Numerical Computation of Quantum Graph Spectra

Chong-Son Dröge, Anna Weller
Department of Mathematics and Computer Science, Division of Mathematics
University of Cologne
droege@math.uni-koeln.de, weller@math.uni-koeln.de

Abstract

In the context of spectral solution methods for partial differential equations on metric graphs, the efficient computation of *quantum graph* spectra is of utmost importance. Under a quantum graph, we understand a metric graph equipped with a differential operator and for which suitable coupling conditions at the nodes apply. The differential operator of our interest is the negative second order derivative acting on each edge. The spectrum of the quantum graph is then understood as the spectrum of the differential operator acting on the metric graph.
The special case where all edges in the graph have the same length (*equilateral graphs*) has been discussed in [AW] using a well-known connection of quantum and combinatorial graph spectra. Unfortunately, these simplifications do not apply for graphs with different edge lengths. Here, some more work has to be done in order to resolve the eigenvalues and corresponding eigenfunctions.
The simplest situation where all edges have integer lengths can be treated using the observation that the spectrum of a quantum graph does not change when we insert vertices with degree two on the edges. Thus, one can simply modify the graph to an equilateral *extended graph*. For the general case with real, positive edge lengths, we show that we can relate the spectrum to a so-called *Nonlinear Eigenvalue Problem* (NEP): Find eigenvalues $\lambda > 0$ such that a nontrivial $\mathbf{v}$ with

$$\mathbf{H}(\lambda)\mathbf{v} = 0$$

exists. Interestingly, the size of the matrix $\mathbf{H}$ is given by the number of vertices of the graph and the information on the edge lengths only contributes to the entries of the matrix. Conveniently, the corresponding eigenfunctions can be constructed using $\mathbf{v}$.
The solutions of the NEP can be found as the roots of $\det(\mathbf{H}(\lambda))$, which is a highly nonlinear problem. A popular solution method for NEPs is the Newton-trace method [GT]. However, the key to the efficient application of this method are suitable initial guesses. To find these, we propose two different approaches [DW]: First, we investigate a polynomial approximation of $\mathbf{H}$ and apply standard nonlinear eigenvalue solvers for polynomial problems. Secondly, we present a workflow to approximate non-equilateral graphs by equilateral graphs and use the eigenvalues of these approximations as a first guess and improve them using the Newton-trace iteration.

This work was supported by Hypatia.Science, an initiative for the promotion of young female scientists at the Department of Mathematics and Computer Science of the University of Cologne.

References

[AW] M. Ainsworth, A. Weller, *A spectral Galerkin method for the solution of reaction-diffusion equations on metric graphs*, Oberwolfach Reports, Workshop Report 36, 2021.

[DW] C. Dröge, A. Weller, *Numerical computation of quantum graph spectra as solutions of nonlinear eigenvalue problems,* in preparation.

[GT] S. Güttel, F. Tisseur, *The nonlinear eigenvalue problem*, Acta Numerica, 26, 1-94., 2017.