Time and space generalized diffusion equation on graph/networks

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Random walks and diffusion are one of the most relevant research areas of statistical physics, due to the wide range of phenomena that show a diffusive behavior. Nevertheless, many real systems violate the predictions of standard diffusion, because of the presence of phenomena such as long range interactions or kinetic traps. This *anomalous diffusion* can be identified by looking at the time scaling of magnitudes such as the height of the maximum of the pdf (f_{max}) or the Full Width at Half Maximum (FWHM). In particular, given that f_{max} usually follows a power law ($f_{max} \propto t^{-\gamma}$), exponents $\gamma < 0.5$ can be identified with subdiffusive systems and exponents $\gamma > 0.5$ with superdiffusive ones.

Several tools have been derived to analyze anomalous diffusion, many of them based on continuous time random walks (CTRW) and fractional diffusion equations [1]. However, most of these approaches neglected the networked structure of many of these systems. To overcome this limitation of previous models, we proposed in [2] a generalized diffusion equation for networks, using Caputo time-fractional derivatives and d-path Laplacian operators [3, 4]. As a result, we obtained a simple equation with a fractional derivative parameter α and a nonlocal hopping parameter s. We analytically proved that the solution of this equation is able to recreate diffusive, subdiffusive and superdiffusive scenarios, and found the parameter regimes where the different types of anomalous diffusion appear (figure 1). We also performed computational simulations that qualitatively agree with our analytical predictions (figure 2).
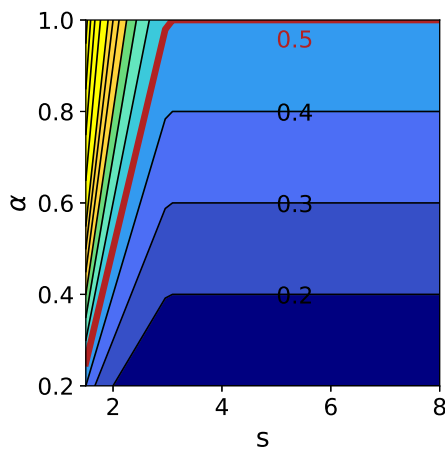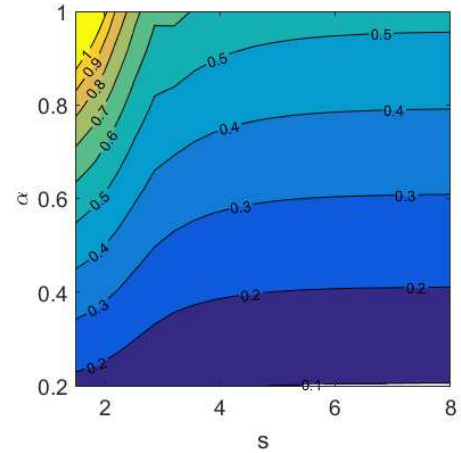

Fig. 2. *Contour plot of the exponent γ of the maximum of the pdf obtained by performing numerical simulations, as a function of the two parameters of the generalized diffusion equation (α and s). Values below $\gamma = 0.5$ correspond to subdiffusion and above $\gamma = 0.5$ correspond to superdiffusion.*

diffusion of proteins along a DNA chain, which is known to exhibit sub- and superdiffusive behaviors [5]. The DNA chain structure can be modelled as a path graph with long-range interactions, and the diffusing proteins can be modelled as particles with time-varying average jump lengths. We find that an alternancy of sub- and superdiffusion allows the proteins to explore more carefully certain regions of the DNA with a faster global exploration. This could represent an advancement in the understanding of protein-DNA interactions.

Proofs and fully detailed explanations of our work can be found in Ref. [2].

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Fig. 1. *Contour plot of the analytical prediction of the exponent γ of the maximum of the pdf as a function of the two parameters of the generalized diffusion equation (α and s). Values below $\gamma = 0.5$ correspond to subdiffusion and above $\gamma = 0.5$ correspond to superdiffusion.*

As as example of the utility of our model, we studied the