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COMPUTING UNSTABLE 2-MANIFOLDS IN 3-DIMENSIONAL PHASE SPACE BY COMPUTING A VOLUME CURVATURE

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This is to certify that I have examined this copy of a technical report by

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and found that it is complete and satisfactory in all respects, and that any and all revisions required by the examining committee have been made.

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Abstract. We develop a numerical method for computing a two dimensional unstable manifold defined in a 3-dimensional "phase space". The method relies on the calculation of a volume formed by a local linear approximation and a local quadratic approximation. We consider mappings on 3-dimensional phase space that preserve volumes under iterations. Approximating these volumes is a natural way of measuring the curvature of a 2-manifold. This calculated volume provides an efficient means of imposing a threshold criteria for refining a manifold; the measure of this volume makes the calculation of curvatures more feasible than approximating curvatures that depend on the direct use of derivatives, especially near cusps and corners. We start by first deriving a method for a 1-manifold embedded in 2-dimensional phase space with an area-preserving map, then apply our findings to the Hénon map. Then we discuss a way to extend this method to 2-manifolds in 3-dimensional phase space.

1. Introduction

Many methods exist for calculating stable or unstable manifolds formed by continuous vector fields in one and two dimensions (e.g. the Lorenz system) ([2], [3]). We present a method for calculating and refining stable or unstable manifolds for a discrete-time system inspired by Henderson's method of computing fat trajectories (Henderson).

Typically when calculating the stable and unstable manifolds of a (discrete) dynamical system defined over a phase space the spacing between points becomes larger with increasing number of iterates of a map. One way to fill in these gaps is to measure the Euclidean distance between points and fill in the gap with a point halfway (depending on the metric used) once the distance gets beyond some threshold, thereby gaining a slightly more resolved manifold. This method can quickly become computationally expensive with higher and higher iterates of a map. One has to keep track of a possibly exponential growth in the number of points for every iterate.

We have developed numerical algorithms that calculate the local curvature of a 1-manifold (2-manifold) based only on a sufficient neighborhood to some points. This method calculates a second order interpolating polynomial local to a few points, measures the area (volume) formed between it and a linear interpolating polynomial defined by the points local to said region, and measures the area (volume) in between (see Figure 1 for the 1-dimensional version, the two dimensional version is similar). If this area (volume) is larger than some threshold we use this quadratic interpolating

polynomial to place a point(s) carefully chosen to minimize the area (volume) of the newly formed quadratic-linear-area (-volume).

2. 1-Dimensional Model

2.1. **Introduction.** The methods developed below were considered in order to refine homoclinic tangles ([1]), though it may be applied to more general circumstances. Therefore, we consider points near the vicinity of a *hyperbolic fixed-point*(see [4] for discussion of related terms); these are points such that $(x_0, y_0) = f(x_0, y_0)$ (for a map f) and the linearization near this point contains two eigenvectors with real eigenvalues, whose magnitudes lie in the domains $|\lambda_1| \in (0, 1)$ and $|\lambda_2| \in (1, \infty)$ respectively.

One often wishes to study these unstable 1-manifolds. These 1-manifolds originate near the vicinity of a hyperbolic fixed-point. To get a good idea of how one would proceed in generating these manifolds we begin, computationally, by placing a point arbitrarily close to the fixed point in the direction of the eigenvector with eigenvalue whose magnitude is greater than 1 - this way we know that f will generate an expansion (the mappings of points in the direction of the eigenvector with eigenvalue whose magnitude is in the domain $(0, 1)$ will contract). We map this point forward, creating two points in space along the eigenvector, the original point and its forward iterate. We call the line-segment between these two points the *fundamental segment*.

Here, one may fill the fundamental segment with a great number of points and map all of them forward a number of times, thereby generating a large set of points that approximate a 1-dimensional curve. This unstable manifold, then, is the topic of much interest.

It becomes computationally expensive to generate a well-resolved manifold at higher and higher iterates using this brute-force method. We have developed a method where one may start with a small number of points and refine as curvatures become "too large". This creates a computationally cheaper alternative to brute-force methods. It also frees up memory in that we no longer need to keep track of as many points.

2.2. **Assumptions.** We consider maps of the form $f : \mathbb{R}^2 \to \mathbb{R}^2$, in other words, a continuous parametrization that also has a continuous inverse, both of which are differentiable at least once. These functions have the following form:

$$(x', y') = f(x, y). \tag{1}$$

2.3. **Setup.** In order to refine a manifold we first consider a parametrization $x = x(s)$ and $y = y(s)$ separately. We begin by considering only $x = x(s)$. All discussions will carry over to $y = y(s)$.

Consider a parabola in $(s, x(s))$-space (see Figure 1). Consider, also, a line that goes through the parabola at two points with s-values s_1 and s_2 with slope m_x. If we consider the difference between the parabola and the secant line just defined we will form a new parabola with roots s_1 and s_2. One more piece remains to be determined in order to define the parabola, and that is to determine the curvature c_x at the vertex. Thus, we have a parametric representation of the quadratic approximation that takes the following form:

$$x(s) = x_1 + (s - s_1)m_x + (s - s_1)(s - s_2)c_x, \tag{2}$$

$$y(s) = y_1 + (s - s_1)m_y + (s - s_1)(s - s_2)c_y. \tag{3}$$

2.4. **Area Calculation.** We need to calculate the area formed by the region between the quadratic approximation in $\mathbb{R}^2$ and the secant line that goes through a pair of points on either side of the vertices. To do this, we need to calculate the following area integral defined in terms of differential forms (see [5] for a detailed discussion of differential forms):

$$\text{Area} = \int_A dx \wedge dy, \tag{4}$$

where A is the region bounded by the parabola and the secant line. Since the domain A is a compact region by construction, we use Stokes' theorem to reduce the above into the following:

$$\text{Area} = \int_A dx \wedge dy \equiv \int_A d\omega = \oint_C \omega, \tag{5}$$

where C is the directed boundary of A. Note that in the above calculation, we may end up with a positive or negative number for the area, depending on the chosen orientation. Computationally, we will only need the absolute value of the above quantity.

We have some freedom in selecting a differential 1-form ω such that $d\omega = dx \wedge dy$. To make calculations easier we choose ω in such a way that the integral along the linear segment vanishes. Consider a vector $\boldsymbol{V}$ tangent to any point on the linear segment of C. A 1-form that sends $\boldsymbol{V}$ to 0

may be defined as follows:

$$\omega = -\frac{(y-y_1)}{2}dx + \frac{(x-x_1)}{2}dy \tag{6}$$

so that for a tangent vector $\boldsymbol{V} = (x - x_1, y - y_1)$, $\forall\,(x, y) \in C_1$ (see Figure 1) we have that

$$\begin{aligned}
\omega(\boldsymbol{V}) &= \frac{1}{2}\left(-(y-y_1)dx + (x-x_1)dy\right)\boldsymbol{V} \\
&= \frac{1}{2}\left(-(y-y_1)dx(\boldsymbol{V}) + (x-x_1)dy(\boldsymbol{V})\right) \\
&= \frac{1}{2}\left(-(y-y_1)(x-x_1) - (x-x_1)(y-y_1)\right) \\
&= 0.
\end{aligned}$$

One may interpret the above as taking the inner-product of two vectors, one tangent to C_1, and one orthogonal to C_1, since $dx(\boldsymbol{V})$ gives the component of $\boldsymbol{V}$ in the x-direction. When we operate d on the above form we find that

$$\begin{aligned}
d\omega &= \frac{1}{2}d\left(-(y-y_1)dx + (x-x_1)dy\right) \\
&= \frac{1}{2}(-dy \wedge dx + dx \wedge dy) \\
&= \frac{1}{2}(2dx \wedge dy) \\
&= dx \wedge dy,
\end{aligned}$$

as expected.

In this way, we have further reduced a double integral into a single integral along the quadratic arc only:

$$\text{Area} = \int_{C_2} \omega = \frac{1}{2}\int_{C_2} (x-x_1)dy - (y-y_1)dx. \tag{7}$$

From equations (2) and (3), we calculate the expression for the pullback of the above form into parameter space, which can be thought of as a substitution of parametric equations for x and y in terms of s alone:

$$\begin{aligned}
\text{Area} = \int_{s_1}^{s_2} \{&[(s-s_1)m_x + (s-s_1)(s-s_2)c_x]\,[m_x + 2(s-\bar{s})c_x] \\
&- [(s-s_1)m_y + (s-s_1)(s-s_2)c_y]\,[m_y + 2(s-\bar{s})c_y]\}ds,
\end{aligned}$$

where $\bar{s} = (s_1 + s_2)/2$. This may be easily integrated to yield the following expression for the area:

$$\text{Area} = \frac{1}{6}[m_x c_y - m_y c_x](s_2 - s_1)^3, \tag{8}$$

or, alternately,

$$\text{Area} = \frac{1}{6}\begin{vmatrix} m_x & m_y \\ c_x & c_y \end{vmatrix}(s_2 - s_1)^3. \tag{9}$$

In this form it looks very similar to the form of the curvature for a 1-manifold embedded in $\mathbb{R}^3$ given by:

$$\kappa = \|\dot{\boldsymbol{x}} \times \ddot{\boldsymbol{x}}\|, \tag{10}$$

where the dot signifies a derivative of the position vector with respect to arc-length. Multiplying by $\Delta s = s_2 - s_1$ to the first row of the determinant in (9) and $(\Delta s)^2$ to the second row yields a quantity proportional to that of equation (10) but restricted to the xy-plane.

The area in equation (9) is very simple to compute. Also, equation (9) may exist whereas the calculation of $\ddot{\boldsymbol{x}}$ may not, causing κ to not exist. This is due to the finite difference technique we use (see Appendix).

3. Application: Hénon Map

3.1. **Defining equations.** Having derived an equation for measuring local curvatures numerically, we show how it performs on a well-known map: the Hénon map. The Hénon map is defined as the following: $f : \mathbb{R}^2 \to \mathbb{R}^2$, where $(x', y') = f(x, y)$, and is expressed as the folloing:

$$x' = y - k + x^2 \tag{11}$$

$$y' = -bx, \tag{12}$$

where b and k are real valued parameters. It can be shown that for parameter value $b = 1$, the Hénon map is area preserving. The Jacobian matrix is given by:

$$\mathsf{J} = \begin{pmatrix} 2x & 1 \\ -b & 0 \end{pmatrix}, \tag{13}$$

whose determinant is equal to b. For area preserving maps, we want the Jacobian determinant to equal 1, hence, $b = 1$.

For this value of b, the fixed point may be found by setting $x' = x$ and $y' = y$:

$$x = y - k + x^2 \tag{14}$$

$$y = -x, \tag{15}$$

Plugging in (15) into (14) we get:

$$0 = x^2 - 2x - k, \tag{16}$$

whose roots are found to be $x = 1 \pm \sqrt{1+k}$. We have shown that the fixed point is given by $(1 \pm \sqrt{1+k}, -1 \pm \sqrt{1+k})$. We pick the right-most fixed point for this study:

$$(x^*, y^*) = \boldsymbol{x}^* = (1 + \sqrt{1+k}, -1 - \sqrt{1+k}). \tag{17}$$

3.2. **Generating the manifold.** We begin with a linearization of the Hénon map near the right-most fixed point. This yields a linear system of the form

$$\boldsymbol{u}' = \mathsf{J}\boldsymbol{u}. \tag{18}$$

This matrix J has two eigenvectors with two eigenvalues. We pick the eigenvector with the corresponding eigenvalue whose magnitude is greater than 1. This will ensure that any point near the fixed point along the direction of this eigenvector will be mapped away from the fixed point. The unstable manifold will be generated here. We call this eigenvector $\boldsymbol{u}^+$.

In order to form the unstable manifold we will first need to construct the fundamental segment. We start by picking a point: $\boldsymbol{x}^* + \delta\boldsymbol{u}^+$, for some small $\delta > 0$. We map that point forward under f. Those two points now define a line, and we fill up the space along the line with points[1]. We then continue to iterate these points forward until we generate an approximation to the unstable manifold.

3.3. **Refining the unstable manifold.** We will iterate the fundamental segment enough times until the forward iterates of the initial set of points, defined as the fundamental segment, begin to spread out in the direction of the manifold. Because of the fact that the Hénon map defined above is area preserving, and the fact that points lying along the unstable manifold tend to expand and separate because of the instability inherent in the map, points lying off the unstable manifold will

[1]It will not matter if the points are equally spaced. One may populate this line segment with as many or as few points as the user may wish.

contract toward the manifold itself. Because of this we do not worry about the numerical errors in interpolating as the map itself reduces the error under further iterations of the map.

After every iteration of the fundamental segment we scan through the newly mapped points forming the newly constructed fundamental segment. We measure the first and second derivatives of every point inside the region of consideration using the formulae calculated in the appendix. We then input the data into equation (9), giving us an area estimate of the region between the secant line approximation and a quadratic one. In this way we approximate the local curvature of the manifold.

If this new measure of curvature is greater than a threshold value that is user-defined, one may add a point midway[2] between, say, the left pair of points used to calculate the second derivative. The location of this new point is placed in $\mathbb{R}^2$ through the quadratic interpolating function constructed in equations (2) and (3). In this manner we add points to locations of greater curvature, and skipping over regions of the manifold where points are, mostly, collinear, or well-resolved enough.

4. Discussion of 2-D Method

In the following we describe a method for approximating the curvature of a 2-manifold locally by calculating the difference between a quadratic approximation to a set of points and a linear (planar) approximation to the same set of points. The method is analogous in almost every way to what we have done above.

4.1. **Introduction and setup.** We begin as before by defining a parameterization $\mathbf{r} = (x^{(2)}, y^{(2)}, z^{(2)}) : \triangle_\alpha \subset \mathbb{R}^2 \to \mathbb{R}^3$, where $(\alpha_1, \alpha_2) \in \triangle_\alpha$ (a triangle in a triangulated parameter space whose vertices are given by $\boldsymbol{\alpha}^i, i = \{1, 2, 3\}$) and $(x, y, z) \in \mathbb{R}^3$, through the following equations:

$$x^{(2)}(\boldsymbol{\alpha}) = \boldsymbol{\alpha} \cdot \mathsf{H}_x \boldsymbol{\alpha} + L_x \cdot \boldsymbol{\alpha} + C_x \tag{19}$$

$$y^{(2)}(\boldsymbol{\alpha}) = \boldsymbol{\alpha} \cdot \mathsf{H}_y \boldsymbol{\alpha} + L_y \cdot \boldsymbol{\alpha} + C_y$$

$$z^{(2)}(\boldsymbol{\alpha}) = \boldsymbol{\alpha} \cdot \mathsf{H}_z \boldsymbol{\alpha} + L_z \cdot \boldsymbol{\alpha} + C_z$$

For future reference, we call H_x, etc... the curvature tensor: which curvature tensor exactly will be clear from the context. Since we have three points in $\triangle_\alpha$ we need three more to solve for all of the above parameters: three independent parameters in H_i, two in κ_i, and one C_i. In order to

[2]The notion of "midway" is determined by the parameter, here being s.

solve for the parameters we must first make a few assumptions about the grid points in each of the (α_1, α_2, x), (α_1, α_2, y), and (α_1, α_2, z) spaces. The base-space $\triangle_\alpha$ is the same for all of these, and we impose a square grid with spacing $\Delta\alpha_1$ in the α_1-coordinate direction, and spacing $\Delta\alpha_2$ in the α_2-coordinate direction. We then compute the a triangulation of this grid, partitioning the fundamental segment into sets of right triangles in our parameter space (see Figure 4). There is now a natural way of picking three points that will allow us to compute the components of the curvature tensor above, that is, we pick the midpoints of each of the sides of partition. This new partition defines one new similar right triangle inscribed inside the larger one. In this way we refine our grid if we do not meet the threshold volume.

To make the computation and the theory easier to understand and compute we split the quadratic interpolating polynomial into two as follows: $x^{(2)} = Q_x + x^{(1)}$, where $x^{(1)}$ is the planar approximation to the triangle (i.e. the plane defined by the three points of the vertices of the triangle), and Q_x is the remaining quadratic approximation defined by $x^{(2)} - x^{(1)}$.

Here we attempt to find the coefficients of the planar approximation, $x^{(1)}$. We anticipate a function of the form:

$$x^{(1)}(\boldsymbol{\alpha}) = \boldsymbol{\kappa}_x \cdot \boldsymbol{\alpha} + a_x. \tag{20}$$

Evaluating the above equation at each of the vertices of a given triangle $\triangle_{\alpha^i}$ we get a system of 3 equation in 3 unknowns. Thus,

$$\begin{aligned} x^{(1)}(\boldsymbol{\alpha}^1) &= x^1 = \kappa_x \cdot \boldsymbol{\alpha}^1 + a_x \\ x^{(1)}(\boldsymbol{\alpha}^2) &= x^2 = \kappa_x \cdot \boldsymbol{\alpha}^2 + a_x \\ x^{(1)}(\boldsymbol{\alpha}^3) &= x^3 = \kappa_x \cdot \boldsymbol{\alpha}^3 + a_x, \end{aligned} \tag{21}$$

or, stated differently,

$$\begin{pmatrix} x^1 \\ x^2 \\ x^3 \end{pmatrix} = \begin{pmatrix} \boldsymbol{\alpha}^1 & 1 \\ \boldsymbol{\alpha}^2 & 1 \\ \boldsymbol{\alpha}^3 & 1 \end{pmatrix} \begin{pmatrix} \kappa_{x,1} \\ \kappa_{x,2} \\ a_x \end{pmatrix}. \tag{22}$$

To gain some geometric insight, we solve for the right hand side column vector of equation (22) using the Cramer's rule algorithm.

$$\kappa_{x,1} = \frac{\begin{vmatrix} x^1 & \alpha_2^1 & 1 \\ x^2 & \alpha_2^2 & 1 \\ x^3 & \alpha_2^3 & 1 \end{vmatrix}}{2 \times \text{Area}(\triangle_{\alpha^i})} = \frac{\begin{vmatrix} x^2 - x^1 & \alpha_2^2 - \alpha_2^1 \\ x^3 - x^1 & \alpha_2^3 - \alpha_2^1 \end{vmatrix}}{2 \times \text{Area}(\triangle_{\alpha^i})}. \tag{23}$$

The above equations may be interpreted as a ratio of projected areas of parallelograms (or triangles) on the principle coordinate planes: the numerator being twice the area of the projection of the triangle upon the $\alpha_2 x$-plane, the denominator being twice the area of the projection of the triangle upon the $\alpha_1\alpha_2$-plane.

Similarly we have that

$$\kappa_{x,2} = \frac{\begin{vmatrix} \alpha_1^1 & x^1 & 1 \\ \alpha_1^2 & x^2 & 1 \\ \alpha_1^3 & x^3 & 1 \end{vmatrix}}{2 \times \text{Area}(\triangle_{\alpha^i})} = \frac{\begin{vmatrix} \alpha_1^2 - \alpha_1^1 & x^2 - x^1 \\ \alpha_1^3 - \alpha_1^1 & x^3 - x^1 \end{vmatrix}}{2 \times \text{Area}(\triangle_{\alpha^i})}. \tag{24}$$

The above equations carry a similar interpretation: it is the ratio of projected areas of parallelograms (or triangles) on the principle coordinate planes: the numerator being twice the area of the projection of the triangle upon the $\alpha_1 x$-plane, the denominator being twice the area of the projection of the triangle upon the $\alpha_1\alpha_2$-plane.

The constant term follows:

$$a_x = \frac{\begin{vmatrix} \alpha_1^1 & \alpha_2^1 & x^1 \\ \alpha_1^2 & \alpha_2^2 & x^2 \\ \alpha_1^3 & \alpha_2^3 & x^3 \end{vmatrix}}{2 \times \text{Area}(\triangle_{\alpha^i})} \tag{25}$$

This last term has the following interpretation, it is the ratio of 6 times the volume of the tetrahedron formed by the origin and the three vertices with twice the area of the projection of the triangle upon the $\alpha_1\alpha_2$-plane.

To calculate Q_x we assume a form that looks like the following

$$Q_x(\boldsymbol{\alpha}) = \boldsymbol{\alpha} \cdot \mathsf{H}_x \boldsymbol{\alpha} + v_x \cdot \boldsymbol{\alpha} - R_x. \tag{26}$$

To make this approximation consistent with what we computed for $x^{(1)}$ we impose the following condition:

$$Q_x(\boldsymbol{\alpha}^i) = 0 = \boldsymbol{\alpha}^i \cdot \mathsf{H}_x \boldsymbol{\alpha}^i + v_x \cdot \boldsymbol{\alpha}^i - R_x. \tag{27}$$

From this we understand that the quadratic interpolant Q_x vanishes at the vertices of the triangles. This is similar to what we did with the linear situation by shearing the secant line through the parabola downward until it lies parallel with the parameter-axis. Hence forth we dismiss the subscript x.

The above condition gives us three equations in three unknowns, one for each vertex:

$$\begin{aligned} 0 &= \boldsymbol{\alpha}^1 \cdot \mathsf{H}\boldsymbol{\alpha}^1 + \boldsymbol{v} \cdot \boldsymbol{\alpha}^1 - R \\ 0 &= \boldsymbol{\alpha}^2 \cdot \mathsf{H}\boldsymbol{\alpha}^2 + \boldsymbol{v} \cdot \boldsymbol{\alpha}^2 - R \\ 0 &= \boldsymbol{\alpha}^3 \cdot \mathsf{H}\boldsymbol{\alpha}^3 + \boldsymbol{v} \cdot \boldsymbol{\alpha}^3 - R. \end{aligned} \tag{28}$$

Since H belongs only to Q_x, we begin to calculate the components of the curvature tensor by assuming a lowest possible order of approximation on the entries. We will use the flat side of the right triangle to calculate the second derivative using a familiar finite-difference formula, and similarly for the vertical side. To calculate the off-diagonal terms we evaluate the difference quotient between the two first derivative approximations: one of the midpoint of one the legs to the midpoint of the hypotenuse and the second from the unused point on the leg in the perpendicular direction of the difference taken in the first part with the point opposite the hypotenuse, (see Figure 5)

For the present discussion we treat only $x = f(\alpha_1, \alpha_2)$. The discussion carries over to the y and z coordinates. We begin with a triangle as shown in Figure 5. Our immediate goal will be to determine the components of the curvature tensor H_x. We drop all subscripts:

$$\mathsf{H} = \begin{pmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{pmatrix}. \tag{29}$$

We calculate the components H_{11} and H_{22} as follows:

$$\mathsf{H}_{11} = \frac{f^{11} - 2f^{21} + f^{31}}{(\Delta\alpha_1)^2} \tag{30}$$

$$\mathsf{H}_{22} = \frac{f^{11} - 2f^{12} - f^{13}}{(\Delta\alpha_2)^2}. \tag{31}$$

The off-diagonal components, being equal [3] , are calculated as follows:

$$\mathsf{H}_{12} = \mathsf{H}_{21} = \frac{\frac{f^{21}-f^{22}}{\Delta\alpha_2} - \frac{f^{11}-f^{12}}{\Delta\alpha_2}}{\Delta\alpha_1} = \frac{f^{21} - (f^{11} + f^{22}) + f^{12}}{\Delta\alpha_1\Delta\alpha_2}. \tag{32}$$

We expect the errors on each of these to be second order in the α spacing. These may be calculated very easily and very efficiently, being the traditional centered-difference formulae from finite difference analysis.

To find the rest of the coefficients of the polynomial Q_x, we subtract equations (28) pair-wise. This way we get three sets of two equations for the two unknowns $\boldsymbol{v}_x$, whose symmetric solution is given by the following:

$$\boldsymbol{v} = \frac{\mathsf{J}}{(\boldsymbol{\alpha}^2 - \boldsymbol{\alpha}^1) \times (\boldsymbol{\alpha}^3 - \boldsymbol{\alpha}^1)} \big((\boldsymbol{\alpha}^3 - \boldsymbol{\alpha}^2)[\boldsymbol{\alpha}^1 \cdot \mathsf{H}\boldsymbol{\alpha}^1] + (\boldsymbol{\alpha}^1 - \boldsymbol{\alpha}^3)[\boldsymbol{\alpha}^2 \cdot \mathsf{H}\boldsymbol{\alpha}^2] + (\boldsymbol{\alpha}^2 - \boldsymbol{\alpha}^1)[\boldsymbol{\alpha}^3 \cdot \mathsf{H}\boldsymbol{\alpha}^3]\big). \tag{33}$$

where

$$\mathsf{J} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \tag{34}$$

Note that the denominator of (33) is actually a scalar. Algorithmically, R may be found by solving (28) for any one of the triangle vertices. We give a symmetric version here, which is easy to prove:

$$3R = (\boldsymbol{\alpha}^1 \cdot \mathsf{H}\boldsymbol{\alpha}^1 + \boldsymbol{\alpha}^2 \cdot \mathsf{H}\boldsymbol{\alpha}^2 + \boldsymbol{\alpha}^3 \cdot \mathsf{H}\boldsymbol{\alpha}^3) + \big(\boldsymbol{v} \cdot (\boldsymbol{\alpha}^1 + \boldsymbol{\alpha}^2 + \boldsymbol{\alpha}^3)\big). \tag{35}$$

5. The Setup of the Volume Integral

Having ascertained the necessary quantities for integration we commence now with the setup of the integral. Given that our map is volume preserving we wish to integrate over a closed volume using the following volume form:

$$\int_V dV = \int_V dx \wedge dy \wedge dz. \tag{36}$$

[3]Since we are evaluating points on a smooth manifold, this condition is guaranteed

where V is defined as before, the region between a quadratic approximation and a secant plane through it.

In order to setup the above integral we pause in order to examine the parts. $\mathbf{r}$ is a vector-valued function of the coordinates x, y, and z, which are in-turn parametrized by (α_1, α_2). We attempt, now, to integrate over the triangle $\triangle_{\alpha^i} \subset \mathbb{R}^2$. In order to do this we make a change of variables from $\mathbb{R}^3$ to $\mathbb{R}^3$ in such a way that would allow us to evaluate the above integral more easily.

We begin this step by defining a new function analogous to x, y, and z; we shall call them X, Y, and Z, and give it the following form:

$$X = X(\boldsymbol{\alpha}, \gamma) = x^{(1)}(\boldsymbol{\alpha}) + \gamma Q_x, \tag{37}$$

$$Y = Y(\boldsymbol{\alpha}, \gamma) = y^{(1)}(\boldsymbol{\alpha}) + \gamma Q_y, \tag{38}$$

$$Z = Z(\boldsymbol{\alpha}, \gamma) = z^{(1)}(\boldsymbol{\alpha}) + \gamma Q_z, \tag{39}$$

where $\gamma \in [0, 1]$. Here, recall that $x^{(1)}$ has the form $x^{(1)}(\boldsymbol{\alpha}) = \boldsymbol{\kappa}_x \cdot \boldsymbol{\alpha} + a_x$. We see that as γ sweeps through the values from 0 to 1 our triangle sweeps through the volume with the vertices fixed, defining a sort of homotopy of surfaces with fixed vertices.

We begin by defining the Jacobian matrix from x, y, z to $\alpha_1, \alpha_2, \gamma$. This will be given by the following:

$$\mathsf{K} = \frac{\partial(X, Y, Z)}{\partial(\alpha_1, \alpha_2, \gamma)} = \begin{pmatrix} \boldsymbol{\kappa}_x + \gamma(2\mathsf{H}_x\boldsymbol{\alpha} + \boldsymbol{v}_x) & |Q_x \\ \boldsymbol{\kappa}_y + \gamma(2\mathsf{H}_y\boldsymbol{\alpha} + \boldsymbol{v}_y) & |Q_y \\ \boldsymbol{\kappa}_z + \gamma(2\mathsf{H}_z\boldsymbol{\alpha} + \boldsymbol{v}_z) & |Q_z \end{pmatrix} \tag{40}$$

The determinant of the above equation is given by the following:

$$\begin{aligned} \det(\mathsf{K}) = Q_x &\left[(\boldsymbol{\kappa}_y + \gamma(2\mathsf{H}_y\boldsymbol{\alpha} + \boldsymbol{v}_y)) \times (\boldsymbol{\kappa}_z + \gamma(2\mathsf{H}_z\boldsymbol{\alpha} + \boldsymbol{v}_z))\right] \\ &+ Q_y \left[(\boldsymbol{\kappa}_z + \gamma(2\mathsf{H}_z\boldsymbol{\alpha} + \boldsymbol{v}_z)) \times (\boldsymbol{\kappa}_x + \gamma(2\mathsf{H}_x\boldsymbol{\alpha} + \boldsymbol{v}_x))\right] \\ &+ Q_z \left[(\boldsymbol{\kappa}_x + \gamma(2\mathsf{H}_x\boldsymbol{\alpha} + \boldsymbol{v}_x)) \times (\boldsymbol{\kappa}_y + \gamma(2\mathsf{H}_y\boldsymbol{\alpha} + \boldsymbol{v}_y))\right]. \end{aligned} \tag{41}$$

All we need is a first-order approximation to the volume. In the integral we have terms with linear error with respect to the spacing of the α grid points. We also have the Q_i terms in front of each term in the Jacobian determinant sum above, this contributes another linear order to the integrand. This gives us freedom to neglect the extra linear terms in the above sum in equation

(41). We may ignore all terms proportional in γ and still maintain quadratic error. Since we will have left over an integral in γ with limits between 0 and 1, we may evaluate it without any change. Thus, the Jacobian determinant now takes the following approximate form:

$$\det(\mathsf{K}) = Q_x\,[\boldsymbol{\kappa}_y \times \boldsymbol{\kappa}_z] + Q_y\,[\boldsymbol{\kappa}_z \times \boldsymbol{\kappa}_x] + Q_z\,[\boldsymbol{\kappa}_x \times \boldsymbol{\kappa}_y] + O(Q^2), \tag{42}$$

or,

$$\det(\mathsf{K}) \approx \mathbf{Q} \cdot \mathbf{n}, \tag{43}$$

where $\mathbf{Q} = (Q_x, Q_y, Q_z)$, a vector of the quadratic approximations, and $\mathbf{n} = (n_x, n_y, n_z)$, a normal vector to the triangle in $\mathbb{R}^3$. Note that we have made the following identification:

$$\begin{aligned} n_x &= \boldsymbol{\kappa}_y \times \boldsymbol{\kappa}_z \\ n_y &= \boldsymbol{\kappa}_z \times \boldsymbol{\kappa}_x \\ n_z &= \boldsymbol{\kappa}_x \times \boldsymbol{\kappa}_y. \end{aligned} \tag{44}$$

Equation (36) now can be written as

$$\int_V dV = \int_V dx \wedge dy \wedge dz \approx \int_{\triangle_{\alpha^i} \times [0,1]} \mathbf{Q} \cdot \mathbf{n}\, d\alpha_1 \wedge d\alpha_2 \wedge d\gamma. \tag{45}$$

Notice that $\gamma \in [0,1]$ and that the integrand does not depend on γ. Therefore, by Fubini's theorem [4], we can evaluate the integral with respect to γ first, giving $\int_{[0,1]} d\gamma = 1$. Now we express $\mathbf{Q}$ in terms of functions and constants we have evaluated in the beginning:

$$\mathbf{Q} = \boldsymbol{\alpha} \cdot \mathsf{H}_i \boldsymbol{\alpha} + \boldsymbol{v}_i \cdot \boldsymbol{\alpha} - R_i, \tag{46}$$

where we express the above vector using index notation, and $i = x, y, z$, so that our integral takes the form

$$\int_V dV \approx \int_{\triangle_{\alpha^i}} (\boldsymbol{\alpha} \cdot \mathsf{H}_i \boldsymbol{\alpha} + \boldsymbol{v}_i \cdot \boldsymbol{\alpha} - R_i) \cdot \mathbf{n}\, d\alpha_1 \wedge d\alpha_2. \tag{47}$$

[4]The function $\mathbf{Q} \cdot \mathbf{n}$ contains polynomials in α_1 and α_2, so $\mathbf{Q}$ is integrable.

We make another pair of substitutions,

$$\bar{\mathsf{H}} = \sum_{i=\{x,y,z\}} \mathsf{H}_i n_i \tag{48}$$

$$\bar{\boldsymbol{v}} = \sum_{i=\{x,y,z\}} \boldsymbol{v}_i n_i \tag{49}$$

$$\bar{R} = \sum_{i=\{x,y,z\}} R_i n_i \tag{50}$$

so that the final form of the volume integral in $\mathbb{R}^3$ looks like the following:

$$\int_V dV \approx \int_{\triangle_{\alpha^i}} \left(\boldsymbol{\alpha} \cdot \bar{\mathsf{H}}\boldsymbol{\alpha} + \bar{\boldsymbol{v}} \cdot \boldsymbol{\alpha} - \bar{R}\right)\, d\alpha_1 \wedge d\alpha_2. \tag{51}$$

6. The Evaluation of the Volume Integral

To begin evaluating the integral above we first break it up into pieces. The three equations below will be done one at a time:

$$\int_{\triangle_{\alpha^i}} \boldsymbol{\alpha} \cdot \bar{\mathsf{H}}\boldsymbol{\alpha}\, d\alpha_1 \wedge d\alpha_2, \tag{52}$$

$$\int_{\triangle_{\alpha^i}} \bar{\boldsymbol{v}} \cdot \boldsymbol{\alpha}\, d\alpha_1 \wedge d\alpha_2, \tag{53}$$

and,

$$\int_{\triangle_{\alpha^i}} \bar{R}\, d\alpha_1 \wedge d\alpha_2 \tag{54}$$

Equation (54) is simply a constant times the area of the triangle in question in (α_1, α_2)-space. This is simple enough.

Equation(53) may be thought as $\bar{\boldsymbol{v}}$ dotted into the coordinates for the barycenter of the triangle $\triangle_{\alpha^i}$. This, too, is simple since $\bar{\boldsymbol{v}}$ is determined and does not depend on any other parameter values.

We will devote the rest of this section to tackling equation (52). To begin, we make a coordinate transformation, setting $\boldsymbol{\beta} = \sqrt{\bar{\mathsf{H}}}\boldsymbol{\alpha}$, which will give us the following

$$\int_{\tilde{\triangle}_{\alpha^i}} \|\boldsymbol{\beta}\|^2 \, \frac{d\beta_1 \wedge d\beta_2}{\sqrt{\det\bar{\mathsf{H}}}} = \frac{1}{\sqrt{\det\bar{\mathsf{H}}}} \int_{\tilde{\triangle}_{\alpha^i}} \|\boldsymbol{\beta}\|^2 \, d\beta_1 \wedge d\beta_2, \tag{55}$$

where $\tilde{\triangle}$ is the new triangle in $(\boldsymbol{\beta}_1, \boldsymbol{\beta}_2)$-space, the square-root in front of the integral in the right most term in equation (55) is the Jacobian factor. We make the observation that the integral may be interpreted to be the moment of inertia of a triangular lamina with unit density. Thus, it can

be shown that equation (55) becomes

$$\frac{1}{\sqrt{\det\bar{\mathsf{H}}}}\int_{\tilde{\triangle}_{\alpha^i}} \|\boldsymbol{\beta}\|^2\, d\beta_1\wedge d\beta_2 = \frac{1}{12\sqrt{\det\bar{\mathsf{H}}}}\left[\boldsymbol{\beta}^3\times\boldsymbol{\beta}^2+\boldsymbol{\beta}^2\times\boldsymbol{\beta}^1+\boldsymbol{\beta}^1\times\boldsymbol{\beta}^3\right]\times \tag{56}$$
$$\left[\boldsymbol{\beta}^1\cdot(\boldsymbol{\beta}^1-\boldsymbol{\beta}^3)+\boldsymbol{\beta}^2\cdot(\boldsymbol{\beta}^2-\boldsymbol{\beta}^1)+\boldsymbol{\beta}^3\cdot(\boldsymbol{\beta}^3-\boldsymbol{\beta}^2)+6\left\|\frac{\boldsymbol{\beta}^1+\boldsymbol{\beta}^2+\boldsymbol{\beta}^3}{3}\right\|^2\right],$$

where arrive at the last term in the above expression by using Steiner's Parallel-Axis Theorem. Note, the terms with the cross-products are all scalars since $\boldsymbol{\beta}$ is a two-dimensional vector. Having evaluated the integral we attempt to express the results in terms of quantities we will have access to more readily: (α_1,α_2), $\bar{\mathsf{H}}$, etc... We attempt to rewrite the cross-products in matrix notation. Recall equation (34). We note that for any two-dimensional vector, say $\boldsymbol{\eta}_i$, $\boldsymbol{\eta}_i\times\boldsymbol{\eta}_j = -\boldsymbol{\eta}_i\mathsf{J}\boldsymbol{\eta}_j$. Recall also that $\boldsymbol{\beta}=\sqrt{\bar{\mathsf{H}}}\boldsymbol{\alpha}$, and that $\bar{\mathsf{H}}^t=\bar{\mathsf{H}}$. Making this coordinate transformation, noting that $\boldsymbol{\alpha}^i$ is the vector from the origin to the vertex i of the triangle, we find that the integral takes the following form

$$\frac{1}{\sqrt{\det\bar{\mathsf{H}}}}\int_{\tilde{\triangle}_{\alpha^i}} |\boldsymbol{\beta}\|^2\, d\beta_1\wedge d\beta_2 = \frac{-1}{12\sqrt{\det\bar{\mathsf{H}}}}\left[\boldsymbol{\alpha}^3\sqrt{\bar{\mathsf{H}}}\mathsf{J}\sqrt{\bar{\mathsf{H}}}\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^2\sqrt{\bar{\mathsf{H}}}\mathsf{J}\sqrt{\bar{\mathsf{H}}}\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^1\sqrt{\bar{\mathsf{H}}}\mathsf{J}\sqrt{\bar{\mathsf{H}}}\boldsymbol{\alpha}^3\right]\times \tag{57}$$

$$\left[\boldsymbol{\alpha}^1\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^1-\boldsymbol{\alpha}^2)+\boldsymbol{\alpha}^2\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^2-\boldsymbol{\alpha}^3)+\boldsymbol{\alpha}^3\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^3-\boldsymbol{\alpha}^1)+6\left(\frac{\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^3}{3}\right)\cdot\bar{\mathsf{H}}\left(\frac{\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^3}{3}\right)\right].$$

Since,

$$\sqrt{\bar{\mathsf{H}}}^{-1}\mathsf{J}\sqrt{\bar{\mathsf{H}}} = \left(\sqrt{\det\bar{\mathsf{H}}}\right)\bar{\mathsf{H}}^{-1}\mathsf{J} \tag{58}$$

or multiplying by a factor of $\bar{\mathsf{H}}$

$$\sqrt{\bar{\mathsf{H}}}\mathsf{J}\sqrt{\bar{\mathsf{H}}} = \left(\sqrt{\det\bar{\mathsf{H}}}\right)\mathsf{J}. \tag{59}$$

So we find that we have

$$\frac{1}{\sqrt{\det\bar{\mathsf{H}}}}\int_{\tilde{\triangle}_{\alpha^i}} \|\boldsymbol{\beta}\|^2\, d\beta_1\wedge d\beta_2 = \frac{-1}{12}\left[\boldsymbol{\alpha}^3\mathsf{J}\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^2\mathsf{J}\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^1\mathsf{J}\boldsymbol{\alpha}^3\right]\times \tag{60}$$

$$\left[\boldsymbol{\alpha}^1\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^1-\boldsymbol{\alpha}^2)+\boldsymbol{\alpha}^2\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^2-\boldsymbol{\alpha}^3)+\boldsymbol{\alpha}^3\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^3-\boldsymbol{\alpha}^1)\ +6\left(\frac{\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^3}{3}\right)\cdot\bar{\mathsf{H}}\left(\frac{\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^3}{3}\right)\right].$$

Because of the fact that

$$\frac{-1}{12}\left[\boldsymbol{\alpha}^3\mathsf{J}\boldsymbol{\alpha}^2+\boldsymbol{\alpha}^2\mathsf{J}\boldsymbol{\alpha}^1+\boldsymbol{\alpha}^1\mathsf{J}\boldsymbol{\alpha}^3\right]=\frac{1}{6}\mathrm{Area}(\triangle_{\alpha^i}), \tag{61}$$

a little bit of algebraic manipulation gives the following final expression for the approximating volume:

$$\int_V dV \approx \frac{1}{18}\mathrm{Area}(\triangle_{\alpha^i})\left\{\boldsymbol{\alpha}^1\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^2-\boldsymbol{\alpha}^1)+\boldsymbol{\alpha}^2\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^3-\boldsymbol{\alpha}^2)+\boldsymbol{\alpha}^3\cdot\bar{\mathsf{H}}(\boldsymbol{\alpha}^1-\boldsymbol{\alpha}^3)\right\}, \tag{62}$$

where $\boldsymbol{\alpha}^i$ is the coordinate of the ith vertex of the triangle $\triangle_{\alpha^i}$ in parameter space, and $\bar{\mathsf{H}}$ can be computed from equation (48).

6.1. **Implementation.** As before with the one-dimensional Hénon map when we calculated the area difference between the linear and quadratic approximations to the manifold, so too in this case we calculate the volume difference between the linear and quadratic approximations. In the one-dimensional case, when we detected an area that was beyond our threshold-area, we constructed a quadratic interpolating function to add a point "half-way" (defined parametrically) between two points. Here in the two-dimensional case, when we detect a volume that is "too large" we add three points in the parameter space, one in the middle of the side of a given triangle in consideration (as in Figure 5). In this way we add inscribe a new triangle that is geometrically similar to the parent triangle, this in order to be able to continue the application of the algorithm developed in section 4.1.

This method cuts back on potentially large computation times that usually result from brute-force computations of 2-dimensional manifolds. It is computationally cheaper to add points only where the volume difference between the linear and quadratic approximations is "too large"; refining a portion of the surface that has a greater curvature, as approximated by this volume difference, saves computation time and memory.

7. Conclusion

We have developed a method for computing the area (or volume) difference between a quadratic approximation to a manifold and a secant line (or plane) through a set of nearby points as a means of approximating the local curvature of a 1-manifold (or 2-manifold) embedded in a 2-dimensional

(or 3-dimensional) volume-preserving phase space. No existing method of computing 2-manifolds in this manner is known to the author. It also has the advantage of being easy to compute.

We demonstrated how this method would work for a 1-manifold embedded in a 2 dimensional phase space using the Hénon map as our volume-preserving diffeomorphism. We refined a portion of a manifold that was not well-resolved by measuring the area (volume) between the local linear and quadratic approximations in order to determine if the area (volume) is beyond a user-selected threshold. If so, we added points to the appropriate location in parameter space, then used an already constructed quadratic interpolating function to map the added point(s) in parameter space to phase space.

By using this method we discussed how we avoid unnecessarily large brute-force computations and memory for storing points in space simply by refining only regions of "large enough" curvature. In doing this we avoid oversampling a region of a manifold that is locally flat.

8. Appendix

8.1. **Finite-Difference formulae for the first and second derivatives with non-equal spacing.** In order to determine the constants m_x, m_y, c_x, and c_y in equations (2) and (3) we need to develop an algorithm for determining the first and second derivatives of functions where the spacing in the domain is uneven. Maps that are nonlinear do not normally preserve distances between a pair of points, so even if one starts with a set of points that are evenly spaced, there is no guarantee they will stay that way in further iterates.

We start by considering three points: $\{(x-h),(x),(x+h)\}$, where h and k are positive distances from x to the left and to the right respectively. We wish to construct formulae for the derivatives at the point x. Therefore we make two Taylor expansions, one about $-h$ and another about k:

$$f(x+k)-f(x) = kf'(x) + \frac{1}{2}k^2 f'' + O(k^3)$$
$$f(x-h)-f(x) = -hf'(x) + \frac{1}{2}h^2 f'' + O(h^3).$$

This equation may be written as a linear system of equations in the following way:

$$\begin{pmatrix} f(x+k)-f(x) \\ f(x-h)-f(x) \end{pmatrix} = \begin{pmatrix} k & k^2/2 \\ -h & h^2/2 \end{pmatrix} \begin{pmatrix} f'(x) \\ f''(x) \end{pmatrix}.$$

Solving this system yields the following:

$$\begin{pmatrix} f'(x) \\ f''(x) \end{pmatrix} = \frac{2}{kh^2 + hk^2} \begin{pmatrix} h^2/2 & -k^2/2 \\ h & k \end{pmatrix} \begin{pmatrix} f(x+k) - f(x) \\ f(x-h) - f(x) \end{pmatrix},$$

or,

$$f'(x) = \frac{h}{h+k} \frac{f(x+k) - f(x)}{k} + \frac{k}{h+k} \frac{f(x) - f(x-h)}{h}, \tag{63}$$

and

$$f''(x) = \frac{2}{hk(h+k)} \left[hf(x+k) - (h+k)f(x) + kf(x-h) \right]. \tag{64}$$

Note that for $h = k$, equation (63) reduces to the familiar leap-frog formula:

$$f'(x) = \frac{f(x+h) - f(x-h)}{2h},$$

and that equation (64) reduces to the familiar centered-difference formula:

$$f''(x) = \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}.$$

Both of equations (63) and (64) have errors that vary linearly with the spacing for small values of h and k, but vary wildly for larger spacings. The errors vary with the spacing squared when $h = k$, as is known.

9. References

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[5] Arnold, V., "Mathematical Methods in Classical Mechanics, Second Edition", *Springer*,(1989).

10. Figures

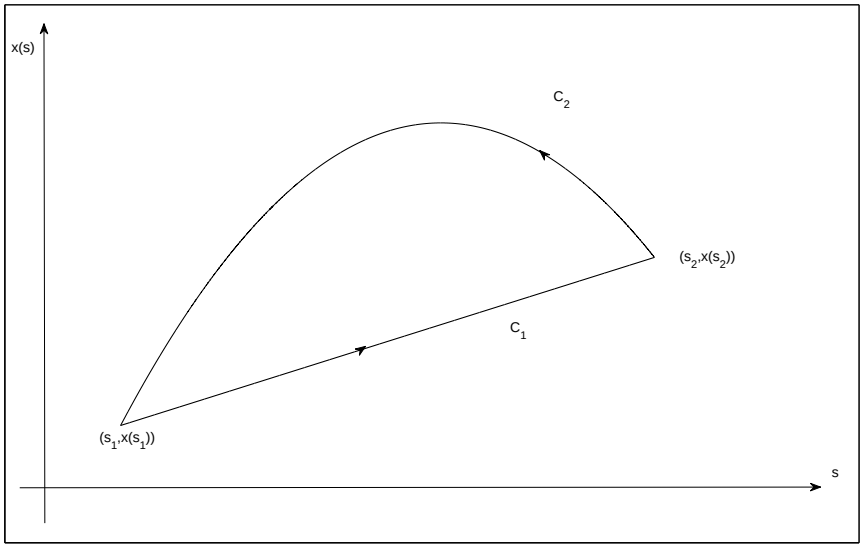

FIGURE 1. A general quadratic in the one-dimensional parameter space.

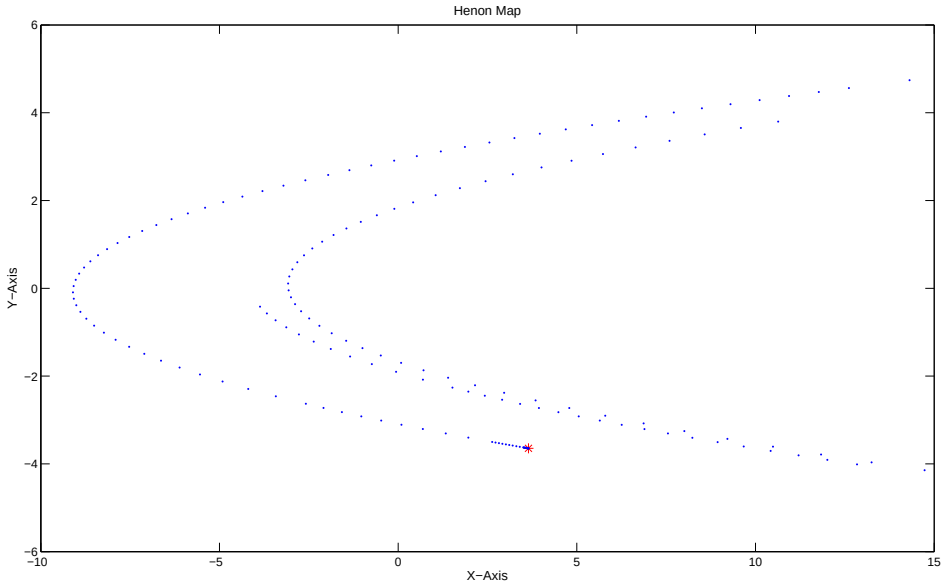

FIGURE 2. Fundamental Segment under a small number of iterates. Note the larger density of points where curvature is largest. Fixed point in red.

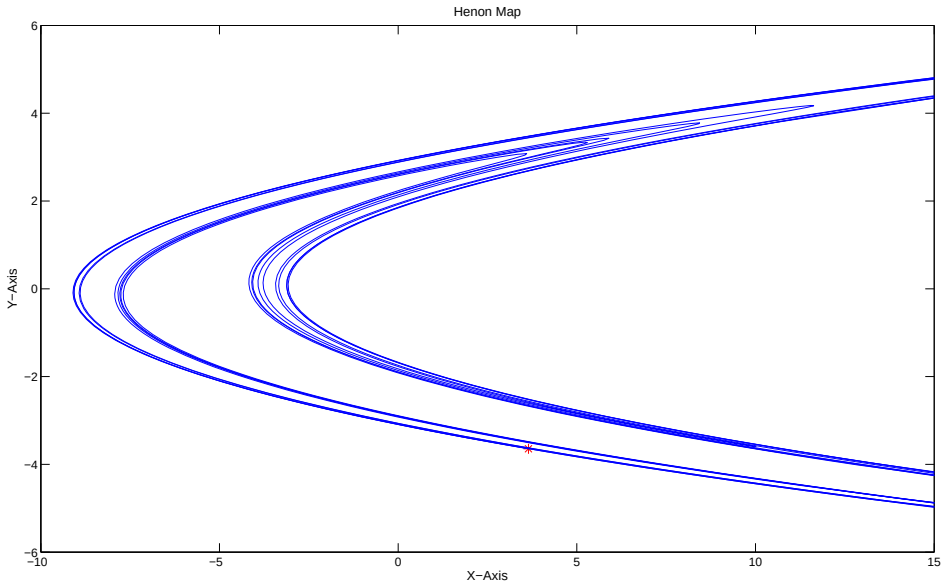

FIGURE 3. Fundamental Segment under a larger number of iterates. Fixed point in red.

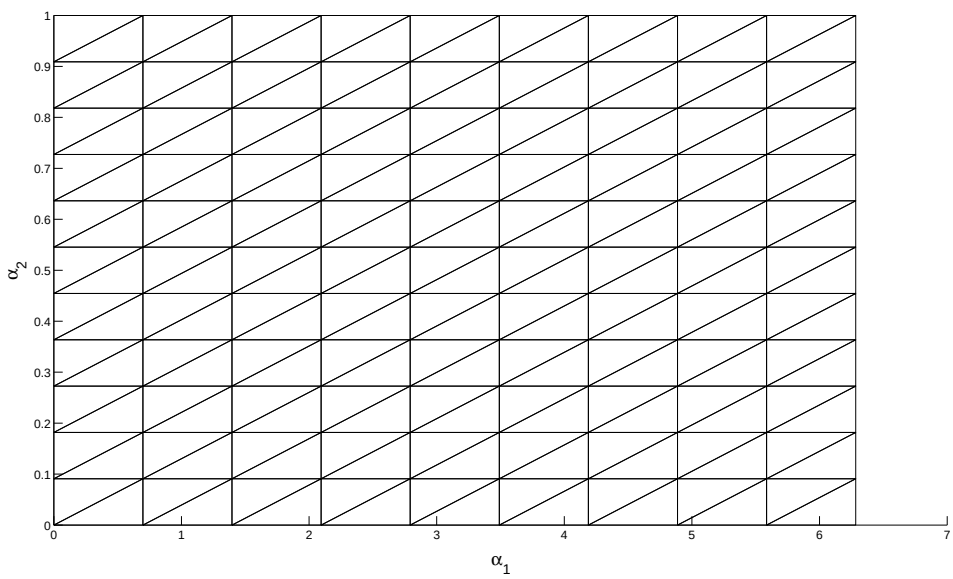

FIGURE 4. A sample 10×12 grid in parameter space, $\alpha_1 \in [0, 2\pi]$ and $\alpha_2 \in [0, 1]$

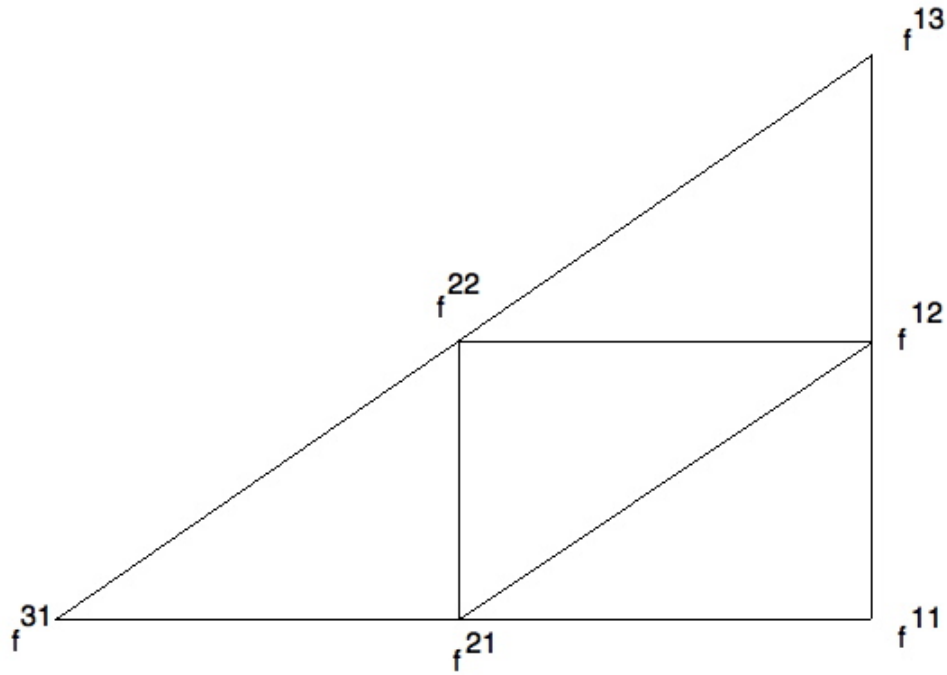

FIGURE 5. Triangle on which we evaluate the entries of the curvature tensor H