Improving numerical continuation for complex delay models of structured populations

Alessia Andò

CDLab – Computational Dynamics Laboratory
Department of Mathematics, Computer Science and Physics
University of Udine

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Population dynamics

Renewal equations (RE) for the birth rate of a consumer of the form

$$b(t) = \int_{a_{\text{mat}}}^{a_{\text{max}}} \overbrace{\beta(a)}^{\text{fertility}} \underbrace{\overbrace{\mathcal{F}(a)}^{\text{survival rate}} \quad b(t-a)}_{\text{individuals of age } a} \, da$$

coupled with delay differential equations (DDE) for the density of a resource of the form

$$S'(t) = f(S(t)) - \int_{0}^{a_{\text{max}}} \overbrace{\gamma(a)}^{\text{consumption}} \underbrace{\overbrace{\mathcal{F}(a)}^{\text{survival rate}} \quad b(t-a)}_{\text{individuals of age } a} \, da.$$

Pseudospectral discretization

In [1] a pseudospectral approach is suggested to discretize delay equations by a finite number of ODEs. Stability and bifurcations can then be investigated by available tools such as MatCont, based on parameter continuation.

The method is particularly promising for complex models where, e.g., vital rates are given through the solution of external ODEs, which themselves depend on model parameters.

Problem: computational time.

[1] Breda D., Diekmann O., Gyllenberg M., Scarabel F. and Vermiglio R., *Pseudospectral discretization of nonlinear delay equations: new prospects for numerical bifurcation analysis*, SIAM J. Appl. Dyn. Syst., 15(1):1-23, 2016.

Example: Daphnia [2]

$$\begin{cases} b(t) = \int_{a_{\text{mat}}(S_t)}^{a_{\max}} \beta(\xi(a; a, S_t), S(t))\mathcal{F}(a; a, S_t) b(t-a)da \\ S'(t) = f(S(t)) - \int_0^{a_{\max}} \gamma(\xi(a; a, S_t), S(t))\mathcal{F}(a; a, S_t) b(t-a)da \end{cases}$$

where $S_t(\theta) = S(t+\theta)$ for $\theta \leq 0$.

In particular, ξ and $\mathcal{F}$ are each solution of an external ODE:

$$\begin{cases} \xi'(\alpha; a, S_t) = g(\xi(\alpha; a, S_t), S_t(\alpha - a)) \\ \mathcal{F}'(\alpha; a, S_t) = \mu(\xi(\alpha; a, S_t), S_t(\alpha - a))\mathcal{F}(\alpha; a, S_t) \end{cases}$$

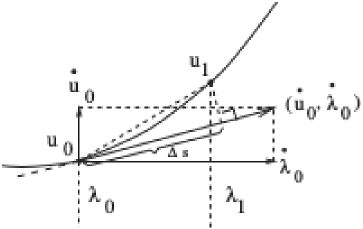
for $\alpha \in [0, a]$, $\xi(0; a, S_t) = \xi_0$ and $\mathcal{F}(0; a, S_t) = \mathcal{F}_0$.

[2] Diekmann O., Gyllenberg M., Metz J.A.J., Nakaoka S., and de Roos A.M., *Daphnia revisited: local stability and bifurcation theory for physiologically structured population models explained by way of an example*, J. Math. Biol., 61:277-318, 2010.

Numerical Continuation

Let $\mathbf{u}' = F(\mathbf{u}, \lambda)$ be the ODEs obtained through the pseudospectral discretization with λ a model parameter. This system is given to MATCONT through its RHS F, which can only be expressed through solutions of external ODEs.

Take, e.g., the problem of continuing an equilibrium curve $\mathbf{u}(\lambda)$, i.e., $F(\mathbf{u}(\lambda), \lambda) = 0$. By numerical continuation, the curve is approximated by a sequence $\{(\mathbf{u}_n, \lambda_n)\}_n$.



Since MATCONT does not know where F comes from, there is no other way than solving the external ODEs from scratch for every λ_n.

Internal continuation

We propose to include the solution of the external ODEs into the continuation framework. In this sense we talk about *internal* continuation, as opposed to the *external* continuation used so far.

To focus on investigating this idea experimentally, we first drop all the technicalities of the Daphnia, whose equilibrium condition reads

$$1 = \int_{a_{\text{mat}}(\bar{S})}^{a_{\max}} \beta(\xi(a,\bar{S}),\bar{S})\mathcal{F}(a,\bar{S})da.$$

Thus we concentrate on continuing the curve $x(\lambda)$ for the prototype problem

$$\int_0^1 f(a,x,\lambda)da = 0,$$

where $f(a,x,\lambda) = \varphi(a;a,x,\lambda)$ with

$$\begin{cases} \varphi'(\alpha;a,x,\lambda) = g(\varphi(\alpha;a,x,\lambda),a,x,\lambda), & \alpha \in [0,a] \\ \varphi(0;a,x,\lambda) = \varphi_0 \end{cases}$$

Clenshaw-Curtis Quadrature

We approximate the integral by Clenshaw-Curtis quadrature

$$\int_0^1 f(a, x, \lambda) da \approx \sum_{j=0}^{N} w_j f(a_j, x, \lambda),$$

where $0 = a_0 < \cdots < a_N = 1$ are the Chebyshev extrema in $[0, 1]$.

This allows us to express the prototype problem in the form $G(\mathbf{u}, \lambda) = 0$ as follows.

Polynomial collocation

For every quadrature node a_j, $j = 1, \ldots, N$, we look for an n-degree polynomial $p^{(j)}(\alpha) := p(\alpha; a_j, x, \lambda)$ such that

$$\begin{cases} p^{(j)\prime}(\alpha_i^{(j)}) = g(p^{(j)}(\alpha_i^{(j)})), \text{ for } i = 1, \ldots, n \\ p^{(j)}(\alpha_0^{(j)}) = \varphi_0. \end{cases}$$

for given points $0 = \alpha_0^{(j)} < \cdots < \alpha_n^{(j)} = a_j \in [0, a_j]$.

All the collocation variables are included in the continuation framework $G(\mathbf{u}, \lambda) = 0$ by setting

$$\mathbf{u} = (p^{(1)}(\alpha_1^{(1)}), \ldots, p^{(1)}(\alpha_n^{(1)}), \ldots, p^{(N)}(\alpha_1^{(N)}), \ldots, p^{(N)}(\alpha_n^{(N)}), x).$$

This also eliminates the classic problem of searching for a suitable initial guess to start the iterative solution by Newton's method.

Internal collocation

Now the collocation equations together with the quadrature formula constitute the continuation problem $G(\mathbf{u}, \lambda) = 0$ for

$$\mathbf{u} = (p^{(1)}(\alpha_1^{(1)}), \ldots, p^{(1)}(\alpha_n^{(1)}), \ldots, p^{(N)}(\alpha_1^{(N)}), \ldots, p^{(N)}(\alpha_n^{(N)}), x).$$

and $G(\mathbf{u}, \lambda)$ given by

$$\begin{cases} p^{(j)\prime}(\alpha_i^{(j)}) - g(p^{(j)}(\alpha_i^{(j)})), \text{ for } i = 1, \ldots, n \text{ and } j = 1, \ldots, N \\ p^{(j)}(\alpha_0^{(j)}) - \varphi_0 \text{ for } j = 1, \ldots, N \\ \sum_{j=0}^{N} w_j p^{(j)}(\alpha_n^{(j)}) \text{ (Clenshaw-Curtis quadrature).} \end{cases}$$

Notice that the dimension is, in this case, $\mathcal{O}(nN)$.

External collocation

Alternatively, as done so far, we can consider $\mathbf{u} = x$ and define

$$G(x, \lambda) = \sum_{j=0}^{N} w_j p^{(j)}(a_j)$$

in the sense that, for each a_j, the components $p^{(j)}(a_j)$ must be computed externally from scratch for every value of λ.

A Python tool

Firstly we compare internal and external continuation both based on collocation. Then since collocation is not the best choice to solve the IVPs externally, we compare also with an external continuation where the IVPs are solved by the Python ODE solver from the `scipy` package, `scipy.integrate.odeint`.

It is based on lsoda from the FORTRAN library ODEPACK. The function starts with nonstiff (Adams) methods initially and, while monitoring data, it may switch to stiff (BDF) methods.

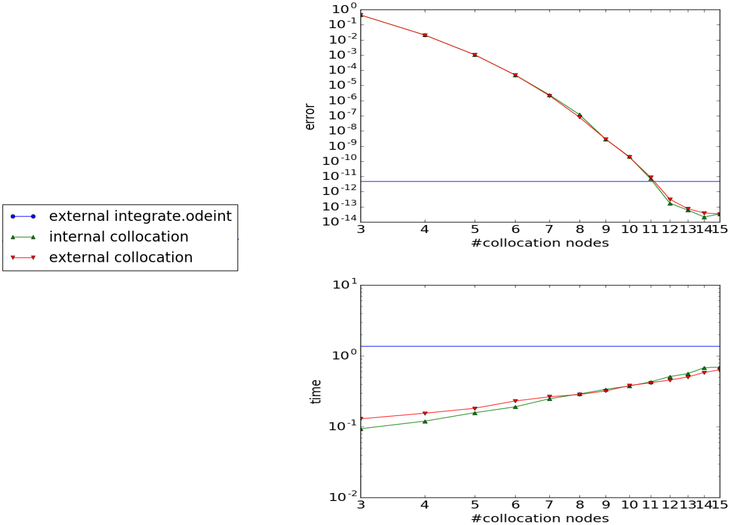
Numerical tests

We compare the three continuation alternatives on either

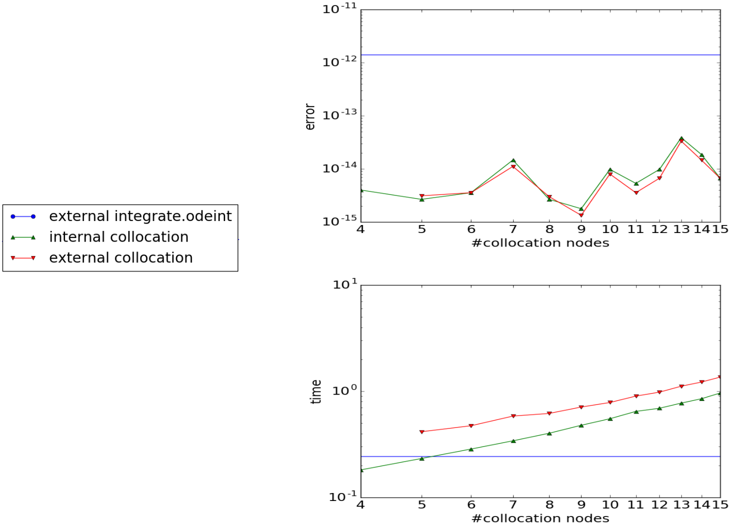
- $g(\varphi(\alpha; a, x, \lambda), a, x, \lambda) = \lambda\varphi(\alpha; a, x, \lambda) + xe^{-\lambda a}$ (linear) or
- $g(\varphi(\alpha; a, x, \lambda), a, x, \lambda) = -2\sqrt{\lambda^4 - 4xa(\varphi_0 - \varphi(\alpha; a, x, \lambda))}$ (nonlinear),

for which we know the exact solution of the external ODE as well as the exact expression of the continuation curve. In this way we can evaluate the true error on the continuation curve by varying the number of collocation and quadrature nodes while running a fixed number of continuation steps.

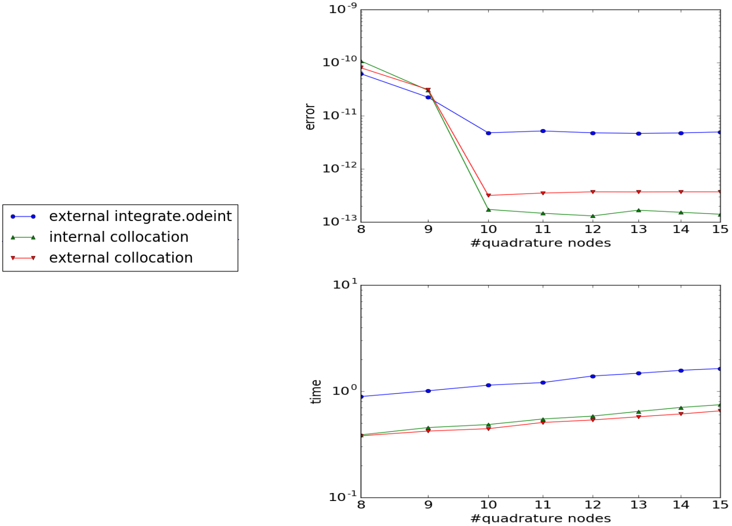
Linear case, $N = 10$



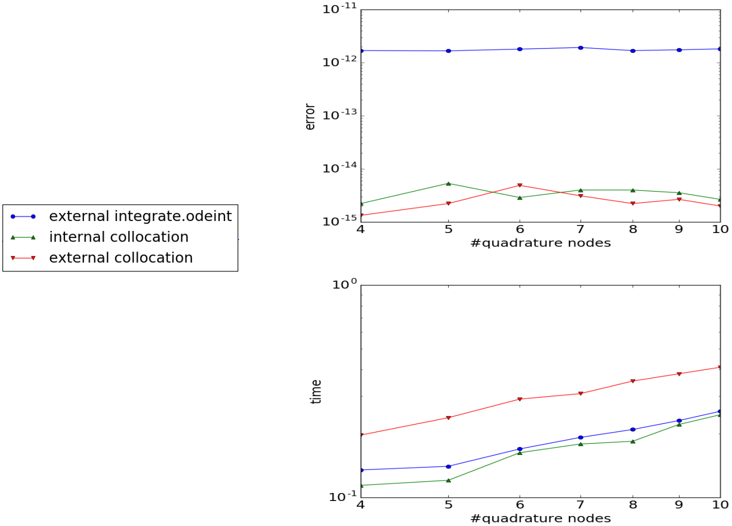
Nonlinear case, $N = 10$



Linear case, $n = 12$



Nonlinear case, $n = 5$



Conclusions

Given these preliminary yet encouraging results, the plan is now to continue our study on prototype models, in particular:

- move to multi-dimensional systems of ODEs
- readd "complications" that have been temporarily removed (e.g., state-dependent integration).

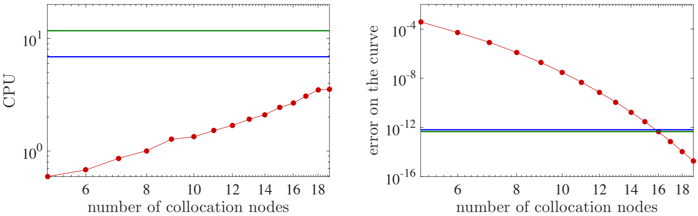
We will also work on improving the collocation method, for example by using piecewise polynomials and possibly an adaptive strategy.

Finally, we will try to exploit the structure of the resulting jacobian in the solution of the Newton's step.

preview on state-dependent

$$\begin{cases} \displaystyle\int_{\bar{a}}^{1} f(a,x,\lambda)da = 0 \\ f(\bar{a},x,\lambda) = \varphi_A \\ \varphi'(\alpha) = g(\varphi(\alpha),a,x,\lambda),\ \alpha \in [0,a],\ \varphi(0)=\varphi_0,\ f(a,x,\lambda) := \varphi(a) \end{cases}$$

- three alternatives, all continuing the first above:
  - external: maturation condition and ODEs outside
  - mixed: maturation condition inside, ODEs outside
  - internal: maturation condition and collocation of ODEs inside



thanks for your attention