Appendix C

Finding cycles

(C. Chandre)

C.1 Newton-Raphson method

C.1.1 Contraction rate

Consider a d-dimensional map $x' = f(x)$ with an unstable fixed point x_*. The Newton-Raphson algorithm is obtained by iterating the following map

$$x' = g(x) = x - (J(x) - 1)^{-1} (f(x) - x) .$$

The linearization of g near x_* leads to

$$x_* + \epsilon' = x_* + \epsilon - (J(x_*) - \mathbf{1})^{-1} (f(x_*) + J(x_*)\epsilon - x_* - \epsilon) + O\left(\|\epsilon\|^2\right),$$

where $\epsilon = x - x_*$. Therefore,

$$x' - x_* = O\left((x - x_*)^2\right).$$

After n steps and if the initial guess x_0 is close to x_*, the error decreases super-exponentially

$$g^n(x_0) - x_* = O\left((x_0 - x_*)^{2^n}\right).$$

C.1.2 Computation of the inverse

The Newton-Raphson method for finding n-cycles of d-dimensional mappings using the multi-shooting method reduces to the following equation

$$\begin{pmatrix} \mathbf{1} & & & -Df(x_n) \\ -Df(x_1) & \mathbf{1} & & \\ & \cdots & \mathbf{1} & \\ & & -Df(x_{n-1}) & \mathbf{1} \end{pmatrix} \begin{pmatrix} \delta_1 \\ \delta_2 \\ \cdots \\ \delta_n \end{pmatrix} = - \begin{pmatrix} F_1 \\ F_2 \\ \cdots \\ F_n \end{pmatrix}, \tag{C.1}$$

where $Df(x)$ is the $[d \times d]$ Jacobian matrix of the map evaluated at the point x, and $\delta_m = x'_m - x_m$ and $F_m = x_m - f(x_{m-1})$ are d-dimensional vectors. By some starightforward algebra, the vectors δ_m are expressed as functions of the vectors F_m:

$$\delta_m = -\sum_{k=1}^{m} \beta_{k,m-1} F_k - \beta_{1,m-1} \left(\mathbf{1} - \beta_{1,n}\right)^{-1} \left(\sum_{k=1}^{n} \beta_{k,n} F_k \right), \tag{C.2}$$

for $m = 1, \ldots, n$, where $\beta_{k,m} = Df(x_m)Df(x_{m-1}) \cdots Df(x_k)$ for $k < m$ and $\beta_{k,m} = \mathbf{1}$ for $k \geq m$. Therefore, finding n-cycles by a Newton-Raphson method with multiple shooting requires the inversing of a $[d \times d]$ matrix $\mathbf{1} - Df(x_n)Df(x_{n-1}) \cdots Df(x_1)$.

C.2 Hybrid Newton-Raphson / relaxation method

 Consider a d-dimensional map $x' = f(x)$ with an unstable fixed point x_*. The transformed map is the following one:

$$x' = g(x) = x + \gamma C(f(x) - x),$$

where $\gamma > 0$ and C is a $d \times d$ invertible constant matrix. We note that x_* is also a fixed point of g. Consider the stability matrix at the fixed point x_*

$$A_g = \left. \frac{dg}{dx} \right|_{x=x_*} = 1 + \gamma C(A_f - 1).$$

The matrix C is constructed such that the eigenvalues of A_g are of modulus less than one. Assume that A_f is diagonalizable: In the basis of diagonalization, the matrix writes:

$$\tilde{A}_g = 1 + \gamma \tilde{C}(\tilde{A}_f - 1),$$

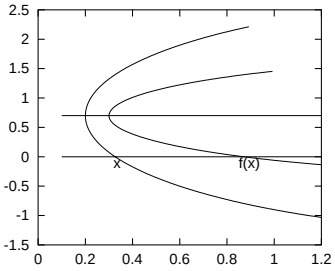

Figure C.1: Illustration of the optimal Poincaré surface. The original surface $y = 0$ yields a large distance $x - f(x)$ for the Newton iteration. A much better choice is $y = 0.7$.

where $\tilde{A}_f$ is diagonal with elements μ_i. We restrict the set of matrices $\tilde{C}$ to diagonal matrices with $\tilde{C}_{ii} = \epsilon_i$ where $\epsilon_i = \pm 1$. Thus $\tilde{A}_g$ is diagonal with eigenvalues $\gamma_i = 1 + \gamma\epsilon_i(\mu_i - 1)$. The choice of γ and ϵ_i is such that $|\gamma_i| < 1$. It is easy to see that if $\mathrm{Re}(\mu_i) < 1$ one has to choose $\epsilon_i = 1$, and if $\mathrm{Re}(\mu_i) > 1$, $\epsilon_i = -1$. If λ is chosen such that

$$0 < \gamma < \min_{i=1,\ldots,d} \frac{2|\mathrm{Re}(\mu_i) - 1|}{|\mu_i - 1|^2},$$

all the eigenvalues of A_g have modulus less that one. The contraction rate at the fixed point for the map g is then $\max_i |1 + \gamma\epsilon_i(\mu_i - 1)|$. If $\mathrm{Re}(\mu_i) = 1$, it is not possible to stabilize x_* by the set of matrices γC.
From the construction of C, we see that 2^d choices of matrices are possible. For example, for 2-dimensional systems, these matrices are

$$C \in \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix} \right\}.$$

For 2-dimensional dissipative maps, the eigenvalues satisfy $\mathrm{Re}(\mu_1)\mathrm{Re}(\mu_2) \leq \det Df < 1$. The case $(\mathrm{Re}(\mu_1) > 1, \mathrm{Re}(\mu_2) > 1)$ which is stabilized by $\left(\begin{smallmatrix} -1 & 0 \\ 0 & -1 \end{smallmatrix}\right)$ has to be discarded. The minimal set is reduced to three matrices.

C.2.1 Newton method with optimal surface of section

(F. Christiansen)

In some systems it might be hard to find a good starting guess for a fixed point, something that could happen if the topology and/or the symbolic dynamics of the flow is not well understood. By changing the Poincaré section one might get a better initial guess in the sense that x and $f(x)$ are closer together. In figure C.1 there is an illustration of this. The figure shows a Poincaré section, $y = 0$, an initial guess x, the corresponding $f(x)$ and pieces of the trajectory near these two points.

If the Newton iteration does not converge for the initial guess x we might have to work very hard to find a better guess, particularly if this is in a high-dimensional system (high-dimensional might in this context mean a Hamiltonian system with

3 degrees of freedom.) But clearly we could easily have a much better guess by simply shifting the Poincaré section to $y = 0.7$ where the distance $x - f(x)$ would be much smaller. Naturally, one cannot see by eye the best surface in higher dimensional systems. The way to proceed is as follows: We want to have a minimal distance between our initial guess x and the image of this $f(x)$. We therefore integrate the flow looking for a minimum in the distance $d(t) = |f^t(x) - x|$. $d(t)$ is now a minimum with respect to variations in $f^t(x)$, but not necessarily with respect to x. We therefore integrate x either forward or backward in time. Doing this we minimize d with respect to x, but now it is no longer minimal with respect to $f^t(x)$. We therefore repeat the steps, alternating between correcting x and $f^t(x)$. In most cases this process converges quite rapidly. The result is a trajectory for which the vector $(f(x) - x)$ connecting the two end points is perpendicular to the flow at both points. We can now choose to define a Poincaré surface of section as the hyper-plane that goes through x and is normal to the flow at x. In other words the surface of section is determined by

$$(x' - x) \cdot v(x) = 0. \tag{C.3}$$

Note that $f(x)$ lies on this surface. This surface of section is optimal in the sense that a close return on the surface is a local minimum of the distance between x and $f^t(x)$. But more importantly, the part of the stability matrix that describes linearization perpendicular to the flow is exactly the stability of the flow in the surface of section when $f(x)$ is close to x. In this method, the Poincaré surface changes with each iteration of the Newton scheme. Should we later want to put the fixed point on a specific Poincaré surface it will only be a matter of moving along the trajectory.