Penalizing loops that deviate from the True Path.

Evangelos Siminos*

School of Physics

Georgia Institute of Technology,

Atlanta, GA 30332-0430, U.S.A

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Abstract

A variational method for periodic orbits searches in a general flow is developed. The method is based on penalizing the misorientation of the tangent vector of a guess-loop to the velocity field of the given flow. The loop is continuously evolved into a periodic orbit by a fictitious time flow.

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*Electronic address: gtg083n@mail.gatech.edu

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CHAOS, AND WHAT TO DO ABOUT IT

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I. INTRODUCTION

The goal of this project is to improve the variational method for finding periodic orbits introduced in refs. [1, 2]. The method evolves an initial guess in the form of a closed loop towards a true periodic orbit of a given flow $f^t(x)$ defined by:

$$\frac{dx}{dt} = v(x), \; x \in \mathbb{R}^d \,. \tag{1}$$

Given a loop parameterized by a parameter s, this is achieved by minimizing the misorientation of the tangent vector $\tilde{v}(x) = dx/ds$ of the loop to the velocity vector (1). In other words minimizing the cost functional

$$\overline{F}^2 = \frac{1}{S} \oint \left(\tilde{v}(x) - \lambda(x)\, v(x)\right)^2 \, ds \,, \tag{2}$$

where the integration is performed along the loop, $\lambda(x)$ an auxiliary undetermined function which compensates for the fact that not only the direction, but also the magnitude of the two fields is different at a point, and S is a normalization factor.

The improvement that will be pursued here is to replace the simple Euclidean metric δ_{ij} that is used in (2) with a metric $g_{ij}(x)$ that would carry information about the flow, that is minimize the functional

$$\overline{F}^2 = \frac{1}{S} \oint \left(\tilde{v} - \lambda v\right)_i \, g_{ij} \, \left(\tilde{v} - \lambda v\right)_j \, ds \,. \tag{3}$$

II. VARIATIONAL SEARCHES FOR PERIODIC ORBITS

In this project any smooth, closed curve in a $d-$dimensional space is referred to as a loop. In general a loop is not a solution of (1), in contrast to a periodic orbit, which satisfies the periodic orbit condition $f^T(x) = x$, where T the period. The tangent vector of the loop $\tilde{v}$ will not in general be parallel to $\hat{v}$. Thus, if we could continously deform the loop in such a way that its tangent becomes parallel to the velocity field we would end up with a true periodic orbit. In ref. [2] it is shown that this corresponds to minimizing (2) and that one can write down a partial differential equation (PDE) for the evolution of the loop towards a periodic orbit[4]. Numerically solving this PDE provides the periodic orbit of the system "closest"[5] to the initial loop.

The method is conceptually more complicated, harder to program and generally slower than Newton or multiple-shooting methods for the search of periodic orbits. On the other hand it has an advantage when one tries to find long or extremely unstable periodic orbits, or when one deals with hard to visualize high-dimensional systems. For multiple-shooting to converge one needs a large number of Poincaré sections in order to control local instability. Thus one needs a great deal of information about the qualitative dynamics of the flow to make a clever choice of those sections. In high-dimensional flows this information is usually not available and multiple shooting methods can easily fail to find the longer cycles. In the variational method described here Poincaré sections play no role and guesses with roughly the correct topology can lead to long cycles.

The extension of the method that will be attempted here is to use a metric that penalizes variations from a true periodic orbit in the unstable eigendirections of the flow more than it does in the stable ones. The hope is that in a high-dimensional flow in which only a few of the these eigendirections are significant, so one can concentrate only on them, effectively reducing the dimensionality of the problem and the computational load.

III. CANDIDATES FOR THE ROLE OF METRIC

A. A Jacobian Matrix for a Loop

The Jacobian matrix $\mathbf{J}^t(x_o)$ describes the deformation of the neighborhood of a point x_o under a flow f^t, in the linear approximation. It can be defined by means of the time-ordered product

$$\begin{aligned}\mathbf{J}^t(x_o) &\equiv \mathbf{T}e^{\int_0^t d\tau \mathbf{A}(f^\tau(x_o))} \\ &\equiv \lim_{m\to\infty} \prod_{n=m}^{1} e^{\Delta t\, \mathbf{A}\left(f^{n\Delta t}(x_o)\right)}\,,\end{aligned} \tag{4}$$

where $\Delta t = t/m$ and $\mathbf{A}$ the matrix of variations defined by

$$A_{ij}(x) = \frac{\partial v_i}{\partial x_j}\,. \tag{5}$$

Along a periodic orbit

$$\mathbf{J}_p \equiv \mathbf{J}^{T_p}(x_o) = \mathbf{T}e^{\oint d\tau \mathbf{A}(f^\tau(x_o))} \,. \tag{6}$$

$\mathbf{J}_p$ describes the local deformation of the neighborhood of the periodic orbit under the flow, for finite times, while its eigenvalues are known to be independent of the initial point x_o on the periodic orbit and provide the local measure of instability of the system.

Thus we would like to use $\mathbf{J}$ as our metric tensor. Yet, a loop is not a solution of the equations of the flow and we cannot calculate the Jacobian along it. Inspired by the time-ordered product (4) though, we define the matrix

$$\begin{aligned} \mathbf{J}_L(x_o) &\equiv \mathbf{T}e^{\oint ds \mathbf{A}(x(s)))} \\ &\equiv \lim_{m\to\infty} \prod_{n=m}^{1} e^{\Delta s\, \mathbf{A}(x(n\,\Delta s))} \,, \end{aligned} \tag{7}$$

where $s \in [s_i, s_f]$ parameterizes the loop and $\Delta s = (s_f - s_i)/m$ and $\mathbf{T}$ now reminds us that the integration is ordered with respect to s. We call this matrix a Jacobian for the loop and try to figure out if it could play the role of a metric for the variational method by capturing the essential information about the flow.

Obviously $\mathbf{J}_L$ is a solution of the diferential equation

$$\frac{\mathbf{J}_L^s}{ds} = \mathbf{A}(x(s))\mathbf{J}_L^s. \tag{8}$$

B. Properties of $\mathbf{J}_L$

First we prove that $\mathbf{J}_L$ has the property of $\mathbf{J}_p$ that its eigenvalues do not depend on the initial point on the loop. Definition (7) establishes the group property

$$\mathbf{J}_L^{s+s'}(x_o) = \mathbf{J}_L^{s'}(x(s))\mathbf{J}_L^s(x_o) \,. \tag{9}$$

This is important since it is all we need to prove that the eigenvalues of $\mathbf{J_L}$ do not depend on the initial point x_o on the loop, in exactly the same way this is proved for $\mathbf{J}$ on a cycle, *cf.* Ref. [3], Paragraph 8.2.

We would also like to proove that the eigenvalues of $\mathbf{J}_L$ are invariant under a change of variables, $y = h(x)$. For notational simplicity we temporarilly drop the index L in $\mathbf{J}_L$. Let $\mathbf{K}^s(y_o)$ denote the Jacobian for the loop in the new variables, with $y_o = h(x_o)$. Then, according to the definition of the Jacobian on a loop

$$\frac{\mathbf{K}^s}{ds} = \frac{\partial u}{\partial y}\mathbf{K}^s \, , \tag{10}$$

where

$$\begin{aligned} u_i &= \frac{dy_i}{dt} \\ &= \frac{\partial h_i}{\partial x_j} v_j \, . \end{aligned} \tag{11}$$

For notational compactness we define the matrix

$$H_{ij} = \frac{\partial h_i}{\partial x_j} \, . \tag{12}$$

Then, for the matrix elements of $\partial u/\partial y$ we have

$$\begin{aligned} \frac{\partial u_i}{\partial y_j} &= \frac{\partial u_i}{\partial x_k}\frac{\partial x_k}{\partial y_j} \\ &= \frac{\partial}{\partial x_k}\left(H_{im} v_m\right)\frac{\partial x_k}{\partial y_j} \\ &= \left(\frac{\partial H_{im}}{\partial x_k} v_m + H_{im} A_{mk}\right) H^{-1}_{kj} \, , \end{aligned} \tag{13}$$

where $H^{-1}_{ij} = \partial h^{-1}_i/\partial y_j$.

To relate the eigenvalues of $\mathbf{J}$ and $\mathbf{K}$ we form the matrix

$$\mathbf{N}^s \equiv \mathbf{K}^s(y_o) - \mathbf{H}(x(s))\mathbf{J}^s(x_o)\mathbf{H}^{-1}(x_o) \, , \tag{14}$$

Differentiating with respect to s,

$$\frac{dN^s_{ij}}{ds} = \frac{dK^s_{ij}}{ds} - \frac{dH_{im}}{ds} J^s_{mk} H^{-1}_{kj} - H_{im}\frac{dJ^s_{mk}}{ds} H^{-1}_{kj} \, , \tag{15}$$

or, using (8) and (10),

$$\frac{dN^s_{ij}}{ds} = \frac{\partial u_i}{\partial y_m} K^s_{mj} - \frac{\partial H_{im}}{\partial x_n}\frac{dx_n}{ds} J_{mk} H^{-1}_{kj} - H_{im} A_{mn} J^s_{nk} H^{-1}_{kj} \, . \tag{16}$$

With the use of (13) and renaming of the dummy indices $n \leftrightarrow m$ in the last term, this reads

$$\frac{dN^s_{ij}}{ds} = \left(\frac{\partial H_{in}}{\partial x_k} v_n + H_{in} A_{nk}\right) H^{-1}_{km}(x(s)) K^s_{mj} - \left(\frac{\partial H_{im}}{\partial x_n}\frac{dx_n}{ds} + H_{in} A_{nm}\right) J^s_{mk} H^{-1}_{kj}(x_o) \, . \tag{17}$$

Inserting the identity matrix $\mathbf{1} = \mathbf{H}^{-1}(x(s))\mathbf{H}(x(s))$ in the second term and noting that

$$\frac{\partial H_{in}}{\partial x_k} = \frac{\partial^2 h_i}{\partial x_k \partial x_n} = \frac{\partial H_{ik}}{\partial x_n}\,, \tag{18}$$

we get

$$\frac{dN^s_{ij}}{ds} = \left(\frac{\partial H_{ik}}{\partial x_n} v_n + H_{in}A_{nk}\right) H^{-1}_{km}(x(s))K^s_{mj} - \left(\frac{\partial H_{im}}{\partial x_n}\frac{dx_n}{ds} + H_{in}A_{nm}\right) H^{-1}_{mq} H_{ql} J^s_{lk} H^{-1}_{kj}(x_o)\,. \tag{19}$$

Were it not $\frac{dx}{ds} \neq v$ this could be factored to get $dN^s_{ij}/ds = (\ldots)_{ik} N^s_{kj}$. This would allow us to complete the proof. The proof is valid only if we are computing the Jacobian on a periodic orbit and its remaining part is given in Appendix A.

The Jacobian is not in general a symmetric matrix and thus it is not diagonalizable by a unitary similarity transformation, while its eigenvectors do not form an orthonormal set. Therefore we use the metric

$$\mathbf{M}(x) = \mathbf{J}^T_L(x)\mathbf{J}_L(x)\,, \tag{20}$$

where the superscript T denotes the transpose of a matrix. $\mathbf{M}$ is symmetric and thus diagonalizable by a unitary similarity transformation and possesses a complete set of orthogonal eigenvectors.

C. The variational method

With this choice of metric we consider minimizing the functional

$$\overline{F}^2 = \frac{1}{S}\oint \left(\mathbf{J}_L\,\mathbf{P}\tilde{v}\right)^T \left(\mathbf{J}_L\,\mathbf{P}\tilde{v}\right)\, ds\,, \tag{21}$$

where

$$P_{ij} = \delta_{ij} - \frac{v_i v_j}{v^2} \tag{22}$$

The operator $v_i v_j / v^2$ acting on a vector projects it to the direction parallel to the velocity and thus $\mathbf{P}$ projects a vector on the plane transverse to v. The motivation to act with $\mathbf{P}$ on $\tilde{v}$ is that we are interested in penalizing components of v transverse to the direction of the velocity. We observe that (21) will have the minimum value of zero on a periodic orbit.

$\mathbf{P}$ is obviously symmetric and thus, from (21),

$$\overline{F}^2 = \frac{1}{S}\oint \tilde{v}^T\mathbf{P}\,\mathbf{J}^T_L\mathbf{J}_L\,\mathbf{P}\tilde{v}\, ds\,. \tag{23}$$

D. The Euclidean metric case

As a first step we will try to implement the variational principle in this form with an Euclidean metric and then switch to $\mathbf{g} = \mathbf{J}^T\mathbf{J}$. Thus, we work with the cost functional

$$\overline{F}^2 = \frac{1}{S}\oint (\mathbf{P}\tilde{v})^2 \, ds \,. \tag{24}$$

For a variational method to work this functional has to be minimized monotonically towards zero, while the loop evolves towards a periodic orbit. Thus we need to write a differential equation for the evolution of each point $\tilde{x}(s)$ of the loop. We can think of such an equation as defining a flow in loop space with a parameter τ playing the role of the time variable and thus refered to as *fictitious time*. Therefore each point on the loop will be a function of two variables s and τ. Diferentiating (24) with respect to fictitious time (remember that $\mathbf{P}$ symmetric)

$$\frac{d\overline{F}^2}{d\tau} = \frac{2}{S}\oint (\mathbf{P}\tilde{v})^T \frac{\partial}{\partial\tau}(\mathbf{P}\tilde{v}) \, ds \,. \tag{25}$$

Since there is no principle associated with the fictitious time flow other than the requirement to minimize (24), we are free to define this flow at our convinience. We observe that the simple choice

$$\frac{\partial}{\partial\tau}(\mathbf{P}\tilde{v}) = -(\mathbf{P}\tilde{v}) \,, \tag{26}$$

when substituted in (25) yields

$$\frac{d\overline{F}^2(\tau)}{d\tau} = -\overline{F}^2(\tau) \,, \tag{27}$$

and thus

$$\overline{F}^2(\tau) = \overline{F}^2(0)e^{-\tau} \,. \tag{28}$$

The functional evolves exponentially to zero, as desired.

To get a differential equation for the evolution of the loop under the fictitious time flow, we simply perform the differentiations in (26) explicitly. We have (we use the summation convention of repeated indices)

$$\begin{aligned}
\frac{\partial P_{ij}}{\partial\tau} &= \frac{\partial P_{ij}}{\partial\tilde{x}_k}\frac{\partial\tilde{x}_k}{\partial\tau} \\
&= -\frac{\partial}{\partial\tilde{x}_k}\left(\frac{v_i v_j}{v^2}\right)\frac{\partial\tilde{x}_k}{\partial\tau} \\
&= -\left(A_{ik}\frac{v_j}{v^2} + \frac{v_i}{v^2}A_{jk} - \frac{2\,v_i v_j v_m}{v^4}A_{mk}\right)\frac{\partial\tilde{x}_k}{\partial\tau} \,,
\end{aligned} \tag{29}$$

and thus

$$
\begin{aligned}
\frac{\partial P_{ij}}{\partial \tau}\tilde{v}_j &= -\left(\frac{v_j\tilde{v}_j}{v^2}A_{ik} + \frac{v_i\tilde{v}_j}{v^2}A_{jk} - \frac{2\,v_iv_j\tilde{v}_jv_m}{v^4}A_{mk}\right)\frac{\partial \tilde{x}_k}{\partial \tau} \\
&= -\frac{1}{v^2}\left(v_j\tilde{v}_j\left(\delta_{im} - \frac{v_iv_m}{v^2}\right)A_{mk} + v_i\tilde{v}_j\left(\delta_{jm} - \frac{v_jv_m}{v^2}\right)A_{mk}\right)\frac{\partial \tilde{x}_k}{\partial \tau}\,, \qquad (30)
\end{aligned}
$$

or

$$
\frac{\partial \mathbf{P}}{\partial \tau}\tilde{v} = -\frac{1}{v^2}\left(v.\tilde{v}\,\mathbf{1} + v\otimes\tilde{v}\right)\mathbf{PA}\frac{\partial \tilde{x}}{\partial \tau}\,, \qquad (31)
$$

where $a \otimes b$ denotes the tensor product of vectors a and b.

On the other hand

$$
\mathbf{P}\frac{\partial \tilde{v}}{\partial \tau} = \mathbf{P}\frac{\partial^2 \tilde{x}}{\partial \tau \partial s}\,. \qquad (32)
$$

Gathering everything together in (26) we get

$$
\left(\frac{1}{v^2}\left(v.\tilde{v}\,\mathbf{1} + v\otimes\tilde{v}\right)\mathbf{PA} - \mathbf{P}\frac{\partial}{\partial s}\right)\frac{\partial \tilde{x}}{\partial \tau} = \mathbf{P}\tilde{v}\,. \qquad (33)
$$

This is the PDE that governs the evolution of a loop towards a periodic orbit.

APPENDIX A: EIGENVALUES OF $\mathbf{J}_p$ UNDER SMOOTH CONJUGACIES

From (19) with $s = t$, that is when calculating $\mathbf{N}^t(x_o)$ along a peridic orbit we get

$$
\begin{aligned}
\frac{dN^t_{ij}}{dt} &= \left(\frac{\partial H_{im}}{\partial x_n}v_n + H_{in}A_{nm}\right)H^{-1}_{mq}(x(t))K^t_{qj} - \left(\frac{\partial H_{im}}{\partial x_n}v_n + H_{in}A_{nm}\right)H^{-1}_{mq}(x(t))H_{ql}(x(t))J^t_{lk}H^{-1}_{kj}(x_o) \\
&= \left(\frac{\partial H_{im}}{\partial x_n}v_n + H_{in}A_{nm}\right)H^{-1}_{mq}(x(t))\left(K^t_{qj} - H_{ql}(x(t))J^t_{lk}H^{-1}_{kj}(x_o)\right) \\
&= \left(\frac{\partial H_{im}}{\partial x_n}v_n + H_{in}A_{nm}\right)H^{-1}_{mq}(x(t))N_{qj}\,, \qquad (\mathrm{A1})
\end{aligned}
$$

from the definition (14) of $\mathbf{N}^s$. Thus we have a differential equation of the form $d\mathbf{N}^t/dt = \mathbf{B}(t)\mathbf{N}^t$ where $B_{ij} = \left(\frac{\partial H_{im}}{\partial x_n}v_n + H_{in}A_{nm}\right)H^{-1}_{mj}(x(t))$. The initial condition is found from (14) to be $\mathbf{N}^0 = 0$ and thus the solution will be $\mathbf{N}^t \equiv 0$ for all times. Thus

$$
\mathbf{K}^t(y_o) = \mathbf{H}(x(t))\mathbf{J}^t\mathbf{H}^{-1}(x_o)\,. \qquad (\mathrm{A2})
$$

On a periodic orbit for t equal to the period T_p we have $x(T_p) = x_o$ and thus

$$
\mathbf{K}_p(y_o) = \mathbf{H}(x_o)\mathbf{J}_p\mathbf{H}(x_o)\,, \qquad (\mathrm{A3})
$$

which means that $\mathbf{K}$ and $\mathbf{J}$ are related by a similarity transformation and thus have the same eignevalues.

APPENDIX B: PROJECT PLAN

Tentative schedule:

1. **Tue Apr 19:** Implement variational principle for Rössler and/or KS.
2. **Tue Apr 26:** Fix the last few quirks ...
3. **Tue May 2:** Project deadline

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[1] Y. Lan and P. Cvitanović, Phys. Rev. E **69**, 16217 (2004).

[2] P. Cvitanović and Y. Lan, in *Proceedings of 10th International Workshop on Multiparticle Production: Correlations and Fluctuations in QCD*, edited by N. Antoniou (World Scientific, Singapore, 2003).

[3] P. Cvitanović, R. Artuso, R. Mainieri, G. Tanner, and G. Vattay, *Chaos: Classical and Quantum* (ChaosBook.org, Niels Bohr Institute, Copenhagen, 2004).

[4] As the form of the equation depends on the parameterization of the loop and the question of the most adequate parameterization will be addressed in this project, I prefer not to present this PDE here.

[5] Distance in the space of loops is hard to define. In practice the method converges to a loop with topology "similar" to the initial guess.