Numerical Solution of Singular ODE Eigenvalue Problems Using the `Matlab` Code `bvpsuite`

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We consider boundary value problems for systems in ODEs which exhibit singular points in the interval of integration. In context of eigenvalue problems we deal with the following important problem class:

$$
\begin{aligned}
&z''(t) - 1/t^{\alpha} f(t, z'(t)) - 1/t^{\alpha+1} g(t, z(t)) = \lambda z(t), \quad t \in (0, 1], \\
&g(z(0), z(1)) = 0,
\end{aligned}
$$

where α is non-negative. Depending on the value of α one distinguishes between singularity of the first kind, $\alpha = 1$, and essential singularity, $\alpha > 1$. We first briefly recapitulate the analytical properties of such problems, especially the existence and uniqueness of bounded solutions, an important prerequisite for the well-posedness of the system.

A `Matlab` code `bvpsuite` which can be applied to approximate the above problem class is presented. This solver is based on polynomial collocation, equipped with a posteriori estimates of the global error of the solution $z(t)$, and features an adaptive mesh selection procedure based on the equidistribution of the global error.

Finally, we demonstrate the reliability and efficiency of our code by solving a few problems relevant in applications. Here, our main focus is on the singular eigenvalue problems such as Schrödinger equations, arising in electronic structure computations. In most established standard methods, the generation of the starting values for the computation of eigenvalues of higher index is a critical issue. Our approach comprises two stages: First we generate rough approximations by a *matrix method*, which yields several eigenvalues and associated eigenfunctions simultaneously, albeit with moderate accuracy. In a second stage, these approximations are used as starting values for a collocation method which yields approximations of high accuracy efficiently due to an adaptive mesh selection strategy, and additionally provides reliable error estimates. We successfully apply our method to the solution of the quantum mechanical Kepler, Yukawa and the coupled ODE Stark problems.

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