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Causal Discovery with Quantum Machine Learning

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Detecting statistical dependence between stochastic processes is a core primitive of causal discovery for dynamical systems. State-of-the-art tests compare whole trajectories with the signature kernel, which propagates a static point-similarity kernel through a Goursat PDE and feeds the resulting Gram matrices into kernel independence tests (HSIC, SDCIT). We investigate replacing the classical RBF static kernel with a quantum embedding kernel: a data-reuploading circuit maps each time-augmented path point to a quantum state, and similarity is the state fidelity, read out with the adjoint-circuit trick. Since only the static kernel is swapped, performance differences are attributable to the kernel itself. The circuit angles and an input scale are trained to maximize a standardized-HSIC proxy of test power using SPSA with Adam and held-out validation, avoiding differentiation through the PDE solver. In simulations on linear SDEs, the trained quantum kernel improves HSIC test power over both the classical and the untrained quantum kernel at small sample sizes, while preserving type-I error control, and supports PC-style recovery of multivariate causal graphs with conditional tests. We further study register widths of 4-12 qubits, connecting fidelity concentration to trainability, and note that the ansatz maps natively onto IBM Heron hardware (CRZ as native RZZ plus virtual RZ; 12-qubit heavy-hex loops).

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