Parameter Continuation with COCO

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January 14, 2016

Outline

A Resonance Manifold

When $\varepsilon = 0$, the Langford dynamical system

$$\begin{pmatrix} \dot{y}_1 \\ \dot{y}_2 \\ \dot{y}_3 \end{pmatrix} = \begin{pmatrix} (y_3 - 0.7)y_1 - \omega y_2 \\ \omega y_1 + (y_3 - 0.7)y_2 \\ 0.6 + y_3 - \frac{1}{3}y_3^3 - (y_1^2 + y_2^2)(1 + \rho y_3) + \varepsilon y_1^3 y_3 \end{pmatrix}$$

corresponds to a parallel flow on an invariant torus, corresponding to either torus-covering quasi-periodic trajectories or a continuous family of periodic orbits.

A periodic orbit continuation problem with a fixed Poincaré phase condition results from the commands

```
>> prob = coco_prob();
>> pnames =  { 'om', 'ro', 'eps' };
>> coll_args = { @lang, t0, x0, pnames, p0 };
>> prob = ode_isol2bvp(prob, '', coll_args{:}, @po_bc);
```

Covering Manifolds

Every continuation problem is of the form

$$\Phi(u) = 0$$

in terms of a function $\Phi : \mathbb{R}^n \to \mathbb{R}^m$ for $n \geq m > 0$.

If u^* is regular, then there exists a locally unique solution manifold through u^* of dimension $n - m$, such that

$$\mathcal{T}_{u^*} = \mathcal{N}[\partial_u \Phi(u^*)].$$

For $v \in \mathcal{T}_{u^*}$, $\operatorname{colspan}\{T^\perp\} = \mathcal{N}[\partial_u \Phi(u^*)]^\perp$, and some function $s \mapsto t(s)$ with $t(0) = 0$, there exists a unique function $s \mapsto \lambda(s)$ with $\lambda(0) = \lambda'(0) = 0$, such that the curve segment

$$\gamma : s \mapsto u^* + t(s)v + T^\perp \cdot \lambda(s), s \in [-\varepsilon, \varepsilon], \varepsilon \ll 1$$

lies on the solution manifold.

Covering Manifolds

Suppose that $V^T \cdot V = I_{n-m}$ for some matrix $V \in \mathbb{R}^{n \times (n-m)}$, and let $V^\perp \in \mathbb{R}^{n \times m}$ denote a full-rank matrix, such that $V^T \cdot V^\perp = 0$. Then,

$$\det \begin{pmatrix} \partial_u \Phi(u^*) \\ V^T \end{pmatrix} \neq 0 \Leftrightarrow \det \left(\partial_u \Phi(u^*) \cdot V^\perp \right) \neq 0.$$

Either condition implies that the columns of

$$\begin{pmatrix} \partial_u \Phi(u^*) \\ V^T \end{pmatrix}^{-1} \cdot \begin{pmatrix} 0 \\ I_{n-m} \end{pmatrix}$$

span $\mathcal{T}_{u^*}$.

If $\mathrm{colspan}\{V\} = \mathcal{N}[\partial_u \Phi(u^*)]$, then this product equals V.

Covering Manifolds

There exists a unique function $\lambda : \mathbb{R}^n \to \mathbb{R}^n$, such that $\lambda(u^*) = 0$,

$$\Phi\left(\tilde{u} + V^\perp \cdot \lambda(\tilde{u})\right) = 0,$$

and

$$\det\left(\begin{array}{c} \partial_u \Phi(\tilde{u} + V^\perp \cdot \lambda(\tilde{u})) \\ V^T \end{array}\right) \neq 0$$

for $\tilde{u} \approx u^*$.

The tangent space to solution manifold at $\tilde{u} + V^\perp \cdot \lambda(\tilde{u})$ is spanned by the columns of

$$\left(\begin{array}{c} \partial_u \Phi(\tilde{u} + V^\perp \cdot \lambda(\tilde{u})) \\ V^T \end{array}\right)^{-1} \cdot \left(\begin{array}{c} 0 \\ I_{n-m} \end{array}\right).$$

Covering Manifolds

The point $\tilde{u} + V^\perp \cdot \lambda(\tilde{u})$ is the unique solution to the equation

$$\begin{pmatrix} \Phi(u) \\ V^T \cdot (u - \tilde{u}) \end{pmatrix} = 0$$

It follows that the solution manifold may be locally described by the image of the function

$$\rho \mapsto \tilde{u} + V \cdot \rho + V^\perp \cdot \lambda(\tilde{u} + V \cdot \rho)$$

for some fixed $\tilde{u} \approx u^*$ and $\rho \approx 0$.

In particular,

$$V^T \cdot (u^* - \tilde{u}) \mapsto u^*.$$

Covering Manifolds

Let $s \in \mathbb{R}^{n-m}$, such that $\|s\| = 1$. It follows that

$$\Gamma : h \mapsto \Gamma_h := \tilde{u} + hV \cdot s + V^{\perp} \cdot \lambda(\tilde{u} + hV \cdot s)$$

is a 1-dimensional curve segment through u^* on the solution manifold, and

$$\left(\begin{array}{c} \partial_u \Phi(\Gamma_h) \\ V^T \end{array} \right) \cdot T_h = \left(\begin{array}{c} 0 \\ I_{n-m} \end{array} \right)$$

implies that $T_h \cdot s$ is a tangent vector to Γ at Γ_h.

Γ_h is the unique solution to the equation

$$\left(\begin{array}{c} \Phi(u) \\ V^T \cdot (u - \tilde{u}) - hs \end{array} \right) = 0.$$
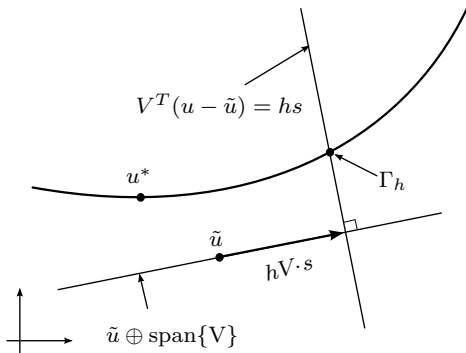
Covering Manifolds

The equation

$$V^T \cdot (u - \tilde{u}) - hs = 0$$

is a *projection condition* in terms of a *base point* $\tilde{u}$, *tangent matrix* V, *direction vector* s, and *step size* h.

Covering Manifolds

Let $\{u, T, \Sigma, R\}$ denote a *chart* based at u, such that

- the columns of T are an orthonormal basis of $\mathcal{T}_u$,
- the elements of Σ are unit tangent vectors at u along curve segments on the solution manifold,
- the scalar R describes the size of the local cover of the solution manifold.

A family of charts is an *atlas*. An *atlas algorithm* generates an atlas from an initial solution guess $\tilde{u}$ and tangent matrix V, through stages of *expansion* and *consolidation*.

During expansion, an atlas algorithm constructs a sequence of charts along a curve segment Γ. During the consolidation, these charts are merged into the atlas by modifying each of the sets Σ.

Covering Manifolds
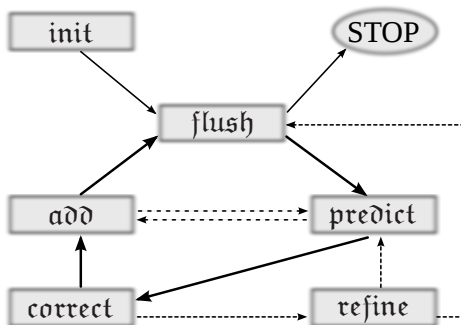
Pseudo-Arclength Continuation

Recall the one-dimensional projection condition

$$v^T \cdot (u - \tilde{u}) - hs = 0$$

in terms of a *base point* $\tilde{u}$, *tangent matrix* v, *direction vector* s, and *step size* h.

Suppose that t^* is a unit tangent vector to $\mathcal{T}_{u^*}$. Let $\tilde{u} = u^*$, $s = \pm 1$, $v = t^*$, and $h = R$, and choose the predictor $\tilde{u} + hsv$. Then, the tangent space at Γ_h is spanned by

$$t_h = \left(\begin{array}{c} \partial_u \Phi(\Gamma_h) \\ t^{*T} \end{array} \right)^{-1} \cdot \left(\begin{array}{c} 0 \\ 1 \end{array} \right).$$

Continuation tracks only the most recently located point on the solution manifold. The atlas algorithm produces an *advancing local cover*.

Accelerated Convergence

Recall the one-dimensional projection condition

$$V^T \cdot (u - \tilde{u}) - hs = 0$$

in terms of a *base point* $\tilde{u}$, *tangent matrix* V, *direction vector* s, and *step size* h.

Suppose that t^* is a unit tangent vector to $\mathcal{T}_{u^*}$. Let $\tilde{u} = u^*$, $s = \pm 1$,

$$v = \left(\begin{array}{c} \partial_u \Phi(u^* + \theta R s t^*) \\ t^{*T} \end{array} \right)^{-1} \cdot \left(\begin{array}{c} 0 \\ 1 \end{array} \right),$$

and $h = R v^T \cdot t^*$, and choose again the predictor $\tilde{u} + hsv$.

The choice $\theta = 0$ yields the pseudo-arclength algorithm, with $\mathcal{O}(R^2)$ predictor residuals. The choice $\theta = 1/2$ yields $\mathcal{O}(R^3)$ predictor residuals.

An Expanding Boundary

In the advancing local cover algorithms, the atlas is always represented by a single base chart. During expansion, a single additional chart is constructed in the "forward" direction. During consolidation, this chart replaces the base chart in the atlas.

In an expanding boundary algorithm, the atlas is represented by charts on its *boundary* that enclose an expanding 1-dimensional volume along the solution manifold. During expansion, charts are constructed in the "outward" direction. During consolidation, the atlas boundary is appropriately reconstructed.

An advancing local cover algorithm never stops and may result in redundant coverage of closed solution manifolds. An expanding boundary algorithm must stop when the unchartered parts of the solution manifold have been exhausted.

An Expanding Boundary

Suppose that the columns of T^* are an orthonormal basis of $\mathcal{T}_{u^*}$ and that $t = T^* \cdot \sigma$ is a unit vector. Let $\tilde{u} = u^*$,

$$V = \mathrm{orth} \left(\left(\begin{array}{c} \partial_u \Phi(u^* + \theta R t) \\ T^{*T} \end{array} \right)^{-1} \cdot \left(\begin{array}{c} 0 \\ I_{n-m} \end{array} \right) \right)$$

$$s = \frac{V^T \cdot t}{\| V^T \cdot t \|}$$

and $h = R \| V^T \cdot t \|$, and choose the predictor $\tilde{u} + h V \cdot s$.

Initialize Σ in terms of a given collection of points on $\mathbb{S}^{n-m-1}$. Define boundary charts as those whose Σ are nonempty. Remove elements from Σ during consolidation to account for chart overlap.

An Expanding Boundary

Basic algorithm suffers from *premature termination* and *redundant coverage*. The resolution to both ailments lies in Henderson's algorithm.
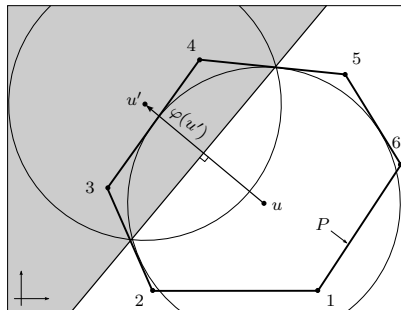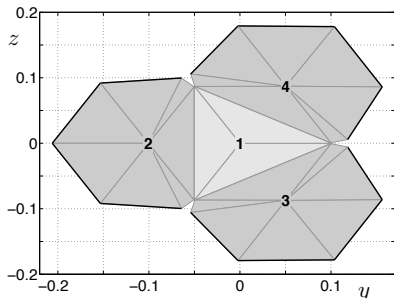

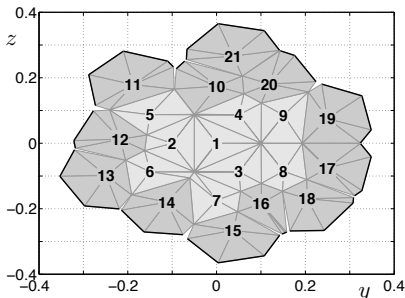(a) Two overlapping charts.
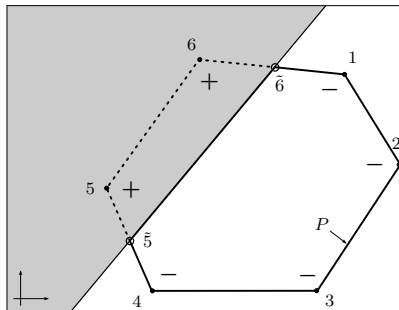
(b) Subtracting a half-space from P.

An Expanding Boundary

Basic algorithm suffers from *premature termination* and *redundant coverage*. The resolution to both ailments lies in Henderson's algorithm.

(a) After 4 steps.

(b) After 21 steps.

The ATLAS-KD toolbox

The current release of COCO includes a multi-dimensional atlas algorithm for arbitrary manifold dimension, modeled on Mike Henderson's MULTIFARIO package and developed jointly with Mike and Erika Fotsch.

The algorithm handles step-size adaptivity along the solution manifold, continuation from computational domain boundaries, and large variations in curvature.

The algorithm does not handle adaptive zero problems. Problems with adaptive discretization (e.g., moving temporal meshes, adaptive finite-element discretizations, or updated phase conditions) break the logic and likely lead to redundant coverage and/or gaps in coverage.

Toolbox Projects

Write a COCO-compatible toolbox for continuation of periodic solutions of delay-differential equations of the form discussed in

Engelborghs, K., Luzyanna, T., and Roose, D., "Numerical bifurcation analysis of delay differential equations using DDE-BIFTOOL," ACM Transactions on Mathematical Software, 28(1), pp. 1-21, 2002

Toolbox Projects

Write a COCO-compatible toolbox for continuation of solutions to differential-algebraic boundary value problems of the form discussed in

> *Ascher, U.M. and Spiteri, R.J., "Collocation software for boundary-value differential-algebraic equations," SIAM Journal on Scientific Computing, 15(4), pp. 938-952, 1994*

Use COCO to implement the method for the computation of isochrones discussed in

> Osinga, H.M. and Moehlis, J., "Continuation-based computation of global isochrones," SIAM Journal of Applied Dynamical Systems 9(4), pp. 1201-1228, 2010

Toolbox Projects

Use COCO to perform continuation of a two-dimensional stable manifold in the Lorenz system using any of the formulations discussed in

> *Krauskopf, B. Osinga, H.M., Doedel, E.J., Henderson, M.E., Guckenheimer, J., Vladimirsky, A., Dellnitz, M., Junge, O., "A survey of methods for computing (un)stable manifolds of vector fields," International Journal of Bifurcation and Chaos in Applied Sciences and Engineering, 15(3), pp. 763-791, 2005*

Toolbox Projects

Use COCO to implement algorithms for the continuation of symmetric periodic orbits as discussed in

> *Wulff, C. and Schebesch, A., "Numerical continuation of symmetric periodic orbits," SIAM Journal on Applied Dynamical Systems, 5(3), pp. 435-475, 2006*

Toolbox Projects

Use COCO to implement the adaptive mesh strategies described in

Budd, C.J., Koomullil, G.P., and Stuart, A.M., "On the solution of convection-diffusion boundary value problems using equidistributed grids," SIAM Journal on Scientific Computing, 20(2), pp. 591-618, 1998

Russell, R.D. and Christiansen, J., "Adaptive mesh selection strategies for solving boundary value problems," SIAM Journal on Numerical Analysis, 15, pp. 59-80, 1978

Toolbox Projects

Use COCO to implement the embedded Runge-Kutta scheme with error control discussed in

> *Dormand, J.R. and Prince, P.J., "A family of embedded Runge-Kutta formulae," Journal of Computational and Applied Mathematics, 6(1), pp. 19-26, 1980*

Additional resources

- *Recipes for Continuation*, SIAM, 2013: principles of continuation, vectorization, and collocation.
- *The 'atlas-kd' toolbox*, SourceForge, 2015: demos for alpha-tested COCO toolbox.
- COCO *tech support*, danko@illinois.edu.
- *No more lectures*, NZMRI, 2016: Thank you for the invitation, wonderful company, and your kind attention!