Delay-Day Hasselt Utrecht Berlin

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Numerical bifurcation analysis of renewal equations via pseudospectral methods

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Delay equations from population dynamics

Renewal equation for population birth rate

$$b(t) = \int_{a_{\mathrm{repr}}}^{a_{\mathrm{max}}} \overbrace{\beta(a)}^{\text{fertility}} \, \overbrace{\mathcal{F}(a)\, b(t-a)}^{\text{ind of age } a} \, da$$

often coupled with a delay-differential equation for the environmental variable (substrate, prey,...)

$$\frac{dS}{dt}(t) = \underbrace{f(S(t))}_{\text{consumer-free}} - \int_0^{a_{\mathrm{max}}} \overbrace{\gamma(a)}^{\text{consumption}} \, \overbrace{\mathcal{F}(a)\, b(t-a)}^{\text{ind of age } a} \, da$$

Bifurcation analyses

- interest in dynamics and bifurcations (rather than time integration)
- often impossible analytical results
- bifurcation software covers ODE and DDE with discrete delays, no distributed delay or integral equations

The goal

Nonlinear delay equation $\rightsquigarrow$  $\rightsquigarrow$ bifurcation analyses

$\uparrow$

ODE approximation
and software for ODE
(`matcont`)

Breda, Diekmann, Gyllenberg, S., Vermiglio, *SIAM J. Appl. Dyn. Syst.*, 2016

- Why? structured models
- What? delay equations
- How? pseudospectral discretization
- A new approach for renewal equations

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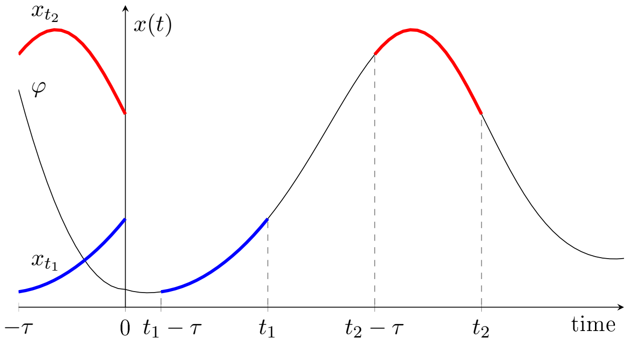
Delay equation: a rule for extending a function given its past

Let $\tau > 0$ be the maximal delay. Given a function x, the history function is

$$x_t \colon [-\tau, 0] \to \mathbb{R}$$
$$x_t(\theta) = x(t+\theta), \quad \theta \in [-\tau, 0]$$



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renewal (RE): $\quad x(t) = F(x_t) \qquad F \colon X \to \mathbb{R}$
$\qquad X = L^1([-\tau, 0], \mathbb{R})$

differential (DDE): $\quad \dot{y}(t) = G(y_t) \qquad G \colon Y \to \mathbb{R}$

The abstract equation

Once provided with an initial condition ψ on $[-\tau, 0]$ and under standard (Lipschitz) assumptions on the rhs, the corresponding initial value problem is equivalent to an Abstract Cauchy Problem for the history function $v(t) \in Y$ (space of functions)

$$\begin{cases} \dot{v}(t) = \mathcal{A}(v(t)) & t \geq 0 \\ v(0) = \psi \end{cases}$$

where $\mathcal{A}$ is the infinitesimal generator of the family of solution operators

$$\mathcal{A}(\psi) = \psi', \quad \psi \in D(\mathcal{A})$$
$$D(\mathcal{A}) = \{\psi \in Y \text{ s.t. } \psi' \in Y \text{ and a "rule for extension"}\}$$

Rule for extension:

- for DDE: $\psi'(0) = G(\psi)$, with $Y = C([-\tau, 0]$
- for RE: $\psi(0) = F(\psi)$, with $Y = L^1([-\tau, 0])$

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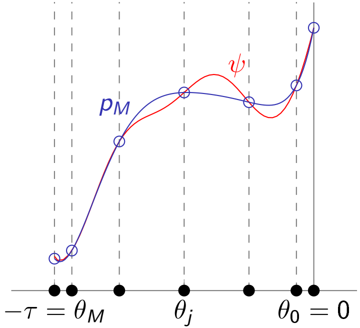
Discretization



Mesh of $M+1$ nodes in $[-\tau, 0]$

$-\tau = \theta_M < \cdots < \theta_0 = 0$

function in Y $\approx$ polynomial of degree M

$$\psi(\theta) \approx p_M(\theta) = \sum_{j=0}^{M} \ell_j(\theta) v_j$$

with v_j values on the nodes, $j = 0, \ldots, M$

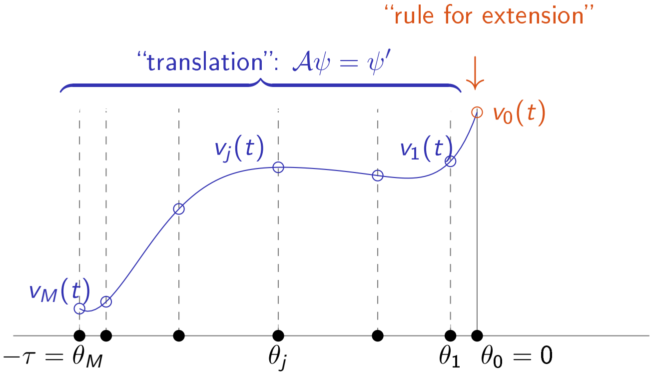
and $\ell_j(\theta)$ Lagrange polynomials:

$$\ell_j(\theta) = \prod_{k \neq j} \frac{\theta - \theta_k}{\theta_j - \theta_k}$$

Collocation

Do to p_M as you would do to ψ (only on $\theta_0, \ldots, \theta_M$)

$\rightarrow$ for DE, we need to describe the abstract equation $\dot{v}(t) = \mathcal{A}(v(t))$



Approximating translation

Recall $v(t)(\theta) \approx p_M(t,\theta) = \sum_{j=0}^{M} v_j(t)\ell_j(\theta)$.

On $\theta_1, \dots, \theta_M$, we approximate the translation $\dot{v}(t) = \mathcal{A}v(t)$ by imposing

$$\frac{\partial}{\partial t} p_M(t,\theta_k) = \frac{\partial}{\partial \theta} p_M(t,\theta_k), \qquad k = 1, \dots M.$$

By linearity, we have:

$$\frac{\partial p_M}{\partial t}(t,\theta_k) = \Big[\frac{\partial}{\partial t} \sum_{j=0}^{M} v_j(t)\ell_j(\theta)\Big]_{\theta=\theta_k} = \sum_{j=0}^{M} \dot{v}_j(t)\ell_j(\theta_k) = \dot{v}_k(t),$$

$$\frac{\partial p_M}{\partial \theta}(t,\theta_k) = \Big[\frac{\partial}{\partial \theta} \sum_{j=0}^{M} v_j(t)\ell_j(\theta)\Big]_{\theta=\theta_k} = \sum_{j=0}^{M} v_j(t)\ell_j'(\theta_k) = \sum_{j=0}^{M} v_j(t) d_{kj}$$

Approximating translation

Hence we get the M equations

$$\dot{v}_k(t) = \sum_{j=0}^{M} v_j(t) d_{kj}, \qquad k = 1, \ldots, M$$

where the coefficients $d_{kj} := \ell'_j(\theta_k)$ are

- completely determined by the nodes
- independent of the specific delay equation

To get a closed system, we need to specify an equation for $v_0(t)$
$\rightarrow$ we do this by imposing the rule for extension (that characterizes the domain of $\mathcal{A}$)

Approximating the rule for extension

- for DDE, the rule for extension is differential ($\psi'(0) = G(\psi)$), and collocation gives:
$$\dot{v}_0(t) = G(p_M(t,\cdot))$$
$\rightarrow$ approximating system of $M+1$ ODE
- for RE, the rule for extension is not differentiated ($\psi(0) = F(\psi)$), and collocation gives:
$$v_0(t) = F(p_M(t,\cdot))$$
$\rightarrow$ approximating system of M ODE, plus algebraic condition for v_0

In any case, the specific right-hand side of the delay equation appears only in the equation for v_0, applied to the interpolating polynomial.

Renewal Equations: the approximating ODE system

Approach in Breda et al, SIADS, 2016

$$v_0(t) = F(p_M)$$

- We can solve the equation for v_0 using a numerical solver for nonlinear equations:

  $$v_0(t) = h(v_1(t), \dots, v_M(t))$$

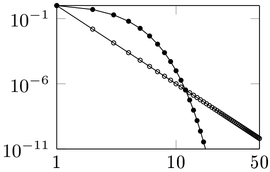
  Plugging into the equations for $\dot{v}_1(t), \dots, \dot{v}_M(t)$, we get a system of M ODE.

- If F is linear (often in models for structured populations, where the unknown describes the population birth rate), we can invert explicitly:

  $$v_0(t) = (I - F\ell_0) \sum_{j=1}^{M} v_j(t) F\ell_j$$

Theoretical convergence for equilibria

- one-to-one correspondence of equilibria
- $\tau < \infty$ and Chebyshev extremal nodes: characteristic roots converging with spectral accuracy, i.e., $O(M^{-k})$ for all k

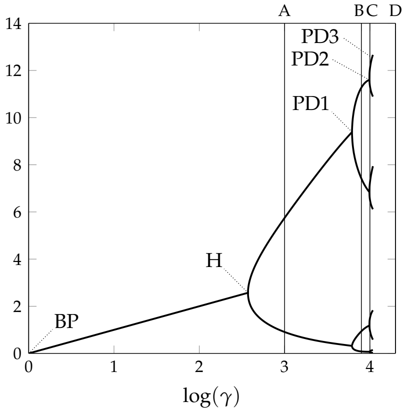


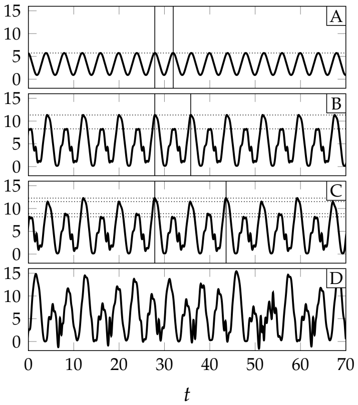
Breda, Maset, Vermiglio, *SIAM J. Sci. Comput.*, 2005
Breda, Getto, Sánchez Sanz, Vermiglio, *SIAM J. Sci. Comput.*, 2015
Breda, Diekmann, Gyllenberg, S., Vermiglio, *SIAM J. Appl. Dyn. Syst.*, 2016

It works! Example: a cannibalism equation

$$b(t) = \frac{\gamma}{2} \int_1^{\tau} b(t-s)\, \mathrm{e}^{-b(t-s)}\, \mathrm{d}s, \quad t \geq 0,$$

Bifurcation analysis and periodic orbits obtained with Matcont, $\tau = 3$, $M = 20$





Limitations

- the nonlinear algebraic equation must be solved at every evaluation of the right-hand side of the ODE system: despite available efficient methods, computationally expensive
- the natural state space of RE is L^1, where point-evaluation is not well defined. In practice, solutions are continuous for $t > \tau$, but approximating L^1 functions with polynomials seems unnatural

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A new approach using the integrated state

In preparation with Rossana Vermiglio (Udine) and Odo Diekmann (Utrecht)

Main idea

Approximate the integrated state (element of AC) rather than the original state (in L^1), via the mapping

$$\begin{aligned} L^1([-\tau,0]) &\to AC([-\tau,0]) \\ \varphi &\mapsto -\int_{\cdot}^{0} \varphi(s)\,\mathrm{d}s \end{aligned}$$

where AC is interpreted as a subspace of NBV,

$$NBV := \{\psi \in BV : \psi(0) = 0,\ \psi \text{ continuous from the right on } (-\tau, 0]\}$$

A dynamical system for the integrated state

Given a renewal equation $b(t) = F(b_t)$, $t > 0$, consider

$$B(t) := \int_0^t b(s)\,\mathrm{d}s$$

and define the state

$$v(t)(\theta) := B(t+\theta) - B(t), \qquad \theta \in [-\tau, 0].$$

Note that $v(t)(0) = 0$ and $\frac{\partial}{\partial\theta} v(t) = b_t$. For $\theta \in [-\tau, 0)$, we have

$$\begin{aligned}
\left(\frac{\mathrm{d}}{\mathrm{d}t} v(t)\right)(\theta) &= \frac{\partial}{\partial t} B(t+\theta) - \frac{\partial}{\partial t} B(t) \\
&= \frac{\partial}{\partial\theta} B(t+\theta) - b(t) \\
&= \frac{\partial}{\partial\theta} v(t)(\theta) - F\left(\frac{\partial}{\partial\theta} v(t)\right), \qquad \theta \in [-\tau, 0)
\end{aligned}$$

The abstract equation

We can represent the dynamical system as abstract equation in NBV:

$$\frac{\mathrm{d}}{\mathrm{d}t} v(t) = \mathcal{A}v(t) - F(\mathcal{A}v(t)),$$

where $\mathcal{A}$ is the operator

$$\begin{aligned} &\mathcal{A}\psi = \psi', \qquad \psi \in D(\mathcal{A}) \\ &D(\mathcal{A}) = \{\psi \in NBV \colon \psi' \in NBV\}. \end{aligned}$$

Note that $D(\mathcal{A}) \subset X \subset NBV$ with

$$X := \{\varphi \in AC([-\tau, 0]) \colon \varphi(0) = 0\}$$

$\mathcal{A}$ is the generator of the semigroup of solution operators, which is not strongly continuous in NBV, but it is in X

The perturbation theory in NBV is developed in

Diekmann, Verduyn Lunel, Twin semigroups and delay equations, submitted

Collocation

We approximate $v(t)$ with a polynomial p_M such that $p_M(0) = 0$, hence

$$p_M(t, \theta) = \sum_{j=1}^{M} v_j(t)\ell_j(\theta)$$

We want to approximate

$$\dot{v}(t) = \frac{\partial}{\partial\theta} v(t) - F\left(\frac{\partial}{\partial\theta} v(t)\right)$$

Using collocation on $\theta_1, \ldots, \theta_M$, we have

$$\dot{v}_k(t) = \sum_{j=1}^{M} d_{kj} v_j(t) - F(\sum_{j=1}^{M} v_j(t)\ell_j'), \qquad k = 1, \ldots, M$$

The approximating ODE system

$$\dot{v}_k(t) = \sum_{j=1}^{M} d_{kj} v_j(t) - F\Big(\sum_{j=1}^{M} v_j(t)\ell_j'\Big)$$

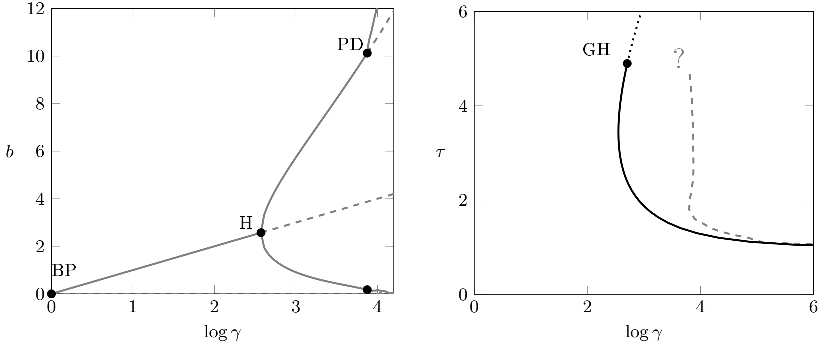
- system of M ODE
- no need to solve a nonlinear equation, but only evaluate the function F
- the solution of the RE can be recovered by

$$b(t) \approx F\Big(\sum_{j=1}^{M} v_j(t)\ell_j'\Big)$$

Example: the cannibalism equation

$$b(t) = \frac{\gamma}{2} \int_1^\tau b(t-s)\, \mathrm{e}^{-b(t-s)}\, \mathrm{d}s, \quad t \geq 0,$$

Performed with Matcont, $M = 20$, $\tau = 3$.



Improved computation times allowed us to study the two-parameter plane.
However, computations are numerically unstable sometimes.

Comparison of computation times

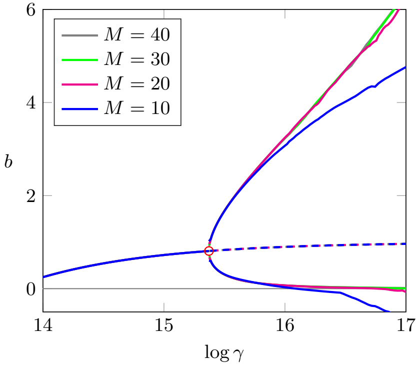
Computation time (seconds) for a 100-point continuation of the branch of positive equilibria and periodic solutions.

Equilibrium				Periodic solutions			
M	[SIADS]	[in progress]	Ratio	M	[SIADS]	[in progress]	Ratio
15	15.65	1.27	12.32	15	2704	198	13.66
16	16.60	1.40	11.86	16	2889	259	11.15
17	17.62	1.52	11.59	17	3066	298	10.29
18	18.75	1.66	11.30	18	3265	301	10.85
19	19.79	1.77	11.18	19	3437	302	11.38
20	21.07	1.91	11.03	20	3659	344	10.64

An SIRS equation

$$b(t) = \gamma \left(1 - \int_0^1 b(t-s)\,\mathrm{d}s\right) \int_0^1 k(s) b(t-s)\,\mathrm{d}s$$

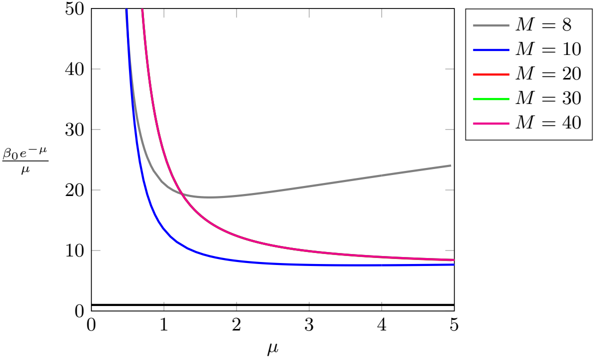
where k is a Gamma-type kernel.



Bifurcation diagram w.r.t. $\log\gamma$ with Hopf bifurcation

(truncated) Nicholson's blowflies equation

$$b(t) = \beta_0 \, e^{-\int_1^\tau b(t-s)\, e^{-\mu s}\, ds} \int_1^\tau b(t-s)\, e^{-\mu s}\, ds$$

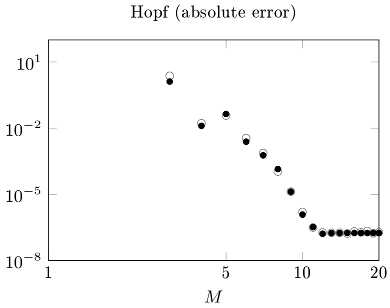


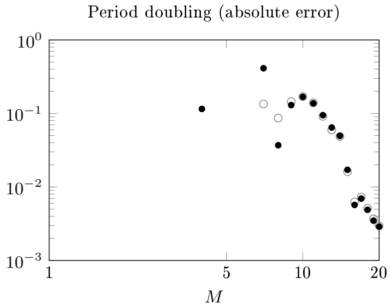
Hopf bifurcation curve in two parameters, $\tau = 10$

Can we really trust the dynamical behavior of the ODE system?

Errors varying M

Errors in approximated Hopf and period doubling bifurcation points (cannibalism equation)





Methods: inversion algebraic condition (SIADS 2016, $\circ$) and integrated state (in progress, $\bullet$).

One-to-one correspondence of equilibria

- If $\overline{b}$ is an equilibrium of
$$b(t) = F(b_t),$$
then $\overline{x} \in \mathbb{R}^M$ with
$$\overline{x}_j = \overline{b}\,\theta_j, \qquad j = 1, \dots, M, \tag{1}$$
is an equilibrium of the approximating ODE system.
- Vice versa, every equilibrium $\overline{x}$ of the ODE system is such that $\overline{b} = \overline{x}_j/\theta_j$ does not depend on j and satisfies $\overline{b} = F(\overline{b})$.
- Discretization and linearization around an equilibrium commute

To study approximation of stability, we focus on linear(ized) equations

Linear equations

Consider a linear equation

$$b(t) = \int_0^\tau k(a) b(t-a)\,\mathrm{d}a \qquad \text{(LRE)}$$

where k is a bounded measurable function on $[0,\infty)$ with support in $[0,\tau]$.

To write the approximating system in compact form, introduce the matrix $D_M \in \mathbb{R}^{M\times M}$ and the row vector K_M,

$$(D_M)_{kj} = d_{kj}$$
$$(K_M)_j = \int_0^\tau k(a) \ell_j'(-a)\,\mathrm{d}a, \qquad j = 1,\dots,M$$

Then, for $V(t) = (v_1(t),\dots,v_M(t))^T \in \mathbb{R}^M$, we can write

$$\dot v_k(t) = \underbrace{\sum_{j=1}^M d_{kj} v_j(t)}_{(D_M V)_k} - F(\underbrace{\sum_{j=1}^M v_j(t)\ell_j'}_{K_M V})$$

$$\dot V = D_M V - (K_M V)\,\mathbf{1} \qquad \text{(LODE)}$$

Characteristic equations

The stability of the zero solution of (LRE) is determined by the real part of the roots of the characteristic equation

$$0 = 1 - \int_0^\tau k(a)\,\mathrm{e}^{-\lambda a}\,\mathrm{d}a =: \chi(\lambda)$$

We can similarly define the characteristic equation of (LODE)

$$0 = 1 - K_M(D_M - \lambda I)^{-1}\mathbf{1} =: \chi_M(\lambda)$$

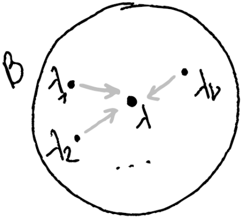
For $\lambda \in \mathbb{C}$, we have $\chi_M(\lambda) \to \chi(\lambda)$

Convergence of characteristic roots

For each characteristic root λ with multiplicity ν contained in a ball B, there exists $\overline{M}(B)$ such that, for $M \geq \overline{M}(B)$, there exist ν characteristic roots $\lambda_1, \ldots, \lambda_\nu$ of the discrete characteristic equation with

$$\max_{j=1,\ldots,\nu} |\lambda - \lambda_j| \to 0 \qquad \text{as } M \to \infty,$$

and the convergence is spectral: $O(M^{-k})$ for any $k \in \mathbb{N}$.



A "bonus": convergence of resolvent operators

Consider

$$\psi = (\lambda I - \mathcal{A})^{-1}\varphi$$

and the corresponding discrete operators

$$p_M = P_M(\lambda I - D_M)^{-1}R_M\varphi,$$

where R_M and P_M denotes restriction on $\theta_1, \ldots, \theta_M$ and interpolation (with 0 in 0), respectively

- $\|p_M - \psi\|_{NBV}$ is bounded by the uniform interpolation error of ψ'
- convergence to zero if $\psi' \in NBV$ (e.g., $\varphi \in D(\mathcal{A})$)
- the order of convergence depends on the regularity of ψ': the smoother the function, the higher the order of convergence
- although resolvent operators are not necessary for the convergence of stability, they are useful for studying solution operators

Final remarks

Specific to the new approach for RE:

- improved computation times compared to the approximation in L^1
- elegant approximation in the space AC, where point evaluation is well defined and interpolation converges on Chebyshev points
- proof techniques and convergence results similar to the original method in L^1 (SIADS)

More general about pseudospectral approximation:

- flexible and general (DDE, RE, ∞-delay, SD delay)
- easy to implement
- low dimensional
- exploits pre-existing software for ODE (hence possible to analyze periodic solutions and their bifurcations)
- no need to linearize

Open problems

- preliminary numerical tests show that periodic orbits are problematic in terms of approximating multipliers and hence bifurcations as M increases
- large computation times beyond equilibria (periodic solutions and bifurcations)
- preservation of the dimension of the unstable manifold for large M
- convergence of solution operators ongoing: exploits representation as Laplace transform of the resolvent operator
- convergence of bifurcations: for DDE, Hopf bifurcation and its direction approximated with spectral accuracy (de Wolff, S., Verduyn-Lunel, Diekmann, *submitted*)
- Krylov's convergence result for $\varphi \in AC$,

$$\|(I - \mathcal{L}_M)\varphi\|_\infty \to 0 \qquad \text{if } M \to \infty,$$

  is proved for Chebyshev zeros. We would like to extend the result to Chebyshev extrema

Thanks for your attention!

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