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Supplementary Material

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1. Simplification analysis

For extremely topologically rich datasets it is often necessary to simplify branches of small edge weights to aid in the eBDG comparison step as discussed in Section 6.4. To this end, we plot the computation time against several levels of simplification of the EMDB-1603 dataset. At few levels, the number of edges of the join tree are shown as well.

2. Perturbation analysis

Herein are some additional plots for different datasets illustrating the stability of the BDT against noise. The y-axis denotes the cost of comparing the full BDT with a noisier version of itself, normalized by the total weight of the original BDT. The x-axis represents the noise levels in % values of the maximum function range of the dataset. In each plot 20 samples are plotted for every noise level and edge weight type. The choice of edge-weight type significantly influence the stability of the BDT as discussed in Section 6.2.



Figure 1: Simplification analysis.



Figure 2: *Perturbation analysis on the time-dependent Cylinder dataset for* T = 75*.*



Figure 3: Perturbation analysis on the Benzene dataset.



Figure 4: Perturbation analysis on the Nucleon dataset.

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