

MATRIX-FREE NUMERICAL CONTINUATION AND BIFURCATION¹

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Abstract. A numerical continuation method traces solution branches of a nonlinear system

$$H(\lambda, x) = 0, \quad H : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$$

which is typically obtained by discretizing a parameter dependent operator equation. The method is called matrix-free if the Jacobian of H is not calculated explicitly, but its action on a vector is given via a difference approximation of a directional derivative. In connection with modern (transpose-free) iterative linear solvers, this is a suitable approach for large systems. We give an introduction into the technique of matrix-free numerical continuation and analyze those recent approaches to numerical bifurcation which permit a matrix-free approach. A sequence of MATLAB codes, which can be viewed as a blueprint for the numerical implementation of this approach, is currently under construction and will be made available on the internet. Parts of this manuscript are based on the 200 page article [2].

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AMS subject classifications. 65H20, 37M20, 49M15

1 Matrix-Free Iterative Methods

Given a nonlinear system of equations $F(x) = 0$ where $F : \mathbb{R}^N \rightarrow \mathbb{R}^N$, we call an iterative method for finding its solution *matrix-free* if the Jacobian $F'(x)$ at a point x is only implemented through its action on a vector v . That is, only an implementation of the function $(x, v) \mapsto F'(x)v$ is exploited. An example is the forward difference approximation

$$F'(x)v \approx \frac{F(x + \epsilon v) - F(x)}{\epsilon}$$

for an $\epsilon > 0$ of suitable size. This is a viewpoint that enjoys increasing popularity for large systems. Sparseness is automatically taken into account.

A suitable iterative solver of $F(x) = 0$ could be an inexact Newton's method:

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take initial guess x_1
 for $k = 1, 2, \dots$ until convergence
 find Δx_k such that $\|F(x_k) + F'(x_k)\Delta x_k\| \leq \eta_k \|F(x_k)\|$
 set $x_{k+1} := x_k + \Delta x_k$,

where Δx_k is determined via an iterative (transpose-free) linear solver such as GMRES, CGS, or TFQMR. Also Broyden's method can be implemented in a matrix-free context.

Let us describe this situation by saying that the solution to $F(x) = 0$ is numerically approximated in a *matrix-free double loop*. The outer loop is represented by the Newton iteration, the inner loop is represented by the iterative linear solver, and the *essential* numerical expense of one step of the inner loop consists of one call of the function F .

In the following, we describe how a matrix-free approach can be used in the context of numerical continuation and bifurcation. In Section 2 we describe the standard steps of following a solution branch which is implicitly given by a system $H(x) = 0$ where $H : \mathbb{R}^{N+1} \rightarrow \mathbb{R}^N$. In Section 3 we show how to find a special point on the solution branch characterized by one additional nonlinear equation. In Section 4 we locate a point on the curve that is characterized as a local minimal point with respect to a function. In particular, fold points are of this type. In Section 5 we investigate how simple bifurcation points can be detected and approximated in a matrix-free approach, and in Section 6 we turn our attention to simple Hopf bifurcation points. In Section 7 we discuss preconditioners. It turns out that for Hopf bifurcation, preconditioning the matrix-free approach is a difficult problem that needs further investigation. Finally, in Section 8, we discuss how higher derivatives of the solution curve can be obtained in a matrix-free setting.

2 Matrix-Free Predictor-Corrector Methods

One of the primary applications of continuation methods involves the numerical solution of nonlinear eigenvalue problems. Such problems are likely to have arisen from a discretization of an operator equation in a Banach space context which also involves an additional bifurcation parameter. As a result of the discretization and the wish to maintain a reasonably low truncation error, the corresponding finite dimensional problem

$$H(\lambda, x) = H(u) = 0$$

where $H : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$, may require that N be quite large. Other applications may view λ as a homotopy or a penalty and smoothing parameter. This then leads to the task of solving large scale continuation problems.

The aim is to approximate a branch of solutions

$$s \mapsto u(s) = (\lambda(s), x(s))$$

where s is a suitable parameter, e.g., arc-length. The parameter s is usually not explicitly used.

A numerical continuation (predictor-corrector) method repeats two steps:

1. A predictor step generates an approximate point further along the solution curve, typically by linear extrapolation.
2. A corrector step finds a point approximately on the solution curve and close to the predicted point, typically by Newton-like steps.

Figure 1 illustrates this situation.

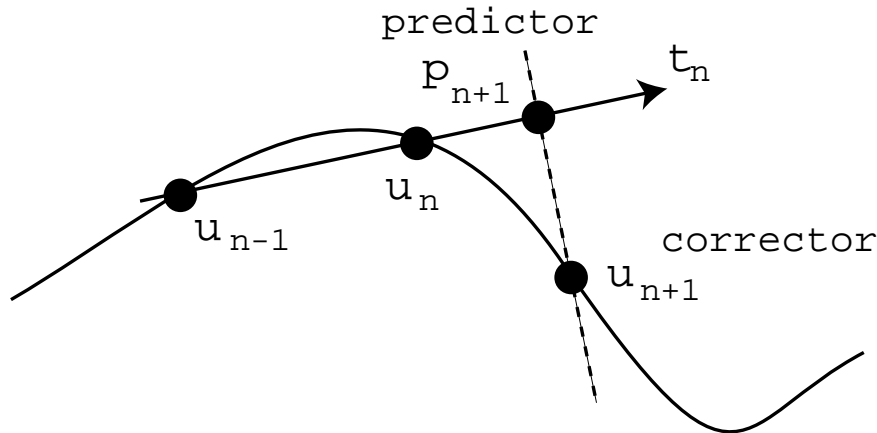


Figure 1: A Predictor-Corrector Step

The following algorithm sketches a possible implementation of this idea. Here and in the following $(\cdot)^*$ denotes the transpose.

Algorithm 2.1 (Matrix-Free Predictor-Corrector).

1. **Initialization**

- choose initial point u_0 such that $H(u_0) = 0$
- choose initial direction t_0 such that $H'(u_0)t_0 \approx 0$, $\|t_0\| = 1$
- choose initial step size $h_0 > 0$
- choose small reduction factor $1 \gg \eta > 0$

2. for $n = 0, 1, 2, \dots$

(a) **Predictor**

$$p_{n+1} := u_n + h_n t_n$$

(b) **Corrector**

find Δp_{n+1} such that

$$\left\| \begin{pmatrix} H(p_{n+1}) \\ 0 \end{pmatrix} + \begin{pmatrix} H'(p_{n+1}) \\ t_n^* \end{pmatrix} \Delta p_{n+1} \right\| \leq \eta \left\| \begin{pmatrix} H(p_{n+1}) \\ 0 \end{pmatrix} \right\|$$

via a transpose-free iterative linear solver

$$u_{n+1} := p_{n+1} + \Delta p_{n+1}$$

(c) **Step-length control**

determine h_{n+1}

(d) **Approximate tangent**

$$t_{n+1} := \frac{u_{n+1} - u_n}{\|u_{n+1} - u_n\|}$$

Remark 2.1. The corrector step solves approximately

$$\begin{pmatrix} H(u) \\ t_n^*(u - p_{n+1}) \end{pmatrix} = 0$$

for u . In our example, we used one corrector step which often is sufficient. However, more corrector steps (e.g., until convergence) can be employed.

Remark 2.2. A new approximate tangent can also be found by solving the linear system

$$\begin{pmatrix} H'(u_{n+1}) \\ t_n^* \end{pmatrix} t = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

for t and then setting $t_{n+1} := t/\|t\|$. This can be done in a matrix-free single loop. Figure 2 illustrates a tangential predictor-corrector step.

3 Finding a Special Point: $\varphi(u(s)) = 0$

When tracing the solution branches of a nonlinear eigenvalue problem, an engineer or scientist usually is particularly interested in special points on this branch. They can be of various types. We begin with the simplest case: Let $\varphi : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}$. We seek a point \bar{u} on the solution branch such that $\varphi(\bar{u}) = 0$. For example, this could be a solution for a particular λ -value, in which case $\varphi(u) := \varphi(\lambda, x) = \lambda - \lambda_0$.

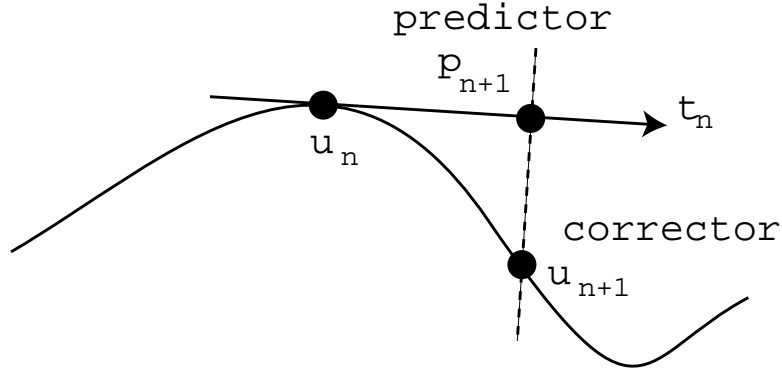


Figure 2: A Tangential Predictor-Corrector Step

The approach is straightforward: During the numerical continuation, we monitor the sign of φ . Assume that a situation $\varphi(u_{n-1})\varphi(u_n) < 0$ is encountered. Then we introduce the approximate tangent

$$T := \frac{u_n - u_{n-1}}{\|u_n - u_{n-1}\|}$$

and the linear approximations

$$p(s) = u_{n-1} + sT \approx u(s)$$

and

$$\psi(s) = \varphi(u_{n-1}) + s \frac{\varphi(u_n) - \varphi(u_{n-1})}{\|u_n - u_{n-1}\|} \approx \varphi(u(s)).$$

If we define \bar{s} via $\psi(\bar{s}) = 0$, then $p(\bar{s})$ is a quadratic approximation of \bar{u} .

We have two options for approximating \bar{u} more precisely:

3.1 Finding a Special Point: $\varphi(u(s)) = 0$: Global approach

Solve

$$\begin{pmatrix} H(u) \\ \varphi(u) \end{pmatrix} = 0$$

via an iterative nonlinear solver, starting at the interpolated point $p(\bar{s})$. Note that this is generally a very good starting point. The method is implemented as a matrix-free double loop.

3.2 Finding a Special Point: $\varphi(u(s)) = 0$: Path-Following Approach

Now let $q(s)$ be the solution of

$$\begin{pmatrix} H(q) \\ T^*(q - p(s)) \end{pmatrix} = 0 .$$

Hence, $q(s)$ can be viewed as the corrector-point to the predictor point $p(s)$. Note that $q(0) = u_{n-1}$ and $q(\|u_n - u_{n-1}\|) = u_n$. Clearly, $q(s)$ can be approximated via an iterative nonlinear solver using a matrix-free double loop. We now find a zero of the function $s \mapsto \varphi(q(s))$ via a secant-like method (e.g., Brent's Method).

This method is implemented as a matrix-free triple loop, the outer loop being the secant-like method. Hence it seems that this is inferior to the method proposed in the last subsection. However, a modification of this second approach can be implemented into the numerical continuation method as a steplength strategy. See Allgower and Georg [2, Section 8.1] for details. This modification permits a matrix-free implementation consisting of a double loop.

4 Finding a Special Point: $\min_s \varphi(u(s))$

The next more complicated situation is a fold-point, as illustrated in Figure 3.

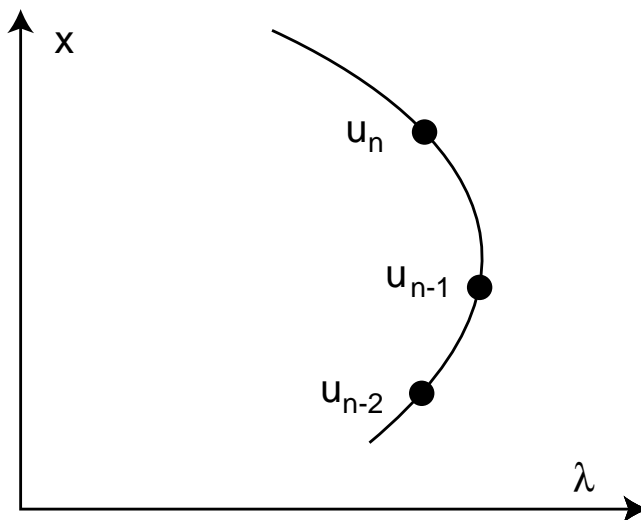


Figure 3: Detecting a Foldpoint

We describe the situation somewhat more generally: Let $\varphi : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}$. We seek a point \bar{u} on the solution branch such that $\varphi(\bar{u})$ has a local minimal value.

We proceed as follows: During the numerical continuation, we monitor for the occurrence of the situation $\varphi(u_{n-2}) > \varphi(u_{n-1}) < \varphi(u_n)$. If this is observed, then we have detected a local minimal point \bar{u} .

We again introduce an approximate tangent

$$T := \frac{u_n - u_{n-2}}{\|u_n - u_{n-2}\|}$$

and the linear approximation

$$p(s) = u_{n-2} + sT \approx u(s) .$$

Next, we find the projection $p(s_1)$ of u_{n-1} onto the line $p(s)$:

$$s_1 = T^*(u_{n-1} - u_{n-2}) .$$

Next, let $r(s)$ be a quadratic polynomial in s with coefficients in $\mathbb{R} \times \mathbb{R}^N$ such that $r(0) = u_{n-2}$, $r(s_1) = u_{n-1}$, and $r(\|u_n - u_{n-2}\|) = u_n$, and let $\psi(s)$ be a quadratic polynomial in s with coefficients in \mathbb{R} such that $\psi(0) = \varphi(u_{n-2})$, $\psi(s_1) = \varphi(u_{n-1})$, and $\psi(\|u_n - u_{n-2}\|) = \varphi(u_n)$. Then ψ has a unique minimal point \bar{s} , and

$$\bar{u} \approx r(\bar{s}) \tag{4.1}$$

is a quadratic approximation of \bar{u} .

We have two options for approximating \bar{u} more precisely:

4.1 Finding a Special Point: $\min_s \varphi(u(s))$: Global Approach

Define a tangent field $t(u)$ as the solution of the linear equations

$$\begin{pmatrix} H'(u) \\ T^* \end{pmatrix} t(u) = \begin{pmatrix} 0 \\ 1 \end{pmatrix} . \tag{4.2}$$

Note that $t(u)$ can be calculated via a matrix-free single loop. Now solve the nonlinear equations

$$\begin{pmatrix} H(u) \\ \varphi'(u)t(u) \end{pmatrix} = 0. \tag{4.3}$$

The last equation in (4.3) comes from the condition

$$\frac{d}{ds} \varphi(u(s)) = 0.$$

Note that the nonlinear equations again can be solved by a matrix-free nonlinear solver.

This procedure is implemented in a matrix-free triple loop. The two outer loops consist of a matrix-free iterative nonlinear solver for the equation (4.3), and the innermost loop represents the function evaluation of the nonlinear system (4.3) which involves the solution of (4.2).

Note also that the previous quadratic approximation (4.1) gives a good starting point for the preceding method: we take $r(\bar{s})$ and $\dot{r}(\bar{s}) / (T^*\dot{r}(\bar{s}))$ as starting points for u and $t(u)$, respectively.

4.2 Finding a Special Point: $\min_s \varphi(u(s))$: Path-Following Approach

Let $q(s)$ be defined as the solution of

$$\begin{pmatrix} H(q) \\ T^*(q - p(s)) \end{pmatrix} = 0.$$

Note that $q(0) = u_{n-2}$, $q(s_1) = u_{n-1}$, $q(\|u_n - u_{n-2}\|) = u_n$, and that $q(s)$ can be viewed as the corrector point to the predictor $p(s)$. Clearly, $q(s)$ can be approximated via a matrix-free iterative nonlinear solver (a matrix-free double loop).

We have now reduced the problem to a one-dimensional minimization of the function $s \mapsto \varphi(q(s))$ for which there are well-known algorithms. Note that the full approach is now implemented via a matrix-free triple loop, the outer loop being the one-dimensional minimizer.

A modification of this method can be implemented as a steplength strategy into the numerical continuation method, see Allgower and Georg [2, Section 8.2]. This modification permits a matrix-free implementation consisting only of a matrix-free double loop.

5 Simple Bifurcation

Let $H : \mathbb{R} \times \mathbb{R}^N \rightarrow \mathbb{R}^N$, and let $u(s)$ be a solution curve, i.e., $H(u(s)) = 0$. For simplicity, we assume that the parametrization is with respect to arclength, i.e., $\|\dot{u}(s)\|_2 = 1$.

The point $\bar{u} \in \mathbb{R}^{N+1}$ is called a *simple bifurcation point* of the equation $H(u) = 0$ if the following conditions hold: $H(\bar{u}) = 0$, $\dim \ker H'(\bar{u}) = 2$, and

$$\bar{e}^* H''(\bar{u}) \Big|_{(\ker H'(\bar{u}))^2}$$

has one positive and one negative eigenvalue, where $\ker H'(\bar{u})^* = \text{span}(\bar{e})$.

If $\bar{u} = u(\bar{s})$ is a simple bifurcation point, then it can be seen that the determinant

$$\det \begin{pmatrix} H'(u(s)) \\ \dot{u}(s)^* \end{pmatrix}$$

changes its sign at $s = \bar{s}$. Figure 4 illustrates the situation.

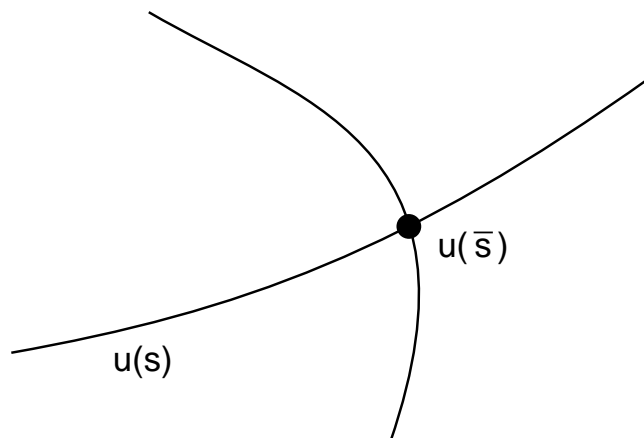


Figure 4: Simple Bifurcation Point

Theorem 5.1. *Let $T \in \mathbb{R} \times \mathbb{R}^N$ be such that $T^* \dot{u}(\bar{s}) > 0$, and let $u(\bar{s})$ be a simple bifurcation point. Then*

$$\det \begin{pmatrix} H'(u(s)) \\ T^* \end{pmatrix}$$

changes its sign at $s = \bar{s}$.

Hence, to observe the sign change, the vector T needs only to be an approximation of the tangent.

Proof: Let $e_{N+1} \in \mathbb{R} \times \mathbb{R}^N$ be the column vector $(0, \dots, 0, 1)^*$. For $s \neq \bar{s}$ and $|s - \bar{s}|$ small we have

$$\begin{aligned} \begin{pmatrix} H'(u(s)) \\ T^* \end{pmatrix} &= \begin{pmatrix} H'(u(s)) \\ \dot{u}(s)^* \end{pmatrix} + e_{N+1}(T - \dot{u}(s))^* \\ &= \begin{pmatrix} H'(u(s)) \\ \dot{u}(s)^* \end{pmatrix} (\mathbf{I} + \dot{u}(s)(T - \dot{u}(s))^*) \end{aligned}$$

The last equation implies the conclusion since the Sherman-Morrison-Woodbury formula implies that

$$\mathbf{I} + \dot{u}(s)(T - \dot{u}(s))^*$$

is invertible and hence its determinant does not change sign at $s = \bar{s}$. ■

The next theorem gives us a test function for a simple bifurcation point.

Definition 5.1. Two m -dim subspaces $U, V \subset \mathbb{R}^k$ are called *acute* iff

$$U \cap V^\perp = \{0\}.$$

Theorem 5.2. Let $\bar{u} = u(\bar{s})$ be a simple bifurcation point, and let $T^* \dot{u}(\bar{s}) > 0$. Let $\text{span}\{c\}$ be acute to the kernel of

$$\begin{pmatrix} H'(u(\bar{s})) \\ T^* \end{pmatrix},$$

and let $\text{span}\{b\}$ be acute to the kernel of

$$\begin{pmatrix} H'(u(\bar{s})) \\ T^* \end{pmatrix}^*.$$

Define $\tau(u)$ via

$$\begin{pmatrix} \begin{pmatrix} H'(u) \\ T^* \end{pmatrix} & b \\ c^* & 0 \end{pmatrix} \begin{pmatrix} \xi(u) \\ \tau(u) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix}. \quad (5.1)$$

Then $\tau(u(s))$ changes sign at $s = \bar{s}$.

The idea of this theorem goes back to Abbott [1] and (in a different context) to Osborne [9].

Proof: By Cramer's Rule we have

$$\tau(u(s)) = \frac{\det \begin{pmatrix} H'(u(s)) \\ T^* \end{pmatrix}}{\det \begin{pmatrix} \begin{pmatrix} H'(u(s)) \\ T^* \end{pmatrix} & b \\ c^* & 0 \end{pmatrix}}.$$

Now we apply Theorem 5.1 and the acuteness conditions satisfied by b, c . It follows that the determinant in the denominator does not change sign at $s = \bar{s}$. ■

Note that (5.1) permits calculating the test function τ in a matrix-free single loop. In practice, we would use the approximation

$$T := \frac{u_n - u_{n-1}}{\|u_n - u_{n-1}\|}$$

in (5.1) to evaluate the test function τ . Hence, by monitoring the sign of τ , a numerical continuation method is able to detect simple bifurcation points.

Once a simple bifurcation point \bar{u} is detected via a change of sign in the test function τ , i.e., $\tau(u_{n-1})\tau(u_n) < 0$, we proceed similarly to Section 3 and define the linear approximations

$$p(s) := u_{n-1} + sT \approx u(s) \quad (5.2)$$

and

$$\psi(s) = \tau(u_{n-1}) + \frac{s}{\|u_n - u_{n-1}\|} (\tau(u_n) - \tau(u_{n-1})) \approx \tau(u(s)) .$$

If we define \bar{s} via $\psi(\bar{s}) = 0$, then $p(\bar{s})$ is a quadratic approximation of the bifurcation point \bar{u} .

We cannot handle this situation in the same way as in Section 3.1 because the nonlinear system

$$\begin{pmatrix} H(u) \\ \tau(u) \end{pmatrix} = 0$$

becomes singular as $u \rightarrow \bar{u}$.

We now describe two possibilities for approximating \bar{u} more precisely:

5.1 Path-Following Approach

We proceed similarly to Section 3.2: Let $q(s)$ be the solution of

$$\begin{pmatrix} H(q) \\ T^*(q - p(s)) \end{pmatrix} = 0.$$

Hence, $q(s)$ can be viewed as the corrector-point to the predictor point $p(s)$. Note again that $q(0) = u_{n-1}$ and $q(\|u_n - u_{n-1}\|) = u_n$, and that $q(s)$ can be approximated via a matrix-free iterative nonlinear solver (a matrix-free double loop). We now find a zero of the function $s \mapsto \tau(q(s))$ via a secant-like method. The full method is implemented as a matrix-free triple loop, the outer loop being the secant-like method.

Again, a modification of this approach can be implemented into the numerical continuation method as a steplength strategy, see Allgower and Georg [2, Section 8.1], resulting in a matrix-free double loop. However, we already noted above that this method runs into a singularity, so \bar{u} cannot be determined very precisely in this way.

5.2 Global approach

Since $H'(u)$ has rank deficiency 2 at a simple bifurcation point $u = \bar{u}$, we need at least two additional equations and one additional unknown in order to extend the system $H(u) = 0$ into a regular characterization of a bifurcation point.

Such systems are called minimally extended systems. As an example, we choose the minimally extended system of Allgower and Schwetlick [3]. Early numerical bifurcation methods are found in [11] and [12]. The first minimally extended system for simple bifurcation points appears to go back to Griewank and Reddien [7]. See Allgower and Georg [2, Section 24.2] for a detailed bibliographical account.

Let $u = \bar{u}$ be a simple bifurcation point.

Given fixed vectors $w, r \in \mathbb{R} \times \mathbb{R}^N$ and $d \in \mathbb{R}^N$, it is not difficult to see that the matrices

$$\begin{pmatrix} H'(u) + dr^* \\ w^* \end{pmatrix}, \quad \begin{pmatrix} H'(u) + dw^* \\ r^* \end{pmatrix} \quad (5.3)$$

are nonsingular at $u = \bar{u}$ if $\text{span}(d)$ is acute to $\ker(H'(\bar{u}))^*$ and $\text{span}\{r, w\}$ is acute to $\ker(H'(\bar{u}))$. Let us assume in the following that the vectors w, r and d are in such general position.

We now define in a neighborhood of \bar{u} the vector fields $v_1(u)$ and $v_2(u)$ via the linear equations

$$\begin{pmatrix} H'(u) + dr^* \\ w^* \end{pmatrix} v_1(u) = e_{N+1}, \quad \begin{pmatrix} H'(u) + dw^* \\ r^* \end{pmatrix} v_2(u) = e_{N+1}. \quad (5.4)$$

Note that these vector fields are obtained via two matrix-free single loops. It can be seen that $\mu = 0$ and $u = \bar{u}$ is a regular zero point of the minimally extended system

$$\begin{pmatrix} H(u) + \mu d \\ r^* v_1(u) \\ w^* v_2(u) \end{pmatrix} = 0. \quad (5.5)$$

The simple bifurcation point \bar{u} can now be approximated precisely and in a numerically stable way via a matrix-free triple loop. The two outer loops consist of a matrix-free iterative nonlinear solver for the equation (5.5), and the innermost loop represents the function evaluation of the nonlinear system (5.5) which involves the solution of the two equations (5.4).

There is an efficient implementation of Newton's method for (5.5), see, e.g., Allgower and Georg [2, Algorithm 24.2], which also yields the two tangent vectors at the bifurcation point \bar{u} . However, this method uses the solving of 3 linear equations involving $H'(u)$ and one involving $H'(u)^*$ per Newton step, and hence this approach cannot be implemented in our matrix-free sense.

If the bifurcation point \bar{u} is detected via a change of sign $\tau(u_{n-1})\tau(u_n) < 0$, then (5.1) furnishes some good starting guesses for the iterations concerning (5.4) and (5.5):

$$\mu = 0, \quad v_2 \approx T, \quad r \approx T, \quad v_1 \approx \frac{\eta(\bar{s})}{\|\eta(\bar{s})\|}, \quad w \approx \frac{\eta(\bar{s})}{\|\eta(\bar{s})\|}, \quad u \approx p(\bar{s}).$$

Recall that $p(\bar{s})$ is defined after equation (5.2). In the same way, we can interpolate

$$\eta(s) = \xi(u_{n-1}) + \frac{s}{\|u_n - u_{n-1}\|} (\xi(u_n) - \xi(u_{n-1})) \approx \xi(u(s))$$

to obtain $\eta(\bar{s})$.

5.3 Switching Branches at a Bifurcation Point

After a bifurcation point $\bar{u} = u(\bar{s})$ has been detected along the path, we also are given a vector ξ orthogonal to the current direction $t \approx \dot{u}(\bar{s})$, see (5.1). Note that the span of t and ξ approximate the kernel of $H'(\bar{u})$.

A point on the bifurcating (new) branch can now be obtained via the equation

$$\begin{pmatrix} H(u) \\ \xi^*(u - (\bar{u} + \epsilon \xi / \|\xi\|)) \end{pmatrix} = 0$$

for some small (but not too small) $\epsilon > 0$. This equation can be viewed as a corrector equation for the predictor point $\bar{u} + \epsilon \xi / \|\xi\|$, and can be solved in a matrix-free double loop.

Figure 5 illustrates the idea.

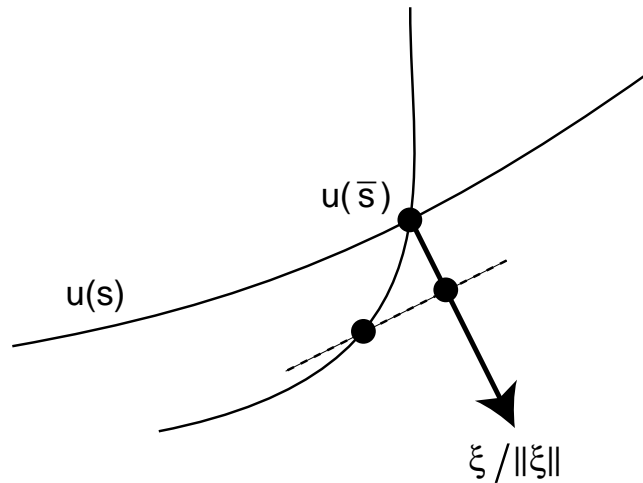


Figure 5: Finding a Second Point on the New Branch

Once we have two points on the new branch, we can proceed with the usual predictor-corrector steps to trace this branch.

5.4 Approach via Perturbation (Sard's Theorem)

A famous perturbation theorem of Sard [10] guarantees that if an $\epsilon > 0$ and a vector $d \in \mathbb{R}^N$ of norm 1 is chosen at random, i.e., if ϵd is outside a set of measure zero, then the equation $H(u) = \epsilon d$ has only regular solutions, i.e., $H'(u)$ has rank N for all u such that $H(u) = \epsilon d$. Hence the resulting solution curves u_ϵ do not have a bifurcation point. We say that the bifurcation point is unfolded.

Figure 6 illustrates a perturbation of a simple bifurcation point. Note that the other special points we consider here (i.e., Sections 3,4,6) are stable under such perturbations!

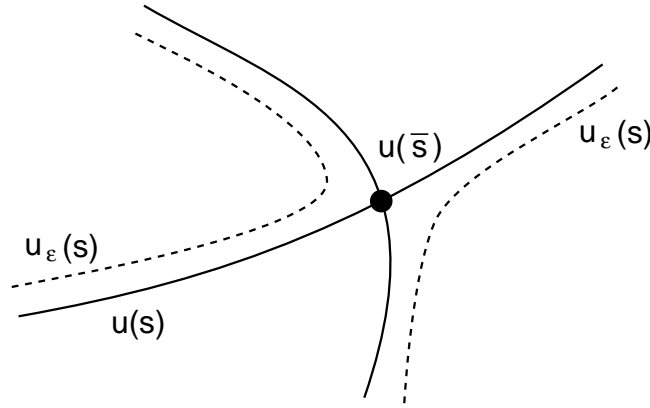


Figure 6: Perturbation of a Simple Bifurcation Point

A very simple idea now is to follow both solution branches $u(s)$ and $u_\epsilon(s)$ for detecting bifurcation points and branching off at such point. This simple idea works astonishingly well, and modifications thereof have been analyzed in several papers, see Allgower and Georg [2, Section 24.1] for a detailed bibliographical account. In [6] it is shown that this idea can also be combined in a robust way with Broyden updates.

6 Hopf bifurcation points

We consider Hopf bifurcation with respect to the dynamical system $\dot{x} = H(\lambda, x)$. Let $u(s) = (\lambda(s), x(s))$ as usual be a solution curve of $H(u) = 0$. A point $\bar{u} = (\bar{\lambda}, \bar{x}) = (\lambda(\bar{s}), x(\bar{s}))$ is a simple Hopf bifurcation point iff for small $|s - \bar{s}|$ there is a complex conjugate pair of simple eigenvalues $\rho(s) \pm i\omega(s)$ of $\partial_2 H(\lambda(s), x(s))$ crossing the imaginary axis for $s = \bar{s}$, i.e., $\rho(\bar{s}) = 0$, $\dot{\rho}(\bar{s}) \neq 0$, $\omega(\bar{s}) \neq 0$, and such that $\partial_2 H(\lambda(\bar{s}), x(\bar{s}))$ has no other eigenvalues on the imaginary axis. The value $\bar{\nu} = (\omega(\bar{s}))^2$ is called the Hopf number.

The following theorem, on which we base our numerical approach, is due to Werner [13] but has some closely related predecessors [4, 5], see [13] for a detailed bibliographical account. Let us introduce the notations

$$A(u) := \partial_2 H(u), \quad \bar{A} := A(\bar{u}), \quad \bar{\nu} := (\omega(\bar{s}))^2.$$

Theorem 6.1. *Let \bar{u} be a simple Hopf bifurcation point. Let $l, r \in \mathbb{R}^N$ be such that $\text{span}\{\bar{A}^*l, l\}$ is acute to $\text{kernel}(\bar{A}^2 + \bar{\nu})$, and $\text{span}\{\bar{A}r, r\}$ is acute to $\text{kernel}(\bar{A}^2 + \bar{\nu})^*$. Then the following linear system is nonsingular for $u \approx \bar{u}$ and $\nu \approx \bar{\nu}$:*

$$\begin{pmatrix} A^2(u) + \nu & A(u)r & r \\ l^*A(u) & 0 & 0 \\ l^* & 0 & 0 \end{pmatrix} \begin{pmatrix} \xi(u, \nu) \\ \alpha(u, \nu) \\ \beta(u, \nu) \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \quad (6.1)$$

Note that for $\nu = \bar{\nu}$ and $u = \bar{u}$ we have $\alpha(\bar{u}, \bar{\nu}) = \beta(\bar{u}, \bar{\nu}) = 0$, and $\xi(\bar{u}, \bar{\nu})$ is a particular vector in the two-dimensional kernel of $\bar{A}^2 + \bar{\nu}$.

Furthermore, $\beta(u, \nu) = 0$ implicitly defines $\nu(u)$, i.e., $\partial_2 \beta(\bar{u}, \bar{\nu}) \neq 0$, and $\tau_H(u(s)) := \alpha(u(s), \nu(u(s)))$ changes sign at $s = \bar{s}$. Hence, $\tau_H(u)$ can be regarded as a test function for Hopf bifurcation.

In order to efficiently calculate the test function $\tau_H(u)$, we use a secant-like method to find a solution $\nu(u)$ of $\beta(u, \nu) = 0$, while evaluating the function $u, \nu \mapsto \beta(u, \nu)$ via (6.1) in a matrix-free loop. Hence $\tau_H(u) = \alpha(u, \nu(u))$ can be calculated via a matrix-free double loop, the outer loop being a secant-like solver, and the inner loop the linear solver for (6.1). However, it may be a problem to find a good starting value ν .

Once a Hopf bifurcation point \bar{u} has been detected via a change of sign: $\tau_H(u_{n-1})\tau_H(u_n) < 0$, we can proceed to approximate \bar{u} with high precision in the sense of Section 3.

7 Preconditioners

As we are aiming at large (and/or sparse) nonlinear systems, we have to take into consideration the fact that the iterative linear solvers of Krylov subspace type often only give acceptable results in combination with a preconditioner B . We take here the point of view that the choice of such a preconditioner B is problem dependent and has to be supplied by the user of the method together with the implementation of H .

Hence, for the most part of this paper, we can view the system H as being already preconditioned, i.e., we assume that the map $u \mapsto H(u)$ is replaced by the map $u \mapsto B^{-1}H(u)$.

Note that the solution branch and the special points in Sections 3,4,5 are unchanged by this preconditioning. However, there is one exception to this

rule, namely, Hopf bifurcation is destroyed by this preconditioning. The situation is similar to the preconditioning problem for eigenvalue solvers based on Krylov subspace techniques. Here, we need much further investigations into the problem of finding good preconditioners for the linear system (6.1).

8 Higher Derivatives of the Solution Curve

It is possible to obtain higher derivatives of the solution curve with matrix-free methods. This possibility may be useful in certain problems, e.g., to obtain high-order predictors. We outline the idea:

Let us assume that u_0 is a fixed solution point: $H(u_0) = 0$. Let $t_0 \in \mathbb{R} \times \mathbb{R}^N$ be such that $H'(u_0)t_0 = 0$ and $t_0^*t_0 = 1$. We parametrize the solution curve $u(s)$ with respect to the direction t_0 : Let $u(s)$ be the solution of

$$\begin{pmatrix} H(u) \\ t_0^*(u - (u_0 + st_0)) \end{pmatrix} = 0, \quad (8.1)$$

see Figure 7 for an illustration.

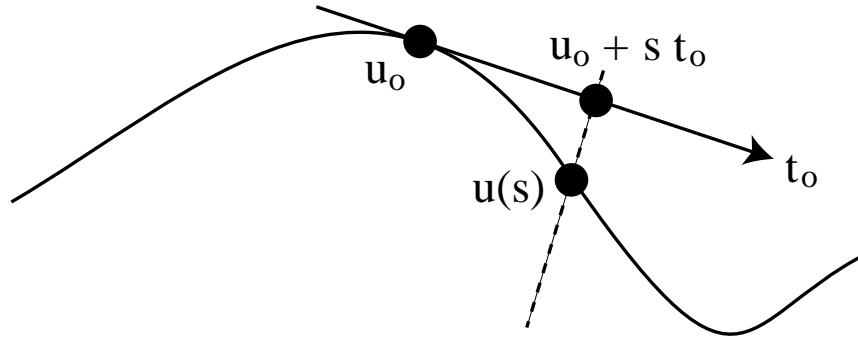


Figure 7: Parametrization of the Solution Curve

Then, by differentiating (8.1) twice with respect to s , we see that the linear systems

$$\begin{pmatrix} H'(u) \\ t_0^* \end{pmatrix} t(u) = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} H'(u) \\ t_0^* \end{pmatrix} a(u) = \begin{pmatrix} -H''(u)[t(u), t(u)] \\ 0 \end{pmatrix}$$

define vector fields $t(u)$ and $a(u)$ such that

$$\dot{u}(s) = t(u(s)), \quad \ddot{u}(s) = a(u(s)).$$

Note that $H''(u)[t(u), t(u)]$ can be approximated via finite difference formulas, e.g.,

$$H''(u)[t(u), t(u)] = \frac{1}{\epsilon^2} (H(u + \epsilon t(u)) - 2H(u) + H(u - \epsilon t(u))) + \mathbf{O}(\epsilon^2).$$

Hence $t(u)$ can be determined in a matrix-free single loop, and an additional matrix-free single loop approximates $a(u)$ such that the truncation error has the same order (in ϵ) as the difference approximation of $H''(u)[t(u), t(u)]$.

Using a trick of Mackens [8], this idea can be generalized to higher derivatives such that each additional derivative is obtained in a matrix-free single loop, see also Allgower and Georg [2, Section 11].

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