GRADIENT FLOWS ON FINITE STATE MARKOV CHAINS

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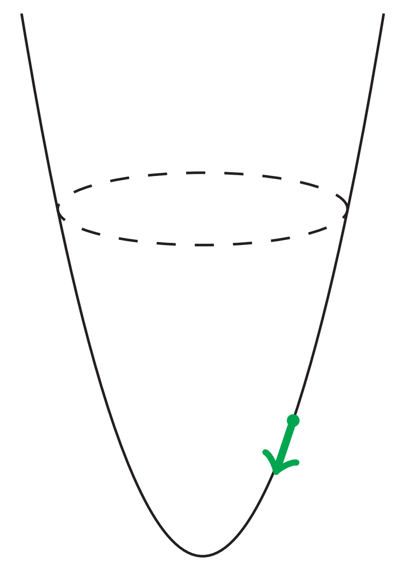
MOTIVATION

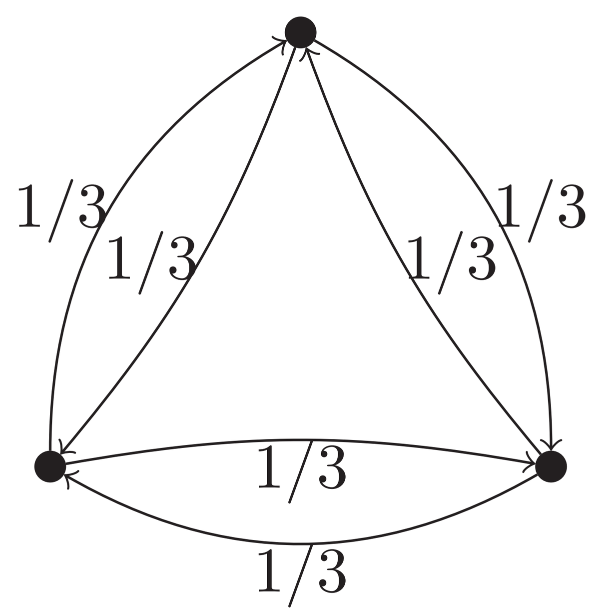


Jordan, Kinderlehrer, and Otto (1998) identified the Fokker-Planck equation

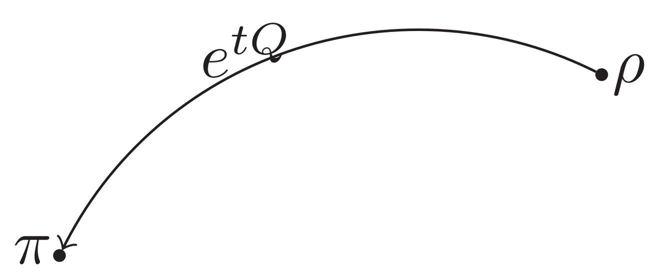
$$\partial_t u - \nabla \cdot (\nabla u + u \nabla V) = 0$$

as *gradient flow* in $E := \mathcal{P}_2(\mathbb{R}^d)$ using the Wasserstein $\mathcal{W}_2$ distance.

CONSTRUCTION BY MAAS

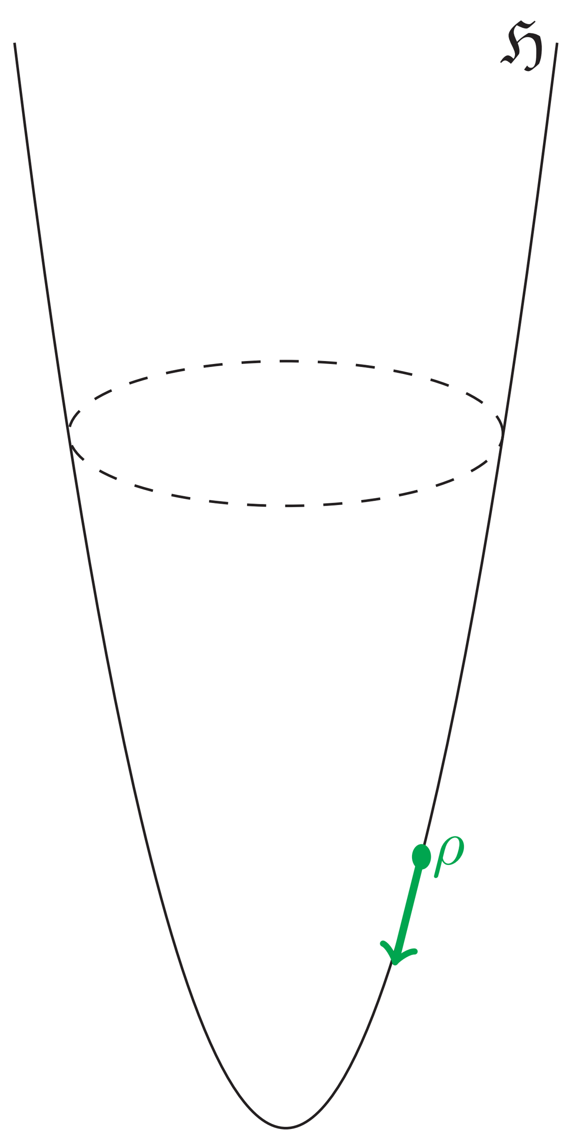


Let $\mathcal{X} = \{0, \dots, d\}$ be a finite state space and K the transition matrix of a Markov chain.
Then the semigroup e^{tQ} with generator $Q = K - I$ converges to the equilibrium π. Is this a gradient flow?



For a gradient flow of the potential $\mathfrak{F}$, we need a Riemannian metric g identifying the cotangent vector $-\mathrm{d}\mathfrak{F}$ with the tangent vector $\partial_t \rho$.
Maas (2011) showed that if K is time-reversible, then e^{tQ} is the gradient flow of the relative entropy

$$\mathfrak{H}(\rho) = \sum_{i \in \mathcal{X}} \rho_i \log \frac{\pi_i}{\rho_i}.$$



The constructed metric cannot come from the Wasserstein distance $\mathcal{W}_2$. Still the metric is motivated by the Wasserstein metric, but the transportation cost depends on the current state.

CHARACTERISATION

When can the semigroup e^{tQ} be written as gradient flow?

Assuming C^2 potential and C^1 metric we show

- e^{tQ} is a gradient flow of the relative entropy $\mathfrak{H}$ only if Q is time-reversible,
- e^{tQ} is a gradient flow of some functional $\mathfrak{F}$ if and only if Q is real diagonalisable.

The proof idea is to expand the flow around the equilibrium distribution π.

Together with Maas' construction this shows:

> The semigroup e^{tQ} can be written as gradient flow of the relative entropy $\mathfrak{H}$ if and only if Q is time-reversible.

UNIQUENESS OF THE METRIC

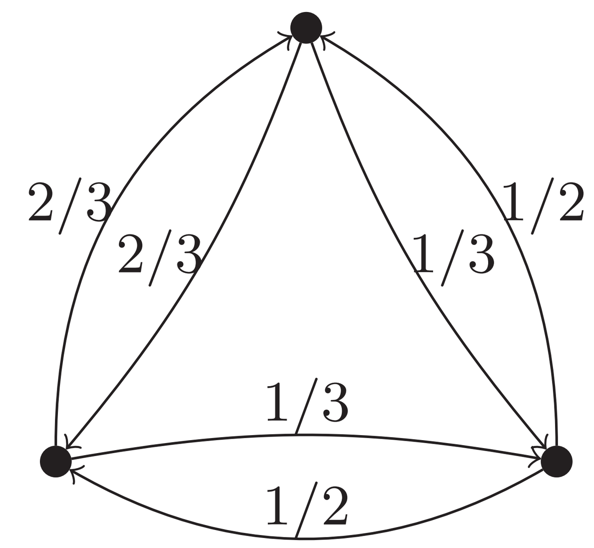
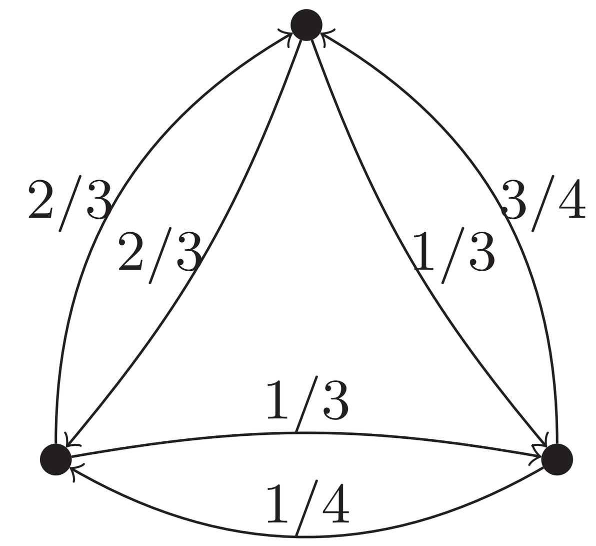
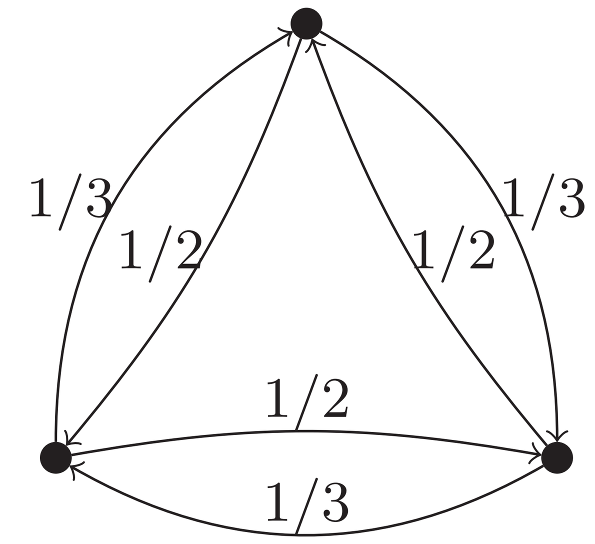
If $d \geq 2$, then the Riemannian metric g identifying e^{tQ} as gradient flow is unique at the equilibrium π. For $\rho \neq \pi$, there exists another metric g' still identifying the semigroup with the gradient flow but $g \neq g'$ at ρ.

DECREASING FUNCTIONAL

From the heat flow analogy the relative entropy $\mathfrak{H}$ is a natural functional for the gradient flow.

Moreover, if $\mathfrak{F}_\pi : \mathcal{P}(\mathcal{X}) \mapsto \mathbb{R}$ is a potential such that every irreducible, time-reversible Markov chain converging to π is a gradient flow with respect to it, then $\mathfrak{F}_\pi$ equals $\mathfrak{H}$ up to quadratic order around π (ignoring rescaling).

EXAMPLES

	Gradient flow of $\mathfrak{H}$	Gradient flow of some $\mathfrak{F}$
	✓	✓
	✗	✓
	✗	✗

REFERENCES

[1] Richard Jordan, David Kinderlehrer, and Felix Otto. The variational formulation of the Fokker-Planck equation. *SIAM J. Math. Anal.*, 29(1):1–17, 1998.

[2] Jan Maas. Gradient flows of the entropy for finite Markov chains. *J. Funct. Anal.*, 261(8):2250–2292, 2011.

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