Hamiltonian Monte Carlo

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Machine Learning Summer School
London, United Kingdom
July 23, 2019

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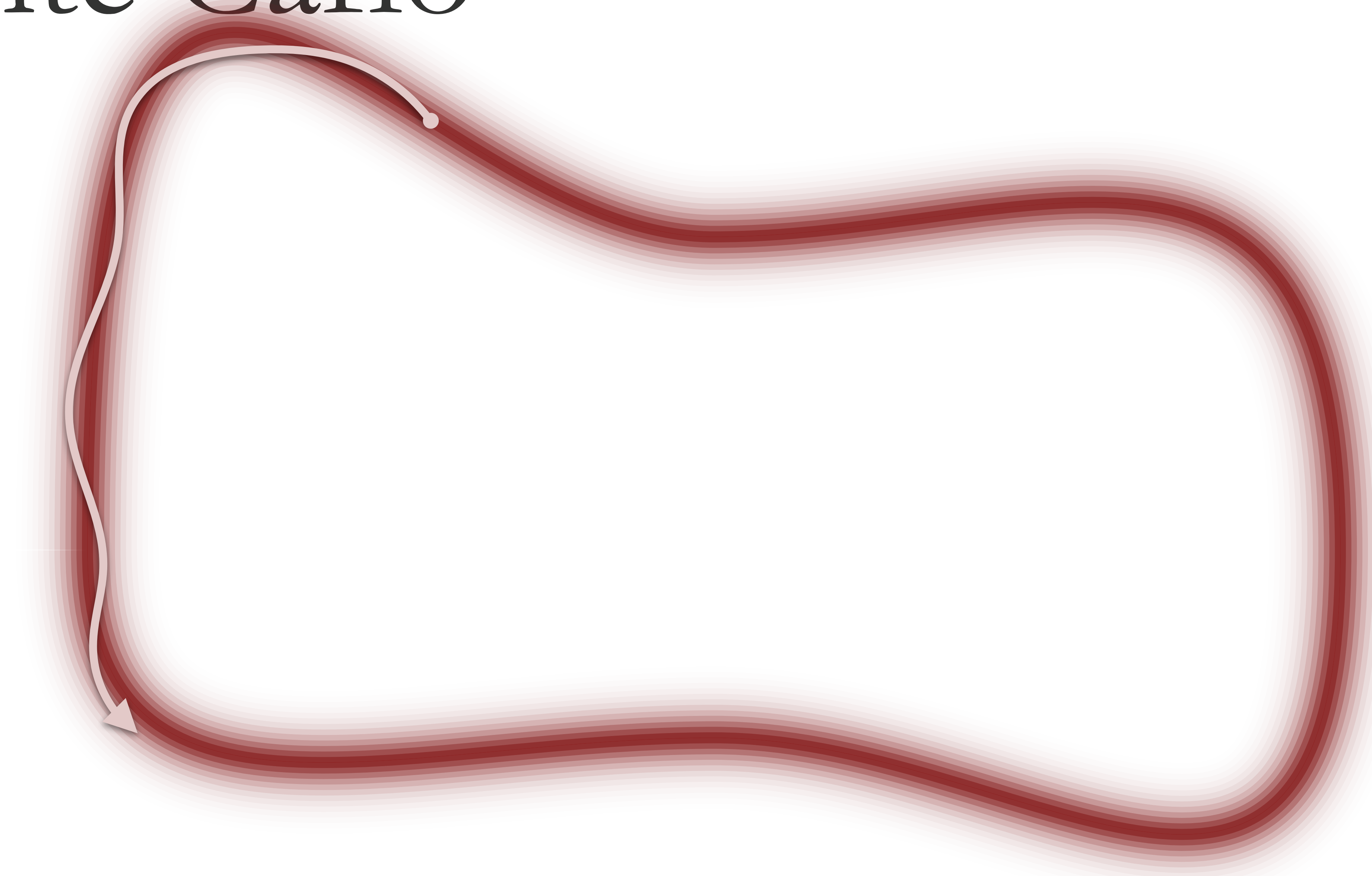

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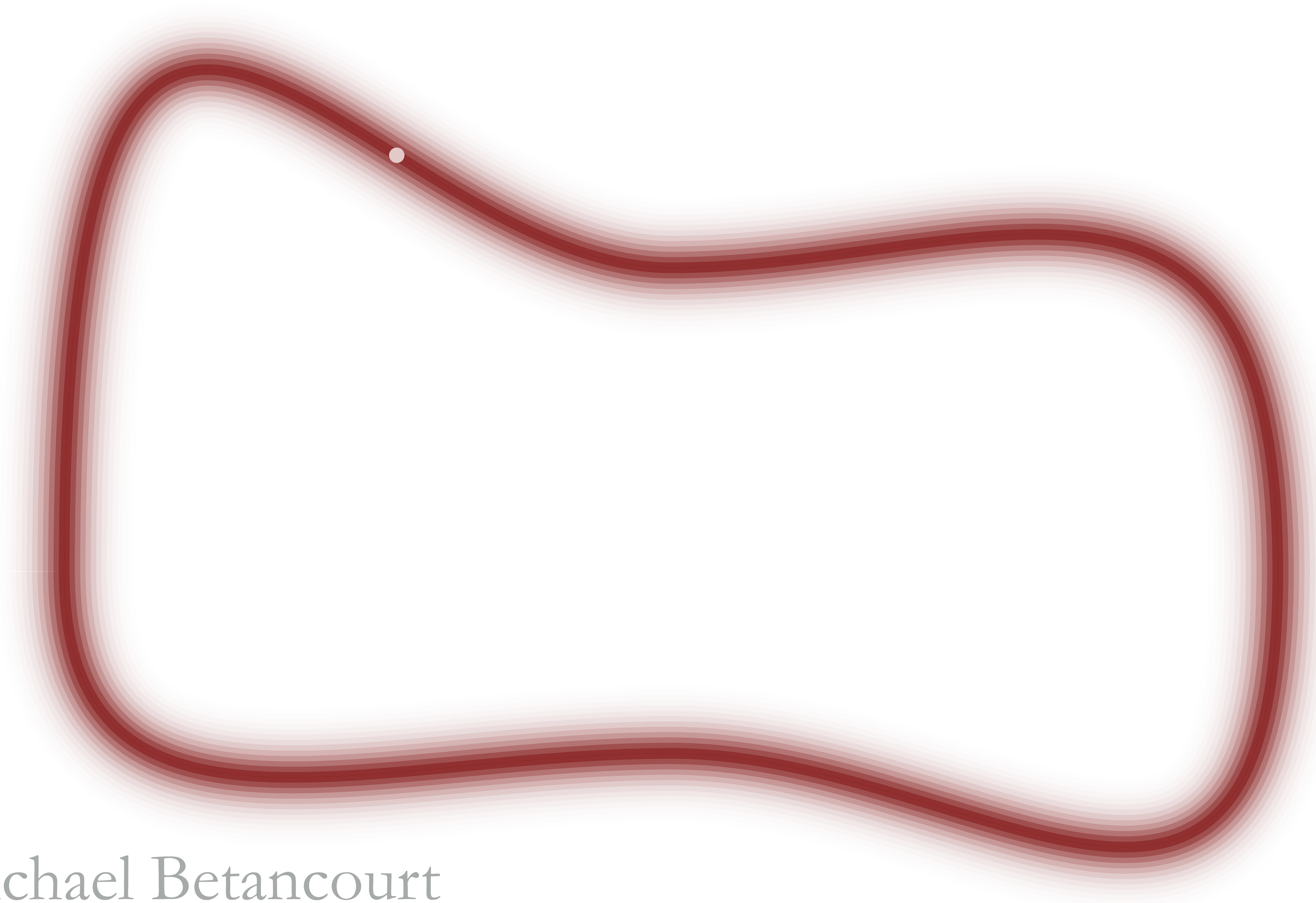
In order to efficiently scale to complex posteriors, MCMC needs *coherent* exploration of the typical set.



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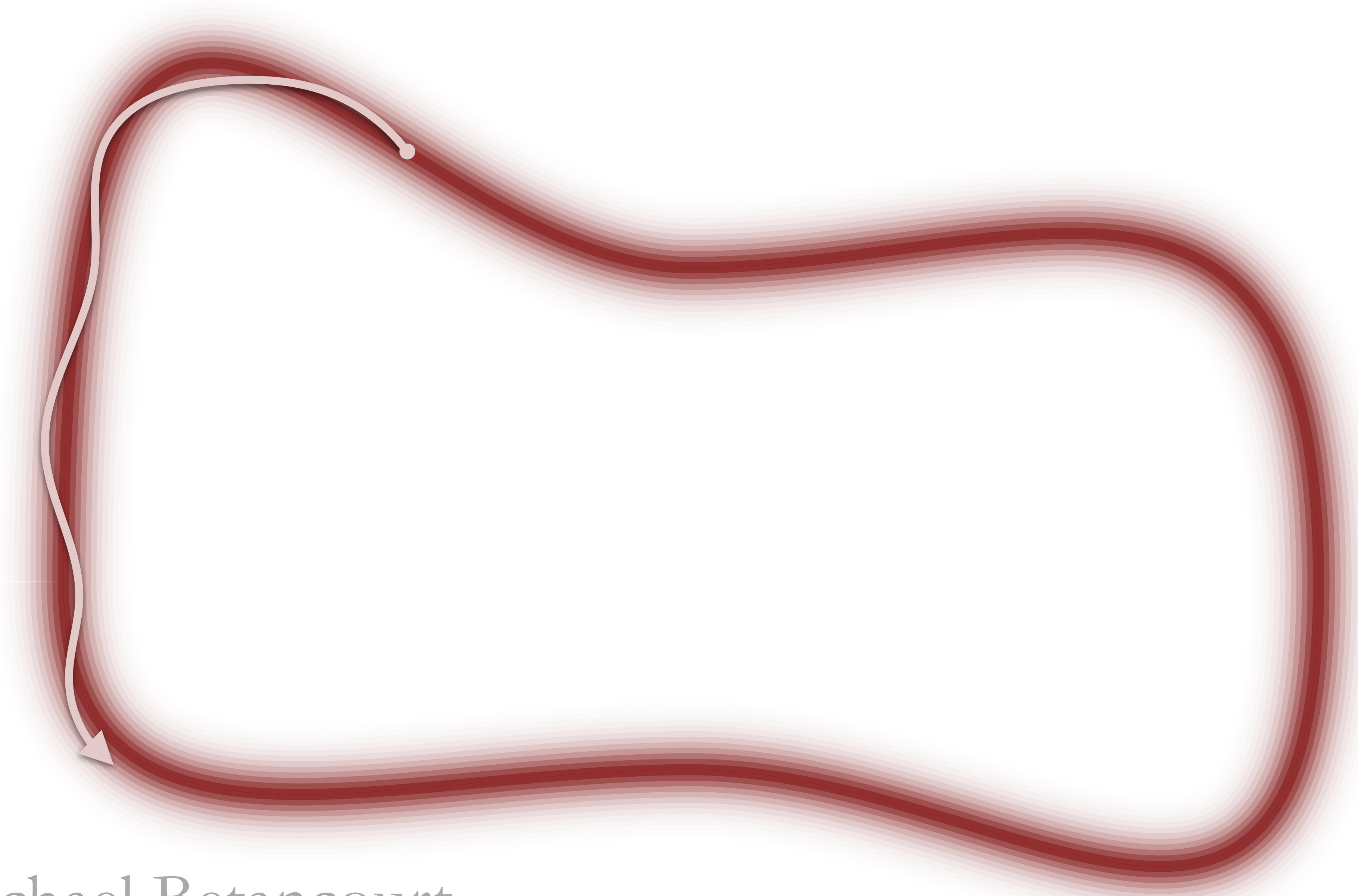

Exploration of the typical set is generated by measure-preserving maps over parameter space.

$$\phi_t : Q \to Q$$

$$\left(\pi \circ \phi_t^{-1} \right) (A) = \pi(A)$$

Coherency of that exploration requires equipping a space of maps with the structure of a Lie group to give a *flow*.

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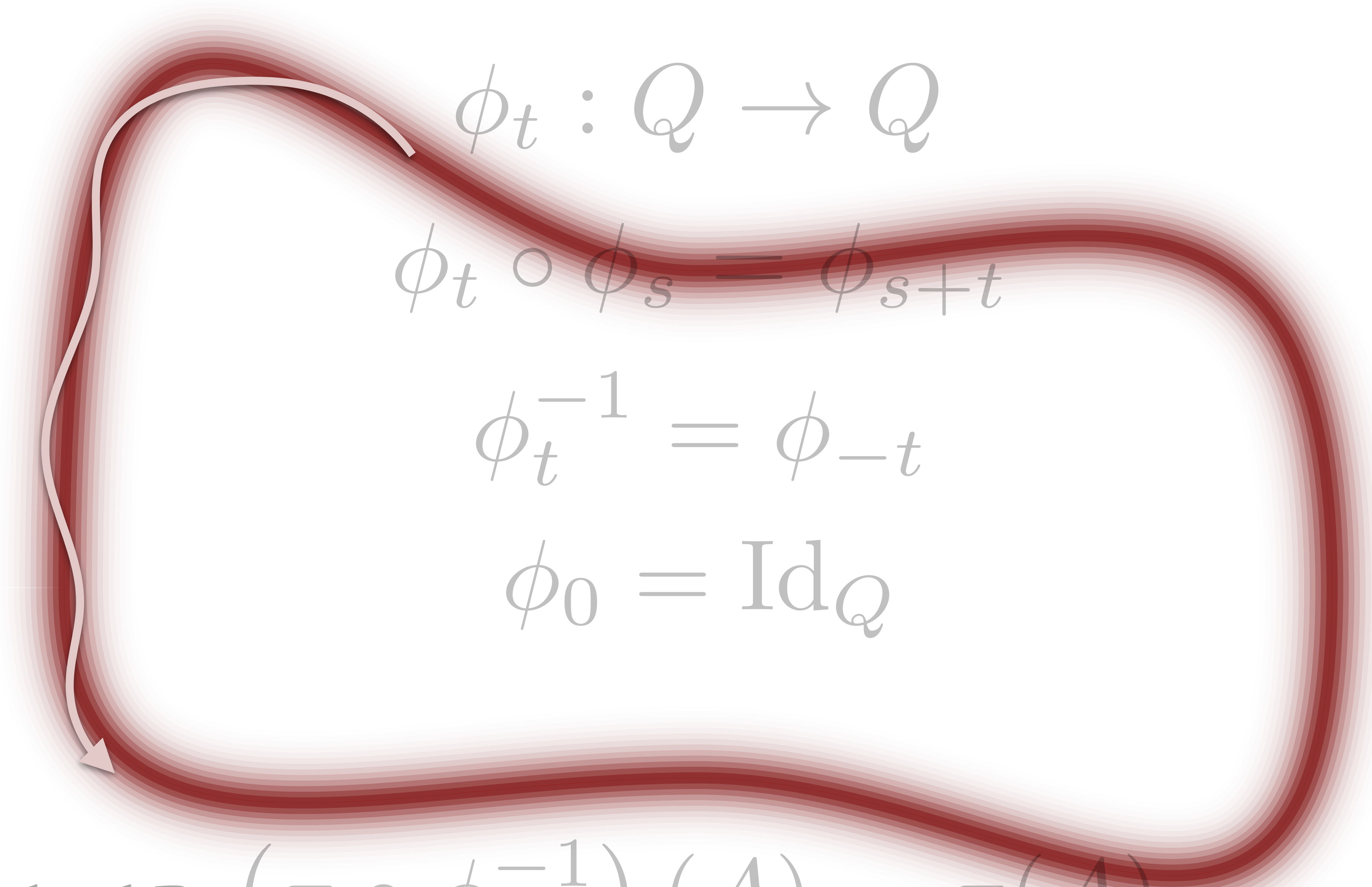

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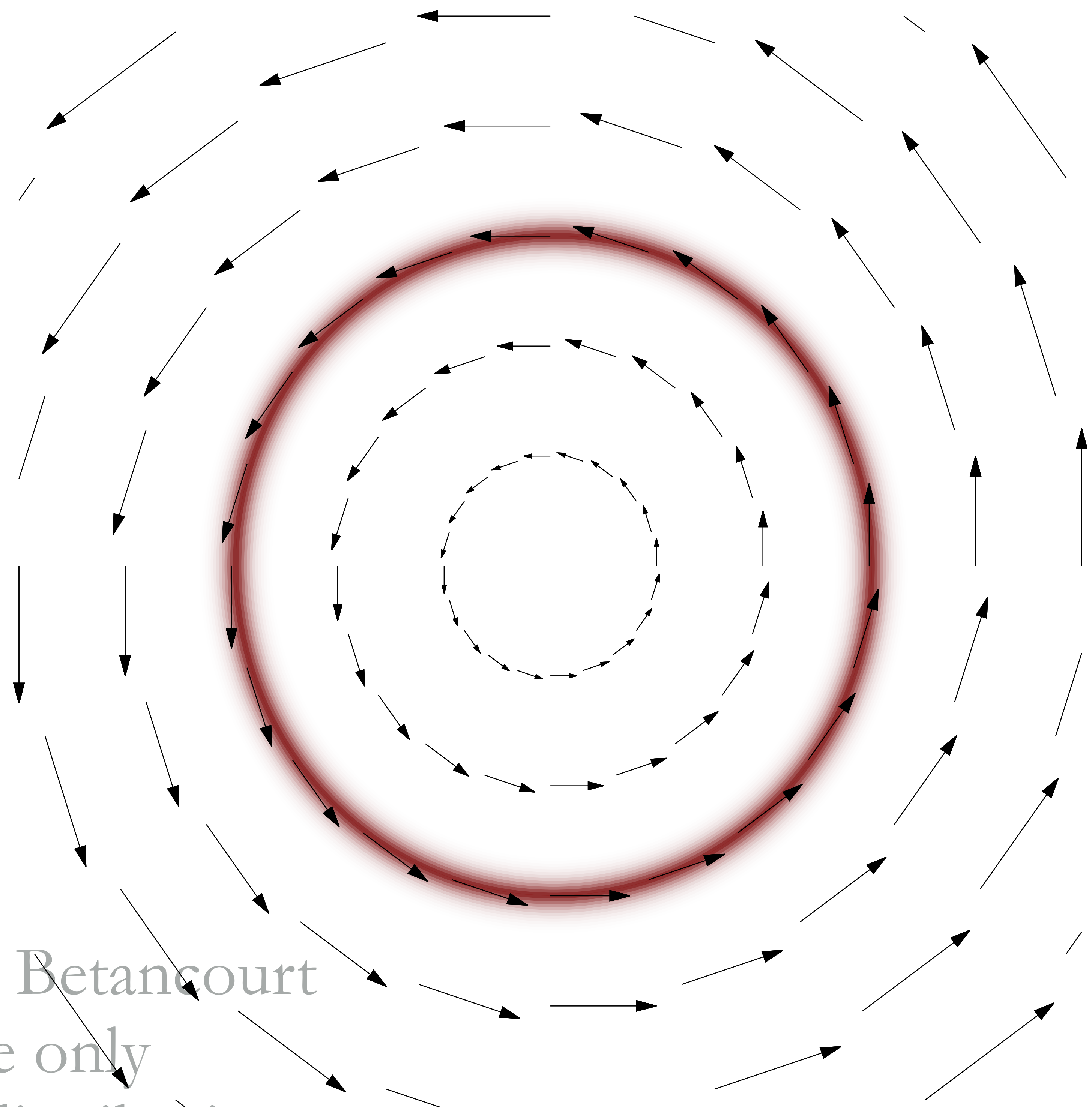

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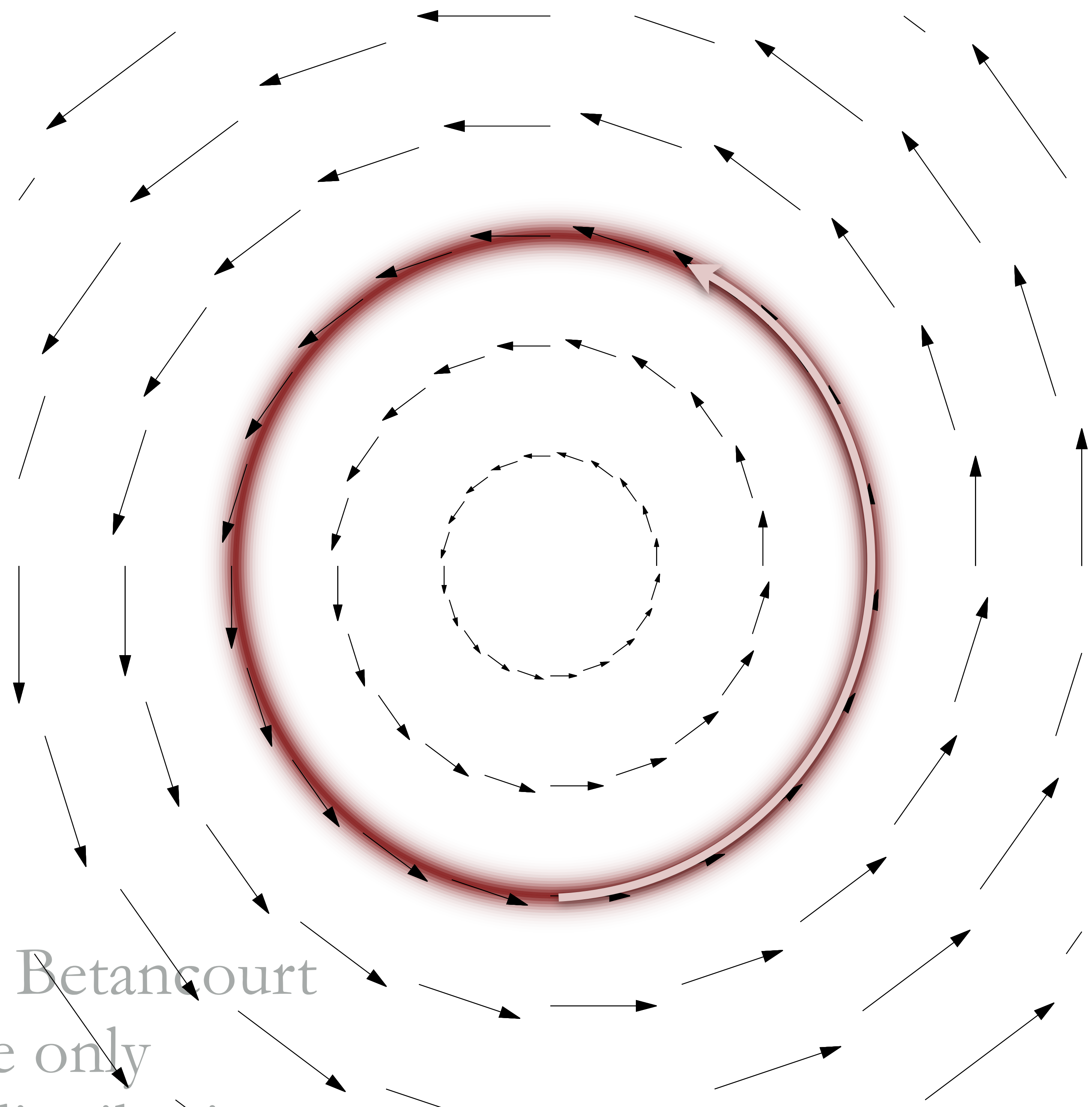
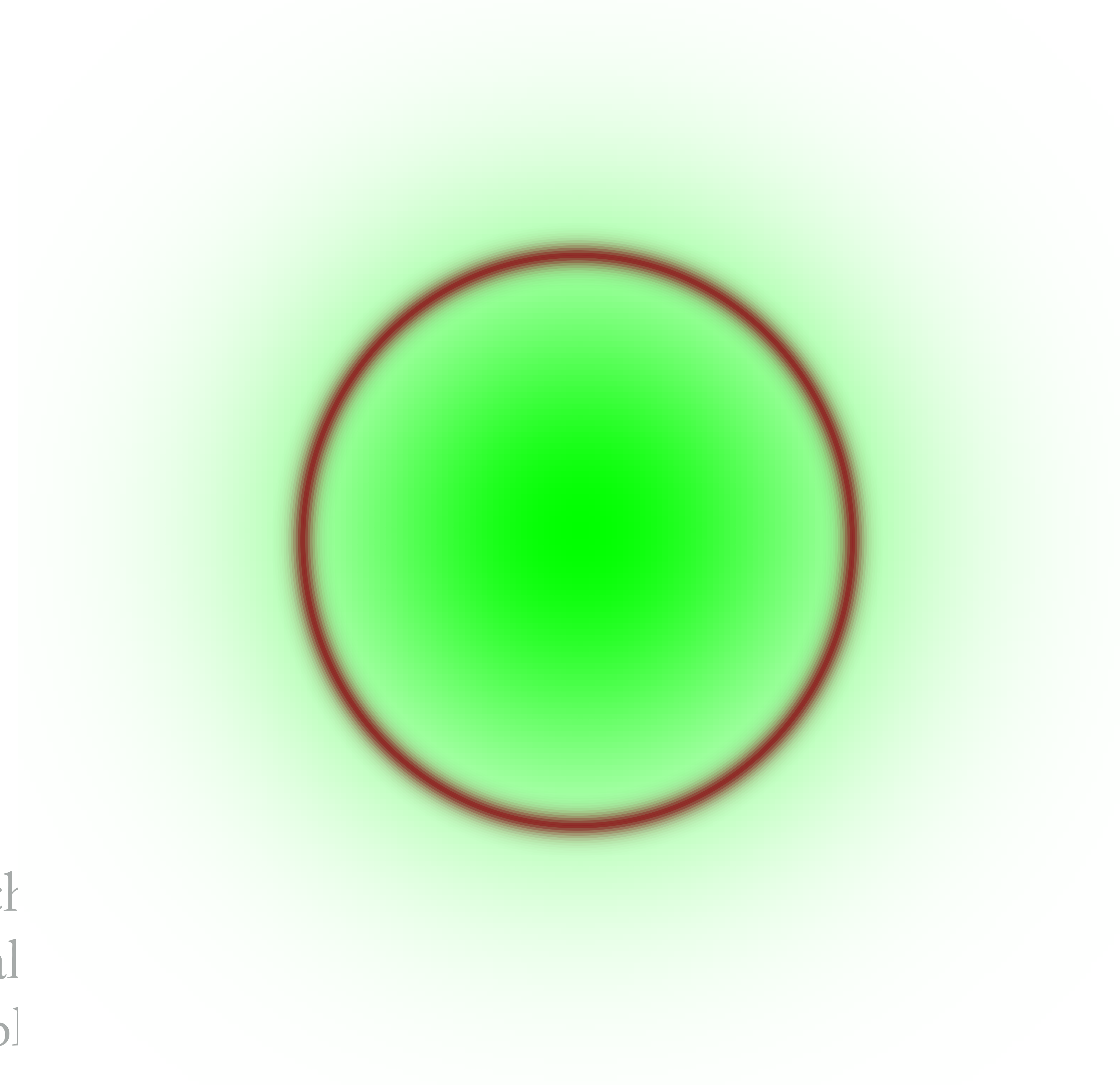


Creating the desired vector field requires transforming available vector fields, such as the gradient.



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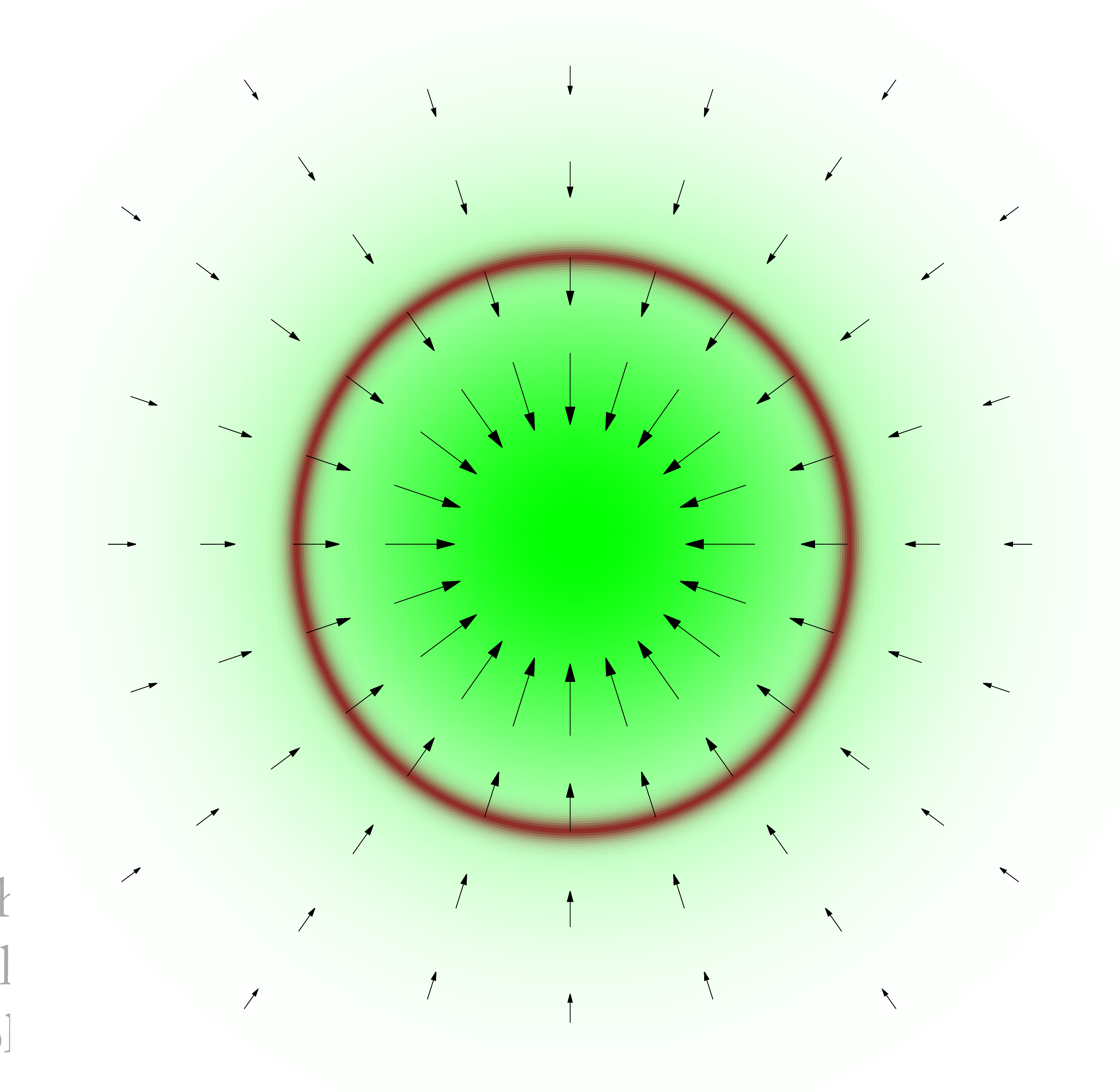

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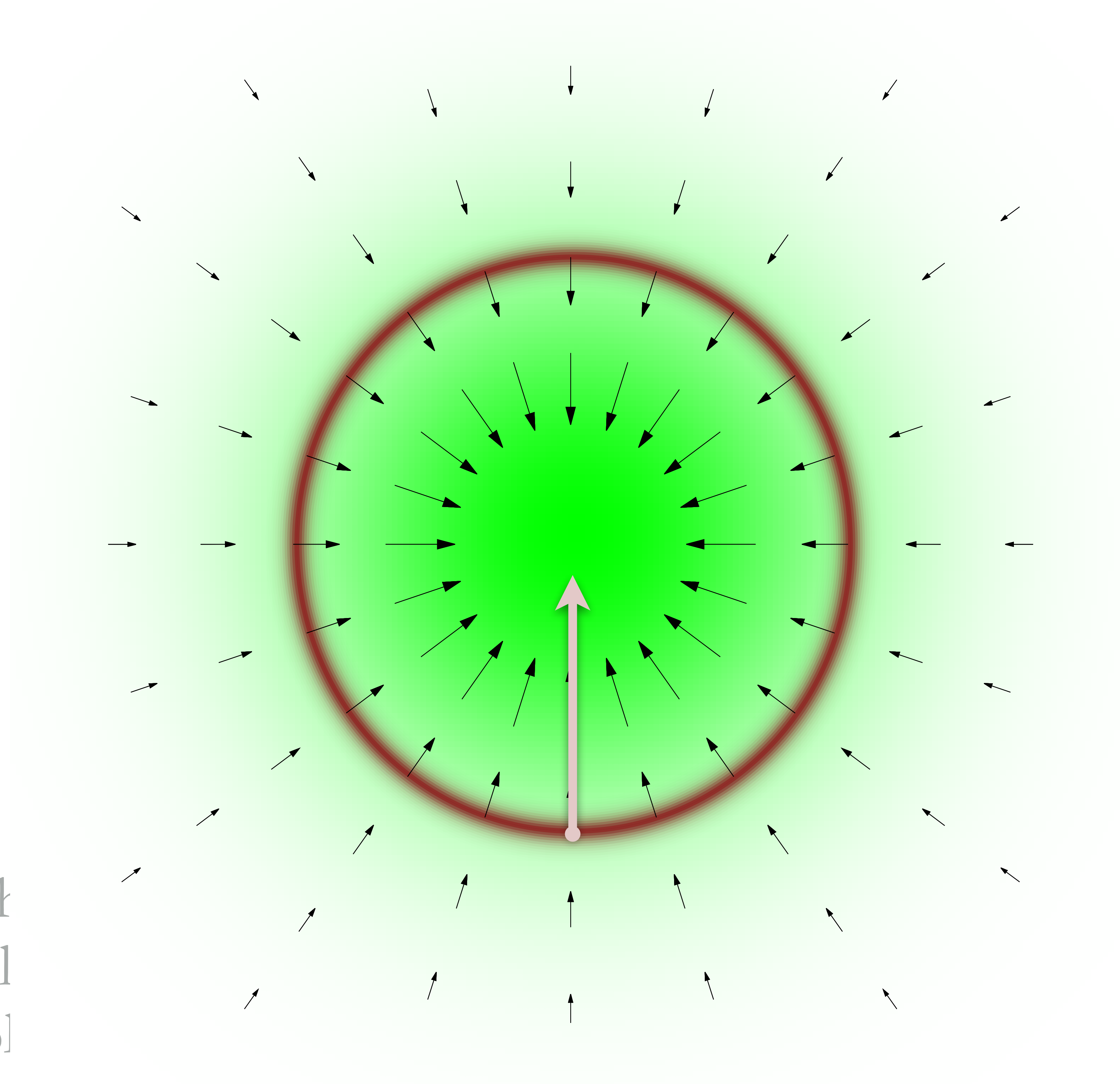

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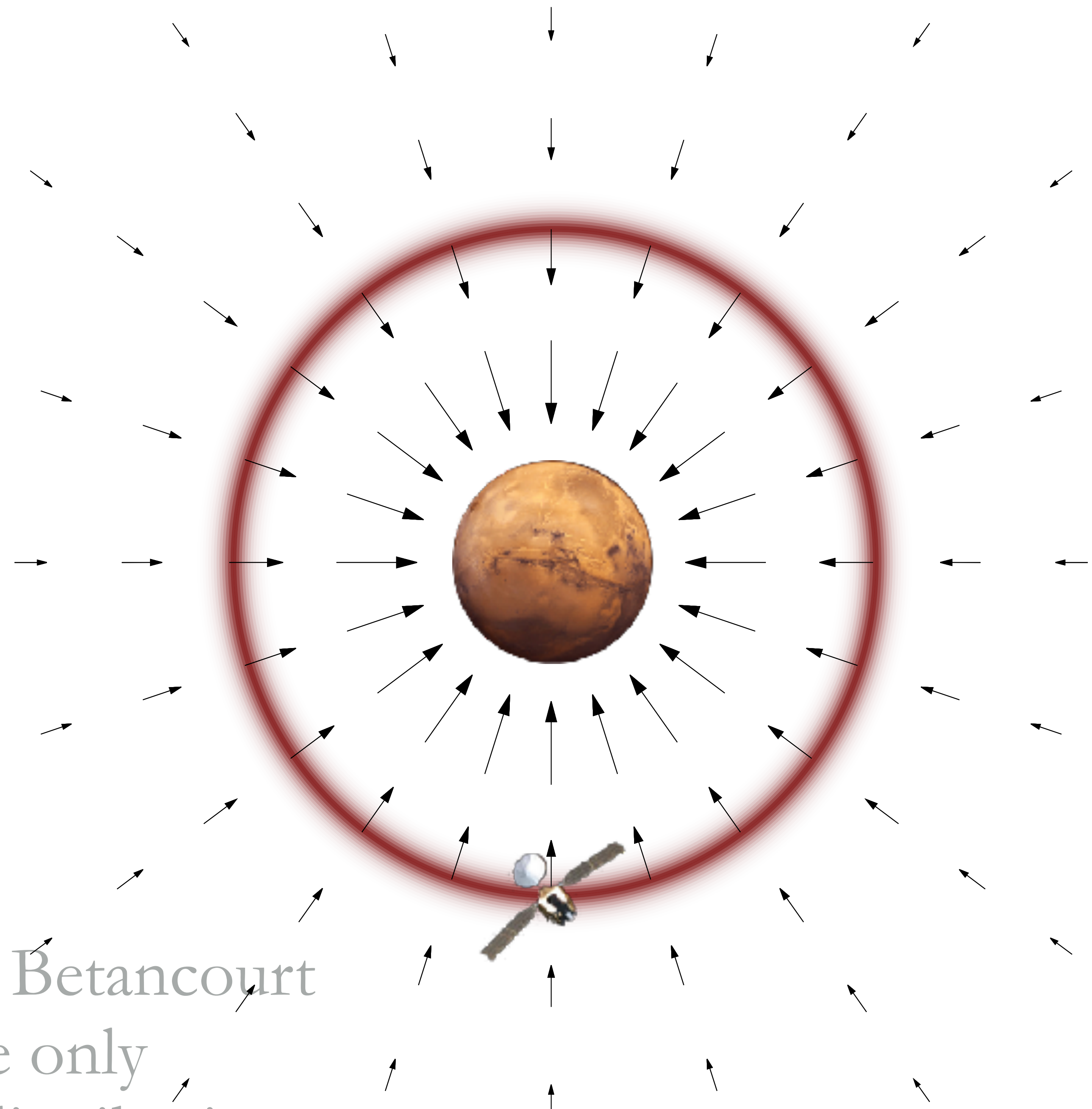
Differential geometry informs this transformation, although a physical analogy can be more intuitive.



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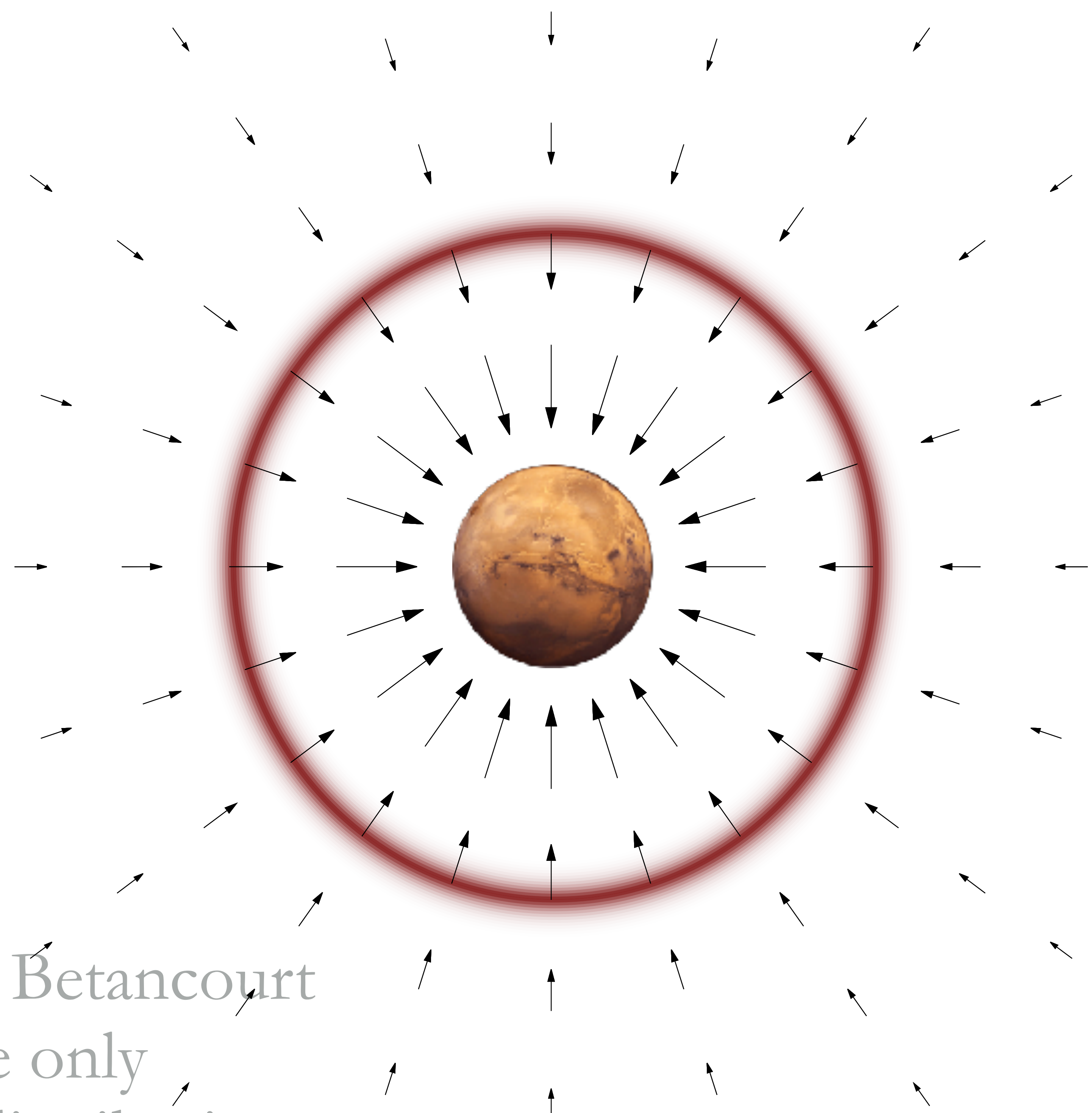

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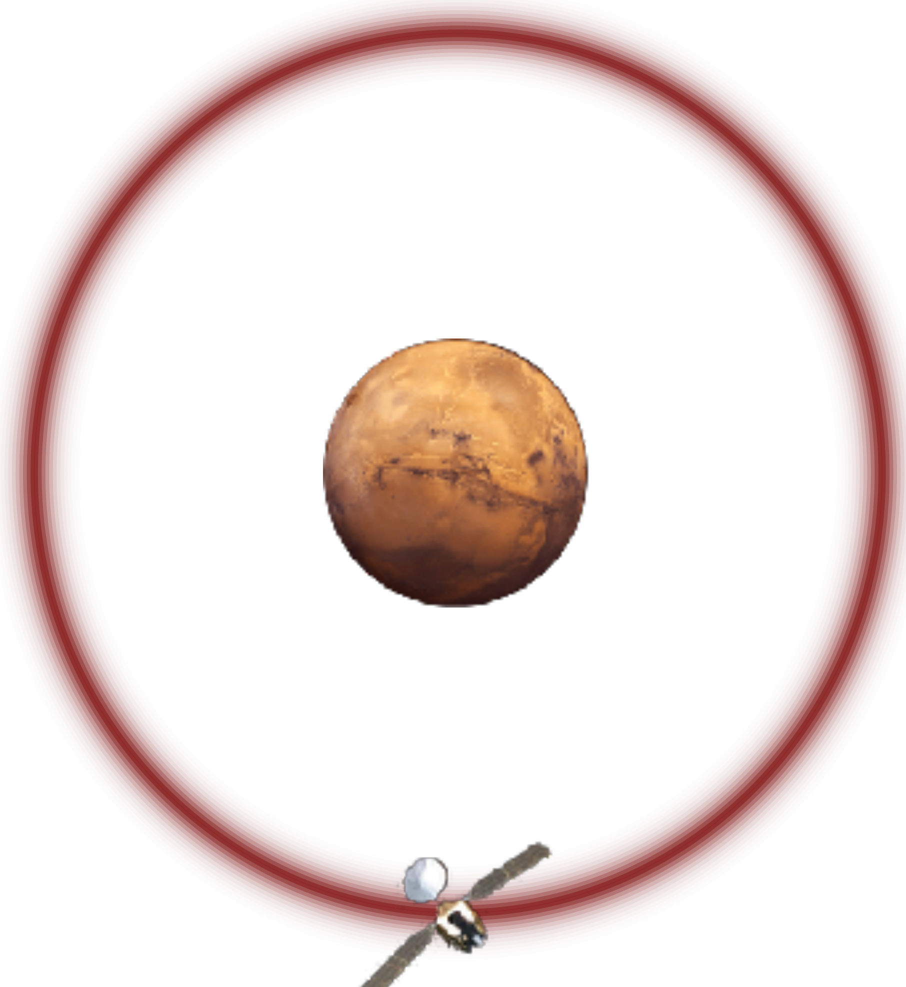
Too little and we still crash into the planet.



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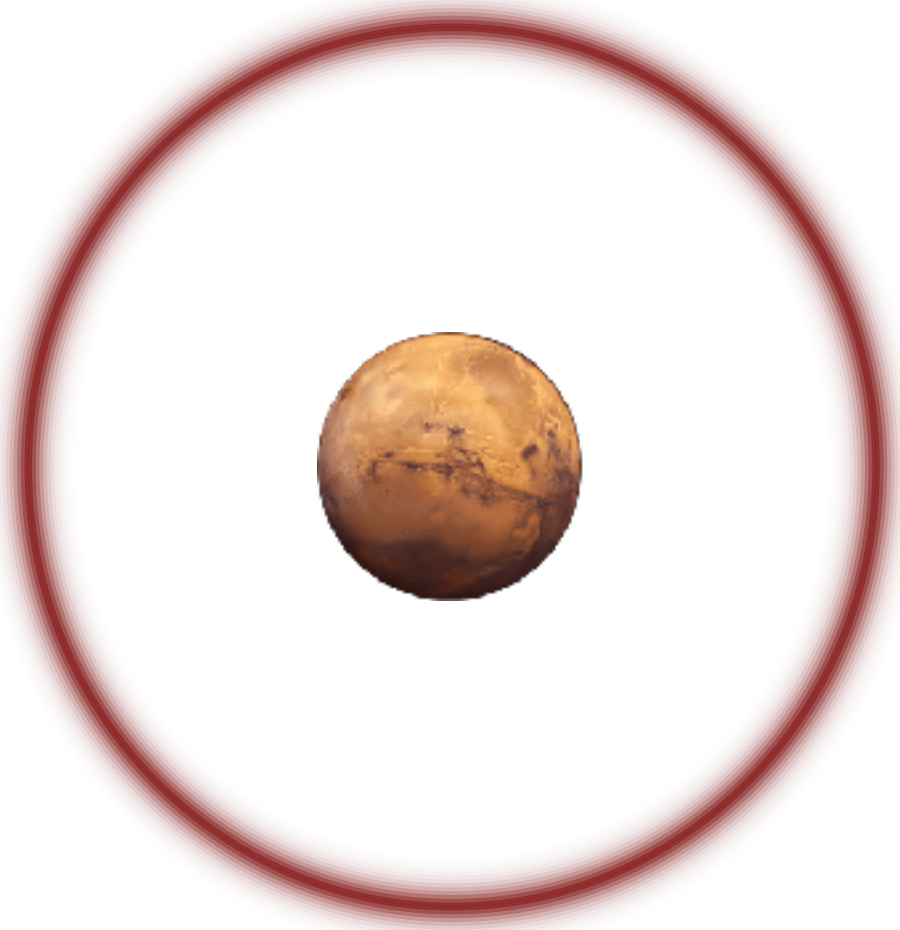

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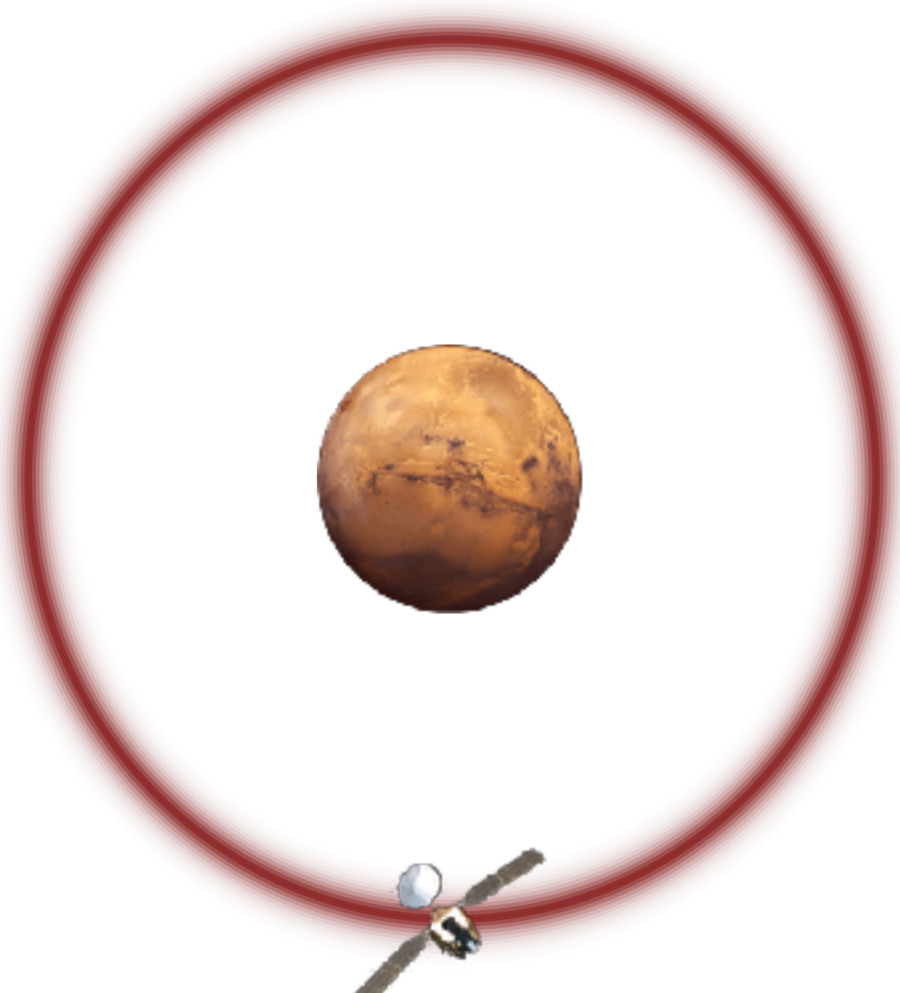

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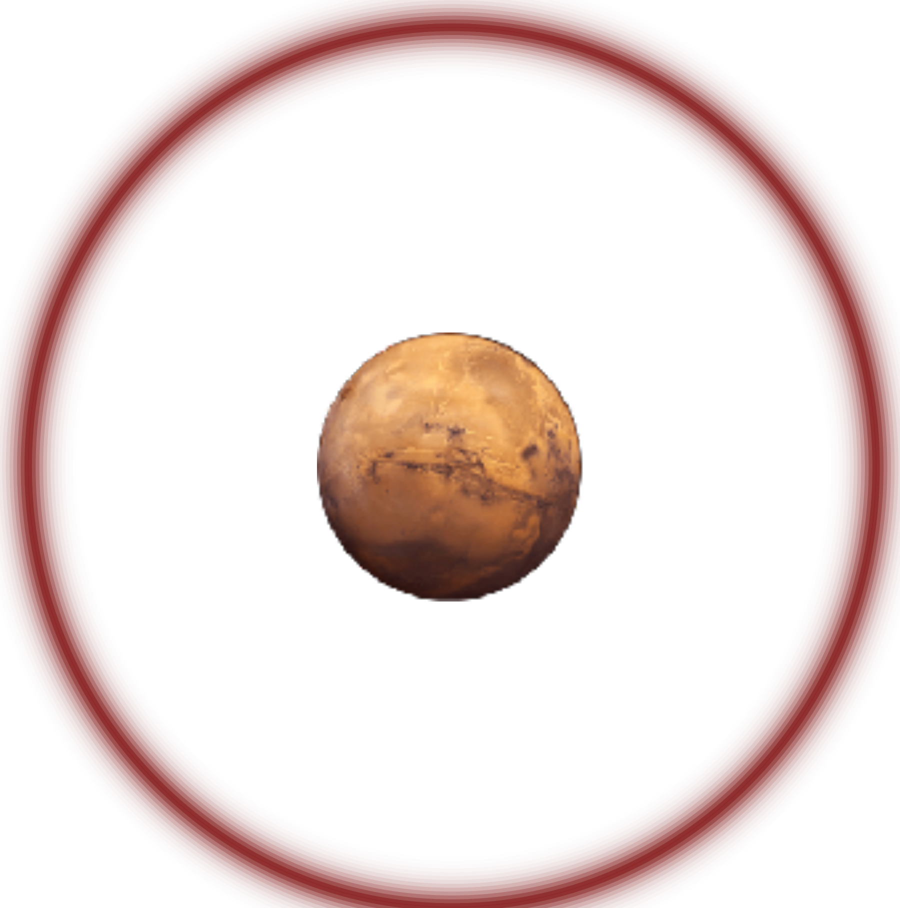
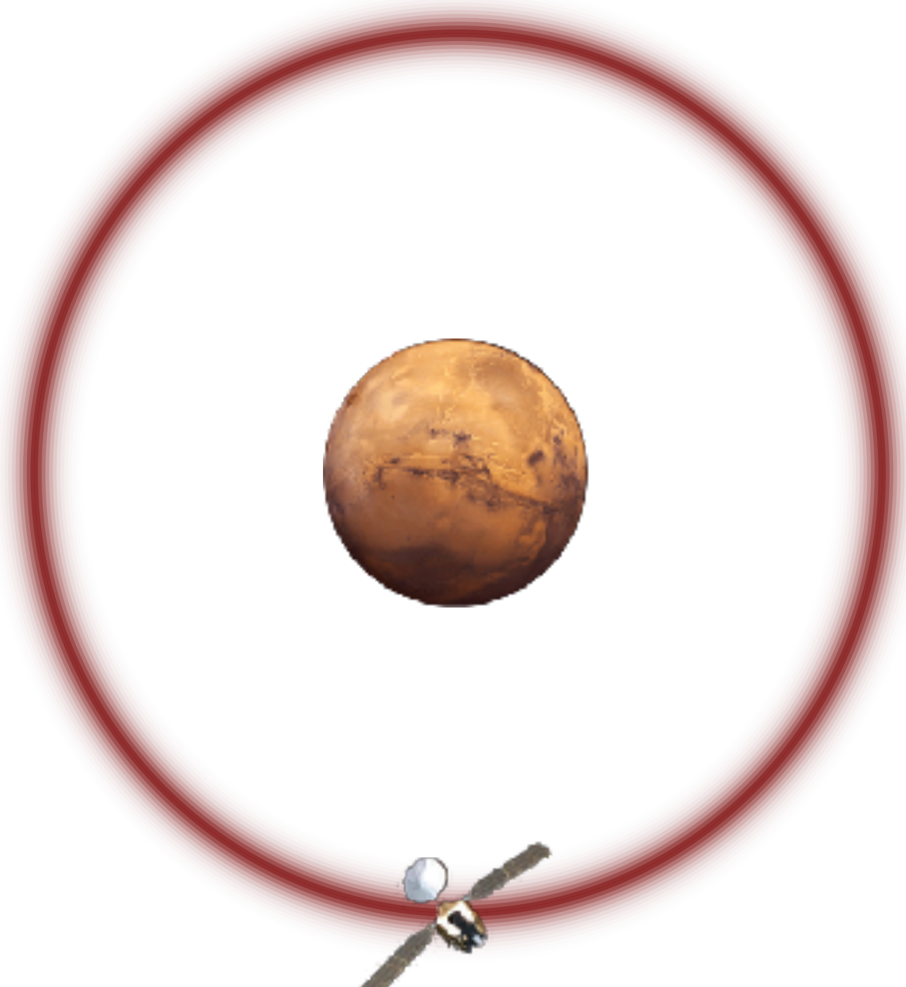


Just enough, however, aligns the gradients with the typical set and yields the desired orbital trajectory.



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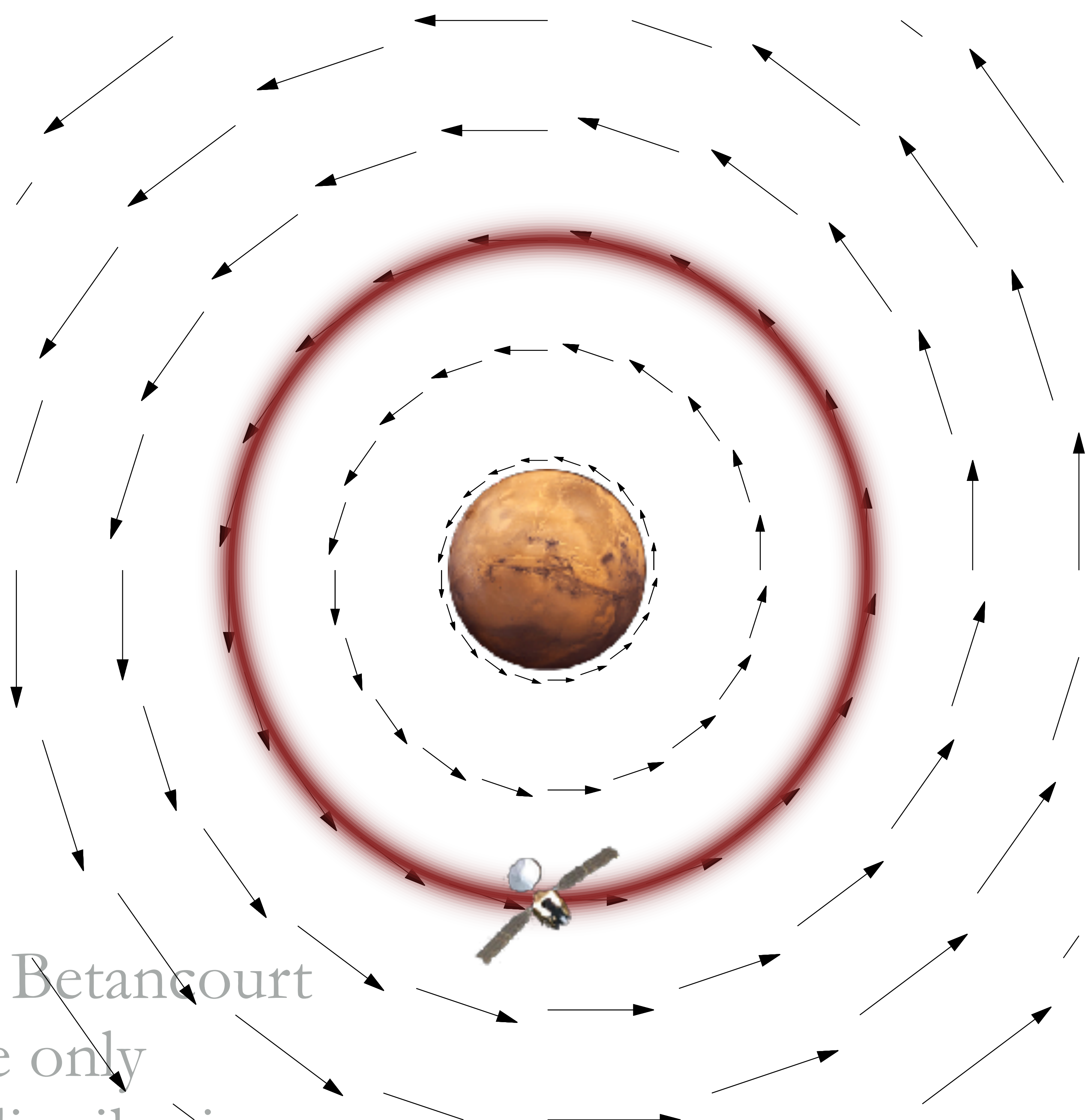

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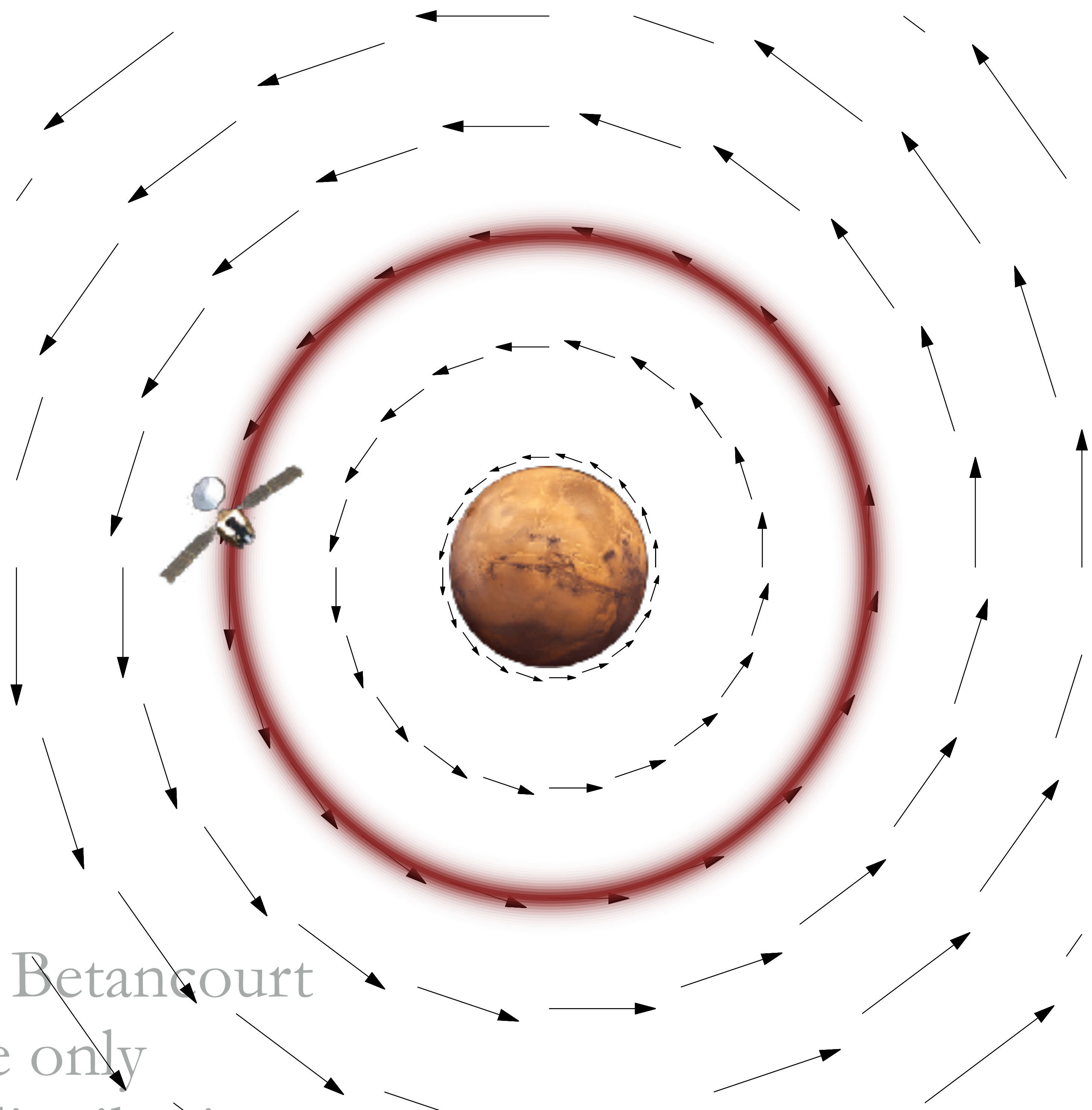

Hamiltonian Monte Carlo is the formal procedure for adding momentum to generate coherent exploration.

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$$q \to (q, p)$$

$$\pi(q) \to \pi(q, p) = \pi(p \mid q)\, \pi(q)$$

Lifting the target distribution gives a *Hamiltonian* that decomposes into a *potential energy* and a *kinetic energy*.

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Any choice of kinetic energy generates coherent exploration through the expanded phase space.

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial K}{\partial p}$$

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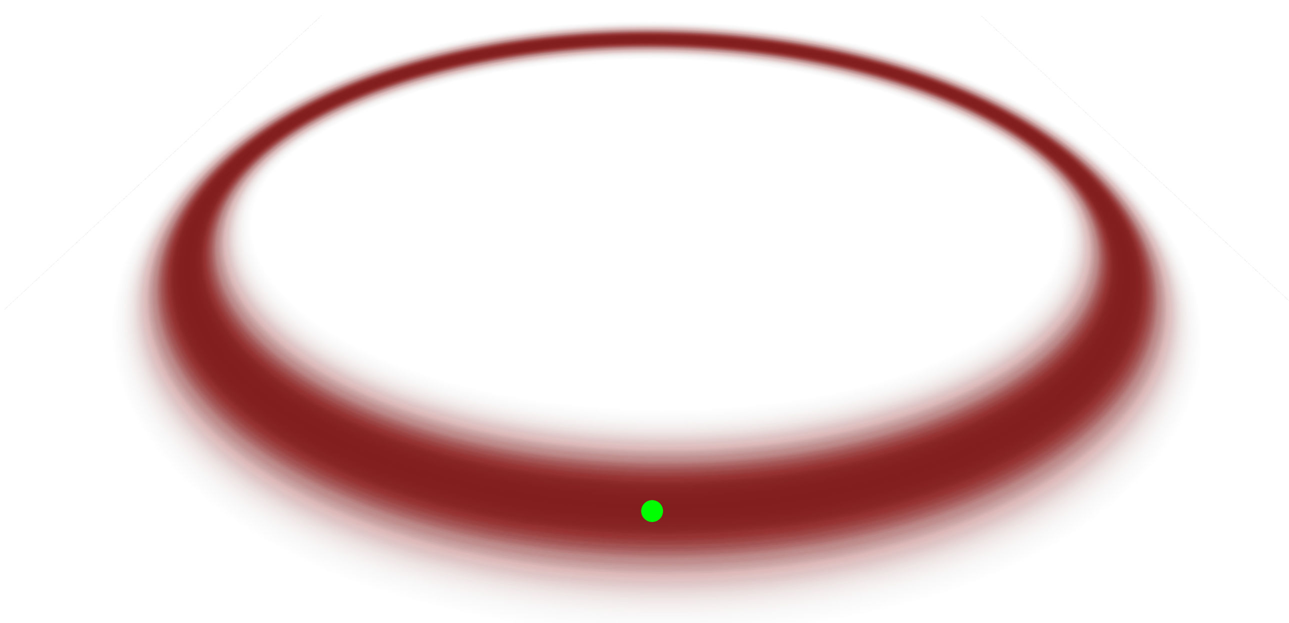
We then construct a Markov transition by lifting into, exploring, and projecting from the expanded space.



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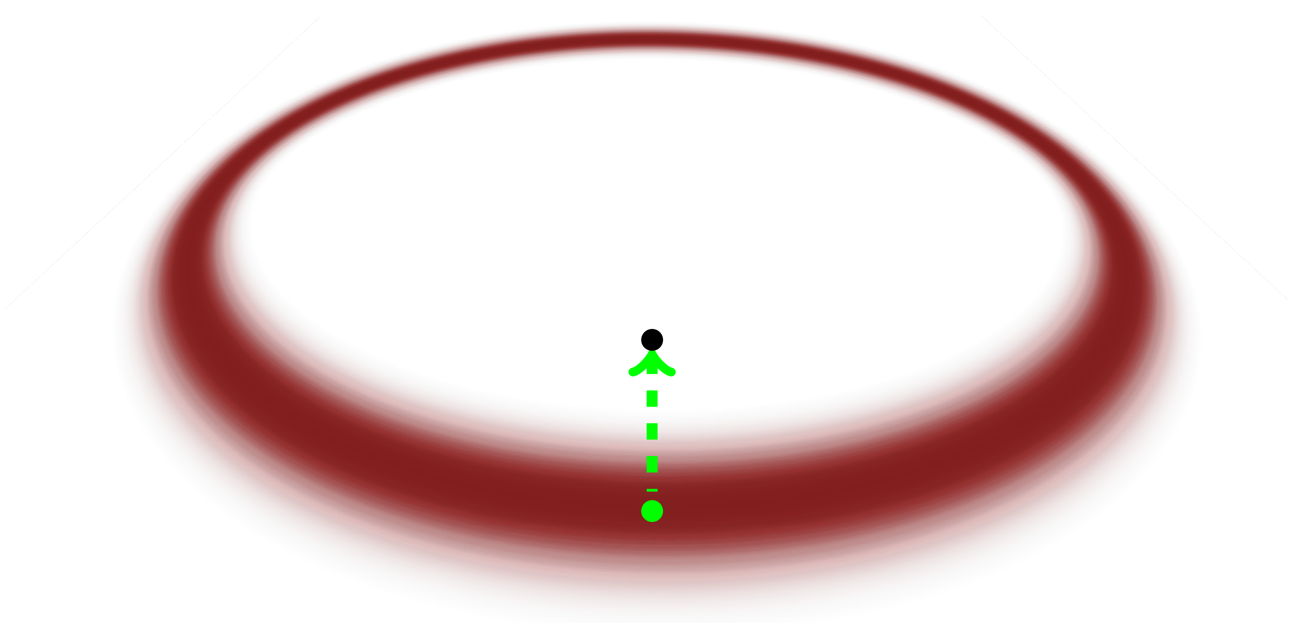

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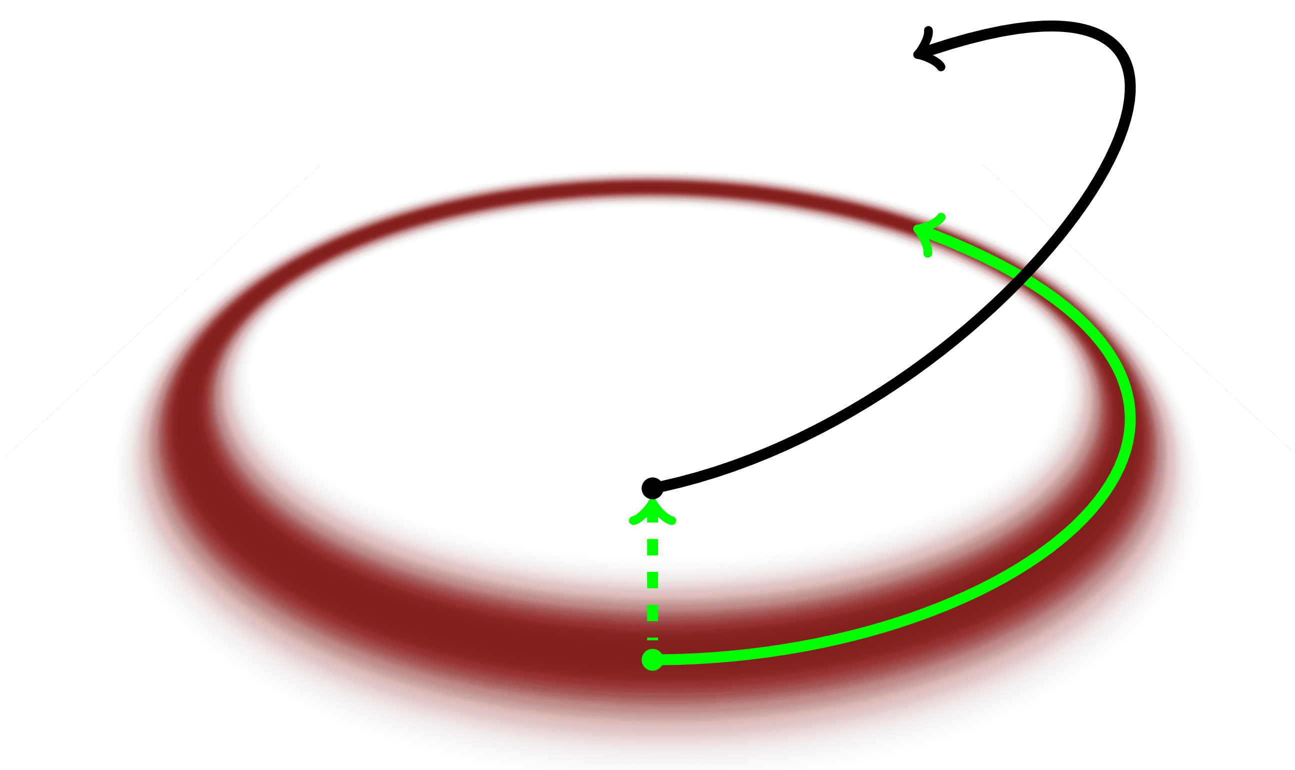

$$p \sim \pi(p \mid q)$$

$$t \sim U[0, T]$$

$$(q', p') \rightarrow \phi_t(q, p)$$

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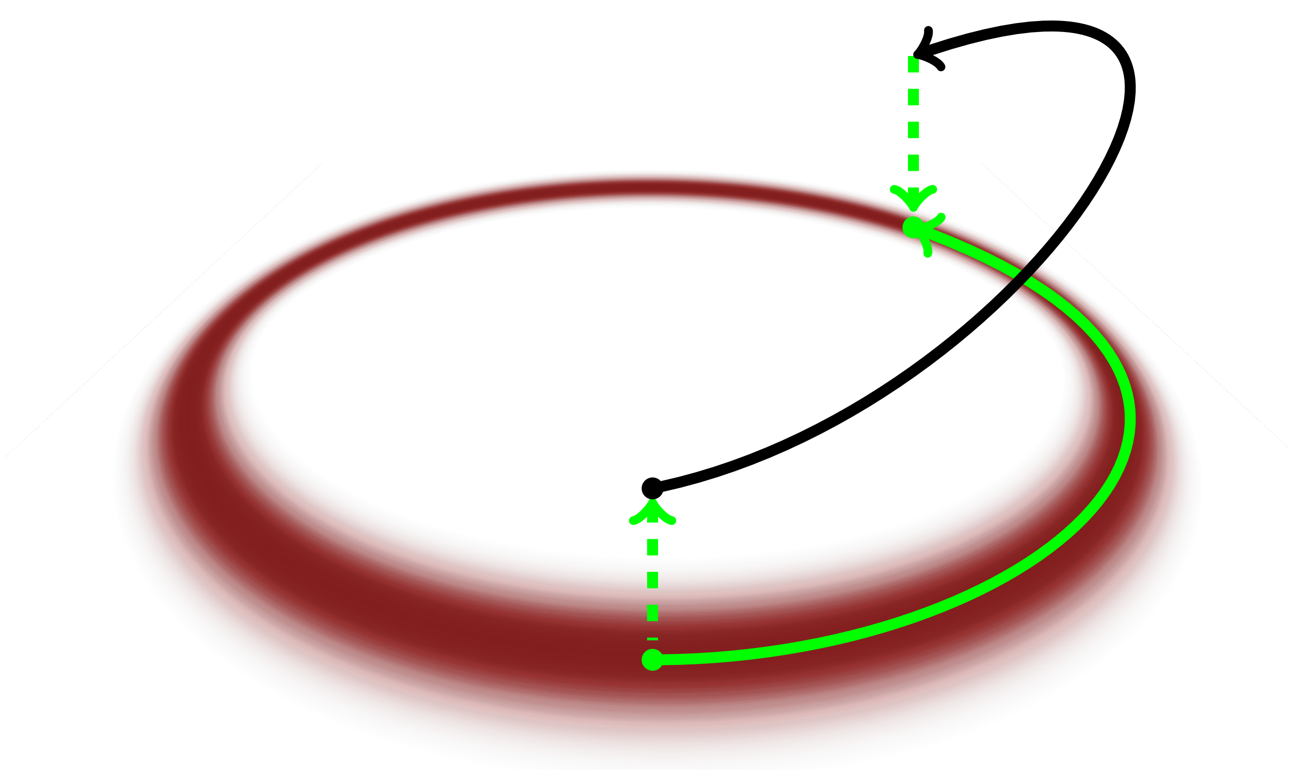

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In practice we have to approximate the exact Hamiltonian trajectories with numerical trajectories.

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$$q \to q + \epsilon \frac{\partial K}{\partial p}$$

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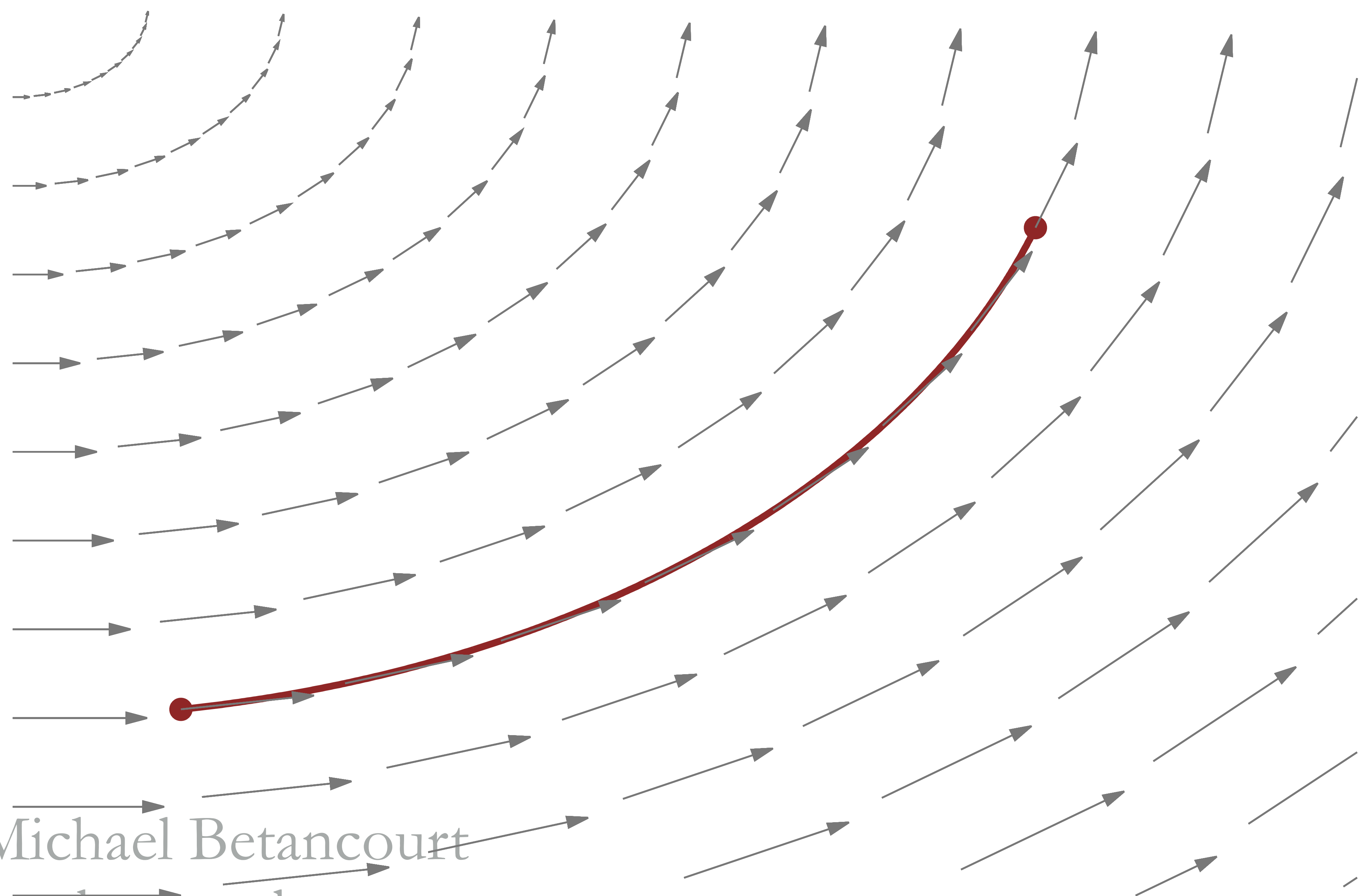
Naive numerical integrators drift away from the exact trajectory, limiting the time for which we can explore.



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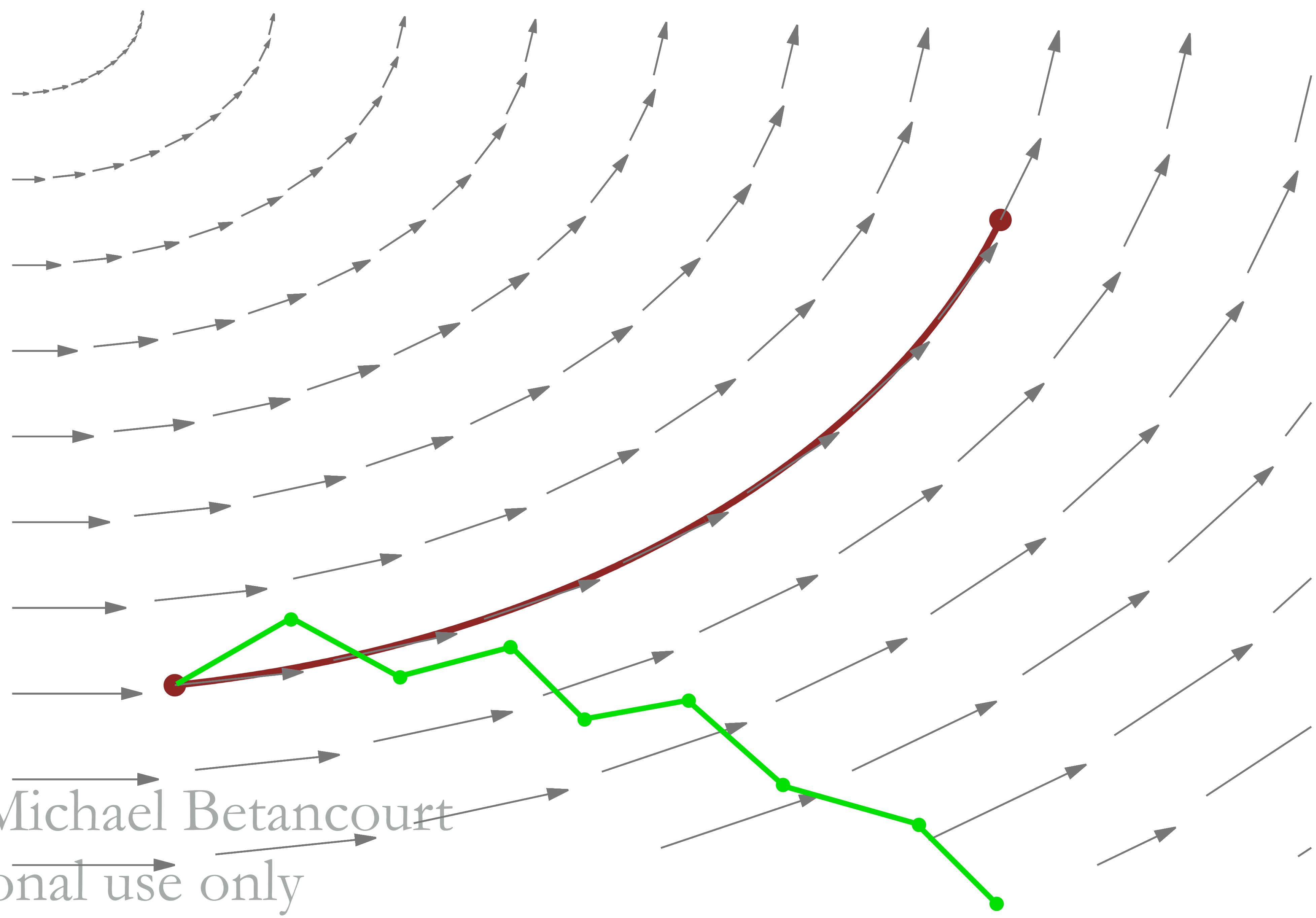
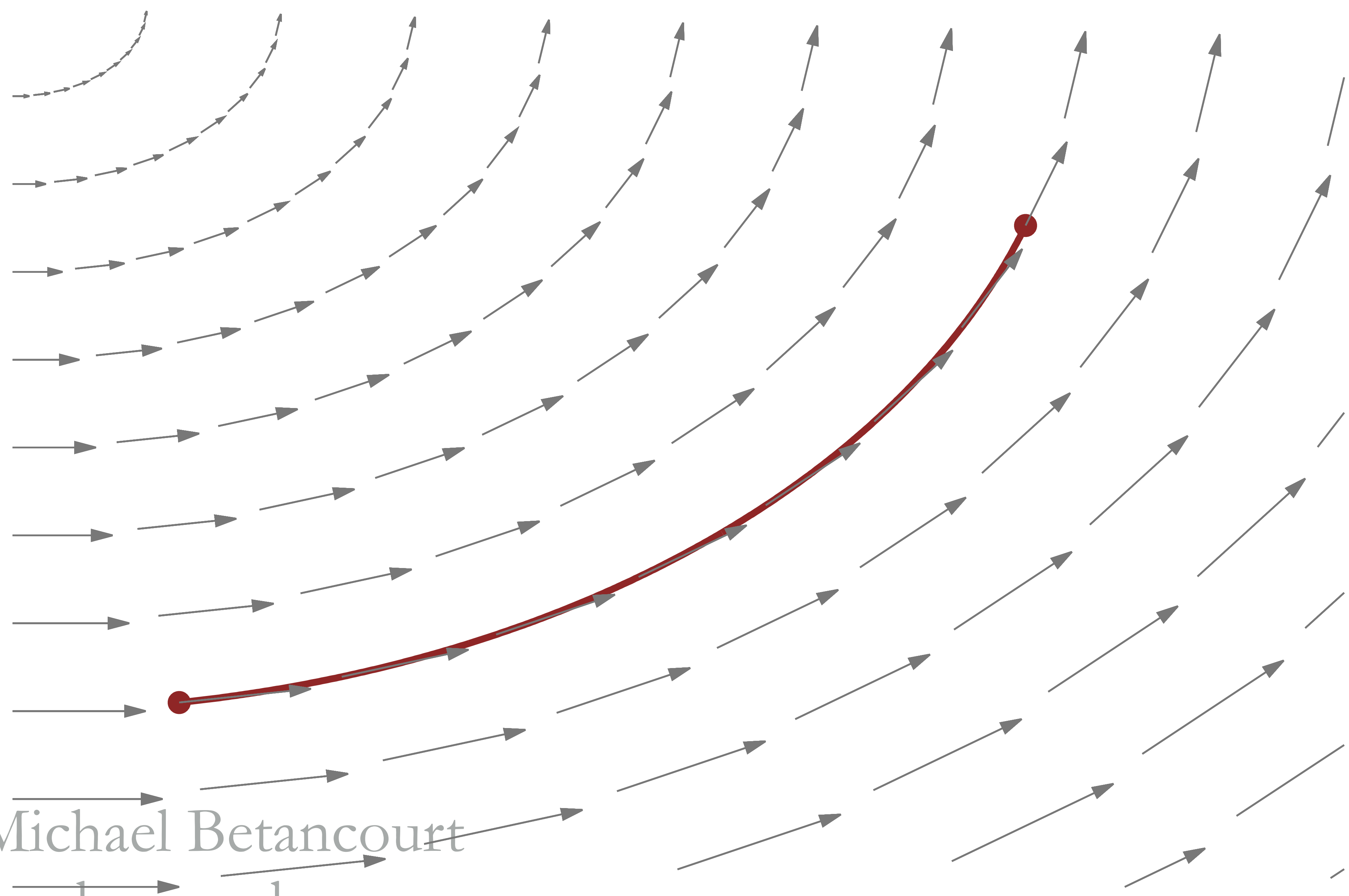


Symplectic integrators very accurately simulate these Hamiltonian systems, even in high dimensions.



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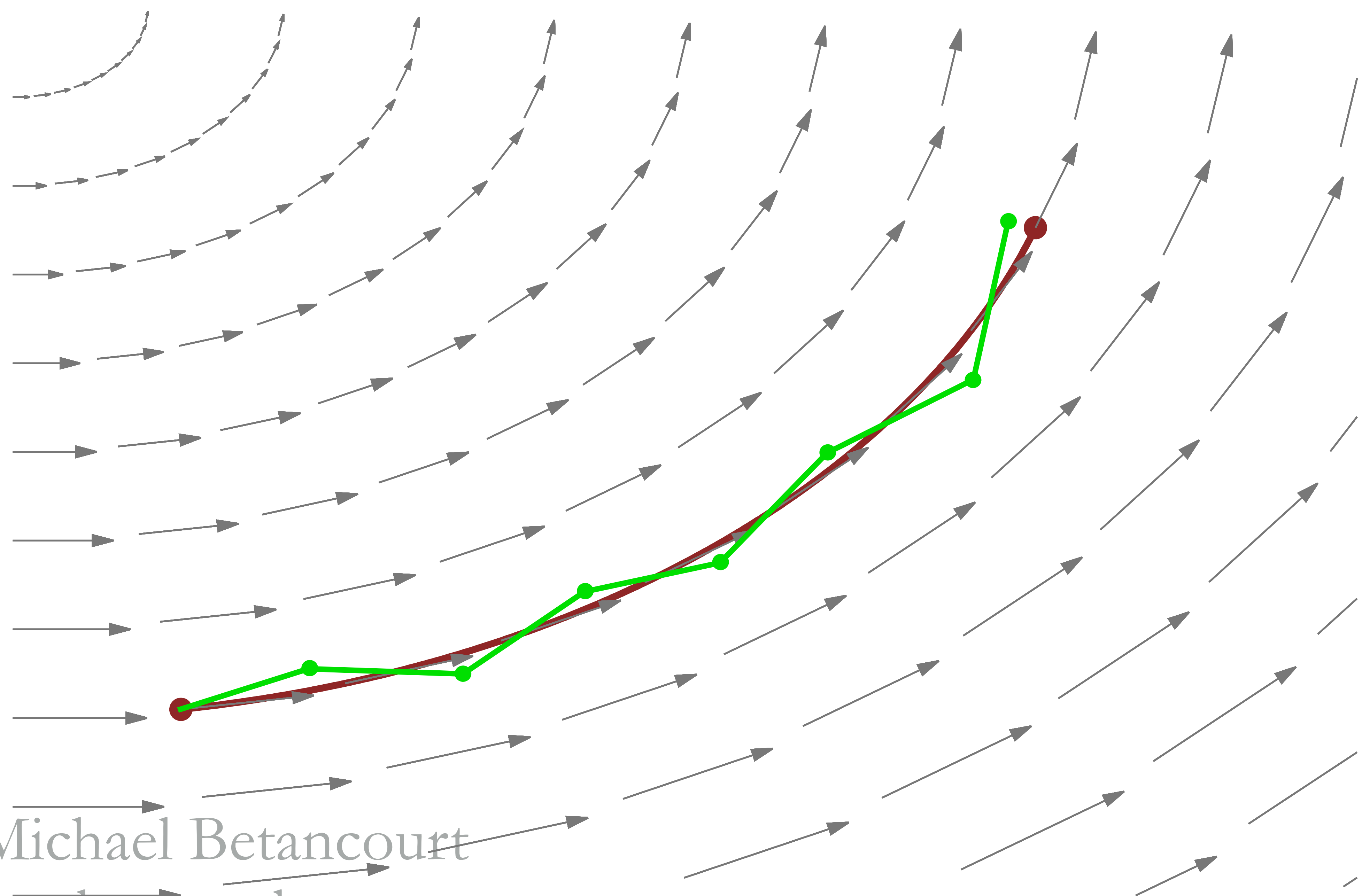

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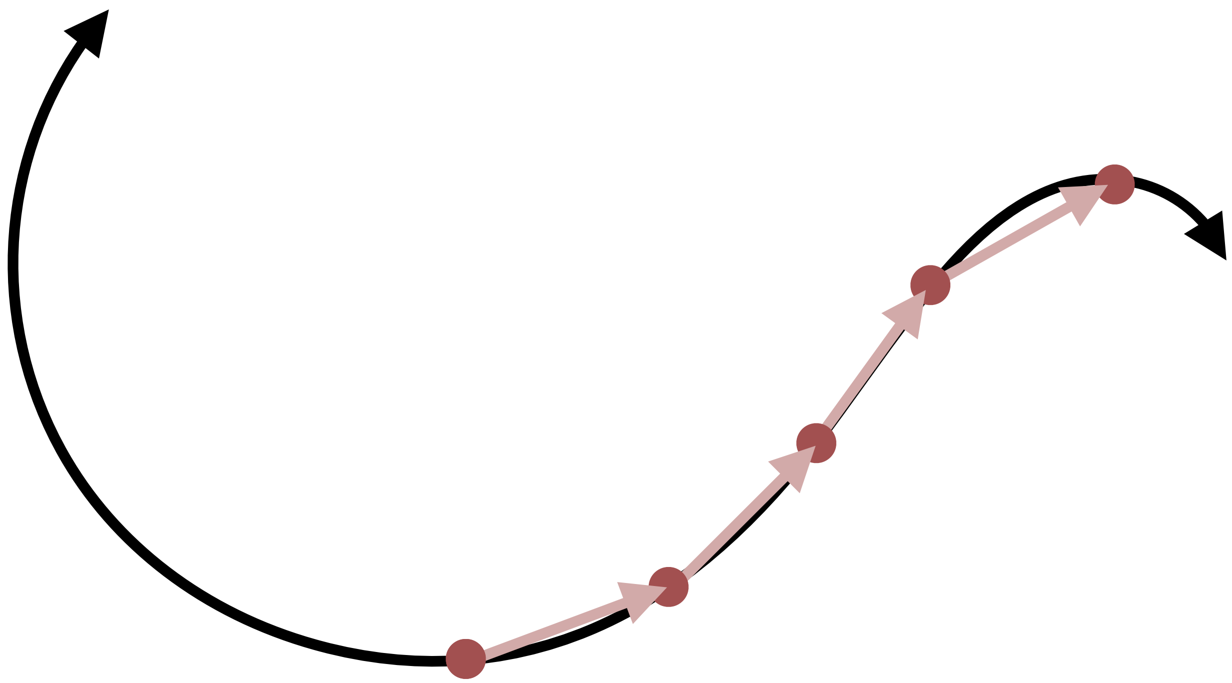

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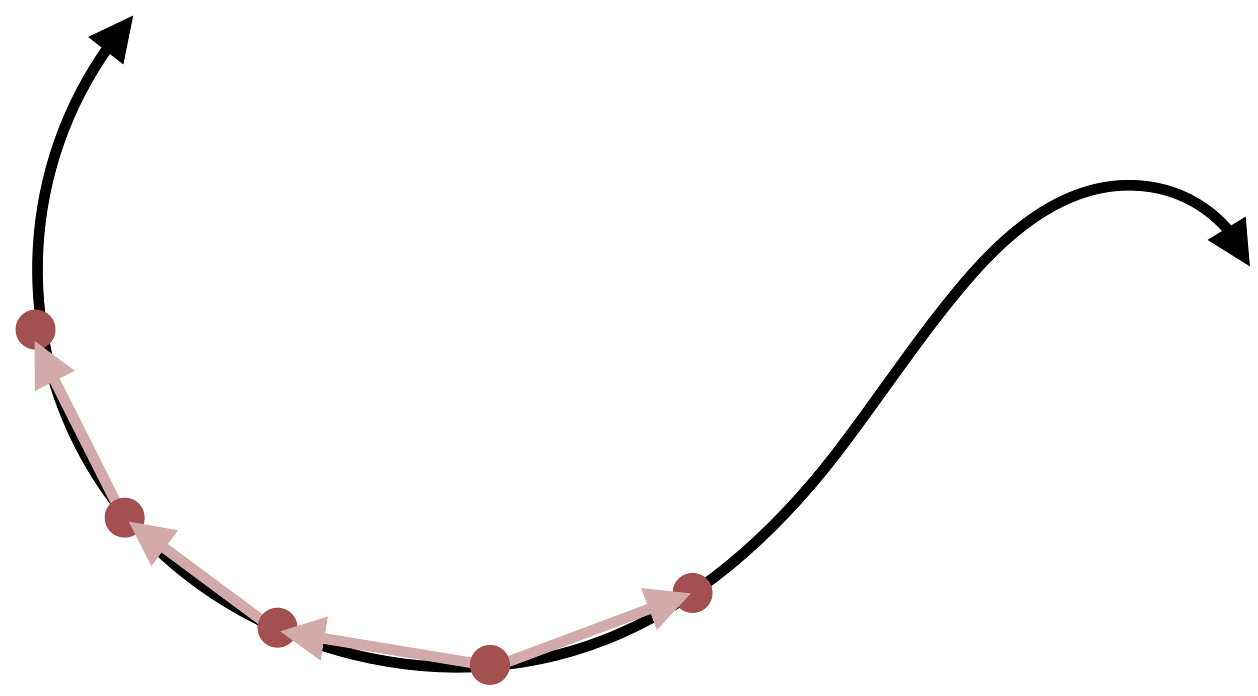

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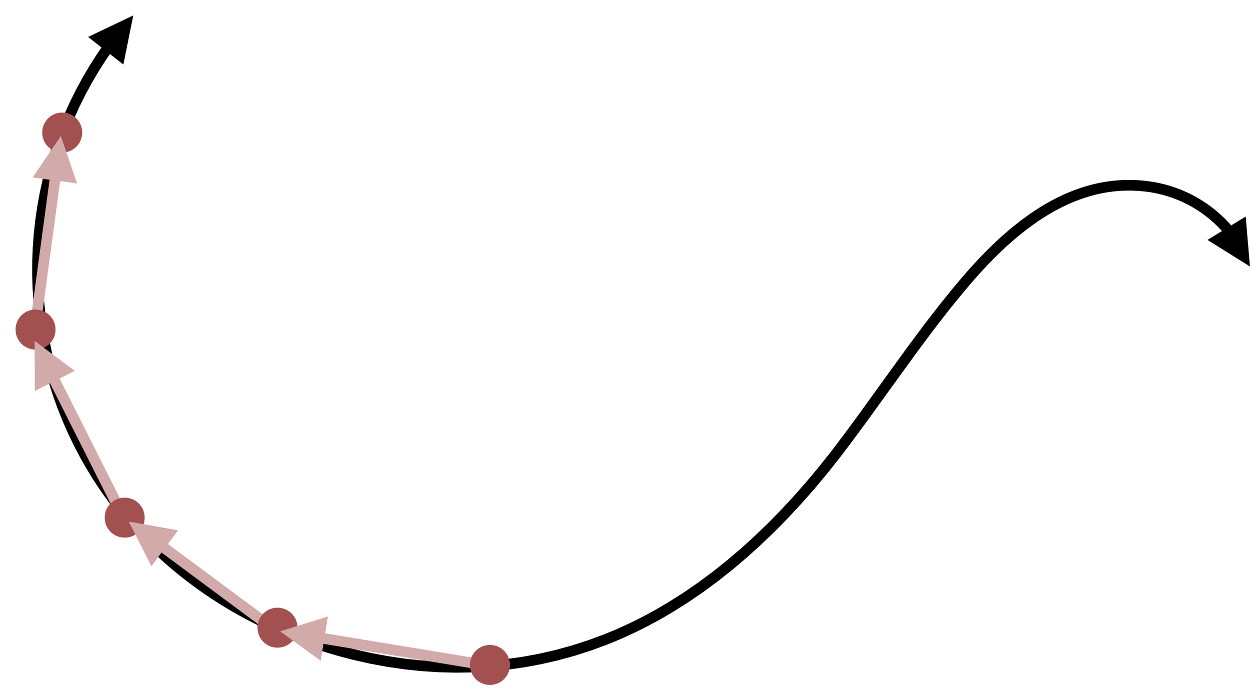

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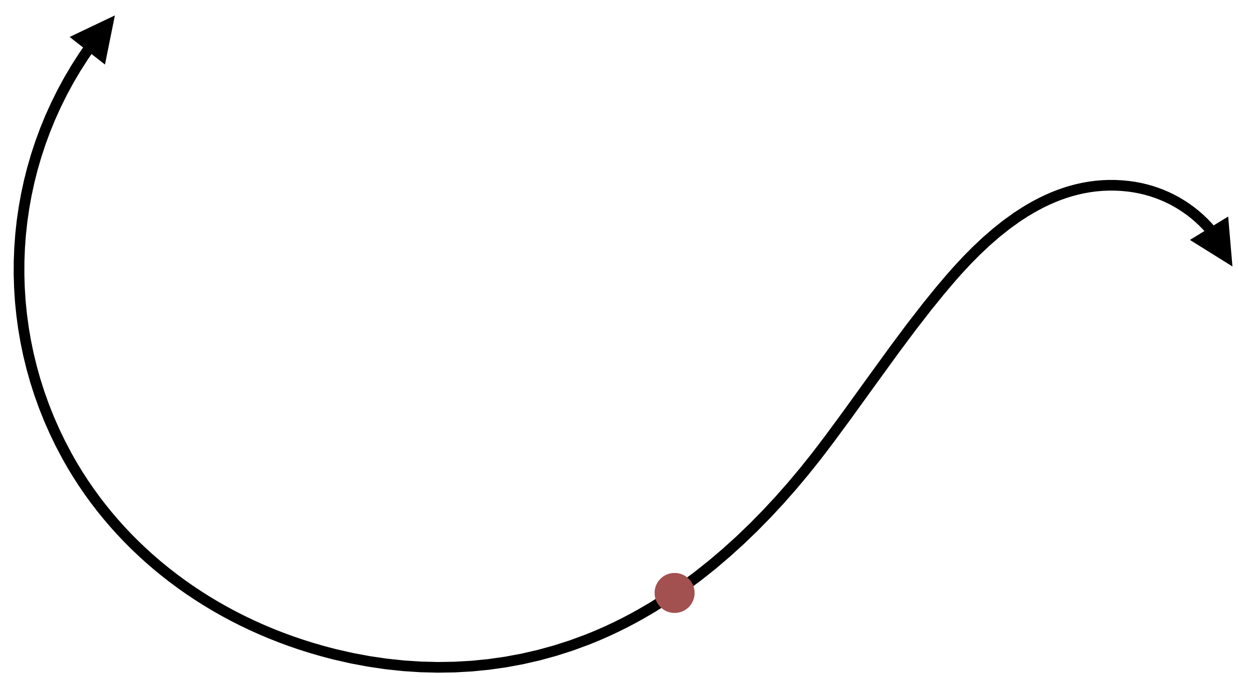

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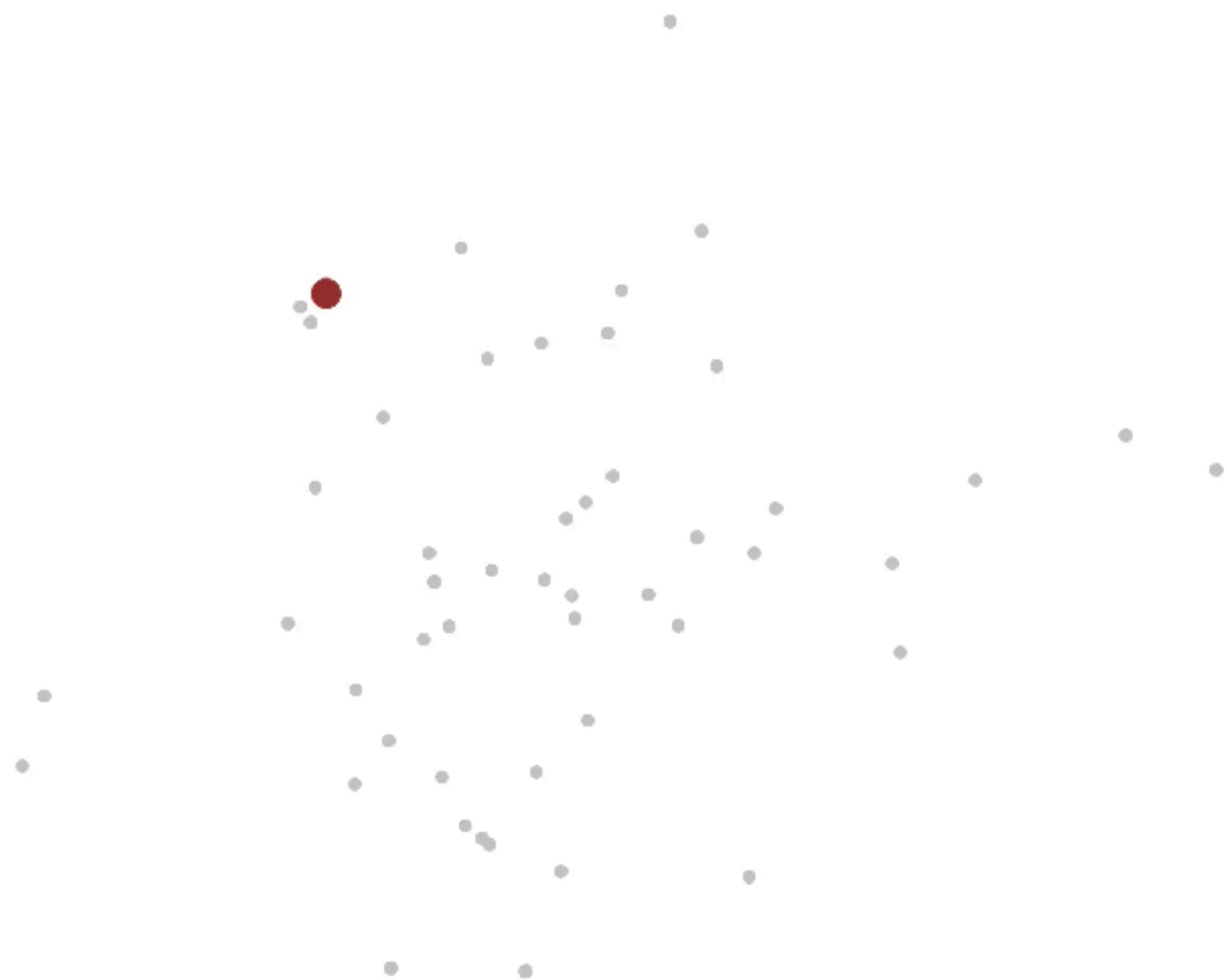
Hamiltonian Monte Carlo yields fast, and *robust*, exploration of the distributions common in practice.



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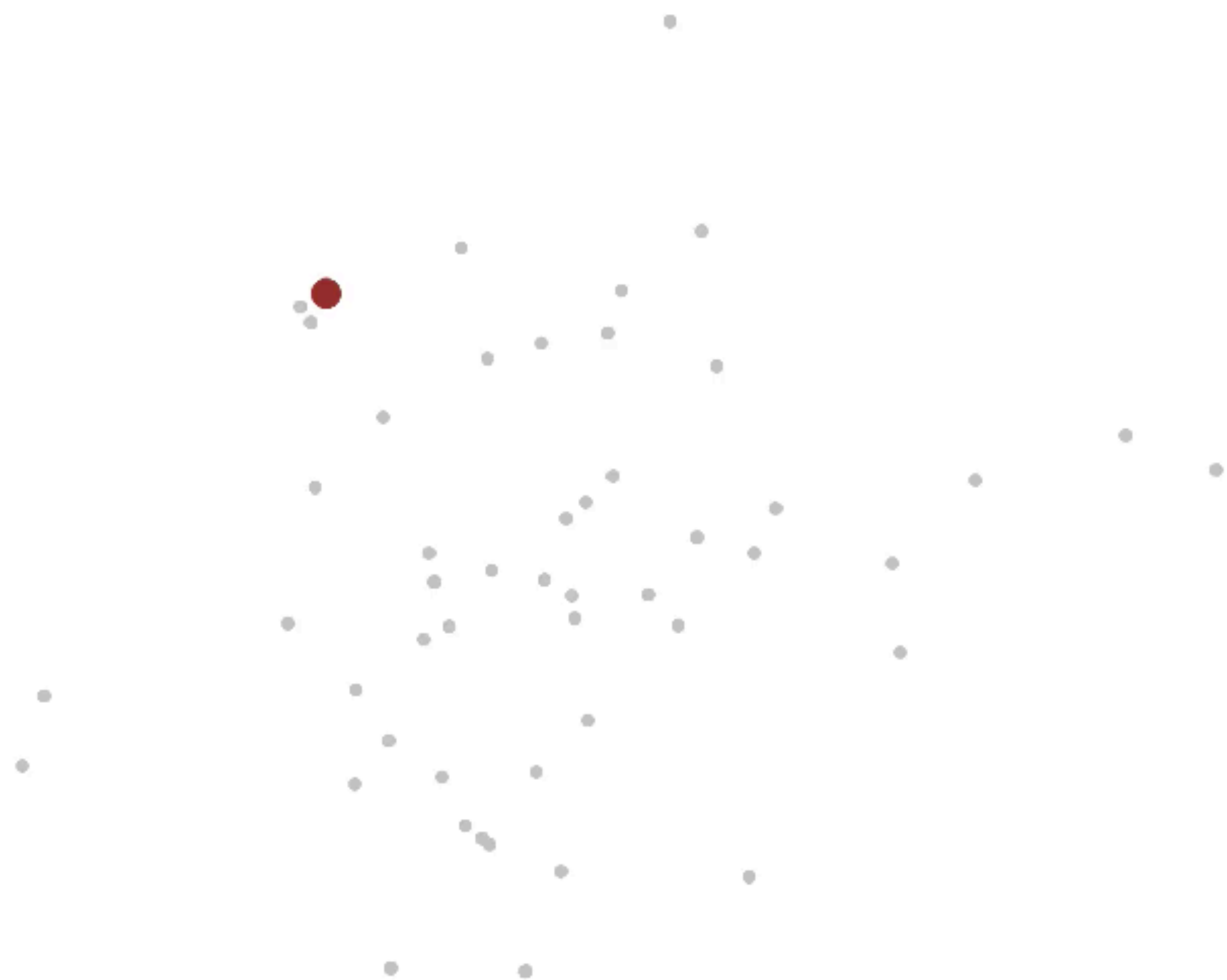

Theory motivates optimal implementations of the many degrees of freedom in this procedure.

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