A Multi-Dimensional Atlas Algorithm for Variable-Mesh Boundary-Value Problems

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Summary. In development since 2007, the MATLAB-based, object-oriented, software platform COCO provides general-purpose support for construction of nonlinear constraints and, in applications to optimization, the corresponding adjoint conditions. COCO atlas algorithms implement continuation strategies that grow constraint manifolds successively from an initial solution guess. Until recently, an alpha implementation in COCO of the multi-dimensional MULTIFARIO package in the `atlas-kd` atlas algorithm was unable to handle problems with changing dimension and/or interpretation of variables and constraints, e.g., boundary-value problems with adaptive meshes. This paper describes a recent upgrade to the `atlas-kd` atlas algorithm that not only provides a resolution to this conundrum, but makes problem-dependent implementation straightforward and consistent with the existing COCO paradigm for construction of constraints and monitor functions. Here, in lieu of a definition of an inner product on an underlying infinite-dimensional vector space, the manifold geometry is characterized using the Euclidean inner product on a suitably-defined finite-dimensional projection. Several examples are considered from the theory of periodic orbits in autonomous and periodically-excited nonlinear dynamical systems.

Fundamentals

The trajectory collocation problem

Following [1], consider the autonomous differential equation $\dot{y} = f(y,p)$ on the interval $[0,T]$ for some positive real number T. Here, the vector field $f : \mathbb{R}^n \times \mathbb{R}^q \mapsto \mathbb{R}^n$ is parameterized by a vector of problem parameters $p \in \mathbb{R}^q$. Choose the integers N and m and the sequence $\{\kappa_j\}_{j=1}^N$ such that $\sum_{j=1}^N \kappa_j = N$. Let $u = \big(\upsilon_{bp}, T, p\big) \in \mathbb{R}^{Nn(m+1)+1+q}$, where

$$\upsilon_{bp}^\top = \begin{pmatrix} \cdots & \upsilon_{(m+1)(j-1)+1}^\top & \cdots & \upsilon_{(m+1)j}^\top & \cdots \end{pmatrix} \tag{1}$$

and j ranges from 1 to N. Then,

$$\tilde{y}(t) = \sum_{i=1}^{m+1} \mathcal{L}_i\left(\frac{2N}{T\kappa_j}\left(t - \frac{T}{N}\sum_{k=1}^{j-1}\kappa_k\right) - 1\right)\upsilon_{(m+1)(j-1)+i} \tag{2}$$

is a candidate approximant for $y(t)$ on the interval $\frac{T}{N}\left(\sum_{k=1}^{j-1}\kappa_k + [0,\kappa_j]\right)$ for every $j = 1,\ldots,N$. Here, $\mathcal{L}_i$ is the i-th Lagrange polynomial of degree m defined on the uniform partition of $[-1,1]$. We obtain a system of $(N-1)n + Nnm$ nonlinear equations by imposition of continuity on $\tilde{y}$ and the collection of collocation conditions

$$0 = \frac{d\tilde{y}}{dt}\left(\frac{T}{N}\left(\sum_{k=1}^{j-1}\kappa_k + \frac{\kappa_j}{2}(1+z_l)\right)\right) - f\left(\tilde{y}\left(\frac{T}{N}\left(\sum_{k=1}^{j-1}\kappa_k + \frac{\kappa_j}{2}(1+z_l)\right)\right), p\right) \tag{3}$$

for $j = 1,\ldots,N$ and $l = 1,\ldots,m$, where z_l is the l-th root of the Legendre polynomial of degree m on the interval $[-1,1]$. Provided that a solution u^* to these equations is regular, there exists an $n+q+1$-dimensional manifold through u^* so that every local solution lies on this manifold. The imposition of up to $n+q+1$ additional constraints (satisfied by u^*) then reduce consideration to lower-dimensional submanifolds of the original solution manifold. The conditions

$$\upsilon_1 - \upsilon_{N(m+1)} = 0 = \tilde{\upsilon}^\top \cdot \upsilon_{bp} \tag{4}$$

for some suitably constructed $\tilde{\upsilon}$ reduce consideration to a local q-dimensional manifold of periodic orbits.

Continuation with a variable mesh

The periodic-orbit problem in the previous section is characterized by the integers N and m, corresponding to the number of mesh intervals and polynomial degree, respectively, the sequence $\{\kappa_j\}_{j=1}^N$ of scaled interval widths, and the reference discretization $\tilde{\upsilon}$, all of which may change during analysis of the collection of solutions obtained for different values of the problem parameters p. Indeed, $\tilde{\upsilon}$ is usually updated before each new solution is sought, using a discretization υ_{bp} from a previously located, nearby solution. Similarly, N and $\{\kappa_j\}_{j=1}^N$ (and, less often, m) may be updated every so often in order to satisfy a desired error tolerance. Each such choice restricts attention to a particular variable space, with its unique interpretations and numbers of problem variables and problem constraints (but identical manifold dimension). As long as one is not concerned with global comparisons between solutions obtained at different stages of the analysis, sequences of solutions may be generated iteratively through a predictor-corrector framework as implemented in an *atlas algorithm*, wherein interpolation is used by the predictor to accommodate changes to N or $\{\kappa_j\}_{j=1}^N$. When global comparisons are of concern, as is the case for closed one-dimensional manifolds and all manifolds of dimension ≥ 2, these may additionally be implemented on the approximant $\tilde{y}$ rather than on the problem discretizations (cf. [2]). Alternatively, as proposed recently in [3], comparisons may be performed in a projected space in terms of invariantly defined solution properties, sufficient in number to ensure a regular embedding of the solution manifold for the underlying infinite-dimensional problem.

A software implementation

The COCO (https://sourceforge.net/projects/cocotools/) software development originates in an effort to provide general-purpose, problem-independent support for i) the construction of *composite continuation problems* (i.e., decomposable into glued-together subproblems with an excess of unknowns relative to the total number of constraints) without concern for the sought manifold dimensionality, and ii) the subsequent analysis of the solution manifold for a given choice of dimension. COCO's construction paradigm allows for solution properties to be defined in terms of subsets of problem variables defined at different stages of construction, for example, the difference between the periods of the individual solutions to two coupled periodic-orbit problems. For variable-mesh problems, such solution properties are said to be invariantly defined if they correspond to a discretized evaluation of a property of the solution to the underlying infinite-dimensional problem, e.g., the mean of a variable or the magnitude of a complex-valued Fourier coefficient. In a recent upgrade to COCO, an implementation of the MULTIFARIO (https://sourceforge.net/projects/multifario/) package for multi-dimensional continuation [4] in the `atlas-kd` atlas algorithm that previously offered no support for variable-mesh continuation problems now provides such support, independently of the nature of the original problem. This functionality is achieved by performing global comparisons in a projection onto a finite-dimensional Euclidean space in terms of invariantly defined solution properties that may be constructed solely in terms of individual discretizations. As an example, Fig. 1 depicts the two-dimensional frequency-amplitude response surface of a hardening Duffing oscillator obtained with `atlas-kd` by performing all global comparisons in the five-dimensional projection onto the excitation period T, excitation amplitude A, first-harmonic Fourier coefficients (scaled by $T/2$), and first-harmonic Fourier amplitude $|c_1|$ (scaled by $T/2$).

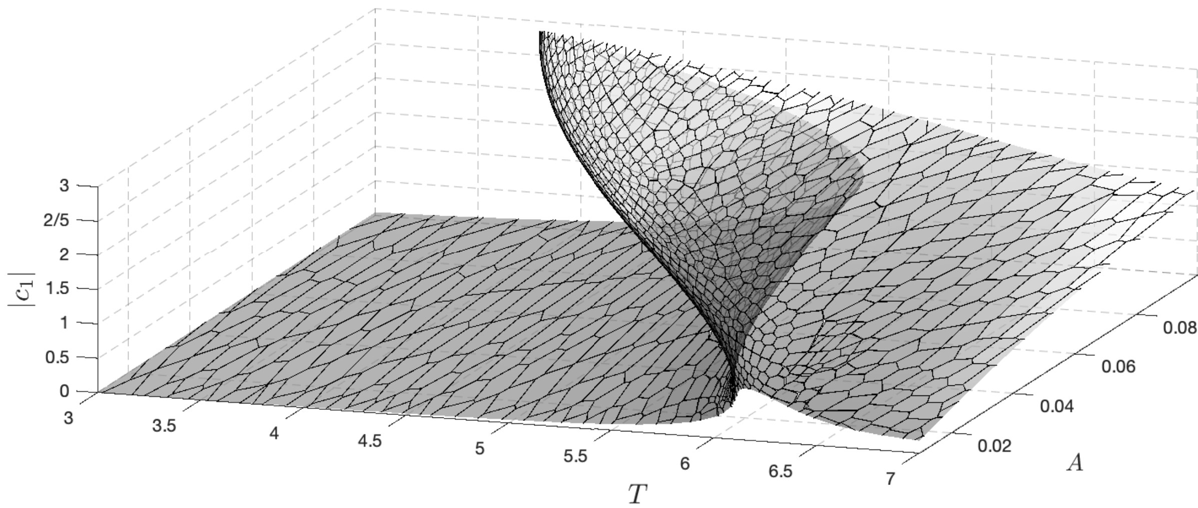

Figure 1: Two-dimensional frequency-amplitude response surface for a hardening Duffing oscillator.

Conclusions

The COCO construction paradigm provides general-purpose support for the definition of small numbers of solution properties that can be used for detecting special points during continuation. Remarkably, the same functionality supports a low-complexity approach for multi-dimensional continuation of variable-mesh boundary-value problems without requiring a user-defined inner product in terms of pairs of discretizations with different interpretations and numbers of problem variables and constraints. The COCO-compatible `atlas-kd` atlas algorithm implements this new paradigm with only minimal modifications to the algorithms inherited from MULTIFARIO.

References

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