Numerical Continuation of Bifurcations — An Introduction, Part I

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Outline

- Continuation — motivation
- pseudo-arclength continuation
- Boundary value problems
- Periodic orbits
- Detection of bifurcations (later)
- Continuation of bifurcations (later)
- Further reading/software
Motivation for Using Continuation Techniques

(see Krauskopf/Lenstra: *Fundamental Issues of Nonlinear Laser Dynamics*, 2000)

- Problem: discover UK mainland, classify into England, Wales, Schottland

- Alternative A: ‘Simulation’, test on a fine grid of points

- Alternative B: ‘Continuation’,
  - start in point you know (L),
  - go ahead, always checking were you are
  - detect borders
  - go along borders
  - detect cross points
  - branch off at cross points

→ flip through animation on next slide
Newton iteration

▶ Solve nonlinear system of equations

\[ f(x) = 0, \quad f : \mathbb{R}^n \mapsto \mathbb{R}^n, \quad x \in \mathbb{R}^n, \quad p \in \mathbb{R} \]

▶ Initial guess \( x_0 \in \mathbb{R}^n \) → iteration

\[ x_{k+1} = x_k - [\partial f(x_k)]^{-1} f(x_k) \]

▶ Assumption: Solution \( x_* \) exists, is regular

\[ \iff \det \partial f(x_*) \neq 0 \]

▶ Pro: good convergence

▶ Con: \( x_0 \approx x_* \) required
Parameter Continuation

- Find \( x \in \mathbb{R}^n \) s.t.
  \[
f(x, p) = 0, \quad f : \mathbb{R}^n \times \mathbb{R} \mapsto \mathbb{R}^n, \quad p \in \mathbb{R}
  \]

- Assumption:
  solution for \( p_0 \) known: \( f(x_0, p_0) = 0, \partial_1 f(x_0, p_0) \) regular

- Implicit Function Theorem \( \implies \)
  solution curve \( x(p) \) for \( f(x(p), p) = 0 \)

- Iterate:
  1. choose \( p_{k+1} \approx p_k \)
  2. old solution \( x_k \) initial guess for \( f(x, p_{k+1}) = 0 \)
  3. solve \( f(x, p_{k+1}) = 0 \) with Newton iteration \( \implies x_{k+1} \)

- points \( (x_k, p_k) \) on solution curve \( x(p) \)

- fails if \( \partial_1 f(x_0, p_0) \) not regular
Pseudo-arclength continuation

Find $y \in \mathbb{R}^{n+1}$ s.t.

$$f(y) = 0, \quad f : \mathbb{R}^{n+1} \rightarrow \mathbb{R}^n$$

Assumption: $y_0, z_0 \in \mathbb{R}^{n+1}$ s.t.

$$f(y_0) = 0, \quad \dim \text{rg } \partial f(y_0) = n, \quad \partial f(y_0)z_0 = 0.$$

Implicit function theorem $\implies$ solution curve $y(s)$ ($s \in (-\delta, \delta)$), s.t.

$$f(y(s)) = 0, \quad y(0) = y_0, \quad y'(0) = z_0.$$
**Iteration**

1. **predictor step**
   \[ y_{k+1}^P = y_k + h z_k \]

2. **corrector step**
   
   Newton iteration for \( y_{k+1} \)
   
   \[
   \begin{align*}
   0 &= f(y_{k+1}) \\
   0 &= z_k^T (y_{k+1} - y_{k+1}^P)
   \end{align*}
   \]
   
   with initial guess \( y_{k+1} = y_{k+1}^P \)

3. **new tangent**
   
   \[
   \begin{align*}
   0 &= \partial f(y_{k+1}) z_{k+1} \\
   1 &= z_k^T z_{k+1}
   \end{align*}
   \]

**if** \( y_k \) **is on solution curve**

\( \implies \) Jacobian \( \in \mathbb{R}^{(n+1) \times (n+1)} \)

regular

\[
\begin{bmatrix}
\partial f(y_k) \\
\vdots \\
\partial f(y_k) \cdot z_k^T
\end{bmatrix}
\]
Geometric illustration

\[ y = (x, p) \]
\[ 0 = f(y) \]
\[ = x^2 + p^2 - 1 \]
Geometric illustration

\[ y = (x, p) \]
\[ 0 = f(y) = x^2 + p^2 - 1 \]
Geometric illustration

\[ y = (x, p) \]
\[ 0 = f(y) = x^2 + p^2 - 1 \]

stepsize \( h \ll 1 \)

corrector step
Newton iteration
orthogonal to tangent
$y = (x, p)$
$0 = f(y) = x^2 + p^2 - 1$

Corrector step
Newton iteration
Orthogonal to tangent
Stepsize $h \ll 1$
Geometric illustration

\[ y = (x, p) \]

\[ 0 = f(y) = x^2 + p^2 - 1 \]

Corrector step
Newton iteration
Orthogonal to tangent
Stepsize \( h \ll 1 \)
$y = (x, p) \quad 0 = f(y) = x^2 + p^2 - 1$

stepsize $h \ll 1$

corrector step
Newton iteration
orthogonal to tangent
Geometric illustration

\[ y = (x, p) \]
\[ 0 = f(y) = x^2 + p^2 - 1 \]

corrector step
Newton iteration
orthogonal to tangent

stepsize \( h \ll 1 \)
Boundary Value Problems (BVP)

- solution \( u(\cdot) \in \mathbb{R}^{n_{\text{dim}}} \) of dimension \( n_{\text{dim}} \)
- parameter \( p \in \mathbb{R}^{n_{\text{cp}}} \) of dimension \( n_{\text{cp}} \)
- \( u \) solves differential equation (ODE) on interval \([0, 1]\)

\[
\dot{u}(t) = f(u(t), p)
\]

- with \( n_{\text{bc}} \) boundary conditions

\[
g(u(0), u(1), p) = 0, \quad g : \mathbb{R}^{2n_{\text{dim}} + n_{\text{cp}}} \rightarrow \mathbb{R}^{n_{\text{bc}}}
\]

- and \( n_{\text{int}} \) integral conditions

\[
\int_0^1 h(u(t), p) \, dt = 0, \quad h : \mathbb{R}^{n_{\text{dim}} + n_{\text{cp}}} \rightarrow \mathbb{R}^{n_{\text{int}}}
\]
initial value problem generates flow map $\Phi$

$$\dot{u}(t) = f(u(t), p), \quad u(0) = x$$

$$\implies u(t) = \Phi(t; x) \quad (\Phi(0; x) = x)$$

BVP is nonlinear system with $n_{\text{dim}} + n_{\text{cp}}$ variables $(x, p)$ and $n_{\text{bc}} + n_{\text{int}}$ equations

$$0 = g(x, \Phi(1; x), p)$$

$$0 = \int_{0}^{1} h(\Phi(t; x), p) \, dt$$

pseudo-arclength continuation for $y = (x, p)$ possible if $n_{\text{dim}} + n_{\text{cp}} = n_{\text{bc}} + n_{\text{int}} + 1$
Discretization

- subdivide interval $[0, 1]$ into $N$ subintervals $I_k$
  
  $0 = t_0 < t_1 < \ldots t_N = 1$

- in each subinterval $I_k = [t_{k-1}, t_k]$: approximate solution $u(t)$ by polynomial of order $m$:

  \[ u(t) \approx q_k(t) \quad \text{for} \quad t \in I_k \]

- $q_k$ satisfies ODE at $m$ points in $I_k$: $t^j_k, j = 1 \ldots m$
  Gauss points (orthogonal collocation)
  \[ \implies \text{error of order } N^{-2m}. \]

- + continuity conditions, boundary conditions, integral conditions
Equations and Variables

▶ Variables:
\[ N \cdot (m + 1) \cdot n_{\text{dim}} \] coefficients of polynomials \( q_k \), 
\[ n_{\text{cp}} \] parameters

▶ Equations:

▶ ODE: \[ \frac{\text{d}}{\text{d}t} q_k(t_k^j) = f(q_k(t_k^j), p) \] for \( j = 1 \ldots m, k = 1 \ldots N \)
\[ \implies N \cdot m \cdot n_{\text{dim}} \] equations

▶ Continuity: \[ q_k(t_k) = q_{k+1}(t_k) \] for \( k = 1 \ldots N - 1 \)
\[ \implies (N - 1) \cdot n_{\text{dim}} \] equations

▶ Boundary conditions: \[ g(q_1(0), q_N(1), p) = 0 \]
\[ \implies n_{\text{bc}} \] equations

▶ Integral conditions: \[ \sum_{k=1}^{N} \int_{I_k} h(q_k(t), p) \, dt = 0 \]
\[ \implies n_{\text{int}} \] equations

\[ \implies N \cdot (m + 1) \cdot n_{\text{dim}} + n_{\text{cp}} \] variables,
\[ \implies N \cdot (m + 1) \cdot n_{\text{dim}} - n_{\text{dim}} + n_{\text{bc}} + n_{\text{int}} \] equations
Continuation of Periodic Orbits

- $u(t)$ is periodic orbit of
  \[ \dot{u}(t) = f(u(t), p) \]
  if it satisfies for some period $T$ the boundary condition
  \[ u(0) - u(T) = 0 \]

- Period $T$ is unknown
- **Phase invariance** $\implies u$ is not unique:
  if $u(t)$ is periodic then $u(t + \delta)$ is periodic
- How to set up a regular BVP?
rescale time:
\[ \dot{u}(t) = T_f(u(t), p) \quad \Leftarrow \text{ODE} \]
\[ 0 = u(0) - u(1) \quad \Leftarrow \text{boundary c.} \]

- \( T \) additional free parameter \( \implies \)
  one additional condition to fix phase
- for example: Poincaré section:
  \( u_k(0) = \text{fixed} \) for some \( k \leq n_{\text{dim}} \)
- computationally optimal for mesh-adaption during continuation

\[
0 = \int_0^1 \dot{u}_{\text{old}}(t)^T u(t) \, dt
\]

where \( u_{\text{old}} \) is the previous solution along the branch
This guarantees

\[
\int_0^1 \| u_{\text{old}}(t) - u(t) \|^2 \, dt \rightarrow \min
\]
Continuation of Periodic Orbits

final form

\[ \dot{u}(t) = T f(u(t), p) \quad \Longleftrightarrow \text{ODE} \]

\[ 0 = u(0) - u(1) \quad \Longleftrightarrow \text{boundary c.} \]

\[ 0 = \int_0^1 \dot{u}_{\text{old}}(t)^T u(t) \, dt \quad \Longleftrightarrow \text{integral c.} \]

- \( n_{\text{bc}} = n_{\text{dim}}, \, n_{\text{int}} = 1 \)
  \( \Longleftrightarrow \) continuation needs \( n_{\text{cp}} = 2 \) parameters:
  \( p \) (one-dimensional) and period \( T \)

- continuation variable \( y \) consists of \((u(\cdot), p, T)\)
Bifurcation detection — equilibria

Special functions (as used by AUTO) for continuation of equilibria

\[ 0 = f(y) = f(x, p) \]

- **Fold (turning point, saddle-node):** \[ z_{k,n+1}/\|z_k\| \]
  (last component of tangent vector)
- **Hopf (equilibria):** imaginary part of complex eigenvalues of \( \partial_1 f(x_k, p_k) \)
- **Branching point:**

\[
\det \begin{bmatrix}
\partial f(y_k) \\
Z_k^T
\end{bmatrix}
\]
Bifurcation detection — periodic orbits

Continuation variable
\[ y = (u([t^j_k, t_k]), p, T) \text{ for } k = 1 \ldots N, \; j = 1 \ldots m \]

overall dimension \( n = N \cdot m \cdot n_{\text{dim}} + n_{\text{cp}} \)

- Fold (for general BVP) \( z_{k,n-n_{\text{cp}}+1}/\|z_k\| \)
  - for periodic orbits \( z_{k,n-1}/\|z_k\| \)

- Branching points: determinant of reduced linearization

- Period doubling, Torus bifurcation: magnitude of Floquet multipliers (excluding one trivial Floquet multiplier 1)

- see Kuznetsov ’04: *Elements of Applied Bifurcation Theory* for alternatives
Continuation of Bifurcations — Equilibria

Fully extended systems (see Kuznetsov ’04 for alternatives):
Fold:

► variables $x, \nu \in \mathbb{R}^n, p \in \mathbb{R}^2$,

► $\nu$ nullvector of linearization

► equations:


\[
\begin{align*}
0 &= f(x, p) \\
0 &= \partial_1 f(x, p) \cdot \nu \\
1 &= \nu^T \nu
\end{align*}
\]

► $\implies 2n + 2$ variables, $2n + 1$ equations
Continuation of Bifurcations — Equilibria

Hopf:

- variables $x, q_r, q_i \in \mathbb{R}^n$, $r_\omega \in \mathbb{R}$, $p \in \mathbb{R}^2$
- $q_r + iq_i$ eigenvector for imaginary eigenvalue $ir_\omega^{-1}$
- equations:

\[
\begin{align*}
0 &= f(x, p) \\
0 &= \begin{bmatrix} r_\omega \partial_1 f(x, p) & I \\ -I & r_\omega \partial_1 f(x, p) \end{bmatrix} \begin{bmatrix} q_r \\ q_i \end{bmatrix} \\
1 &= q_r^T q_r + q_i^T q_i \\
0 &= q_{i,old}^T (q_r - q_{r,old}) - q_{r,old}^T (q_i - q_{i,old})
\end{align*}
\]

- $\implies 3n + 3$ variables, $3n + 2$ equations
- period of periodic solution branch will be $2\pi r_\omega$
Continuation of Bifurcations — Periodic Orbits

Fold (for other bifurcations see AUTO or Kuznetsov):

- variables: \( u(\cdot), v(\cdot) \in \mathbb{R}^n \) on \([0, 1] \), \( p \in \mathbb{R}^2 \), \( T, \beta \in \mathbb{R} \)
- \( v \) generalized eigenvector of Floquet multiplier \( 1 \), \( T \) period
- equations:

\[
\begin{align*}
\dot{u} &= Tf(u, p) & \Leftarrow & \text{ODE} \\
\dot{v} &= T \partial_1 f(u, p) v + \beta f(u, p) & \Leftarrow & \text{ODE} \\
0 &= u(0) - u(1) & \Leftarrow & \text{boundary c.} \\
0 &= v(0) - v(1) & \Leftarrow & \text{boundary c.} \\
0 &= \int_0^1 \dot{u}_{\text{old}}(t)^T u(t) \, dt & \Leftarrow & \text{integral c.} \\
0 &= \int_0^1 \dot{u}_{\text{old}}(t)^T v(t) \, dt & \Leftarrow & \text{integral c.} \\
c &= \int_0^1 v(t)^T v(t) \, dt + \beta^2 & \Leftarrow & \text{integral c.}
\end{align*}
\]
Further software

- **AUTO**
  - current versions: **AUTO97** (fortran), **AUTO2000** (C, python)
  - help for AUTO2000 (and 97): Bart Oldeman

- software performing similar tasks:
  - **MATCONT** (implemented in Matlab), currently maintained at Gent (Belgium), [http://www.matcont.ugent.be](http://www.matcont.ugent.be)
  - **XPPAUT** (simulation package has interface for AUTO) [http://www.math.pitt.edu/~bard/xpp/xpp.html](http://www.math.pitt.edu/~bard/xpp/xpp.html)

- Delay-differential equations: DDE-BIFTOOL, PDDECONT

- invariant manifolds:
  - invariant tori (**Torcont**)
  - 1D stable/unstable manifolds of periodic orbits (part of **DsTool**)

- see [http://www.dynamicalsystems.org/sw/sw/](http://www.dynamicalsystems.org/sw/sw/) for more