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Surrogate models for diffusion on graphs: a high-dimensional polynomial approach

Graphs are an essential mathematical tool used to model real-life complex systems such as social networks and transportation networks. Understanding diffusion processes on graphs is crucial for modelling phenomena such as the propagation of information within a network of individuals or the flux of goods and/or people through a transportation network. Accurately simulating these diffusion processes can be, in general, computationally demanding since it requires the solution of large systems of ordinary differential equations.

Motivated by this challenge, we propose to construct surrogate models able to approximate the state of a graph at a given time from the knowledge of the diffusivity parameters. Specifically, we consider recently introduced high-dimensional approximation methods based on sparse polynomial expansions, which are known to produce accurate, sample-efficient approximations when the function to be approximated has holomorphic regularity. Hence, to justify our methodology, we will theoretically show that solution maps arising from a certain class of parametric graph diffusion processes are indeed holomorphic. Then, we will numerically illustrate that it is possible to efficiently compute accurate sparse polynomial surrogate models from a few random samples, hence empirically showing the validity of our approach.