Demystifying diffusion models via their Markov semigroups

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Markov diffusion processes are a crucial instrument in Bayesian sampling and generative modeling, thanks to their strength in interpolating between distributions. The law of a Markov diffusion process is fully described by its Markov semigroup – a *temporally indexed* family of operators that characterize conditional expectations. Inspecting diffusion processes via the lens of their Markov semigroups yields novel insights.

Diffusion models first reduce an intractable data distribution p_{data} to a noise distribution π via the simulation of a diffusion process, and seek to invert it for sample generation by assessing the scores of the interpolating distributions. We observe that the densities of intermediate noise-corrupted distributions can be regarded as *kernel mean embeddings of* p_{data}, namely, $\int k_t(x, \cdot)\mathrm{d}p_{\mathrm{data}}(\cdot)$, in a *temporally indexed* family of kernels $\{k_t\}$ associated with its Markov semigroup. Moreover, the learning of the mean embedding function at a certain noise level simultaneously approximates those of higher noise levels. Empirically, we manage to generate samples from p_{data} by estimating one singular mean embedding with a flexible kernel-based parametrization, thus disentangling the temporal and spatial effects of black-box score matching paradigms.