Discretisation of Transfer Operators by Sparse Spectral Methods

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Abstract

Eigenvectors of transfer operators play an important role in the calculation of almost-invariant sets[1]. In the case of a flow arising from the solution of an autonomous ordinary differential equation, the transfer operator for the flow at time-t is described by a partial differential equation called the Liouville equation. For stochastic perturbations of the flow, the Fokker-Planck equation takes the role of the Liouville Equation. Each of these equations has an *infinitesimal generator* which is a linear partial differential operator that has the same eigenvectors as the transfer operator being considered[1].

Recently, a discretisation method for general linear partial differential operators was introduced by Olver and Townsend[2, 3] called the *ultraspherical method*. This method is attractive because it results in banded representation matrices for a wide class of linear operators, including some of those mentioned above. This suggests that this discretisation method could be effective for discretising the infinitesimal generator of the Liouville/Fokker-Planck equation to find almost-invariant sets.

Transfer Operators

Consider a bijective function $T : \Omega \to \Omega$. For *non-singular* T with respect to a measure μ, the Frobenius-Perron operator $P_T : L^1(\mu) \to L^1(\mu)$ describes the transfer of measures under T.

$$\int_A P_T f d\mu = \int_{T^{-1}(A)} f d\mu$$

In the case that T_t is the time-t flow map of an autonomous ordinary differential equation $u' = F(u)$, the Frobenius-Perron operator is described by a partial differential equation.

More precisely: subject to some technical restrictions, the functions $\rho(x,t) := P_{T_t} f(x)$ obey the Liouville Equation:

$$\partial_t \rho = -\text{ div } (F\rho)$$

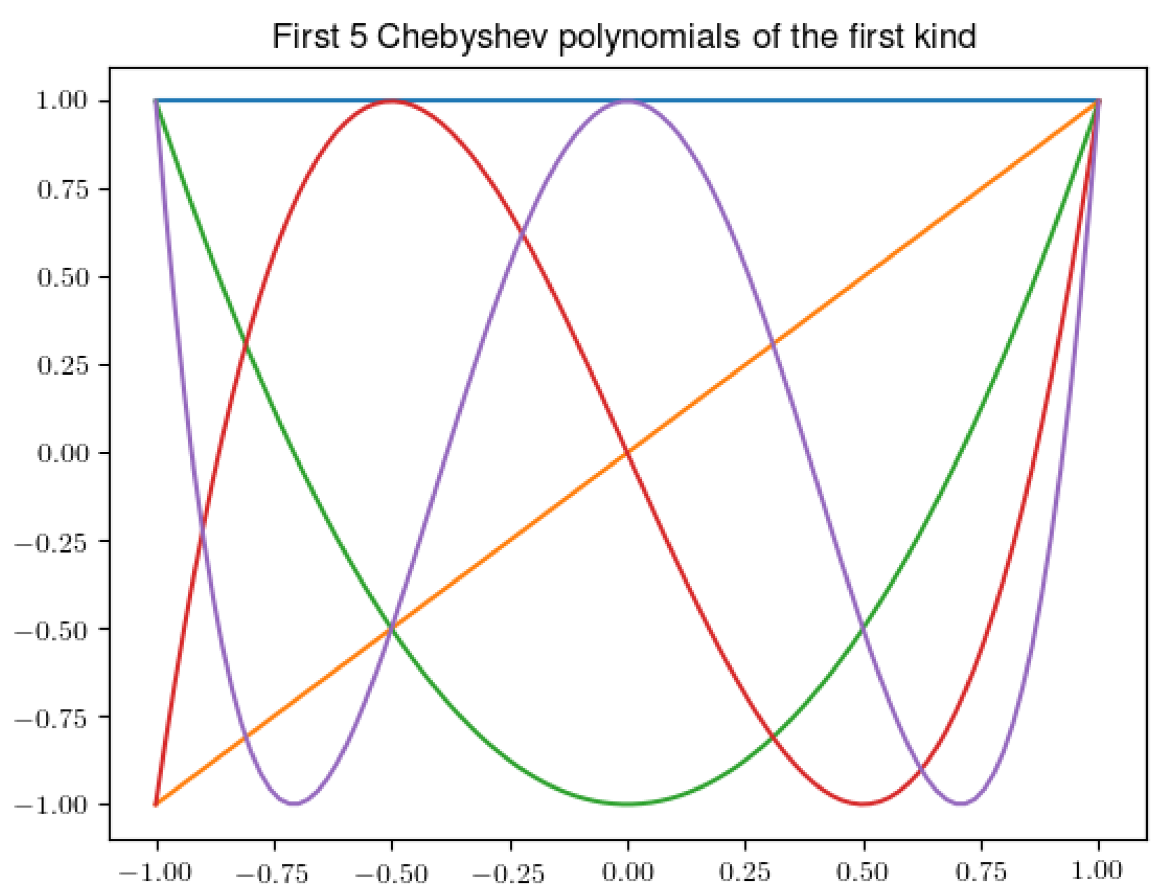
For a stochastic perturbation of the flow, the Liouville Equation is replaced by the Fokker-Planck equation:

$$\partial_t \rho = -\text{ div } (F\rho) + \frac{\epsilon^2}{2}\Delta\rho$$

Eigenvectors of the transfer operators can be used to give information about important features of the flow such as "almost-invariant" sets. [1]. This suggests that discretisations of the Liouville/Fokker-Planck equation can be used to numerically obtain information about almost-invariant sets (see also [1]).

The Ultraspherical Method

- A spectral method, introduced in [2, 3]
- Gives representation matrices for wide class of linear ordinary differential operators.
- Different basis used for domain and range of representation matrix.
- Basis for the domain consists of Chebyshev polynomials of the first kind:



- Basis for the range consists of Ultraspherical-(λ) polynomials ($\lambda \in \mathbb{N}_0$), which are (up to scaling) higher order derivatives of the Chebyshev polynomials of the first kind.
- Both multiplication and differentiation become banded! The resulting representation-matrices (including boundary conditions) can be QR-factorised in linear time[2].
- Higher-dimensional partial differential operators can be discretized using a tensor-product approach (see also [3]).

The Infinitesimal Generator

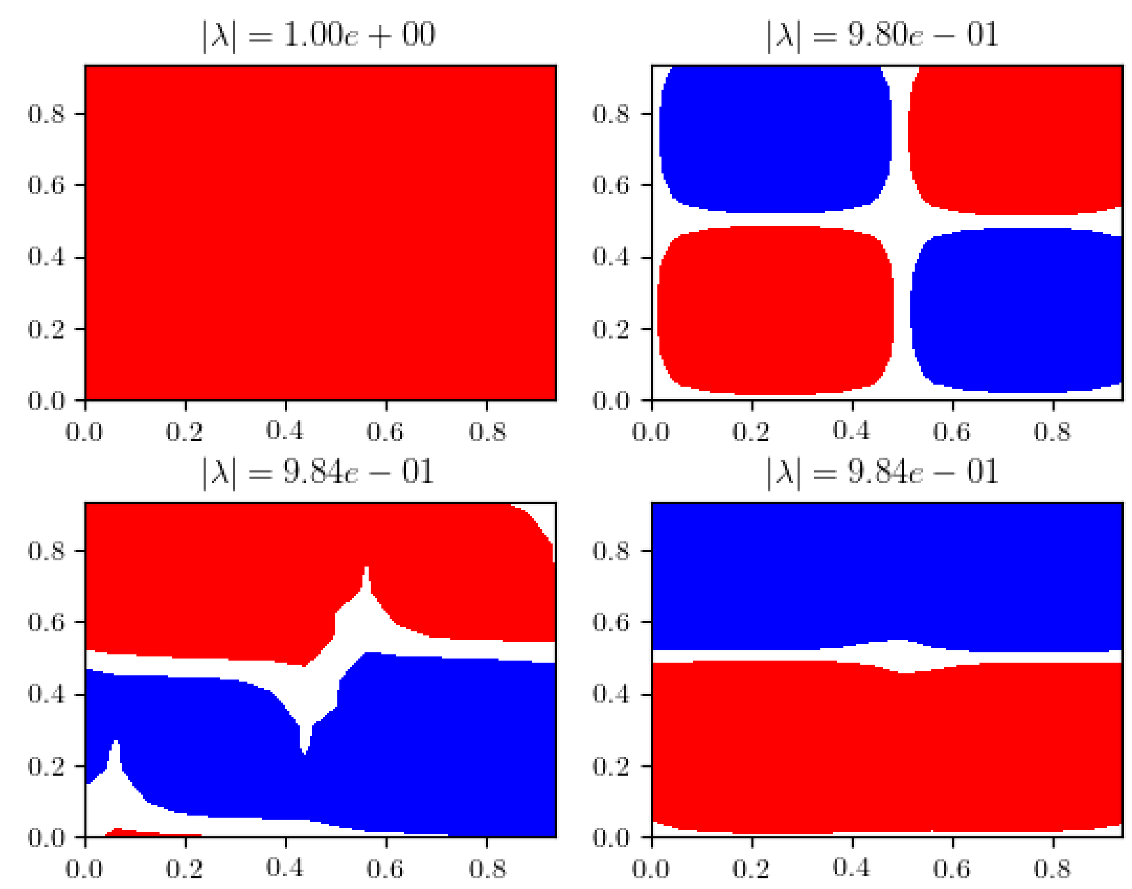
When looking at solutions to the ODE $u' = Au$ with linear A, then the eigenvectors of the solution operator e^{tA} are the same as those of A (spectral mapping theorem). A similar result also holds for the infinite-dimensional setting[1]. Here it is enough to consider the eigenvectors of the operator $\rho \mapsto \text{div}(F\rho)$ instead of looking at the time-t solution operator of the Liouville-Equation. This makes it possible to use discretisation methods like the ultraspherical method for numerically approximating eigenvectors of the transfer operator.

Polynomial Spectral-shifts

- Instead of looking for eigenvectors of discretisation A of the infinitesimal generator, look at those for $p(A)$ where p is a polynomial.
- By spectral mapping theorem, eigenvectors stay the same.
- If $|p(\lambda)| \leq$ for all $\lambda \in \sigma(A)$, and if non-zero eigenvalues of the infinitesimal generator are in the interior of the left-hand side of the complex plane, and $p(0) = 1$, then we can look for small eigenvalues of A by looking for large eigenvalues of $p(A)$. This means power iteration can be applied to find small eigenvectors of A without needing to invert A.
- If p is the stability polynomial for an explicit Runge-Kutta method, then $p(A)$ describes the numerical solution of the Liouville Equation using the method of lines. The requirement $|p(A)| \leq 1$ corresponds to requiring absolute stability for the Runge-Kutta method used in the method of lines.

Numerical Results

- No conclusive results regarding the effectiveness of the ultraspherical method for calculating almost-invariant sets.
- Successful calculation of invariant densities in the 1d case using ultraspherical discretisation.
- The method of polynomial spectral shifts was successfully applied together with a pseudospectral discretisation using the fast Fourier transform to calculate almost invariant sets. However, doing so was not faster than explicitly dealing with the represenation matrix of the discretisation of the infinitesimal generator.



The image above shows the sign of the real part of eigenvectors calculated with pseudospectral method and a polynomial spectral shift using a fourth order Runge-Kutta method.

References

[1] Gary Froyland, Oliver Junge, and Péter Koltai. Estimating long-term behavior of flows without trajectory integration: The infinitesimal generator approach. *SIAM Journal on Numerical Analysis*, 51(1):223–247, 2013.

[2] Sheehan Olver and Alex Townsend. A fast and well-conditioned spectral method. *SIAM Review*, 55(3):462–489, 2013.

[3] Alex Townsend and Sheehan Olver. The automatic solution of partial differential equations using a global spectral method. *Journal of Computational Physics*, 299:106–123, 2015.

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