



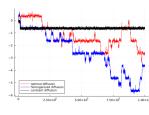


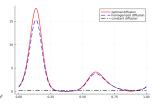


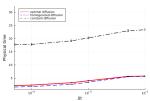
Optimizing overdamped Langevin dynamics

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Markov chains

Diffusion coefficients

Transition times

$$dq_t = \left(-\mathcal{D}(q_t)\nabla V(q_t) + \beta^{-1}\operatorname{div}\mathcal{D}(q_t)\right)dt + \sqrt{2\beta^{-1}\mathcal{D}(q_t)}dW_t$$

Improve sampling efficiency for metastable dynamics

$$\frac{1}{N} \sum_{i=1}^{N} f(q^{i}) \xrightarrow[N \to +\infty]{} \mathbb{E}_{\pi}[f], \quad \pi \propto e^{-\beta V}$$