbb{R})$ defined by

$$\mathcal{M}(n, \theta) = \begin{cases} M(\theta + (n-1)\omega) \cdots M(\theta) & n \geq 1 \\ \mathrm{Id} & n = 0 \\ M^{-1}(\theta + (n+1)\omega) \cdots M^{-1}(\theta) & n \leq 1 \end{cases} \tag{3}$$

Remark In our case $M(\theta) = DF(K(\theta))$

Algorithm

Given $M(\theta)$, compute

$$\widetilde{M}(\theta) = M(\theta + \omega) M(\theta). \tag{4}$$

Set $\widetilde{M} \to M$, $2\omega \to \omega$ and iterate the procedure.

Remark We can compute $\mathcal{M}(2^k, \theta)$ in k operations.

The QR method

Algorithm (Fast computation of cocycles with QR)

Given $M(\theta)$ and a QR decomposition of $M(\theta)$, $M(\theta) = Q(\theta)R(\theta)$, perform the following operations:

1. *Compute* $S(\theta) = R(\theta + \omega)Q(\theta)$
2. *Compute pointwise a QR decomposition of S,* $S(\theta) = \bar{Q}(\theta)\bar{R}(\theta)$.
3. *Compute* $\widetilde{Q}(\theta) = Q(\theta + \omega)\bar{Q}(\theta)$
   - 3.1 $\widetilde{R}(\theta) = \bar{R}(\theta)R(\theta + \omega)$
   - 3.2 $\widetilde{M}(\theta) = \widetilde{Q}(\theta)\widetilde{R}(\theta)$
4. *Set* $M \leftarrow \widetilde{M}$
   - 4.1 $R \leftarrow \widetilde{R}$
   - 4.2 $Q \leftarrow \widetilde{Q}$
   - 4.3 $2\omega \leftarrow \omega$

and iterate the procedure.

Straddle the saddle

Consider a change of coordinates Q so that the cocycle

$$\tilde{M}(\theta) = Q(\theta + \omega)^{-1} M(\theta) Q(\theta)$$

is close to a constant.

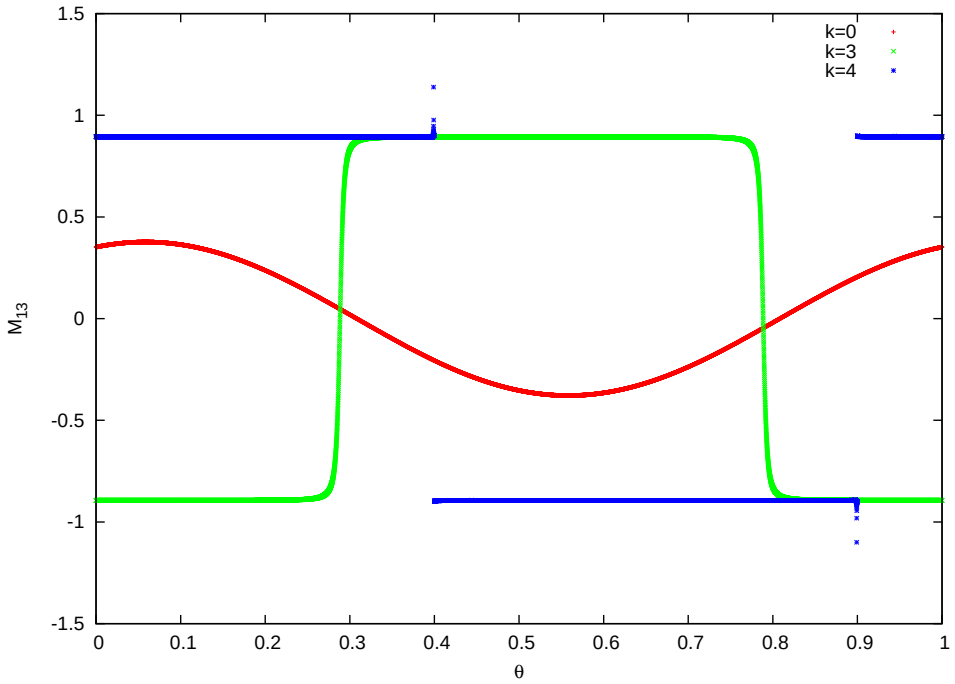

Figure: The straddle the saddle phenomenon. We plot one of the components of the cocycle $\mathcal{M}(2^k, \theta)$ for the values $k = 0, 3, 4$. The case $k = 0$ was scaled by a factor 200.

- Consider we have computed $\mathcal{M}(2^k, \theta)$.
- Compute the QR decomposition of the cocycle $\mathcal{M}(2^k, \theta)$.
- Pick the column of Q ($m(\theta)$) associated to the largest value in the diagonal of R.
- Shift it by an angle $-2^k\omega$.
- We have $M(\theta)m(\theta) = \lambda_{max}(\theta)m(\theta + \omega)$
- Therefore, $\lambda_{max}(\theta) = ([M(\theta)m(\theta)]^T[M(\theta)m(\theta)])^{1/2}$

Primary KAM tori for the Froeschlé Map

4D exact symplectic map defined on the 2-cylinder $\mathbb{R}^2 \times \mathbb{T}^2$.

$$
\begin{aligned}
\bar{p}_1 &= p_1 + \epsilon\left(\frac{\lambda_1}{2\pi}\sin(2\pi q_1) + \frac{\lambda_{12}}{2\pi}\sin(2\pi(q_1+q_2))\right) \\
\bar{p}_2 &= p_2 + \epsilon\left(\frac{\lambda_2}{2\pi}\sin(2\pi q_2) + \frac{\lambda_{12}}{2\pi}\sin(2\pi(q_1+q_2))\right) \\
\bar{q}_1 &= q_1 + \bar{p}_1 \qquad (\mathrm{mod}\ 1) \\
\bar{q}_2 &= q_2 + \bar{p}_2 \qquad (\mathrm{mod}\ 1)
\end{aligned}
$$

Remark: If $\lambda_{12} = 0$, the system consists of two uncoupled standard maps.

Hyperbolic invariant tori of the Froeschlé Map

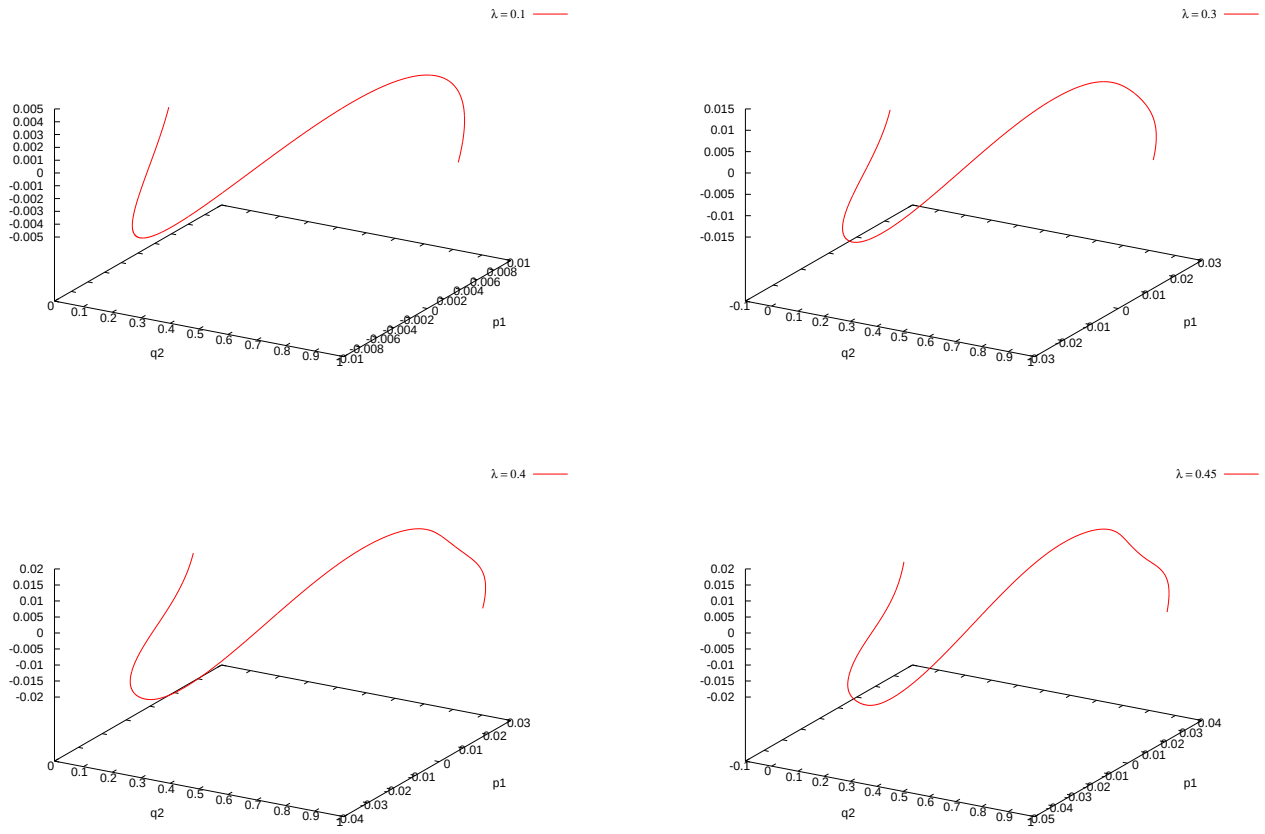

Figure: The $q_1 q_2 p_1$ projection of the primary hyperbolic invariant tori of the Froeschlé map of frequency ω_g for $\lambda_{12} = 0.1, 0.3, 0.4, 0.45$ and $\lambda_2 = 0.5, \lambda_1 = 0.01, \epsilon = 1$. We have used $N = 2^{11}$ Fourier modes.