Quasipolynomial root-finding and applications

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Introduction

We wish to find the roots of the one-variable *quasipolynomial*:

$$P(\lambda) = a_n\lambda^n e^{\tau_n\lambda} + a_{n-1}\lambda^{n-1}e^{\tau_{n-1}\lambda} + \ldots + a_1\lambda e^{\tau_1\lambda} + a_0 e^{\tau_0\lambda} + p(\lambda)$$

where the $a_i s$ are complex constants with rational coefficients, the $\tau_i s$ are constant rational numbers, n is a natural number, and $p(\lambda)$ is a polynomial in λ.

Motivation

Quasipolynomials arise

- in eigenvalue problems associated with systems of delay differential equations
- as the characteristic equation of delay differential equations and partial functional differential equations

Current numerical methods are slow especially when many problems require the computation of a large number of roots.

- `RootFinding[Analytic]` in Maple can find the roots of quasipolynomials (uses a repeated Newton's method)
- Our goal is to develop a numerical method specially designed for quasipolynomials using homotopy continuation

Homotopy Continuation

- Goal: to find all roots of $P(\lambda)$ in a given region of the complex plane.
- Construct the homotopy

$$H(\lambda,\mu) : \mathbf{C} \times [0,1] \mapsto \mathbf{C}$$

s.t. $H(\lambda,0) = Q(\lambda)$ and $H(\lambda,1) = P(\lambda)$

- We use the commonly used homotopy for polynomials:

$$H(\lambda,\mu) = (1-\mu)Q(\lambda) + \mu P(\lambda),\ 0 \le \mu \le 1$$

- As μ varies from 0 to 1, numerical continuation methods trace out the paths from the solutions of $Q(\lambda)$ to the solutions of $P(\lambda)$.

From T.Y. Li (1989), there are three properties required for a good homotopy:

1. **Triviality** - Solutions for $\mu = 0$ are known.
2. **Smoothness** - No singularities along solution paths occur.
3. **Accessibility** - All solutions can be reached by some path originating at $\mu = 0$.

In order to fully define our homotopy, we need a way to determine $Q(\lambda)$ from a given $P(\lambda)$.

Finding $Q(\lambda)$ for quasipolynomials

Proposition: Any two-term quasipolynomial has an analytical solution written in terms of Lambert W or logs.

Proof. Consider the quasipolynomial of two (non-like) terms

$$q(\lambda) = c_1\lambda^{m_1}e^{\alpha_1\lambda} + c_2\lambda^{m_2}e^{\alpha_2\lambda}.$$

Case 1: $\alpha_1 = \alpha_2$

$$\Rightarrow \lambda = \exp\left(\frac{\log\left(-\frac{c_1}{c_2}\right)}{m_2 - m_1}\right)$$

Case 2: $m_1 = m_2$

$$\Rightarrow \lambda = \frac{\log\left(-\frac{c_1}{c_2}\right)}{\alpha_2 - \alpha_1}$$

Case 3: $\alpha_1 \neq \alpha_2,\ m_1 \neq m_2$

$$\Rightarrow \lambda = \exp\left(\frac{m_1 W_{k_1}\left(-\frac{A\exp(\frac{L}{B})}{B}\right) - m_2 W_{k_2}\left(-\frac{A\exp(\frac{L}{B})}{B}\right)}{B} + L\right)$$

where $L = \log\left(-\frac{c_1}{c_2}\right)$, $A = \alpha_1 - \alpha_2$, $B = m_2 - m_1$.

This takes care of all possible cases. □

$\therefore$ Any two-term quasipolynomial satisfies the **Triviality property**. **Smoothness** and **Accessibility** cannot yet be guaranteed.

Determining the homotopy path

- Differentiate $H(\lambda,\mu)$ w.r.t. μ to obtain an ODE
- Solve the ODE with the roots of $Q(y) = 0$ as ICs
- Solution is a parameterized function $\lambda(\mu)$
- Path is $\lambda(\mu)$ as μ varies from 0 to 1
- Each root of $Q(\lambda)$ corresponds to a different path

Algorithm

$$H(\lambda,\mu) = (1-\mu)Q(\lambda) + \mu P(\lambda)$$

$\downarrow$ *Differentiate w.r.t.* μ

ODE in $\lambda(\mu)$

$\downarrow$ *Solve ODE using roots of* $Q(\lambda)$ *as ICs*

$\lambda(\mu)$, *one for each IC*

$\downarrow$ *Evaluate at* $\mu=1$

Estimate for roots

$\downarrow$ *Newton iterations*

Refined estimate for roots

Application in HIV modeling

Quasipolynomial arising in a delay model for HIV infection (Culshaw and Ruan (2000)):

$$P(\lambda) = \lambda^3 e^{\lambda\tau} + 2.7\lambda^2 e^{\lambda\tau} + 0.74\lambda e^{\lambda\tau} - 3.6\times10^{-4} - 0.63\lambda + 0.027e^{\lambda\tau}$$

which has an infinite number of roots.
Consider the region

$$-20 \le Re(\lambda) \le 2, -22 \le Im(\lambda) \le 22.$$

Choose $Q(\lambda) = \lambda^3 e^{\lambda\tau} - 3.6\times10^{-4}$.

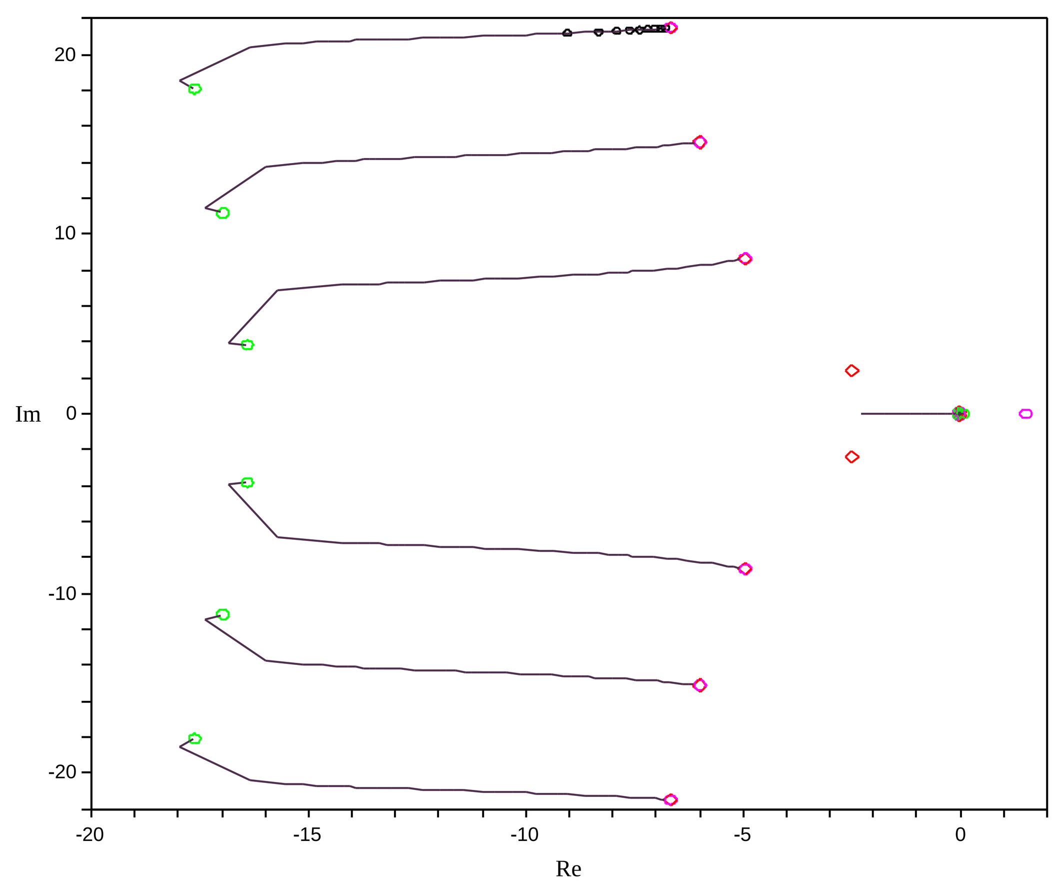

Figure 1

In Figure 1 you can see:

- the roots of $Q(\lambda)$ (in green)
- the roots of $P(\lambda)$ (in pink)
- the one pink root on the real line is actually a false root
- the homotopy paths (in violet)
- points (in black) corresponding to $\mu = 0.1, 0.2, 0.3, \ldots, 0.9$ on the top homotopy path
  → shows that movement along $\lambda(\mu)$ is faster at smaller μ
- two roots not found (in red)
  → **Accessibility** not satisfied
- an incomplete path starting at a root of $Q(\lambda)$ on the positive real line (causes the false root)
  → Singularity encountered - **Smoothness** not satisfied

Problem was redone using $Q(\lambda) = \lambda^3 e^{\lambda\tau} - 0.63\lambda$

- The two roots not found in Figure 1 were found using the new $Q(\lambda)$; however, two other roots found by the old $Q(\lambda)$ were missing instead.

Conclusions

- Movement along $\lambda(\mu)$ is faster at smaller μ
- May encounter singularities when solving the DE
- May need to combine roots resulting from different choices of $Q(\lambda)$ in order to find them all
- Useful method if more efficient than current root-finders used for quasipolynomials

Future work

- Find a systematic way to find $Q(\lambda)$ for general $P(\lambda)$
- Determine smallest starting region in which to look for roots of $Q(\lambda)$ that will find all roots of $P(\lambda)$ in a user-specified region (some roots of $P(\lambda)$ will be found from homotopy paths originating outside desired region)
- Prove that homotopy will find all roots in region
- Write efficient Maple code
- Look at more applications

Summary

A new numerical method based on homotopy continuation has been developed to find the roots of quasipolynomial $P(\lambda)$, a problem often arising in areas involving delay differential equations. The homotopy used is $H(\lambda,\mu) = (1-\mu)Q(\lambda) + \mu P(\lambda),\ 0 \le \mu \le 1$ where $Q(\lambda)$ is chosen to be two terms from $P(\lambda)$. $H(\lambda,\mu)$ is differentiated and the resulting ODE is solved numerically using the roots of $Q(\lambda)$ as initial conditions. The resulting parameterized functions $\lambda(\mu)$ (one for each root of $Q(\lambda)$) define the homotopy paths as μ varies from 0 to 1. $\lambda(1)$ gives the estimate for the corresponding root of $P(\lambda)$. It is still unclear how to systematically choose $Q(\lambda)$ for general $P(\lambda)$. It may be that the roots found using different choices of $Q(\lambda)$ may need to be combined in order to find all roots of $P(\lambda)$.

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