pseudospectral methods for delay equations in population dynamics

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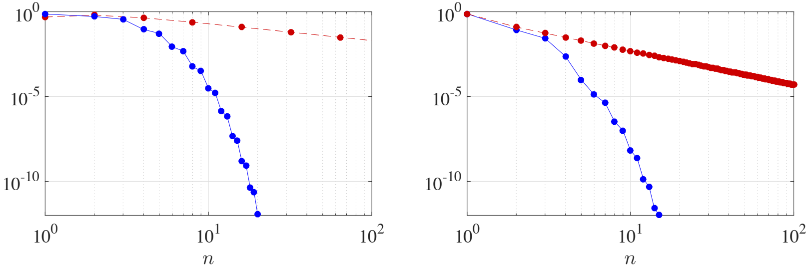
9th workshop
dynamical systems applied to biology and natural sciences
February 7 – 9, 2018 @ Torino (I)

who

- A. Andò @ Udine (I)
- O. Diekmann @ Utrecht (NL)
- P. Getto @ Dresden (D)
- M. Gyllenberg @ Helsinki (FIN)
- D. Liessi @ Udine (I)
- S. Maset @ Trieste (I)
- A. de Roos @ Amsterdam (NL)
- J. Sánchez Sanz @ Bilbao (E)
- F. Scarabel @ Helsinki (FIN)
- R. Vermiglio @ Udine (I)

pseudospectral methods and spectral accuracy

- substitute functions on intervals with interpolating polynomials on given nodes
- fine for smooth functions and good nodes (e.g., Chebyshev)
- example for $f(t) = e^{-t^2}$, $t \in [-1, 1]$:
  – left: approximation of $f'(0)$ via n-degree interpolation (blue) and finite differences with step $2/n$ (red)
  – right: quadrature on $[-1, 1]$ via n-degree interpolation (blue) and trapezoidal rule with step $2/n$ (red)



- error: $O(n^{-n})$ vs $O(n^{-p})$ for some fixed p

daphnia

- a better way to model population dynamics, but lack of tools hinders diffusion
- size-structured consumer b competing for unstructured resource S

$$
\begin{cases}
b(t) = \displaystyle\int_{a_A(S_t)}^{h} \beta(X(a,S_t),S(t))\mathcal{F}(a,S_t)b(t-a)\,da, & b_t \in L^1([-h,0],\mathbb{R}) \\
S'(t) = f(S(t)) - \displaystyle\int_0^h \gamma(X(a,S_t),S(t))\mathcal{F}(a,S_t)b(t-a)\,da, & S_t \in C([-h,0],\mathbb{R}) \\
x'(\alpha) = g(x(\alpha),S_t(\alpha-a)), & \alpha\in[0,a],\ x(0)=x_b,\ \ X(a,S_t):=x(a) \\
\bar{\mathcal{F}}'(\alpha) = -m(x(\alpha),S_t(\alpha-a))\bar{\mathcal{F}}(\alpha), & \alpha\in[0,a],\ \bar{\mathcal{F}}(0)=1,\ \ \mathcal{F}(a,S_t):=\bar{\mathcal{F}}(a)
\end{cases}
$$

- difficulties:
  - functional integro-differential
  - ∞ dimension
  - distributed delays
  - juveniles/adults discontinuities
  - state-dependent: $X(a_A,S_t)=x_A$
  - nonlinear
  - outer ODEs

[Diekmann, Gyllenberg, Metz, Nakaoka, de Roos – JMB 2010]

equilibria

- existence:
  – trivial equilibria $(0, \bar{S})$ satisfy $f(\bar{S}) = 0$, while nontrivial equilibria $(\bar{b}, \bar{S})$ satisfy

$$\begin{cases} 1 = \int_{\bar{a}}^{h} \beta(X(a, \bar{S}), \bar{S}) \mathcal{F}(a, \bar{S}) da \\ 0 = f(\bar{S}) - \int_{0}^{h} \gamma(X(a, \bar{S}), \bar{S}) \mathcal{F}(a, \bar{S}) \bar{b} da \\ X(\bar{a}, \bar{S}) = x_A \\ x'(\alpha) = g(x(\alpha), \bar{S}), & \alpha \in [0, a],\ x(0) = x_b,\ \ X(a, \bar{S}) := x(a) \\ \bar{\mathcal{F}}'(\alpha) = -m(x(\alpha), \bar{S}) \bar{\mathcal{F}}(\alpha), & \alpha \in [0, a],\ \bar{\mathcal{F}}(0) = 1,\ \ \mathcal{F}(a, \bar{S}) := \bar{\mathcal{F}}(a) \end{cases}$$

- computation:
  – Newton or Broyden methods for nonlinear equations
  – Runge-Kutta methods for ODEs (automatic step and event detection for $\bar{a}$)
  – continuation for parameter variation
- stability and bifurcation:
  – infinitesimal generator approach via pseudospectral methods

[B., Getto, Sánchez Sanz, Vermiglio – SISC 2015]
[Sánchez Sanz, Getto – BMB 2016]

linearization

- leads to

$$\begin{bmatrix} b(t) \\ S'(t) \end{bmatrix} = A \begin{bmatrix} b(t) \\ S(t) \end{bmatrix} + \int_{-\bar{a}_A}^{0} B^{(J)}(\theta) \begin{bmatrix} b(t+\theta) \\ S(t+\theta) \end{bmatrix} d\theta + \int_{-h}^{-\bar{a}_A} B^{(A)}(\theta) \begin{bmatrix} b(t+\theta) \\ S(t+\theta) \end{bmatrix} d\theta$$

- difficult and complicated:

$$\begin{aligned} B_{22}^{(J)}(\theta) = & -\frac{\bar{b}(\gamma^+ - \gamma^-)}{g^-} \mathcal{F}(\bar{a}_A, \bar{S}) \mathcal{K}(\bar{a}_A, \bar{a}_A + \theta) \\ & -\bar{b} \int_{\bar{a}_A}^{\min\{-\theta+\bar{a}_A, h\}} \mathcal{F}(\sigma, \bar{S}) \left[\frac{\mu^- - \mu^+}{g^-} \gamma(\sigma) \mathcal{K}(\bar{a}_A, \sigma+\theta) \right. \\ & \left. + \left(\frac{g^+}{g^-} - 1 \right) \left(\gamma_1(\sigma) \mathcal{K}(\sigma, \sigma+\theta) - \gamma(\sigma) \int_{\bar{a}_A}^{\sigma} \mu_1(\rho) \mathcal{K}(\rho, \sigma+\theta) d\rho \right) \right] d\sigma \\ & -\bar{b} \int_{-\theta}^{h} \left[\gamma_1(\sigma) \mathcal{F}(\sigma, \bar{S}) \mathcal{K}(\sigma, \sigma+\theta) + \gamma(\sigma) \mathcal{H}(\sigma, \sigma+\theta) \right] d\sigma \end{aligned}$$

$$\mathcal{K}(\alpha_1, \alpha_2) = e^{\int_{\alpha_2}^{\alpha_1} g_1(\theta) d\theta} g_2(\alpha_2)$$

$$\mathcal{H}(\alpha_1, \alpha_2) = -\mathcal{F}(\alpha_1, \bar{S}) \left(\int_{\alpha_2}^{\alpha_1} \mu_1(\theta) \mathcal{K}(\theta, \alpha_2) d\theta + \mu_2(\alpha_2) \right)$$

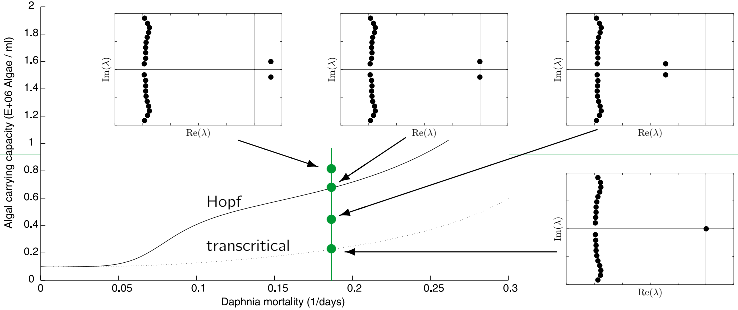
[B., Getto, Sánchez Sanz, Vermiglio – SISC 2015]
[de Roos, Diekmann, Getto, Kirkilionis – BMB 2016]

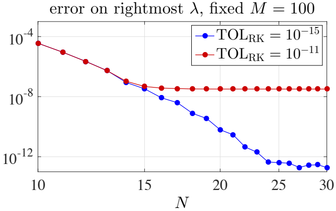
eigenvalues

- ensure spectral convergence: small matrices, high accuracy, fast algorithms
- outer integrals: piecewise quadrature for J/A discontinuities
- piecewise discretization of generator: same quadrature and interpolation nodes
- inner integrals:
  - variable integration intervals
  - split according to J/A discontinuities again
  - about 40 integrals per node!
- evaluation of $\mathcal{A}$ and $\mathcal{B}$'s:
  - no relation between quadrature and RK nodes used for ODEs
  - dense output is mandatory
- possible since $\bar{a}_A$ constant and known: state dependency disappears

[B., Getto, Sánchez Sanz, Vermiglio – SISC 2015]

results and open issues





- convergence w.r.t. tolerance of Newton or Broyden methods
- optimal tuning of discretization parameters
- conditioning of discretized generator
- instability barrier for $\Re(\lambda) < (\log \varepsilon)/h$

curves from [de Roos, Diekmann, Getto, Kirkilionis – BMB 2010]
eigenvalues from [B., Getto, Sánchez-Sanz, Vermiglio – SISC 2015]

periodic solutions

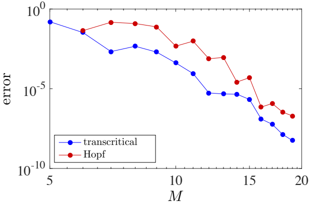
- existence:
  – start from Hopf bifurcations
- computation:
  – as boundary value problem
  – orthogonal collacation
  – continuation
- stability and bifurcation:
  – Floquet theory (ongoing)
  – numerical linearization
  – pseudospectral discretization of monodromy operator

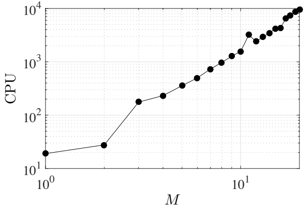
[Engelborghs, Luzyanina, In 't Hout, Roose – SISC 2000]
[Maset – SINUM 2015 – NM 2016]
[B., Diekmann, Liessi, Scarabel – EJQTDE 2016]
[Liessi – PhD thesis 2018]
[B., Liessi – SINUM accepted]

back to ODEs

- pros:
  - – complete and efficient bifurcation tools for ODEs (MATCONT, AUTO,...)
  - – spectral accuracy reasonably implies few (?) ODEs
  - – works well for given and explicit RHS
- daphnia requires black-box RHS for
  - – automatic dense RK solvers for ODEs
  - – automatic adaptive quadrature
  - – automatic detection of $\bar{a}$

  which asks to call external routines every time the bifurcation package evaluates the RHS
- high computational cost/time:
  - – efficient continuation
  - – HPC





[B., Diekmann, Gyllenberg, Scarabel, Vermiglio – SIADS 2016]

Andò – ongoing PhD

two directions

- pseudospectral reduction of nonlinear DEs to ODEs + ODEs tools
  – easy to derive
  – need to optimize computational efficiency
  – lack of convergence proofs
- principle of linearized stability + pseudospectral approximation of spectra:
  – equilibria, cycles,...,chaos
  – need for theoretical background
  – not easy to devise, implement and use
  – more efficient
- example: detect chaos via Lyapunov exponents
  –reduce to ODEs and apply QR methods? [B., Della Schiava – DCDS-B 2018]
  –develope theory and methods ad-hoc? [B. Van Vleck – NM 2014]

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thanks for your attention