Quasipolynomial root-finding: A numerical homotopy method*

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Abstract

Quasipolynomials arise in a number of applications, and in particular as the characteristic equation associated with systems of delay differential equations. Quasipolynomial equations are generally difficult to solve, and most often must be solved numerically. In the non-trivial case, quasipolynomials have an infinite number of roots in the complex plane. We present a new numerical method for finding the roots of any given quasipolynomial that lie in a given region of the complex plane. The method is based on homotopy continuation, a method currently used to solve polynomial systems. A homotopy between two functions Q and P from a space X to a space Y is a continuous map $H(\lambda, \mu)$ from $X \times [0,1] \mapsto Y$ such that $H(\lambda, 0) = Q(\lambda)$ and $H(\lambda, 1) = P(\lambda)$. In our case space X and space Y are both the complex plane and μ is a parameter that varies from 0 to 1. $Q(\lambda)$ represents a problem that is easier to solve (the roots are known or can be easily computed). $P(\lambda)$ is the original quasipolynomial. We begin with the roots of $Q(\lambda)$ (which are the roots of H at $\mu = 0$). As μ increases from 0 to 1, numerical continuation methods trace out the homotopy paths. At $\mu = 1$, the roots of H are also the roots of $P(\lambda)$, the original quasipolynomial. The numerical continuation method used to trace the homotopy paths will be discussed as well as our future work in this area.

1 Introduction

In a given region, R, we wish to find all complex roots of the one-variable *quasipolynomial*:

$$\begin{aligned} P(\lambda) =& a_0\lambda^{n_0}e^{\tau_0\lambda} + a_1\lambda^{n_1}e^{\tau_1\lambda} + ... + a_N\lambda^{n_N}e^{\tau_N\lambda} \\ =& \sum_{i=0}^{N} a_i\lambda^{n_i}e^{\tau_i\lambda} \end{aligned} \tag{1}$$

where the a_is are real constants, the n_is are nonnegative integers, the τ_is are rational numbers, and N is a positive integer.

Quasipolynomial equations appear most commonly as the characteristic equation associated with systems of delay differential equations (see Asl and Ulsoy [1], Bellman and Cooke [2], Chattopadhyay, et al. [4], Culshaw and Ruan [8], Ruan [24], and Wright [28]). In the non-trivial case,

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quasipolynomials have an infinite number of roots in the complex plane. There does exist a numerical procedure `RootFinding[Analytic]` in the Maple computer algebra software is able to compute the complex roots of analytic functions. However, since approximating the solutions to delay differential equations involves the computation of a large number of roots, the need arises for a faster numerical method specifically tailored to quasipolynomials. This is our motivation for developing the numerical method presented in this paper.

2 Homotopy

We want to find all roots of our quasipolynomial, $P(\lambda)$, that lie in R. The idea is to start with an easier problem $Q(\lambda)$ (the roots are known or can by easily computed). A *homotopy* is a continuous parameterized map $H(\lambda, \mu)$ that connects the roots of $Q(\lambda)$ with the roots of $P(\lambda)$.

Much research has been done on using homotopy methods to solve polynomial systems (see Garcia and Zangwill [13], Li [18], Li and Sauer [19] and [20], Li et al. [21] and [22], and Morgan [23]). Polynomial systems have a finite number of solutions. Therefore, analytic functions which allow for an infinite number of roots, make the problem of quasipolynomial homotopy much more difficult.

We need a function $H(\lambda, \mu)$ with $H(\lambda, 0) = Q(\lambda)$ and $H(\lambda, 1) = P(\lambda)$. Consider the homotopy

$$H(\lambda, \mu) = (1 - \mu)Q(\lambda) + \mu P(\lambda) \tag{2}$$

where μ is a parameter which varies from 0 to 1.

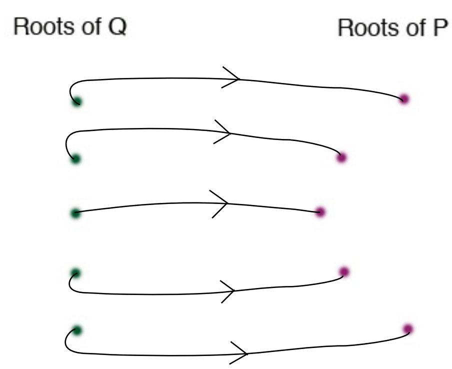

Figure 1: The lines represent the path of the homotopy as the parameter μ is varied from 0 to 1.

A homotopy between two functions Q and P from a space X to a space Y is a continuous map $H(\lambda, \mu)$ from $X \times [0, 1] \mapsto Y$ such that $H(\lambda, 0) = Q(\lambda)$ and $H(\lambda, 1) = P(\lambda)$. In our case, space X and space Y are both the complex plane and μ is a parameter that varies from 0 to 1. $Q(\lambda)$ represents a problem that is easier to solve (the roots are known or can be easily computed). $P(\lambda)$ is the original quasipolynomial. We begin with the roots of $Q(\lambda)$ (which are the roots of H at $\mu = 0$). As μ increases from 0 to 1, numerical continuation methods trace out the homotopy paths.

At $\mu = 1$, the roots of H are also the roots of $P(\lambda)$, the original quasipolynomial. We trace out the homotopy paths using numerical continuation methods.

Li [18] states three properties of a good homotopy:

1. **Triviality** - Roots of $H(\lambda, 0) = Q(\lambda)$ are known.

2. **Smoothness** - No singularities along homotopy paths occur.

3. **Accessibility** - All roots of $H(\lambda, 1) = P(\lambda)$ can be reached by some path originating at the roots of $H(\lambda, 0) = Q(\lambda)$.

In this paper we shall prove that we will always satisfy the Triviality property by choosing $Q(\lambda)$ to be the sum of any two terms from $P(\lambda)$. We will also show how Puiseux series expansions can help lead the homotopy paths away from singularities. Since we are generally dealing with a problem with an infinite number of solutions, the question of Accessibility is related to the region in which we want to find roots of $P(\lambda)$. The reason for this is that the corresponding roots of $Q(\lambda)$ may not lie in the region R. The question then becomes, in what region do all the roots of $Q(\lambda)$ lie which correspond to a root of $P(\lambda)$ in R? And even if we can find this region, how do we know we will still not miss a root of $P(\lambda)$ in R? We will explore each of these questions along with each of the three homotopy properties given above. In the next section, we will explain the numerical continuation method used to trace out the homotopy paths.

3 Numerical continuation method

We need to form paths from the roots of $Q(\lambda)$ to the roots of $P(\lambda)$. We cannot simply trace out the solutions of $H(\lambda, \mu) = 0$ as μ varies from 0 to 1 because eventually we will run back into our original problem as we approach $\mu = 1$, that is, finding the roots of $P(\lambda)$. So that will not get us anywhere. We need another way of finding the roots of $H(\lambda, \mu)$ as μ goes from 0 to 1. The idea is to set $\lambda = \lambda(\mu)$ and turn $H(\lambda(\mu), \mu) = 0$ into a differential equation by differentiating it with respect to μ. This gives a first order differential equation in λ with independent variable μ. Solving this differential equation (numerically) with an initial condition will give us an equation (which may or may not be able to be written explicity) for λ in terms of μ. Evaluating along $\mu = 0$ to $\mu = 1$ forms solution trajectories (paths), one for each initial condition. The initial conditions are non other than the roots of $Q(\lambda)$ which are known. Each initial condition (root of $Q(\lambda)$) corresponds to a solution trajectory (path) taking us from a root of $Q(\lambda)$ at $\mu = 0$ to a root of $P(\lambda)$ at $\mu = 1$. We do not have to worry about homotopy paths crossing since the trajectories of differential equations never cross.

This method is outlined in the following flow chart.

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

Differentiate w.r.t. μ ↓

ODE in $\lambda(\mu)$

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

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

Evaluate at μ=1 ↓

Estimate for roots

Newton iterations ↓

Refined estimate for roots

4 Guaranteeing Triviality of Q

We need a $Q(\lambda)$ with known roots. It makes sense to choose a $Q(\lambda)$ that is somehow related to $P(\lambda)$. Let us choose $Q(\lambda)$ to be the sum of two terms from $P(\lambda)$ (exactly which terms of $P(\lambda)$ will be discussed in the next section).

Consider the general two-term quasipolynomial

$$a_1\lambda^{n_1}e^{\tau_1\lambda} + a_2\lambda^{n_2}e^{\tau_2\lambda} = 0. \tag{3}$$

Note that we cannot have both $n_1 = n_2$ and $\tau_1 = \tau_2$ or we would be able to reduce the problem to a one-term quasipolynomial. We are left with three cases. We will show that in each case, equation (3) can be solved analytically.

Case 1: $\tau_1 = \tau_2 = \tau$

$$\begin{aligned} &a_1\lambda^{n_1}e^{\tau\lambda} = -a_2\lambda^{n_2}e^{\tau\lambda} \\ &\Rightarrow \lambda^{n_2-n_1} = -\frac{a_1}{a_2} \\ &\Rightarrow \lambda = \left(-\frac{a_1}{a_2}\right)^{\frac{1}{n_2-n_1}}. \end{aligned}$$

Also, if $n_1, n_2 \neq 0$ then $\lambda = 0$ is a root of multiplicity $\min\{n_1, n_2\}$. This case simply reduced to a polynomial equation. Therefore, the number of roots is $\max\{n_1, n_2\}$ (counting multiplicity).

Case 2: $n_1 = n_2 = n$

$$
\begin{aligned}
&a_1\lambda^n e^{\tau_1\lambda} = -a_2\lambda^n e^{\tau_2\lambda} \\
&\Rightarrow e^{(\tau_2-\tau_1)\lambda} = -\frac{a_1}{a_2} \\
&\Rightarrow \lambda = \frac{\ln_k\left(-\frac{a_1}{a_2}\right)}{\tau_2-\tau_1}
\end{aligned}
$$

where $k = 0, \pm 1, \pm 2, ...$ denotes the branch of the multivalued logarithm. Therefore, in this case we have an infinite number of solutions. Also, if $n_1 = n_2 = n \neq 0$ then $\lambda = 0$ is a root of multiplicity n.

Case 3: $\tau_1 \neq \tau_2,\ n_1 \neq n_2$

$$
\begin{aligned}
&a_1\lambda^{n_1} e^{\tau_1\lambda} = -a_2\lambda^{n_2} e^{\tau_2\lambda} \\
&\Rightarrow \lambda^{n_1-n_2} e^{(\tau_1-\tau_2)\lambda} = -\frac{a_2}{a_1} \\
&\Rightarrow \left(\lambda^{n_1-n_2} e^{(\tau_1-\tau_2)\lambda}\right)^{\frac{1}{n_1-n_2}} = -\left(\frac{a_2}{a_1}\right)^{\frac{1}{n_1-n_2}} \\
&\Rightarrow \lambda e^{\frac{\tau_1-\tau_2}{n_1-n_2}\lambda} = -\left(\frac{a_2}{a_1}\right)^{\frac{1}{n_1-n_2}} \\
&\Rightarrow \frac{\tau_1-\tau_2}{n_1-n_2}\lambda e^{\frac{\tau_1-\tau_2}{n_1-n_2}\lambda} = -\frac{\tau_1-\tau_2}{n_1-n_2}\left(\frac{a_2}{a_1}\right)^{\frac{1}{n_1-n_2}} \\
&\Rightarrow \frac{\tau_1-\tau_2}{n_1-n_2}\lambda = W_k\left(-\frac{\tau_1-\tau_2}{n_1-n_2}\left(\frac{a_2}{a_1}\right)^{\frac{1}{n_1-n_2}}\right) \\
&\therefore \lambda = \frac{n_1-n_2}{\tau_1-\tau_2} W_k\left(-\frac{\tau_1-\tau_2}{n_1-n_2}\left(\frac{a_2}{a_1}\right)^{\frac{1}{n_1-n_2}}\right)
\end{aligned}
$$

Note that the solution has been written in terms of the Lambert W function (see Corless et al. [7]), which is implicitly defined as the function satisfying

$$
W(z)e^{W(z)} = z
$$

where $z \in \mathbb{C}$. The Lambert W function, like the logarithm, is multivalued. Therefore, in this case we have an infinite number of solutions. Also, if $n_1, n_2 \neq 0$ then $\lambda = 0$ is a root of multiplicity $\min\{n_1, n_2\}$.

This takes care of all possible cases for equation (3). □

Therefore, we know ALL the roots of ANY two-term quasipolynomial, which means that any two-term quasipolynomial satisfies the Triviality property.

5 Smoothness and Accessibility

We have shown that if we choose $Q(\lambda)$ to be the sum of two terms of $P(\lambda)$ then we are guaranteed to satisfy the Triviality property in any region R. However, this does not tell us how to choose *which* two terms of $P(\lambda)$ are to be used for $Q(\lambda)$. We want to guarantee that we do indeed find *every* root of $P(\lambda)$ that lies in the region R. We cannot simply use the roots of $Q(\lambda)$ that lie in R because it is possible that homotopy trajectories originating outside R may lead to points inside R. Therefore, we need a new region in which to look for roots of $Q(\lambda)$, and the number of roots of $Q(\lambda)$ in this region must equal the number of roots of $P(\lambda)$ in R (counting multiplicities).

First, let us state the Argument Principle and Rouché's Theorem.

Argument Principle. *If $P(\lambda)$ is meromorphic in a domain D enclosed by a simple contour Γ, let n be the number of complex roots of $P(\lambda)$ inside Γ, and let p be the number of poles inside Γ, then*

$$n - p = \frac{1}{2\pi i} \oint_{\Gamma} \frac{P'(\lambda)}{P(\lambda)} d\lambda.$$

Rouché's Theorem. *If $Q(\lambda)$ and $P(\lambda) - Q(\lambda)$ are analytic in a simply connected domain D containing a Jordan contour C and $|Q(\lambda)| > |P(\lambda) - Q(\lambda)|$ on C, then $Q(\lambda)$ and $P(\lambda)$ have the same number of roots inside C.*

The idea is to find the number of roots of $P(\lambda)$ in R using the Argument Principle and choose $Q(\lambda)$ such that $|Q(\lambda)| > |P(\lambda) - Q(\lambda)|$ on some Jordan contour C containing the roots of $P(\lambda)$ in R. Then by Rouché's Theorem, $Q(\lambda)$ has the same number of roots as $P(\lambda)$ inside C. Then we would only search for roots of $Q(\lambda)$ inside this Jordan contour C. However, defining this contour C in general, and proving Smoothness and Accessibility in the general case, is quite difficult and still not been done.

Instead, using Rouché's Theorem to guide our intuition, we have come up with a systematic way of choosing $Q(\lambda)$ that has so far survived all of our experimental testing. We propose to choose $Q(\lambda)$ as the dominant two terms of $P(\lambda)$ as $\lambda \to \pm\infty$.

There is also the problem of $Q(\lambda)$ having multiple roots. This is a problem since each root of $Q(\lambda)$ may lead to a different root of $P(\lambda)$. The homotopy paths are generated using the roots of $Q(\lambda)$. Therefore, multiple roots generate the same path, and therefore lead to the same root of $P(\lambda)$, possibly causing other roots of $P(\lambda)$ to be missed. To avoid this, we need to somehow distinguish multiple roots from each other. To do this we use Puiseux series, also known as fractional power series. We expand equation (2) using Puiseux series about the multiple root. At a multiple root of multiplicity m, there corresponds m Puiseux series expansions about that multiple root. At $\mu = 0$, each Puiseux series is equal to zero. Therefore, we evaluate each Puiseux series at a slightly larger value of μ, say $\mu = 0.1$. By $\mu = 0.1$ each Puiseux series has moved away from the multiple root in different directions. Taking a few terms of the Puiseux series at $\mu = 0.1$ in each direction gives us m distinct values to use as initial conditions in our homotopy, thus distinguishing the multiple roots from each other, thus generating different paths.

It turns out that this method of Puiseux series expansions about any $\lambda = 0$ roots also solves the problem of initial singularites at $\lambda = 0$ in the ordinary differential equation whose solutions define the homotopy paths.

For further reading on Puiseux series, see Casas-Alvero [3], Chudnovsky and Chudnovsky [5] and [6], Duval [9], Fine [10], Fischer [11], Fuchs and Levin [12], Hilton [14], Krantz and Parks [16], Kung and Traub [17], Siegel [25], Sturmfels [26], and Vui and So'n [27] .

6 A probabilistic approach for finding the Q root search region

The approach is outlined as follows. Consider a quasipolynomial, $P(\lambda)$. Use the homotopy method described above and compute a finite number of roots of $Q(\lambda)$ and the corresponding roots of $P(\lambda)$. Then draw the smallest possible box in the complex plane that contains all roots of $P(\lambda)$. Then determine the smallest amplification factor required for this box to be enlarged enough that it also contains all roots of $Q(\lambda)$. Do this for many different quasipolynomials and plot the results. Hopefully this will help gain insight for determining the region in which to search for roots of $Q(\lambda)$ so that with high probability, we obtain all roots of $P(\lambda)$ using our homotopy method. This method has no guarantees, but it is computationally faster than computing integrals to determine the number of roots in a region.

7 Implementation

Currently, we have no mathematical proof guaranteeing that the numerical method introduced here will ensure that we are always able to find all roots of a given quasipolynomial in a specified region, R. However, we have implemented this numerical homotopy method in a Maple procedure. The general algorithm used can be found in the Appendix.

In the current implementation we have used a different method for finding the region in which to search for roots of $Q(\lambda)$. First, the user defines a square region (four vertex points) in the complex plane in which they would like to find roots of $P(\lambda)$. Then, we find out in which branch of the analytical solution of $Q(\lambda) = 0$ each of the vertex points lie (see Jeffrey et al. [15] for information on the branches of the Lambert W function). Then we search for roots of $Q(\lambda)$ in the branches in which the vertex points lie and in all branches in between. Usually, this leads to more roots of $P(\lambda)$ than we want, but it is possible that roots of $P(\lambda)$ originate from outer branches, in which case, these roots would be missed.

Upon experimentation with our Maple procedure, we have found that in some problems we miss a root. This problem was solved by multiplying each term of $Q(\lambda)$ by a small random complex number. However, in other problems, multiplying each term of $Q(\lambda)$ by a small random complex number causes roots to be missed that would not have otherwise been missed. It still needs to be determined systematically which quasipolynomials require this and which do not.

It can also be shown that since our definition of a quasipolynomial requires the coefficients of each term to be real, then the distribution of roots of roots in the complex plane is symmetric about the real axis. The proof is as follows:

Show: If all $a_i s$ are real, then $\sum_{i=0}^{N} a_i(x+yi)^{n_i} e^{\tau_i(x+yi)} = 0$ implies $\sum_{i=0}^{N} a_i(x-yi)^{n_i} e^{\tau_i(x-yi)} = 0$.

Proof. First we have

$$\sum_{i=0}^{N} a_i(x+yi)^{n_i} e^{\tau_i(x+yi)} = 0.$$

Take the complex conjugate of both sides:

$$\sum_{i=0}^{N} a_i(x-yi)^{n_i} e^{\tau_i(x-yi)} = 0.$$

This shows that if we have a root of a quasipolynomial, its complex conjugate is also a root. □

This fact may be used to reduce computation time, however, it is not yet implemented in the Maple procedure.

8 Example

Consider the QP

$$P(\lambda) = -9\lambda^3 e^{2\lambda} - 35\lambda^2 e^{\lambda} - 94e^{\lambda} - 68.$$

Choose $Q(\lambda) = -9\lambda^3 e^{2\lambda} - 68$. Construct the homotopy and set $\lambda \to \lambda(\mu)$:

$$\begin{aligned} H(\lambda(\mu), \mu) =& (1-\mu)Q(\lambda(\mu)) + \mu P(\lambda(\mu)) \\ \therefore H(\lambda(\mu), \mu) =& -9\lambda(\mu)^3 e^{2\lambda(\mu)} - 35\mu\lambda(\mu)^2 e^{\lambda(\mu)} - 94\mu e^{\lambda(\mu)} - 68 \end{aligned}$$

Differentiate $H(\lambda(\mu), \mu) = 0$ with respect to μ. This gives an ordinary differential equation with which to construct the homotopy paths between the roots of $Q(\lambda)$ and the roots of $P(\lambda)$. The region R has been chosen to be $-3.0 \leq Re\lambda \leq 0.2$, $-8.1 \leq Im\lambda \leq 8.1$. Graphical results are shown in Figure 2.

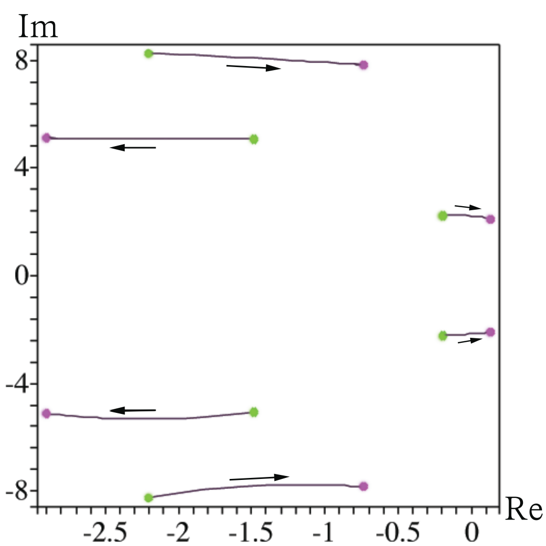

Figure 2: The green and magenta points correspond to the roots of $Q(\lambda)$ and $P(\lambda)$, respectively. The homotopy paths have been drawn and the arrows denote the direction of increasing μ.

9 Future work

A good way of choosing the region in which to search for roots of $Q(\lambda)$ still needs to be decided upon. Also, the problem of missing roots when we multiply the terms of $Q(\lambda)$ by small random numbers in some problems and missing roots when we *don't* multiply the terms of $Q(\lambda)$ by small random numbers in other problems needs to be looked at further. One way will find all the roots. Systematically choosing which way for which problem is something that needs to be explored.

Of course program efficiency can be improved. Using the symmetry in the roots about the real axis is one way. Also, since the homotopy moves the quickest at small μ, by the time we get to $\mu = 0.5$, the homotopy paths have pretty much arrived at their destination. The Maple procedure created uses a command called `dsolve` to solve the ordinary differential equation. Perhaps making the range of `dsolve` go from $\mu = 0$ to $\mu = 0.5$ instead of $\mu = 1$ will speed up computation time.

In addition, the current program only considers multiple roots of $Q(\lambda)$ at $\lambda = 0$ (by far the most common). However, other multiple roots are possible, and this possibility needs to be considered.

Appendix

Algorithm

Inputs: $P(\lambda)$, region R, tolerance
Find d_1 and d_2, the dominant terms of $P(\lambda)$
Set $Q(\lambda) = d_1(\lambda) + d_2(\lambda)$
Find $Q(\lambda)$
Determine region, R_Q, for $Q(\lambda)$
Find analytical solution of $Q(\lambda) = 0$
Find all (non-multiple) roots of $Q(\lambda)$ in R_Q
If $\lambda = 0$ is a root of $Q(\lambda)$ in R_Q then
   Define $H(\lambda, \mu) = (1-\mu)Q(\lambda) + \mu P(\lambda)$
   Using $H(\lambda, \mu)$, find the Puiseux series for λ about $\mu = 0$
   Evaluate each resulting series at some small value of μ, say 0.1 and include these
      values with the roots of $Q(\lambda)$ (number of series will correspond to root multiplicity)
# values of multiple roots other than $\lambda = 0$ are not yet considered
end if
Define $H(\lambda(\mu), \mu) = (1-\mu)(d_1(\lambda(\mu)) + d_2(\lambda(\mu))) + \mu P(\lambda(\mu))$
Define $DE = \frac{d}{d\mu} H(\lambda(\mu), \mu)$
Solve $DE = 0$ with the roots of $Q(\lambda)$ as initial conditions and evaluate at $\mu = 1$
Resulting points are an estimate for the roots of $P(\lambda)$ in R
Pass these points to Newton iteration until desired tolerance is achieved or MAXITS is reached

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