A Newton-Picard method for accurate computation of period doubling bifurcation points of large-scale systems of ODEs

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Abstract

Periodic solutions of certain large scale systems of ODEs can be computed efficiently using a hybrid Newton-Picard scheme, especially in a continuation context. In this paper we describe and analyse a numerical method to accurately compute period doubling bifurcation points using the Newton-Picard approach. The method avoids the computation of the full monodromy matrix, which is present in the determining system for period doubling bifurcation points. Test results are presented that demonstrate the numerical properties.

Keywords : Periodic solutions, period doubling point, Newton-Picard.
AMS(MOS) Classification : Primary : 65N12, Secondary : 35B32, 35B10.

1 Introduction

1.1 Periodic solutions and bifurcation points

This paper is concerned with the efficient computation of period doubling points on branches of periodic solutions of large- (or infinite-) dimensional dynamical systems with low-dimensional long-term dynamics, such as certain systems of parabolic partial differential equations (PDEs). More specifically, we consider the autonomous dynamical system

$$\frac{dx}{dt} = f(x, \lambda), \quad x \in \mathbb{R}^N, \quad \lambda \in \mathbb{R}. \tag{1}$$

with N 'large' and with f derived from a finite element or finite difference spatial discretisation of a PDE system. We will assume that f is C^3-continuous in x and λ in the region of interest. A point on a branch of periodic solutions is then determined by one point $x(0)$ on the limit cycle, its period T and the parameter value λ. These unknowns can be computed from the boundary value problem with boundary conditions

$$\left\{ \begin{array}{l} x(T) - x(0) = 0 \\ s(x(0), T, \lambda) = 0 \\ n(x(0), T, \lambda; \tau) = 0 \end{array} \right. \tag{2}$$

where $s(x(0), T, \lambda) = 0$ is a phase condition needed to eliminate the time translational invariance of periodic solutions of autonomous dynamical systems, and where $n(x(0), T, \lambda; \tau) = 0$ is the parameterizing equation and τ is an artificial parameter. Using a suitable parameterizing equation, this system will be regular in every point on the branch except in transcritical or pitchfork bifurcation points and other higher-order singularities.

The asymptotic stability of the periodic orbit is determined by the monodromy matrix

$$M = \frac{\partial x(T)}{\partial x(0)}. \tag{3}$$

The eigenvalues of this matrix are called the Floquet multipliers. One Floquet multiplier is always one and the corresponding eigenvector is the tangent vector to the limit cycle in $x(0)$. The limit cycle is asymptotically stable if all other Floquet multipliers lie within the unit circle. Bifurcation points occur if one or more non-trivial Floquet multipliers cross the unit circle.

This paper is concerned with the case of the non-degenerate (codimension 1) period doubling point. In such a point a real Floquet multiplier crosses the unit circle transversally at -1 and, except this one and the trivial Floquet multiplier, no other Floquet multiplier has modulus equal to 1. Such points can be computed by replacing the parameterising equation in (2) by one or more equations expressing the conditions for the Floquet multiplier in terms of $x(0)$, T and λ and probably some additional variables. Our method is designed to work well when only a small number of the Floquet multipliers are close to or outside of the unit circle, while all others are clustered around 0.

1.2 Numerical method

The method presented in this paper is based on the shooting method to solve the boundary value problem (2). We restrict the discussion to single shooting, although this approach has its limitations as discussed in [16]. For a given initial condition $x(0)$, we denote the solution of (1) at $t = T$ by $\varphi(x(0), T, \lambda)$. Single shooting solves (2) by computing $x(0)$, T and λ from the $N + 2$-dimensional nonlinear system

$$\left\{ \begin{array}{l} r(x(0), T, \lambda) := \varphi(x(0), T, \lambda) - x(0)) = 0 \\ s(x(0), T, \lambda) = 0 \\ n(x(0), T, \lambda) = 0. \end{array} \right. \tag{4}$$

We denote a solution of (4) with $(x(0)^*, T^*, \lambda^*)$. Remark that the monodromy matrix M^* and the eigenvector b^* corresponding to the trivial Floquet multiplier are given by

$$M^* = \left. \frac{\partial \varphi}{\partial x(0)} \right|_{(x(0)^*, T^*, \lambda^*)}, \qquad b^* = \left. \frac{\partial \varphi}{\partial T} \right|_{(x(0)^*, T^*, \lambda^*)} = f(x(0)^*, T^*, \lambda^*)$$

respectively. The Floquet multipliers are denoted by μ_i^*, $i = 1, \ldots, N$.

Codimension 1 period doubling points can now be computed by replacing the last equation in (4) with a suitable condition, see e.g. [4, 5, 10]. Our approach is based on a system similar to the system proposed in [4] and used in AUTO94 [2]

$$\left\{ \begin{array}{l} r(x(0), T, \lambda) = \varphi(x(0), T, \lambda) - x(0) = 0 \\ s(x(0), T, \lambda) = 0 \\ (M(x(0), T, \lambda) + I)v = 0 \\ d^T v - 1 = 0. \end{array} \right. \tag{5}$$

This is a $(2N + 2)$-dimensional nonlinear systems with unknowns $x(0)$, T, the parameter λ and an additional unknown v. v is an N-dimensional vector and at the solution point the eigenvector for the Floquet multiplier -1. Since $d^T v = 1$ is a normalization condition, ideally, d should lie as much as possible in the direction of the eigenvector corresponding to the eigenvalue -1. System (5) has a structure which we will be able to exploit in our method. In §2.3 we will argue the particular choice of this extended system over systems requiring fewer or no additional unknowns.

(5) can be solved using Newton's method and a direct linear system solver to solve the resulting linear systems. This approach involves the computation of $M = \frac{\partial \varphi}{\partial x(0)}$ and perhaps even its derivatives. The monodromy matrix M can be calculated by numerical differentiation or by solving the variational equations. In the former case, the nonlinear problem (1) would have to be integrated N times with perturbed initial data, and in the latter case an N^2-dimensional linear initial-value problem has to be integrated together with (1). Both approaches are prohibitively expensive when N is large. Note also that M is a full matrix and has no specific structure even if $\frac{\partial f}{\partial x}$ has, so Newton-like approaches

with direct solvers will also require the expensive storage and factorization of full $N \times N$ or larger matrices. Our method avoids the computation and factorization of the monodromy matrix by combining a simple Picard iteration scheme and a direct (Newton) method. The scheme is based on the Newton-Picard method presented in [12, 15] for solving (4). The resulting method is able to accurately compute period doubling points on branches of stable and unstable periodic solutions and also delivers good estimates for the other dominant Floquet multipliers as a natural by-product.

The remainder of this paper is organised as follows. In §2.1 we will derive the Newton-Picard method for period doubling points. This will require the solution of several smaller linear systems. In §2.2 we will prove that all these subsystems are regular for generic period doubling points. In §2.3 we discuss the particular choice for the extended system. The computational aspects of the method are discussed in §3. This includes a detailed discussion of the cost of our method. In §4, we present some numerical results to illustrate the effectiveness of our approach. Finally §5 contains our conclusions.

2 Newton-Picard methods for period doubling bifurcation points

2.1 Derivation

In deriving our method, we start from the nonlinear system (5) which we solve using Newton's method. This requires the solution of the linear system

$$\begin{bmatrix} M-I & \varphi_T & 0 & \varphi_\lambda \\ s_x & s_T & 0 & s_\lambda \\ M_x v & M_T v & M+I & M_\lambda v \\ 0 & 0 & d^T & 0 \end{bmatrix} \begin{bmatrix} \Delta x(0) \\ \Delta T \\ \Delta v \\ \Delta\lambda \end{bmatrix} = - \begin{bmatrix} r(x(0),T,\lambda) \\ s(x(0),T,\lambda) \\ (M(x(0),T,\lambda)+I)v \\ d^T v - 1 \end{bmatrix}, \tag{6}$$

where

$$\begin{bmatrix} M-I & \varphi_T & 0 & \varphi_\lambda \\ s_x & s_T & 0 & s_\lambda \\ M_x v & M_T v & M+I & M_\lambda v \\ 0 & 0 & d^T & 0 \end{bmatrix} = \frac{\partial(r, s, (M+I)v, d^T v)}{\partial(x(0), T, v, \lambda)}.$$

A partial derivative with respect to $x(0)$ is represented with the subscript x. Remark that φ_T can be computed easily from $\varphi_T = f(\varphi(x(0),T,\lambda),T,\lambda)$. For large N the computation of the full matrices M and $M_x v$ is very costly, both with respect to time and memory. The aim of the Newton-Picard method is to avoid this computation.

We will make the same assumptions as in [12], which we repeat here:

Assumption 2.1 *Let $y^* = (x(0)^*, T^*, v^*, \lambda^*)$ denote an isolated solution to (5) and let $\mathcal{B}$ be a small neighbourhood of y^*. Let $M(y) = \frac{\partial \varphi}{\partial x(0)}(y)$ for $y \in \mathcal{B}$ and denote its eigenvalues by μ_i, $i = 1, \ldots, N$. Assume that for all $y \in \mathcal{B}$ precisely p eigenvalues lie outside the disk*

$$C_\rho = \{|z| < \rho\}, \quad 0 < \rho < 1 \tag{7}$$

and that no eigenvalue has modulus ρ, i.e. for all $y \in \mathcal{B}$

$$|\mu_1| \geq |\mu_2| \geq \cdots \geq |\mu_p| > \rho > |\mu_{p+1}|, \ldots, |\mu_N|.$$

Let $V_p \in \mathbb{R}^{N \times p}$ be a basis for the subspace $\mathcal{U}$ of $\mathbb{R}^N$ spanned by the (generalised) eigenvectors of $M(x(0), T, \lambda)$ corresponding to the eigenvalues μ_i, $i = 1, \ldots, p$ and $V_q \in \mathbb{R}^{N \times (N-p)} = \mathbb{R}^{N \times q}$ a basis for $\mathcal{U}^\perp$, the orthogonal complement of $\mathcal{U}$ in $\mathbb{R}^N$. We note that, in general, $\mathcal{U}^\perp$ is not an invariant subspace of $M(x(0), T, \lambda)$. Our method is designed to be efficient for systems with low-dimensional dynamics where $p \lll q$.

We construct orthogonal projectors P and Q of $\mathbb{R}^N$ onto $\mathcal{U}$ and $\mathcal{U}^\perp$ respectively as

$$\begin{aligned} P &:= V_p V_p^T, \\ Q &:= V_q V_q^T = I_N - V_p V_p^T. \end{aligned} \tag{8}$$

Both $\Delta x(0) \in \mathbb{R}^N$ and $\Delta v \in \mathbb{R}^N$ have a unique decomposition

$$\begin{aligned} &\Delta x(0) = V_p \Delta \bar{x}_p + V_q \Delta \bar{x}_q = \Delta x_p + \Delta x_q = P \Delta x(0) + Q \Delta x(0), \\ &\Delta v = V_p \Delta \bar{v}_p + V_q \Delta \bar{v}_q = \Delta v_p + \Delta v_q = P \Delta v + Q \Delta v, \end{aligned} \tag{9}$$

with Δx_p, Δx_q, Δv_p, $\Delta v_q \in \mathbb{R}^N$, $\Delta \bar{x}_p$, $\Delta \bar{v}_p \in \mathbb{R}^p$ and $\Delta \bar{x}_q$, $\Delta \bar{v}_q \in \mathbb{R}^q$.

After substitution of (9) into (5) and multiplying the first and the third set of equations at the left hand side with $\left[\begin{array}{cc} V_q & V_p \end{array}\right]^T$, we get

$$\begin{bmatrix} V_q^T(M-I)V_q & V_q^T M V_p & V_q^T \varphi_T & 0 & 0 & V_q^T \varphi_\lambda \\ V_p^T M V_q & V_p^T (M-I) V_p & V_p^T \varphi_T & 0 & 0 & V_p^T \varphi_\lambda \\ s_x V_q & s_x V_p & s_T & 0 & 0 & s_\lambda \\ V_q^T M_x v V_q & V_q^T M_x v V_p & V_q^T M_T v & V_q^T (M+I) V_q & V_q^T M V_p & V_q^T M_\lambda v \\ V_p^T M_x v V_q & V_p^T M_x v V_p & V_p^T M_T v & V_p^T M V_q & V_p^T (M+I) V_p & V_p^T M_\lambda v \\ 0 & 0 & 0 & d^T V_q & d^T V_p & 0 \end{bmatrix} \begin{bmatrix} \Delta \bar{x}_q \\ \Delta \bar{x}_p \\ \Delta T \\ \Delta \bar{v}_q \\ \Delta \bar{v}_p \\ \Delta \lambda \end{bmatrix} = - \begin{bmatrix} V_q^T r \\ V_p^T r \\ s \\ V_q^T (M+I) v \\ V_p^T (M+I) v \\ d^T v - 1 \end{bmatrix} \tag{10}$$

where we used $V_q^T V_p = 0$, $V_p^T V_q = 0$. Because $\mathcal{U}$ is an invariant subspace of M we have,

$$V_q^T M V_p = 0. \tag{11}$$

And because in the solution point φ_T^* is the eigenvector of M^* corresponding to the eigenvalue $+1$, we can make the following approximation:

$$\begin{aligned} V_q^T\varphi_T &= V_q^T f(\varphi(x(0),T,\lambda),\lambda) \\ &\approx V_q^{*T} f(\varphi(x(0)^*,T^*,\lambda^*),\lambda^*) = V_q^{*T} f(x(0)^*,\lambda^*) = 0. \end{aligned} \tag{12}$$

The matrix of system (10) reduces to

$$\begin{bmatrix} V_q^T(M-I)V_q & 0 & 0 & 0 & 0 & V_q^T\varphi_\lambda \\ V_p^T M V_q & V_p^T(M-I)V_p & V_p^T\varphi_T & 0 & 0 & V_p^T\varphi_\lambda \\ s_x V_q & s_x V_p & s_T & 0 & 0 & s_\lambda \\ V_q^T M_x v V_q & V_q^T M_x v V_p & V_q^T M_T v & V_q^T(M+I)V_q & 0 & V_q^T M_\lambda v \\ V_p^T M_x v V_q & V_p^T M_x v V_p & V_p^T M_T v & V_p^T M V_q & V_p^T(M+I)V_p & V_p^T M_\lambda v \\ 0 & 0 & 0 & d^T V_q & d^T V_p & 0 \end{bmatrix} \tag{13}$$

Matrix (13) is a rank one update of a block-triangular matrix. The similarity with the continuation variant of [12] suggests the use of the Sherman-Morisson formula to solve (10). Here we will follow a different approach similar to one followed in [13], which has somewhat nicer theoretical properties (see §2.2).

To solve the first q equations of (10) we split $\Delta\bar{x}_q$ according to

$$\Delta\bar{x}_q = \Delta\bar{x}_{q,1} + \Delta\lambda\Delta\bar{x}_{q,2}, \tag{14}$$

and solve $\Delta\bar{x}_{q,1}$ and $\Delta\bar{x}_{q,2}$ from

$$\begin{aligned} V_q^T(M-I)V_q\Delta\bar{x}_{q,1} &= -V_q^T r, \\ V_q^T(M-I)V_q\Delta\bar{x}_{q,2} &= -V_q^T\varphi_\lambda. \end{aligned} \tag{15}$$

From assumption (2.1) and the construction of the basis follows that the spectral radius $r_\sigma(V_q^T M V_q) < \rho < 1$, so we can solve (15) approximately using a Picard iteration scheme:

$$\left\{ \begin{array}{l} \Delta\bar{x}_{q,i}^{[0]} = 0, \quad i = 1,2 \\ \Delta\bar{x}_{q,1}^{[j+1]} = V_q^T M \Delta\bar{x}_{q,1}^{[j]} + V_q^T r, \quad j = 0,\ldots,\nu-1 \\ \Delta\bar{x}_{q,2}^{[j+1]} = V_q^T M \Delta\bar{x}_{q,1}^{[j]} + V_q^T\varphi_\lambda, \quad j = 0,\ldots,\nu-1 \\ \Delta\bar{x}_{q,i} = \Delta\bar{x}_{q,i}^{[\nu]}, \quad i = 1,2. \end{array} \right. \tag{16}$$

After left-multiplying all steps of (16) with V_q, we obtain a Picard iteration to compute the N-dimensional vectors $\Delta x_{q,1} = V_q\Delta\bar{x}_{q,1}$ and $\Delta x_{q,2} = V_q\Delta\bar{x}_{q,2}$. The scheme now reads

$$\left\{ \begin{array}{l} \Delta x_{q,i}^{[0]} = 0, \quad i = 1,2 \\ \Delta x_{q,1}^{[j+1]} = QM\Delta x_{q,1}^{[j]} + Qr, \quad j = 0\ldots\nu-1 \\ \Delta x_{q,2}^{[j+1]} = QM\Delta x_{q,2}^{[j]} + Q\varphi_\lambda, \quad j = 0\ldots\nu-1 \\ \Delta x_{q,i} = \Delta x_{q,i}^{[\nu]}, \quad i = 1,2. \end{array} \right. \tag{17}$$

Since $Q = V_qV_q^T = I - V_pV_p^T$, the basis V_q is no longer needed.

Substituting $\Delta x_{q,1}$ and $\Delta x_{q,2}$ in the next $p+1$ equations of (10) gives

$$\begin{aligned}\left[\begin{array}{cc} V_p^T(M-I)V_p & V_p^T\varphi_T \\ s_xV_p & s_T\end{array}\right]\left[\begin{array}{c}\Delta\bar{x}_p \\ \Delta T\end{array}\right] = & -\left[\begin{array}{c} V_p^Tr+V_p^TM\Delta x_{q,1} \\ s+s_x\Delta x_{q,1}\end{array}\right] \\ & -\Delta\lambda\left[\begin{array}{c} V_p^T\varphi_\lambda + V_p^TM\Delta x_{q,2} \\ s_\lambda+s_x\Delta x_{q,2}\end{array}\right].\end{aligned} \tag{18}$$

As in (14) we split $\Delta\bar{x}_p$ and ΔT as

$$\begin{aligned}\Delta\bar{x}_p &= \Delta\bar{x}_{p,1} + \Delta\lambda\Delta\bar{x}_{p,2}, \\ \Delta T &= \Delta T_1 + \Delta\lambda\Delta T_2,\end{aligned}$$

and solve $\Delta\bar{x}_{p,1}$, $\Delta\bar{x}_{p,2}$, ΔT_1 and ΔT_2 from

$$\begin{aligned}&\left[\begin{array}{cc} V_p^T(M-I)V_p & V_p^T\varphi_T \\ s_xV_p & s_T\end{array}\right]\left[\begin{array}{cc}\Delta\bar{x}_{p,1} & \Delta\bar{x}_{p,2} \\ \Delta T_1 & \Delta T_2\end{array}\right] \\ &= -\left[\begin{array}{cc} V_p^Tr+V_p^TM\Delta x_{q,1} & V_p^T\varphi_\lambda+V_p^TM\Delta x_{q,2} \\ s+s_x\Delta x_{q,1} & s_\lambda+s_x\Delta x_{q,2}\end{array}\right],\end{aligned}$$

which is a small $(p+1)\times(p+1)$ system that is easily solved using Gauss elimination with partial or full pivoting.

Similarly we can split

$$\Delta\bar{v}_q = \Delta\bar{v}_{q,1} + \Delta\lambda\Delta\bar{v}_{q,2}$$

and solve $\Delta\bar{v}_{q,1}$ and $\Delta\bar{v}_{q,2}$ from

$$\begin{aligned}V_q^T(M+I)V_q\Delta\bar{v}_{q,1} &= -V_q^T((M+I)v + M_xv(V_p\Delta\bar{x}_{p,1}+\Delta x_{q,1}) + M_Tv\Delta T_1), \\ V_q^T(M+I)V_q\Delta\bar{v}_{q,2} &= -V_q^T(M_\lambda v + M_xv(V_p\Delta\bar{x}_{p,2}+\Delta x_{q,2}) + M_Tv\Delta T_2).\end{aligned} \tag{19}$$

The matrix $V_q^T(M+I)V_q$ is very similar to the matrix $V_q^T(M-I)V_q$ of (16). We again solve the system using a Picard scheme, which we immediately write for the N-dimensional vectors $\Delta v_{q,1} = V_q\Delta\bar{v}_{q,1}$ and $\Delta v_{q,2} = V_q\Delta\bar{v}_{q,2}$.

$$\left\{\begin{array}{l} r_1 = -((M+I)v + M_xv(V_p\Delta\bar{x}_{p,1}+\Delta x_{q,1}) + M_Tv\Delta T_1) \\ r_2 = -(M_\lambda v + M_xv(V_p\Delta\bar{x}_{p,2}+\Delta x_{q,2}) + M_Tv\Delta T_2) \\ \Delta v_{q,i}^{[0]} = 0, \quad i = 1,2 \\ \Delta v_{q,i}^{[j+1]} = -QM\Delta v_{q,i}^{[j]} + Qr_i, \quad j = 0,\ldots,\nu-1, \quad i = 1,2 \\ \Delta v_{q,i} = \Delta v_{q,i}^{[\nu]}, \quad i = 1,2.\end{array}\right. \tag{20}$$

It remains to determine $\Delta\bar{v}_p$ and $\Delta\lambda$ from the last $p+1$ equations. After substituting Δx_q, $\Delta\bar{x}_p$, ΔT and Δv_q in these equations and moving all terms not depending on the unknown $\Delta\lambda$ to the right hand side, we obtain the $(p+1)\times(p+1)$ system

$$\left[\begin{array}{cc} V_p^T(M+I)V_p & g \\ d^TV_p & d^T\Delta v_{q,2}\end{array}\right]\left[\begin{array}{c}\Delta\bar{v}_p \\ \Delta\lambda\end{array}\right] = -\left[\begin{array}{c} h \\ d^T(v+\Delta v_{q,1})-1\end{array}\right] \tag{21}$$

with

$$\begin{aligned} g &= V_p^T(M_\lambda v + M\Delta v_{q,2} + M_T v\Delta T_2 + M_x v(V_p\Delta\bar{x}_{p,2} + \Delta x_{q,2})), \\ h &= V_p^T((M+I)v + M\Delta v_{q,1} + M_T v\Delta T_1 + M_x v(V_p\Delta\bar{x}_{p,1} + \Delta x_{q,1})). \end{aligned} \tag{22}$$

After solving (21) with Gaussian elimination and partial pivoting all unknowns can be fully calculated:

$$\begin{aligned} &\Delta x(0) = V_p\Delta\bar{x}_{p,1} + \Delta x_{q,1} + \Delta\lambda(V_p\Delta\bar{x}_{p,2} + \Delta x_{q,2}), \\ &\Delta T = \Delta T_1 + \Delta\lambda\Delta T_2, \\ &\Delta v = V_p\Delta\bar{v}_p + \Delta v_{q,1} + \Delta\lambda\Delta v_{q,2}. \end{aligned}$$

2.2 Mathematical motivation of the method

To motivate our method, we will now proof that the extended system (5) has a regular Jacobian matrix at the period doubling point and that the subsystems (15), (18), (19) and (21) are regular.

We first give a lemma stating the mathematical condition for transversal crossing of the unit circle by the Floquet multiplier -1.

Lemma 2.1 *Suppose $(x(0), T, \lambda)$ is a period doubling point. Suppose $+1$ and -1 are algebraically simple eigenvalues of $\varphi_x = M(x(0), T, \lambda)$. Suppose w_{-1} and v_{-1} are left and right eigenvalues of φ_x for the eigenvalue -1. The transversality condition is then satisfied iff*

$$k = w_{-1}^T\left[\varphi_{x\,\lambda}v_{-1} - \varphi_{x\,(x,T)}v_{-1}\begin{bmatrix} \varphi_x - I & \varphi_T \\ s_x & s_T \end{bmatrix}^{-1}\begin{bmatrix} \varphi_\lambda \\ s_\lambda \end{bmatrix}\right] \neq 0 \tag{23}$$

where $s(x(0), T, \lambda) = 0$ is any phase condition satisfying $s_x^T\varphi_T \neq 0$.

The proof of this lemma is long and of no particular interest for the remaining of the paper. The condition is very similar to the condition in terms of the Poincaré return map given in [14]. Remark that the coefficient k is independent of the choice of the phase condition s as long as $s_x^T\varphi_T \neq 0$ is satisfied ($s_x^T\varphi_T \neq 0$ is the condition for transversal crossing of the limit cycle and the manifold $s = 0$).

To prove the regularity of the extended system in a non-degenerate simple period doubling point we need an additional lemma.

Lemma 2.2 *Let $A \in \mathbb{R}^{N\times N}$ have an algebraically simple eigenvalue 0 with corresponding eigenvector v. Let $b, c \in \mathbb{R}^N$, $d \in \mathbb{R}$. Suppose $b \notin \mathrm{Range}(A)$. Let*

$$\bar{A} = \begin{bmatrix} A & b \\ c^T & d \end{bmatrix}$$

then $\bar{A}$ is regular iff $c^T v \neq 0$.

Proof 2.2 *$\bar{A}$ is regular $\underline{\text{iff}}$ the only solution to the system*

$$\begin{bmatrix} A & b \\ c^T & d \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}, \quad x \in \mathbb{R}^N, \quad y \in \mathbb{R} \tag{24}$$

is the null vector. The first N equations read $Ax + by = 0$. Since $b \notin \mathrm{Range}(A)$, $y = 0$. From $Ax = 0$ follows $x = kv$, $k \in \mathbb{R}$, and after substitution in the last equation we get $k\, c^T v = 0$. So (24) has only solutions different from the null vector when $c^T v = 0$.

We first proof the regularity of the extended system.

Lemma 2.3 *Suppose the conditions from lemma 2.1 hold and (23) is satisfied. Suppose also $d^T v_{-1} \neq 0$. Then:*

$$E = \begin{bmatrix} \varphi_x - I & \varphi_T & 0 & \varphi_\lambda \\ s_x & s_T & 0 & s_\lambda \\ \varphi_{xx} v_{-1} & \varphi_{xT} v_{-1} & \varphi_x + I & \varphi_{x\lambda} v_{-1} \\ 0 & 0 & d^T & 0 \end{bmatrix}$$

is regular.

Proof 2.3 *Since 1 is an algebraically simple eigenvalue of φ_x, $\varphi_T \notin \mathrm{Range}(\varphi_x - I)$. Furthermore we have $s_x^T \varphi_T \neq 0$. Thus, following lemma 2.3,*

$$\begin{bmatrix} \varphi_x - I & \varphi_T \\ s_x & s_T \end{bmatrix}$$

is regular. According to lemma 2.8 from [8], E is regular $\underline{\text{iff}}$

$$\begin{aligned} E_c &= \begin{bmatrix} \varphi_x + I & \varphi_{x\lambda} v_{-1} \\ d^T & 0 \end{bmatrix} \\ &\quad - \begin{bmatrix} \varphi_{xx} v_{-1} & \varphi_{xT} v_{-1} \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \varphi_x - I & \varphi_T \\ s_x & s_T \end{bmatrix}^{-1} \begin{bmatrix} 0_{N\times p} & \varphi_\lambda \\ 0_{1\times p} & s_\lambda \end{bmatrix} \\ &= \begin{bmatrix} \varphi_x + I & \varphi_{x\lambda} v_{-1} - \varphi_{x\,(x,T)} v_{-1} \begin{bmatrix} \varphi_x - I & \varphi_T \\ s_x & s_T \end{bmatrix}^{-1} \begin{bmatrix} \varphi_\lambda \\ s_\lambda \end{bmatrix} \\ d^T & 0 \end{bmatrix} \\ &= \begin{bmatrix} \varphi_x + I & t \\ d^T & 0 \end{bmatrix} \end{aligned}$$

is regular. The transversality condition $k = w_{-1}^T t \neq 0$ implies that $t \notin \mathrm{Range}(\varphi_x + I)$. Furthermore $d^T v \neq 0$. Therefore E_c and (thus) E are regular.

The above lemmas permit us to show the regularity of all subsystems solved in our method under the condition that they are solved exactly. We will again use M as a shorthand for φ_x.

Lemma 2.4 *Suppose the conditions from lemma 2.3 hold. Furthermore suppose the subsystems (15), (18) and (19) are solved exactly. Then at the period doubling point, the matrices*

$$V_q^T(M-I)V_q, \tag{25}$$

$$\begin{bmatrix} V_p^T(M-I)V_p & V_p^T\varphi_T \\ s_x^T V_p & s_T \end{bmatrix}, \tag{26}$$

$$V_q^T(M+I)V_q \tag{27}$$

and

$$\begin{bmatrix} V_p^T(M+I)V_p & g \\ d^T & d^T\Delta v_{q,2} \end{bmatrix} \tag{28}$$

are regular.

Proof 2.4 *The regularity of*

$$M_1 = \begin{bmatrix} M-I & \varphi_T \\ s_x & s_T \end{bmatrix}$$

follows from the proof of lemma 2.3. Furthermore,

$$V = \begin{bmatrix} V_q & V_p & 0_{N\times 1} \\ 0_{1\times q} & 0_{1\times p} & 1 \end{bmatrix}$$

is an orthonormal matrix, so

$$V^T M_1 V = \begin{bmatrix} V_q^T(M-I)V_q & 0 & 0 \\ V_p^T M V_q & V_p^T(M-I)V_p & V_p^T\varphi_T \\ s_x V_q & s_x V_p & s_T \end{bmatrix}$$

is regular and thus also (25) and (26).

Since $r_\sigma(V_q^T M V_q) < \rho < 1$*, all eigenvalues of (27) lie in a circle with radius* $\rho < 1$ *around 1, thus (27) is also regular.*

The regularity of (28) can be shown as follows. From the transversality condition it follows that

$$t = \left[M_\lambda v_{-1} - M_{(x,T)} v_{-1} \begin{bmatrix} M-I & \varphi_T \\ s_x & s_T \end{bmatrix}^{-1} \begin{bmatrix} \varphi_\lambda \\ s_\lambda \end{bmatrix} \right] \notin \mathrm{Range}(M+I).$$

Since also $d^T v \neq 0$*,*

$$M_2 = \begin{bmatrix} M+I & t \\ d^T & 0 \end{bmatrix}$$

and thus also

$$V^T M_2 V = \begin{bmatrix} V_q^T(M+I)V_q & 0 & V_q^T t \\ V_p^T M V_q & V_p^T(M+I)V_p & V_p^T t \\ d^T V_q & d^T V_p & 0 \end{bmatrix}$$

are regular matrices. This implies (lemma 2.8 from [8], (19) and the regularity of (27)) that

$$\begin{aligned} E_v &= \begin{bmatrix} V_p^T(M+I)V_p & V_p^T t \\ d^T V_p & 0 \end{bmatrix} \\ &- \begin{bmatrix} V_p^T M V_q \\ d^T V_q \end{bmatrix} \left(V_q^T(M+I)V_q\right)^{-1} \begin{bmatrix} 0_{q\times p} & V_q^T t \end{bmatrix} \\ &= \begin{bmatrix} V_p^T(M+I)V_p & V_p^T(t+M\Delta v_{q,2}) \\ d^T V_p & d^T \Delta v_{q,2} \end{bmatrix} \end{aligned}$$

is regular. Since

$$V_p^T(t+M\Delta v_{q,2}) = V_p^T(M_\lambda v + M_x v(V_p \Delta \bar{x}_{p,2} + \Delta x_{q,2}) + M_T v \Delta T_2 + M \Delta v_{q,2}) = g,$$

E_v is just the matrix of the linear system (21).

The regularity is only proved at the solution point and when (15), (18) and (19) are solved exactly. However, regular matrices remain regular under small perturbations, so we have good confidence that the actual subsystems will also be regular. This is confirmed by the test results.

2.3 Discussion of alternatives

Instead of using a determining system of dimension $(2N+1)$, some authors prefer to work with an $(N+2)$-dimensional system

$$\left\{ \begin{array}{l} \varphi(x(0),T,\lambda) - x(0) = 0 \\ s(x(0),T,\lambda) = 0 \\ n(x(0),T,\lambda) = 0, \end{array} \right. \tag{29}$$

where $n(x(0),T,\lambda) = 0$ is a scalar equation expressing the condition for a period doubling point (e.g. $\det(M(x(0),T,\lambda)+I) = 0$). Examples can be found in [10]. However for the evaluation of n one typically needs the full matrix M, which is exactly what we wish to avoid.

Another alternative is obtained from the observation that, in a solution point, all information about v and the Floquet multiplier crossing the unit circle is present in the projected matrix $V_p^T M V_p$. This is so because $v^* \in \mathcal{U}^*$. Therefore our technique (as well as (29)) can be reformulated in terms of the projected matrix. In our case, this would lead to a reduced, $(N+p+1)$-dimensional system

$$\left\{ \begin{array}{l} \varphi(x(0),T,\lambda) - x(0) = 0 \\ s(x(0),T,\lambda) = 0 \\ V_p^T(M(x(0),T,\lambda)+I)V_p \bar{v} = 0. \end{array} \right. \tag{30}$$

There are two problems with (30) and other methods based on the projected matrix. The first problem is that $v = V_p \bar{v}$ is restricted to the subspace $\mathcal{U}$.

Consequently, for a high accuracy of v, V_p needs to be accurate. We will see in §4 that in our method we don't need a very accurate basis to obtain a high accuracy for v. The second problem with the projected matrix is that $\mathcal{U}$ depends on $x(0)$, T and λ. One implicitly or explicitly needs to compute derivatives of V_p with respect to the variables, which requires that the basis changes smoothly (see e.g. [1, 6]).

3 Computational aspects

Our algorithm avoids the use of $\Delta\bar{x}_q$ and $\Delta\bar{v}_q$. As a consequence we do not need the basis V_q. A Q-projection is calculated using $Q = I_N - V_p V_p^T$. Therefore every step of our algorithm requires the calculation (or updating) of the basis V_p and the calculation of a number of matrix vector products with M and partial derivatives of M.

Since the computed v is allowed to have components in the computed $\mathcal{U}$ as well as in $\mathcal{U}^{\perp}$, a very high accuracy for the basis is not needed. We use the same code as in [12] to compute and adapt the basis. This amounts to approximately one subspace iteration step per Newton-Picard iteration.

The work in each Newton-Picard step can be summed up as follows: We need the evaluation of $\varphi(x(0), T, \lambda)$; we need a number of matrix-vector products with M: p in each subspace iteration step, one for the righthand side of (6), $2(\nu - 1)$ in the Picard scheme (17), two for the righthand side of (18), $2(\nu - 1)$ in the Picard scheme (20) and another two in (22); and we need to evaluate the partial derivatives $M_x v(V_p \Delta\bar{x}_{p,1} + \Delta x_{q,1})$, $M_x v(V_p \Delta\bar{x}_{p,2} + \Delta x_{q,2})$, $M_\lambda v$ and $M_T v$.

A matrix-vector product with M is a directional derivative and can be calculated with a finite difference formula. The first-order formula

$$Mv \approx \frac{\varphi(x(0) + \epsilon_1 v, T, \lambda) - \varphi(x(0), T, \lambda)}{\epsilon_1} \tag{31}$$

requires one extra time integration. Second order derivatives can be calculated similarly,

$$\begin{aligned}
M_x v \Delta x &\approx \frac{\varphi(x(0)+\epsilon_1 v+\epsilon_2 \Delta x, T, \lambda)+\varphi(x(0), T, \lambda)-\varphi(x(0)+\epsilon_2 \Delta x, T, \lambda)-\varphi(x(0)+\epsilon_1 v, T, \lambda)}{\epsilon_1 \epsilon_2}, \\
M_\lambda v &\approx \frac{\varphi(x(0)+\epsilon_1 v, T, \lambda+\epsilon_3)+\varphi(x(0), T, \lambda)-\varphi(x(0), T, \lambda+\epsilon_3)-\varphi(x(0)+\epsilon_1 v, T, \lambda)}{\epsilon_1 \epsilon_3}, \\
M_T v &\approx \frac{f(\varphi(x(0), T, \lambda)+\epsilon_4 M v, \lambda)-f(\varphi(x(0), T, \lambda), \lambda)}{\epsilon_4}.
\end{aligned} \tag{32}$$

We remark that a number of terms in these expressions can be reused from (31).

Using the formulas (31) and (32) the total work in each step amounts to $p + 4\nu + 8$ time integrations. This contrasts with the number of N time integrations to compute the full monodromy matrix.

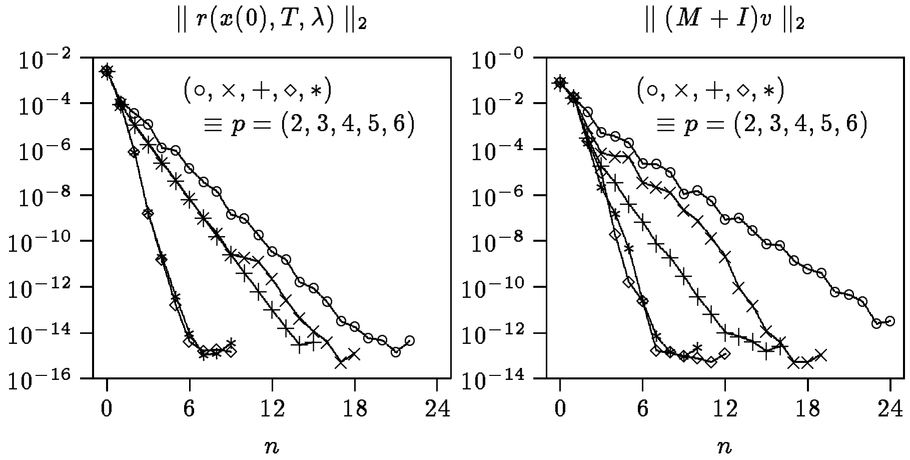

Figure 1: Convergence evolution for different values of the parameter p, using $\nu = 1$. The starting value for v is normalized to one.

4 Numerical results

4.1 Model

The model we used is a reaction-diffusion system studied by Elezgaray and Arneodo in [3].

$$\begin{cases} \frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial^2 x} + \frac{1}{\epsilon}(v - (u^2 + u^3)) \\ \frac{\partial v}{\partial t} = D\frac{\partial^2 v}{\partial^2 x} + \alpha - u \end{cases} \tag{33}$$

with Dirichlet boundary conditions:

$$\begin{cases} u(0,t) \equiv u(1,t) \equiv -2 \\ v(0,t) \equiv v(1,t) \equiv -4 \end{cases}$$

D is used as the bifurcation parameter and ϵ and α are kept constant at 0.01. A bifurcation diagram can be found in [7].

For the space discretization we use the classical second order central difference scheme, which leads to a large system of ordinary differential equations. When using only a small number of discretisation points, the bifurcation diagram is not completely reproduced. This is caused by steep space gradients in the solution.

4.2 Tests

To test the algorithm, we computed a number of period doubling points of (33) on both stable and unstable branches, using 15 respectively 31 discretisation points.

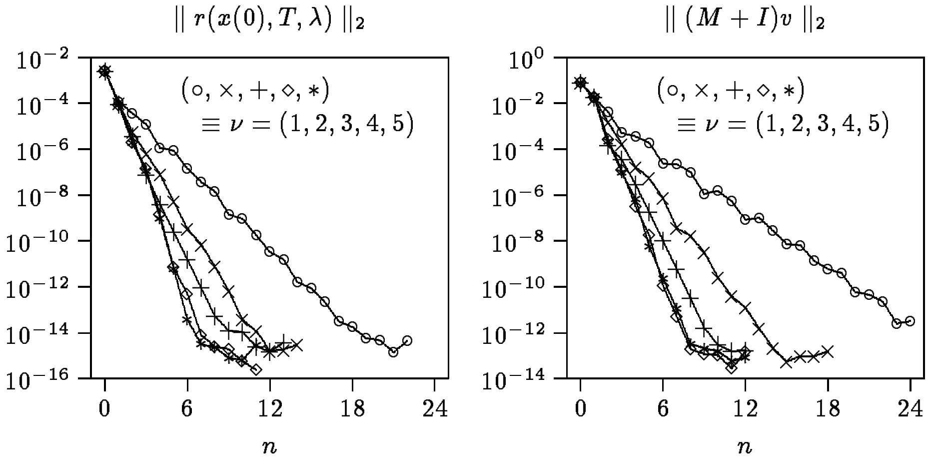

Figure 2: Convergence evolution for different values of the parameter ν, using $p=2$.

As a starting point, we used points on a branch of periodic solutions quite far from the period doubling point. For instance, at the starting point the Floquet multiplier closest to -1 was around 0.9. As a starting value for v, we used the Schur vector corresponding to the Floquet multiplier closest to -1 (although the eigenvector would be a better approximation). Better starting values could have been easily obtained, but this was not necessary for convergence. We also succesfully used starting points with perturbed initial points that are no longer on any branch of periodic orbits. This was done to simulate the effect of a predictor when one is following a branch of period doubling bifurcation points in function of a second parameter.

We will illustrate our results and the influence of the parameters p and ν using a bifurcation point with as largest Floquet multipliers,

$$\begin{aligned}
\mu_1 &= +1.000,\\
\mu_2 &= -1.000,\\
\mu_{3,4} &= +0.173 \pm 0.354i,\\
\mu_5 &= +0.158,\\
\mu_6 &= +0.0136,\\
\mu_7 &= +0.00958,\\
\mu_8 &= +0.000370.
\end{aligned}$$

Figure 1 shows the influence of p (the dimension of $\mathcal{U}$) on the convergence. Figure 2 shows the influence of the parameter ν on the convergence. The overall convergence speed is limited by the convergence of the Picard part, the accuracy of the basis, the accuracy of the calculated second order partial derivatives and second order effects.

The convergence speed was found to be highly dependent on the calculations (32). In our tests we used forward differences but some tuning of the parameters

ϵ_1 and ϵ_2 was necessary. The use of central differences leaves a greater margin in the choice of ϵ_1 and ϵ_2, indicating the presence of large second order terms.

As a final remark we note that at convergence

$$\begin{aligned}
&\|v\|_2 \approx \|v_p\|_2 \approx 1.0133,\\
&\|v_q\|_2 \approx 1.2\ 10^{-6},\\
&\|(M+I)v\|_2 \approx 5.0\ 10^{-14},\\
&\|(M+I)v_p\|_2 \approx 7.8\ 10^{-6}.
\end{aligned}$$

Thus we can conclude that in our method the accuracy of the basis of the invariant subspace will have an influence on convergence speed (due to the neglected term $V_q^T M V_p$) but not on the accuracy of the computed solution point.

5 Conclusions

In this paper we developed a Newton-Picard method for computing period doubling bifurcation points of large-scale systems of ODEs based on a similar method for the computation of periodic solutions [12, 15]. The method is based on an extended system and involves only matrix-vector products with the monodromy matrix and does not require the computation of the monodromy matrix itself. This approach is particularly efficient for systems that exhibit low-dimensional behaviour as is the case in many physically important systems.

The method is based on single shooting. This has the advantage that memory requirements remain low, but the disadvantage that it is hard or even impossible to compute period doubling points on limit cycles with large Floquet multipliers or limit cycles with long period. However, in the forthcoming paper [11] we show how the basic Newton-Picard method can be extended to multiple shooting [9, 16]. We strongly believe that the ideas presented in this paper can also be extended to other types of bifurcation points such as fold points and torus bifurcation points.

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