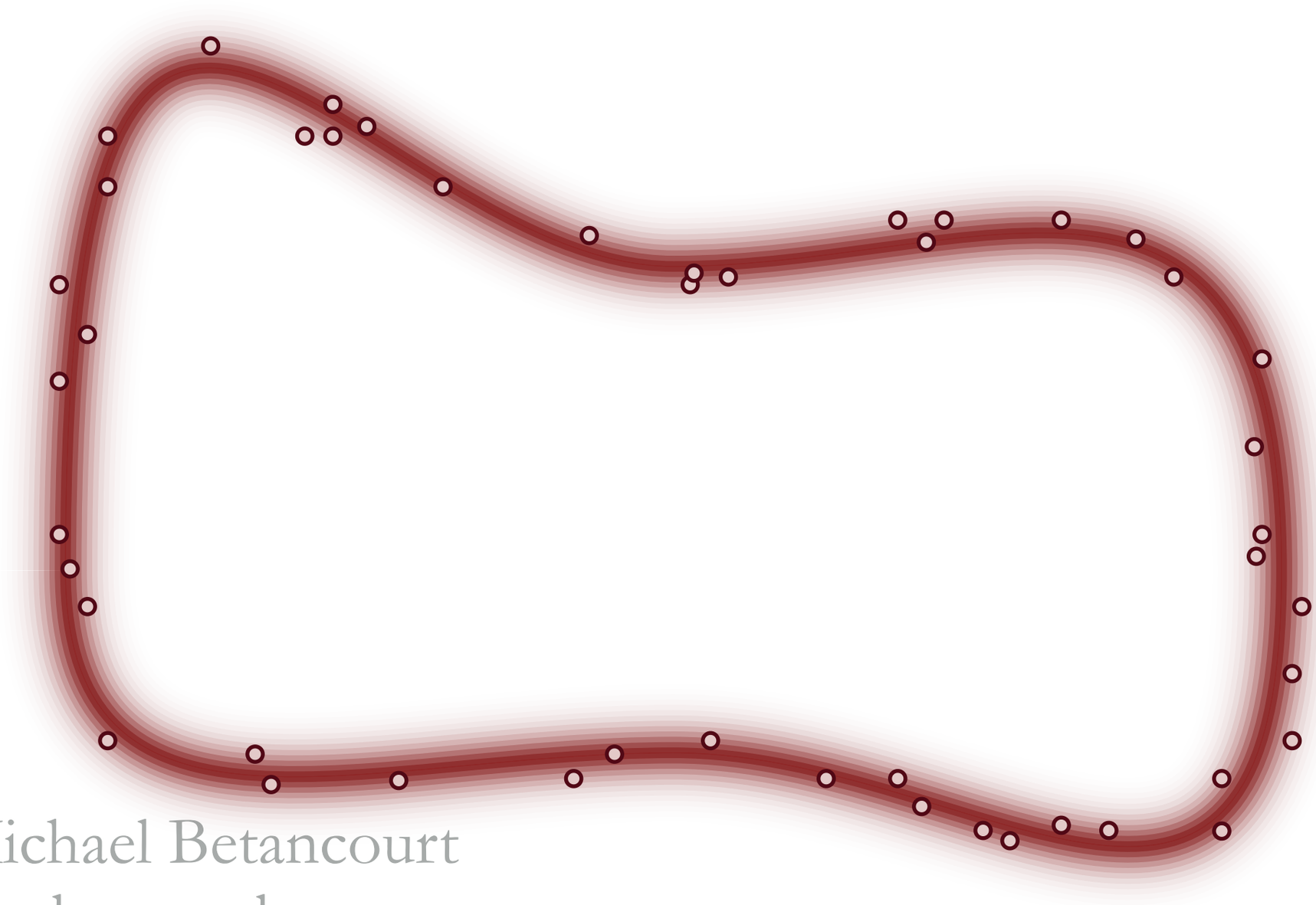
Markov chain Monte Carlo



Michael Betancourt @betanalpha
Symplectomorphic, LLC

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

We can also use it to analyze particular algorithms and build intuition about their robustness, or lack thereof.

Deterministic

Modal Estimators

Laplace Estimators

Variational Estimators

...

Stochastic

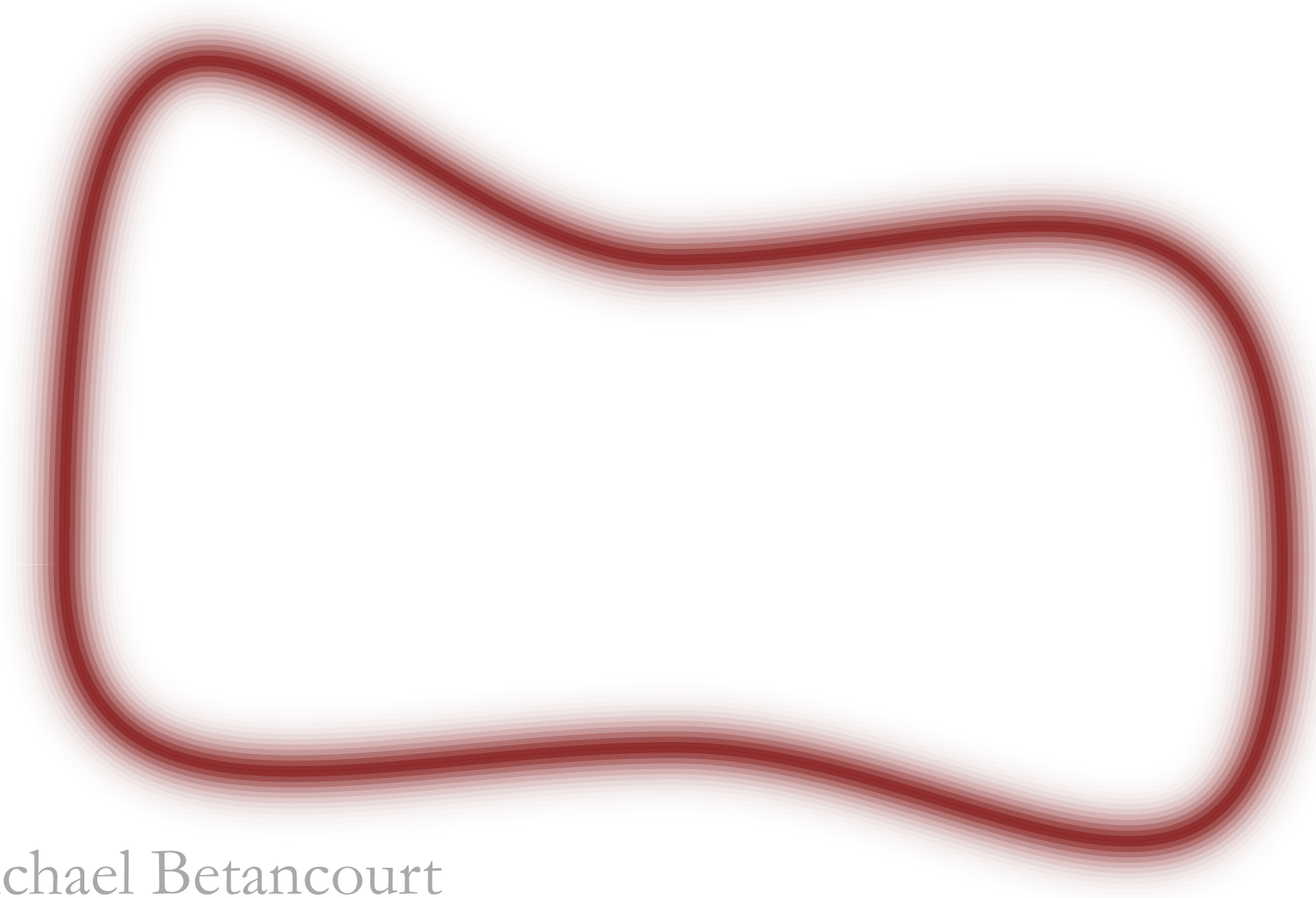
Importance Sampling

Monte Carlo

Markov Chain Monte Carlo

...

Monte Carlo methods quantify the typical set using *exact* samples drawn from the target distribution.



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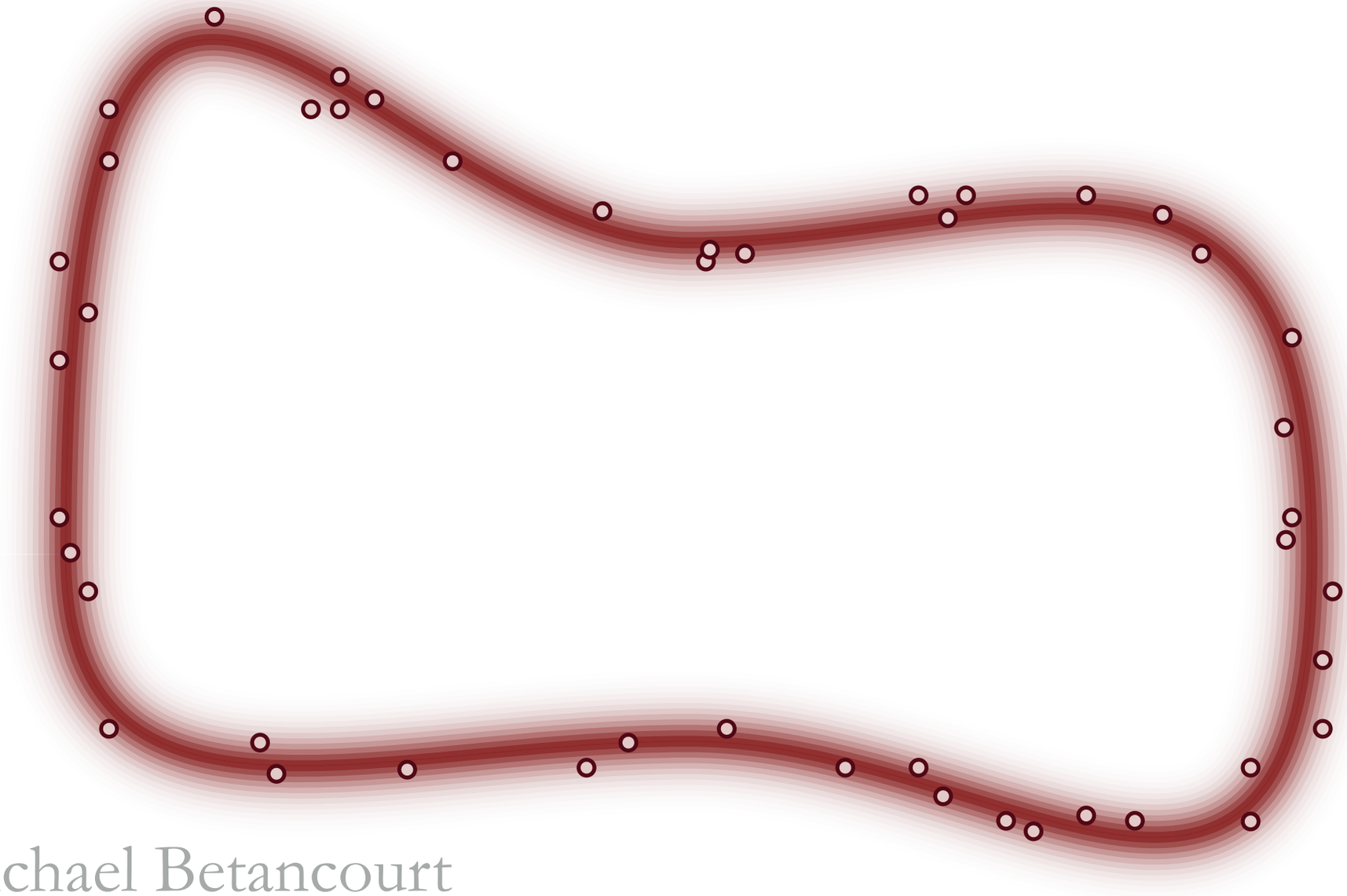

Monte Carlo estimators average a given function over these samples to approximate the expectation value.

$$\hat{f} = \frac{1}{N} \sum_{n=1}^{N} f(\theta_i)$$

Subject to mild conditions on the true expectation values these estimators enjoy a *central limit theorem*.

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While exact samples are typically impractical to generate we can extend this approach to *Markov chain Monte Carlo*.

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Variational Estimators
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$$T(\theta \mid \theta')$$

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$$\pi_S(\theta \mid \tilde{y}) = \int \mathrm{d}\theta' \, \pi_S(\theta' \mid \tilde{y}) \, T(\theta \mid \theta')$$

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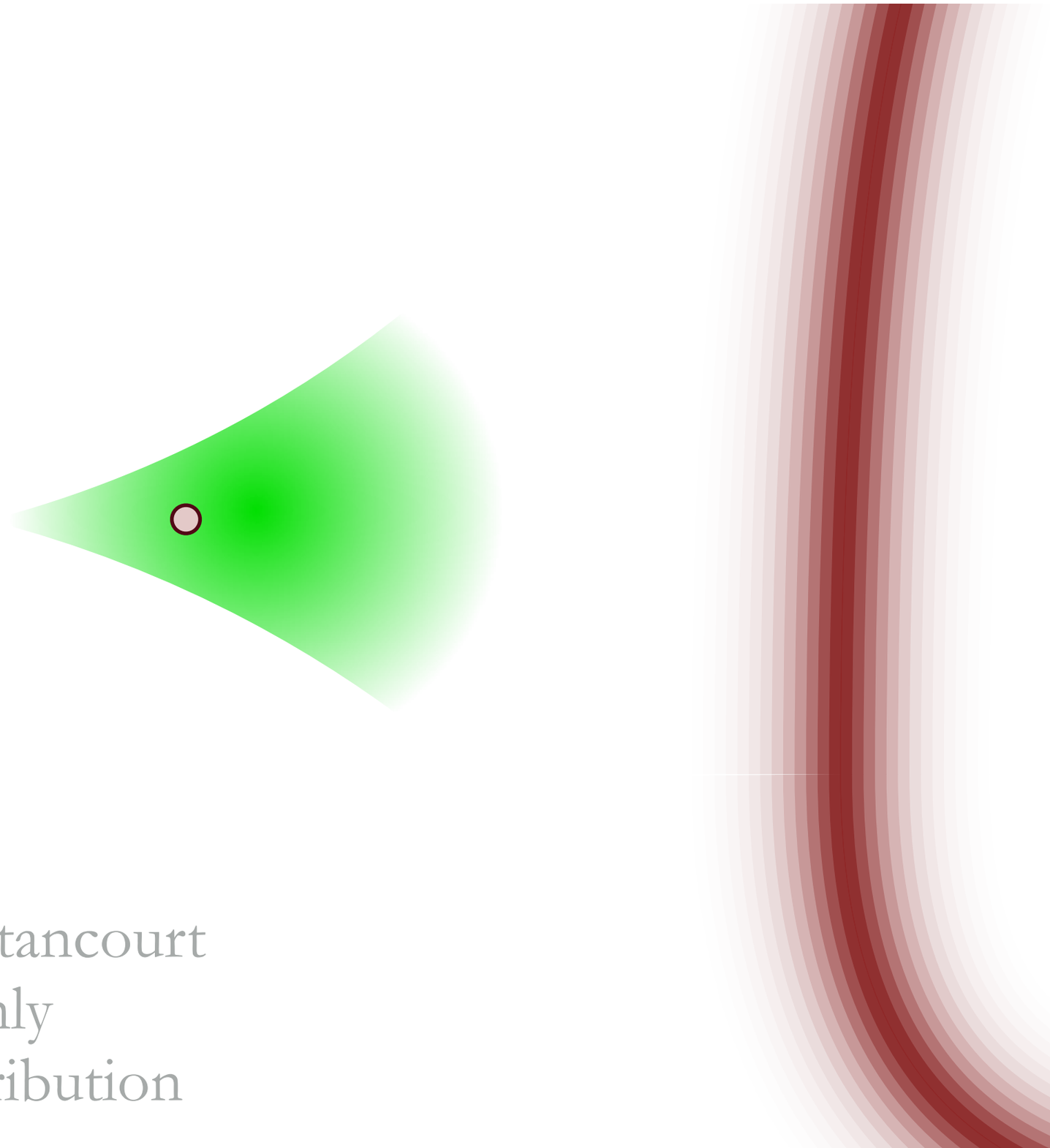

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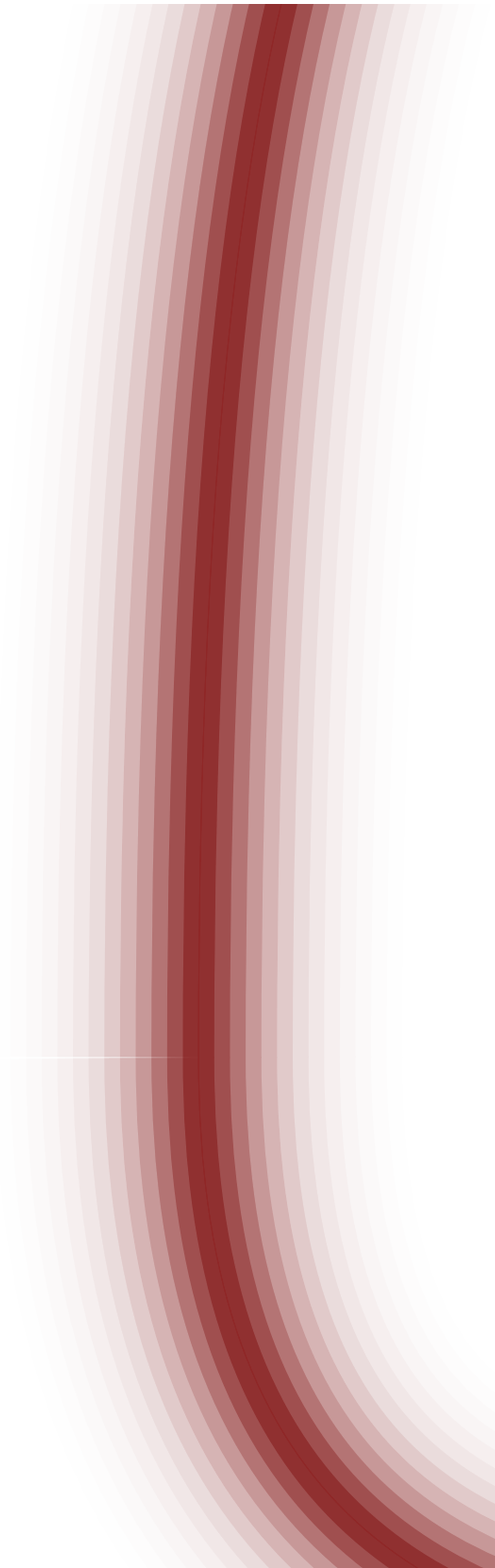

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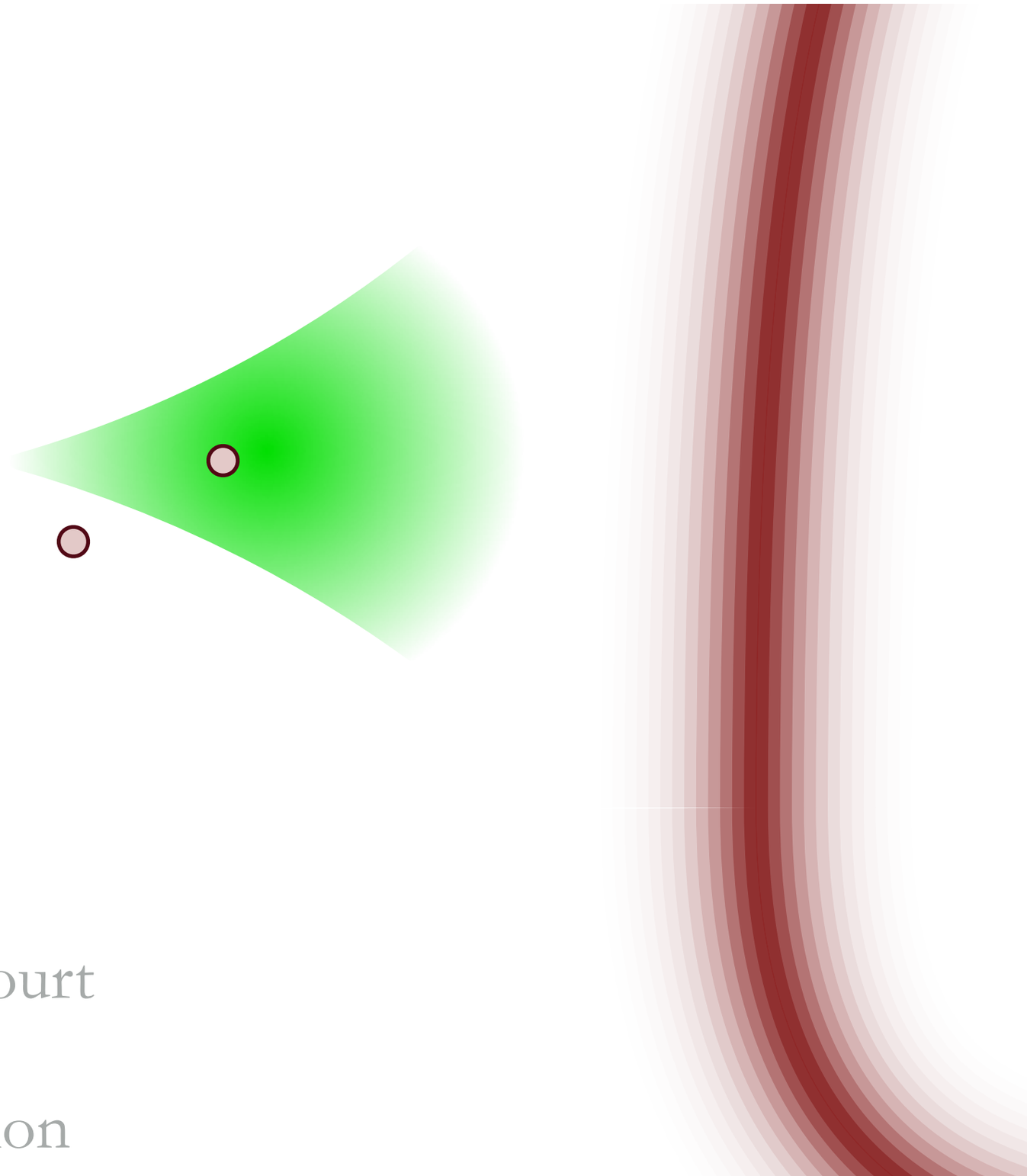
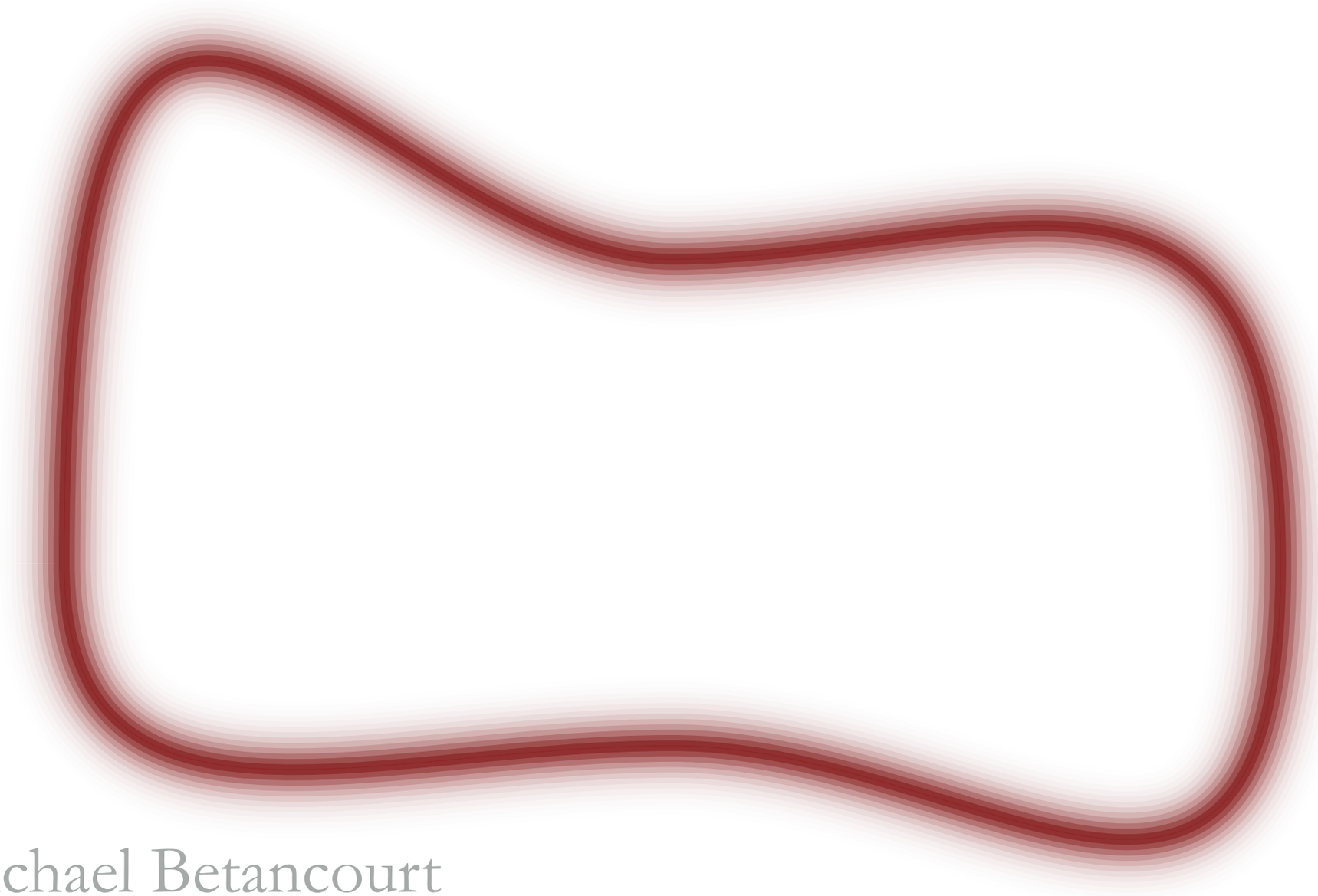


We can then exploit the subsequent *Markov chains* as a generic scheme for finding and exploring typical sets.



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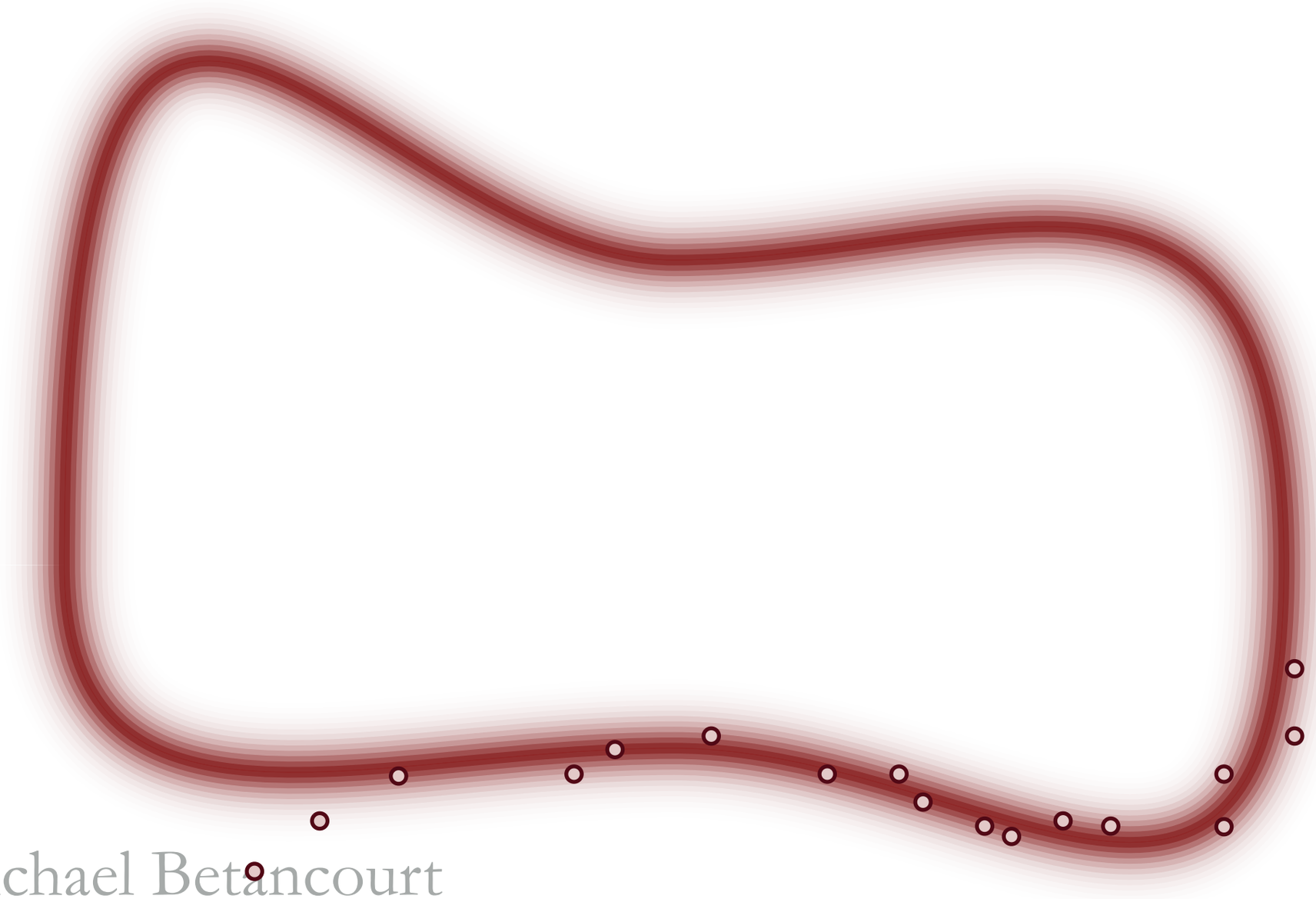
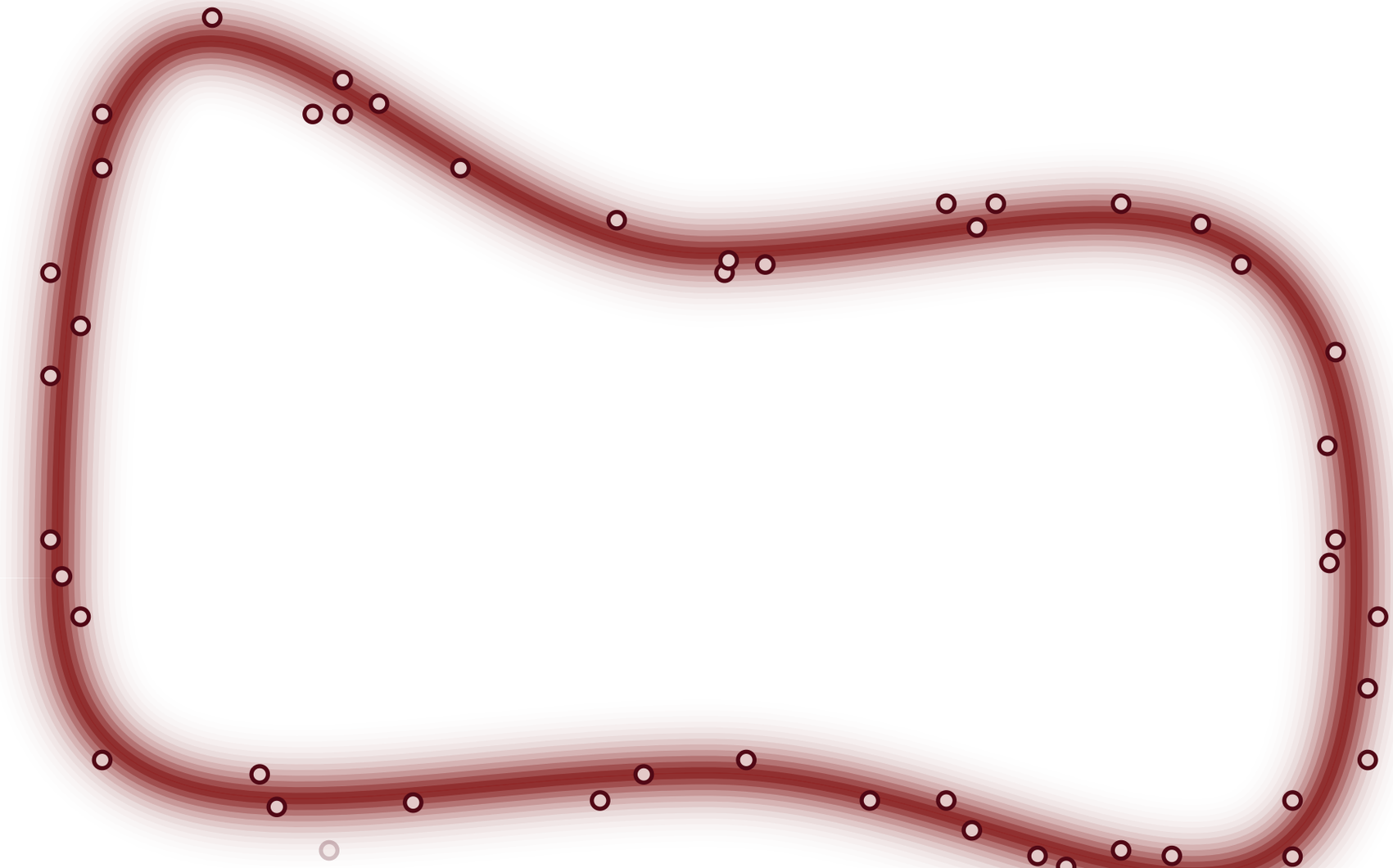


Each Markov chain defines an asymptotically consistent *Markov Chain Monte Carlo estimator*.



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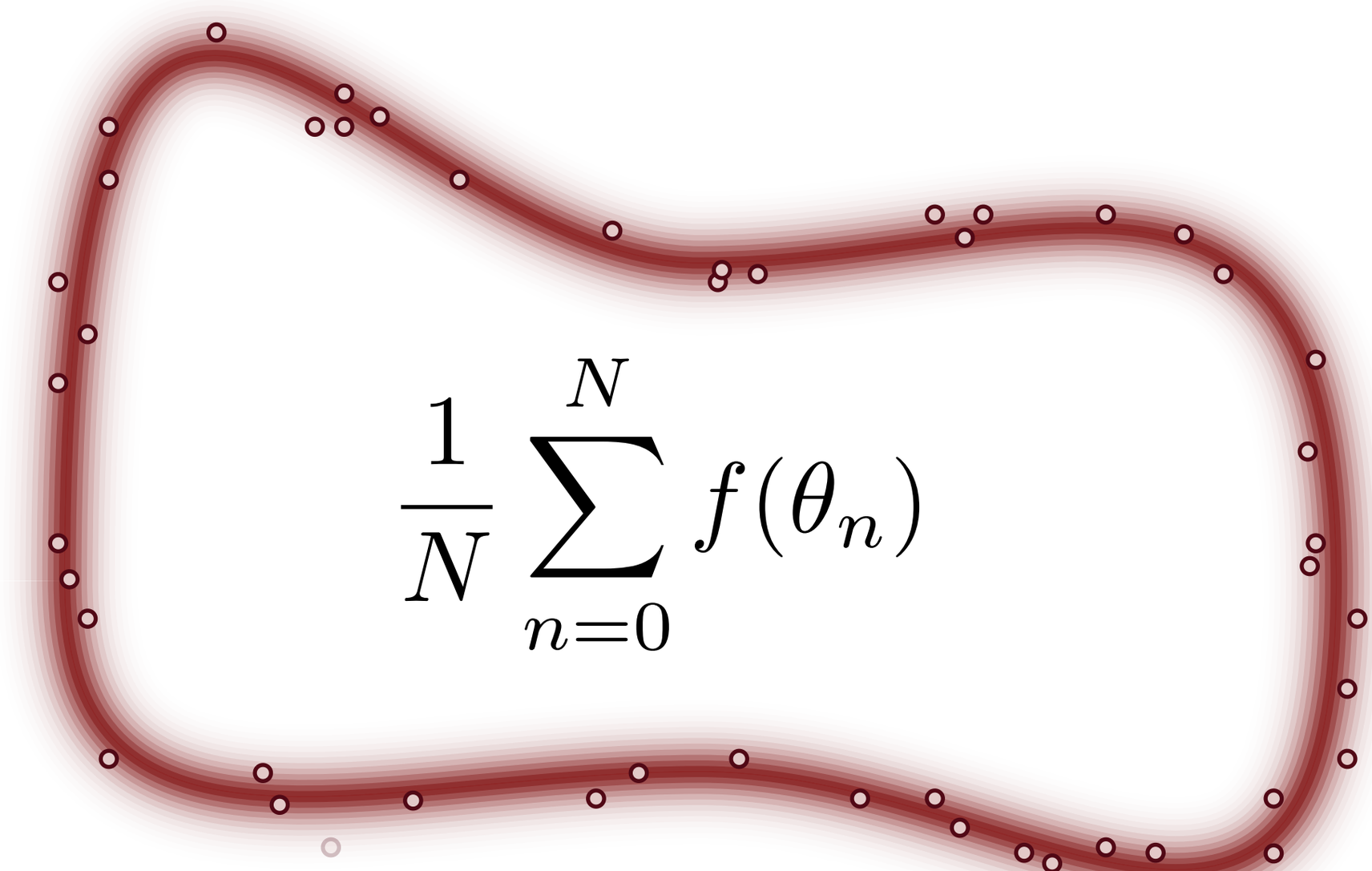

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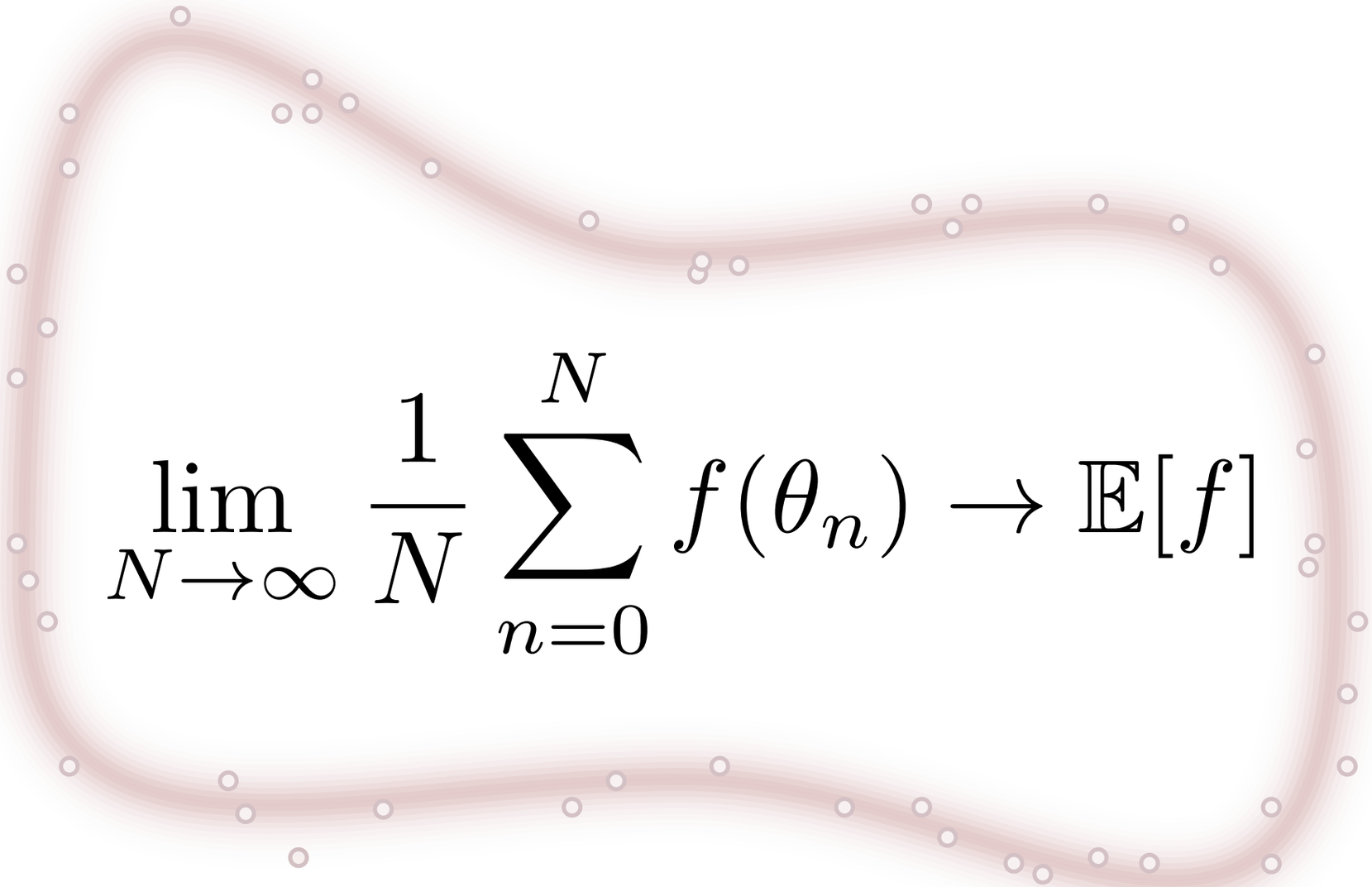
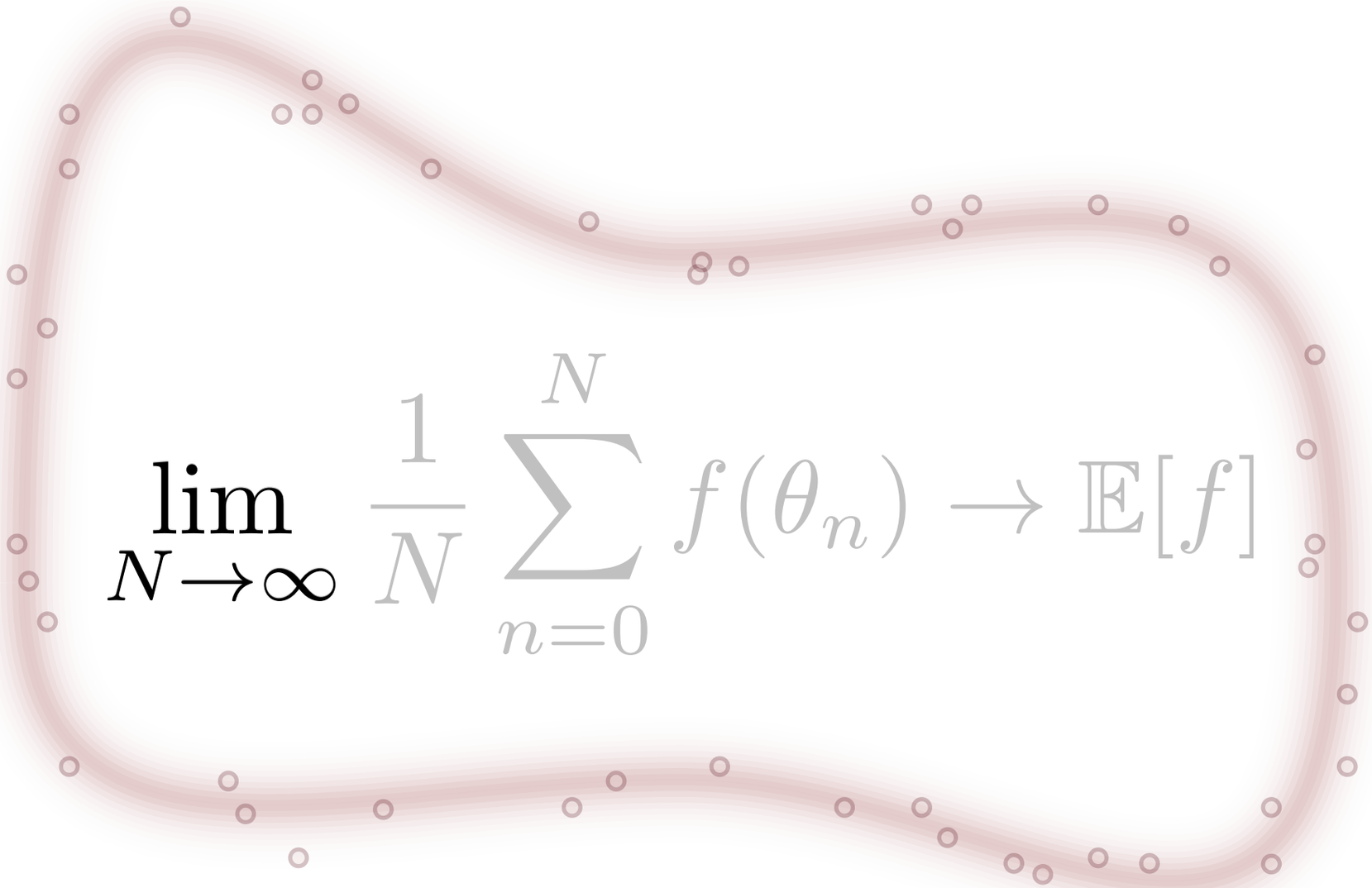


$$\lim_{N \to \infty} \frac{1}{N} \sum_{n=0}^{N} f(\theta_n) \to \mathbb{E}[f]$$

Unfortunately this asymptotic consistency makes no guarantees on the *finite time* behavior of the estimators.



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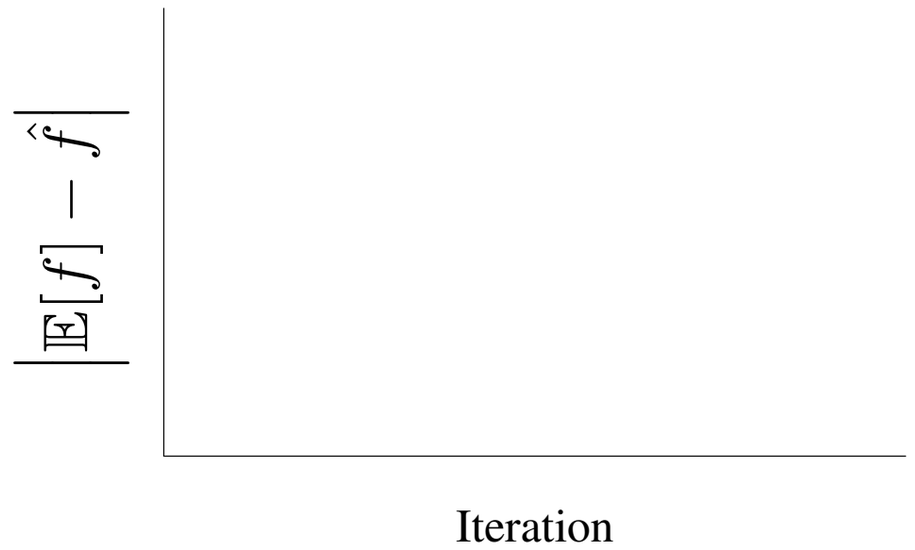

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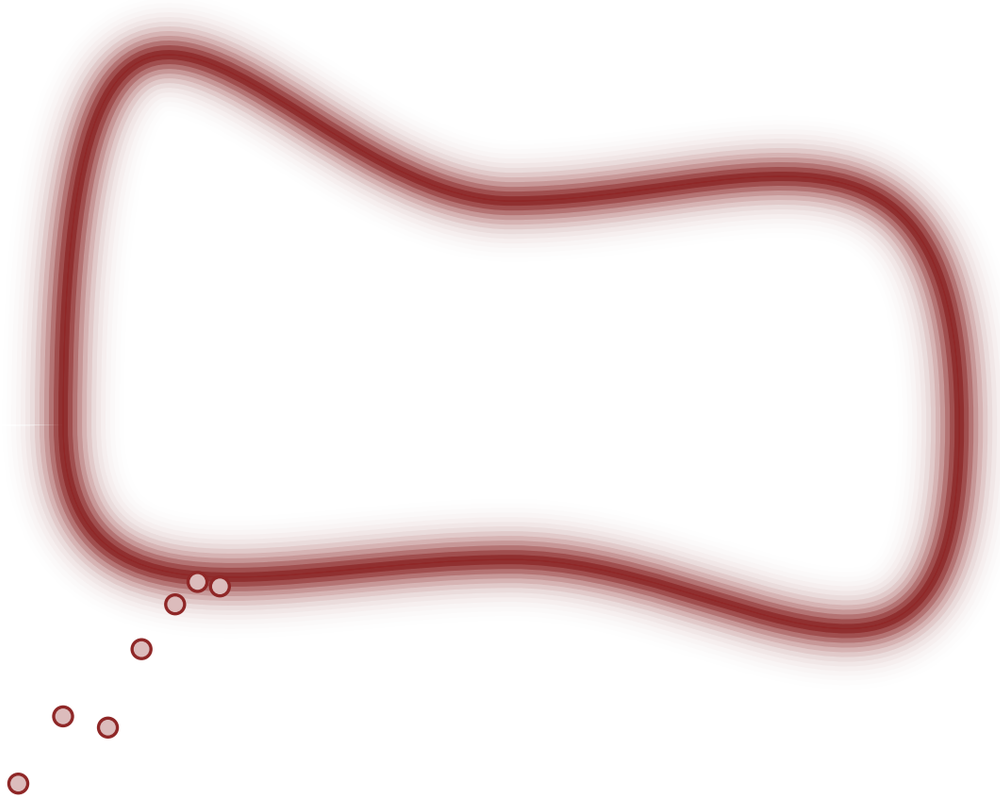

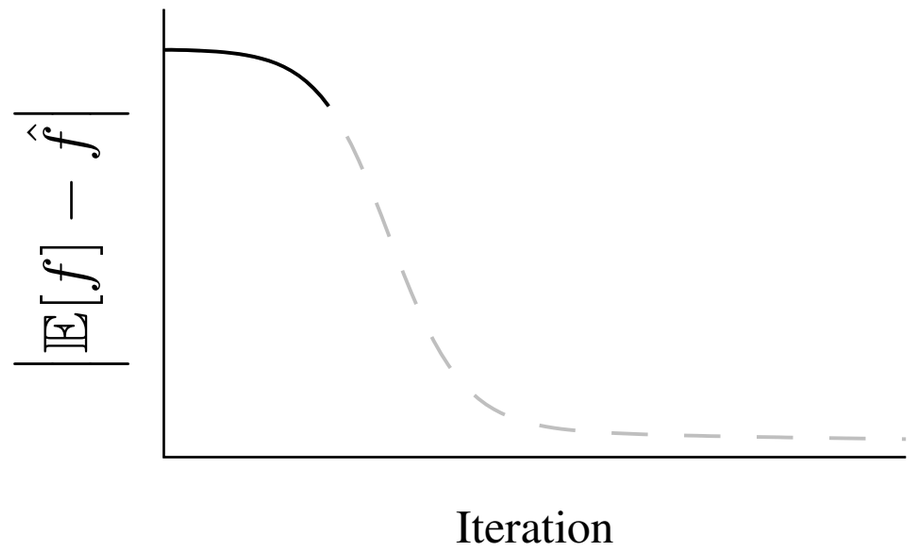

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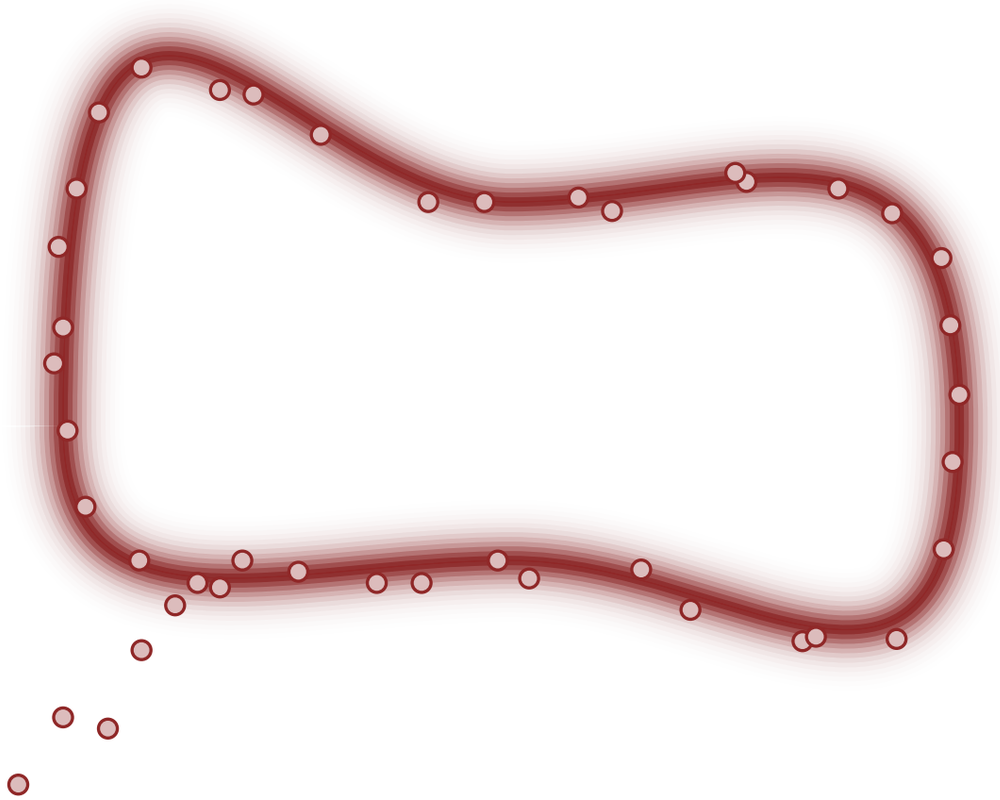

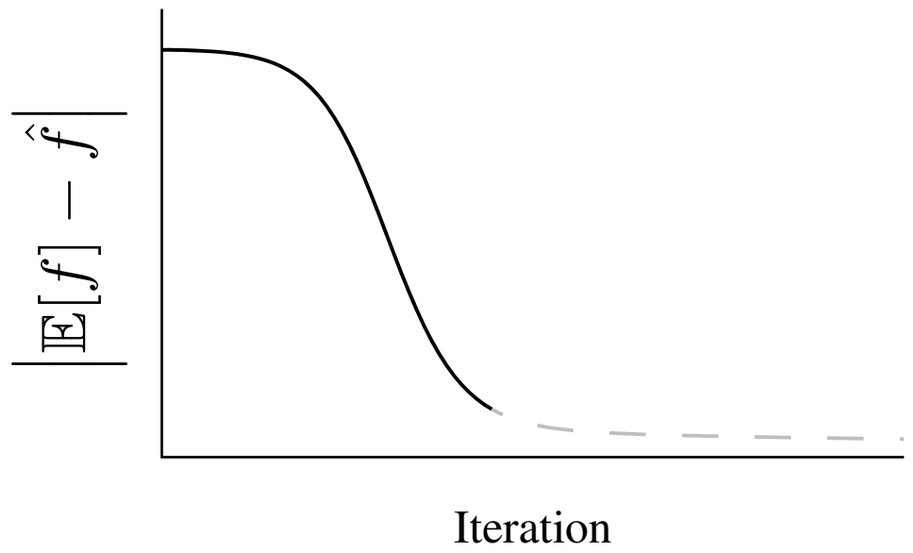

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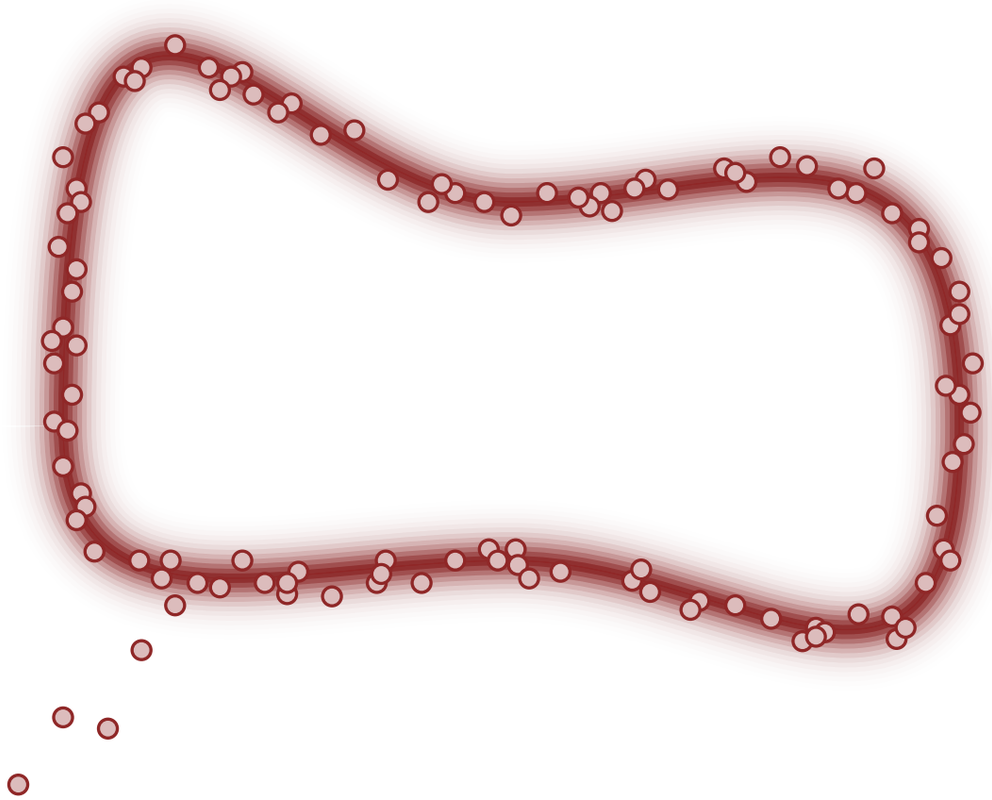
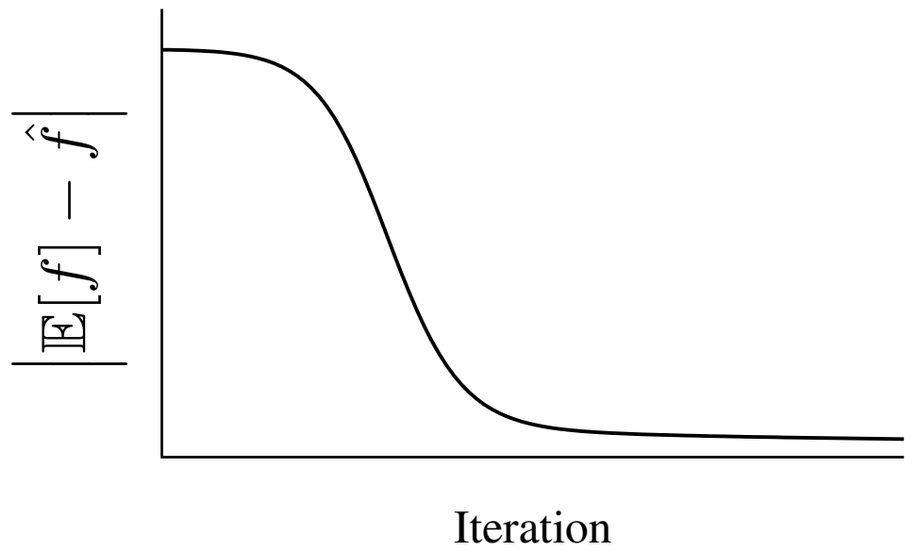
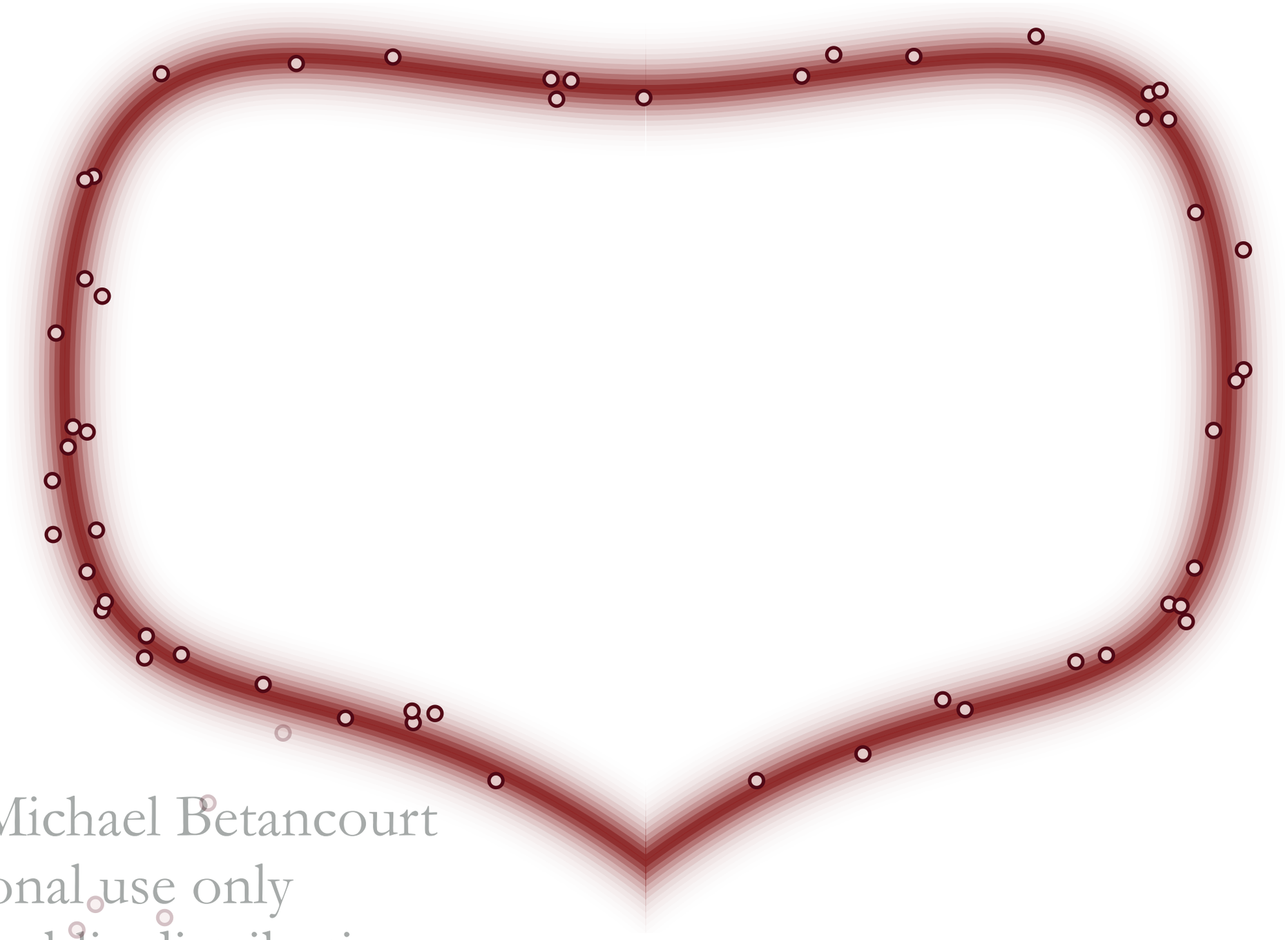




There are pathological interactions between the transition and target, however, that can spoil these ideal conditions.



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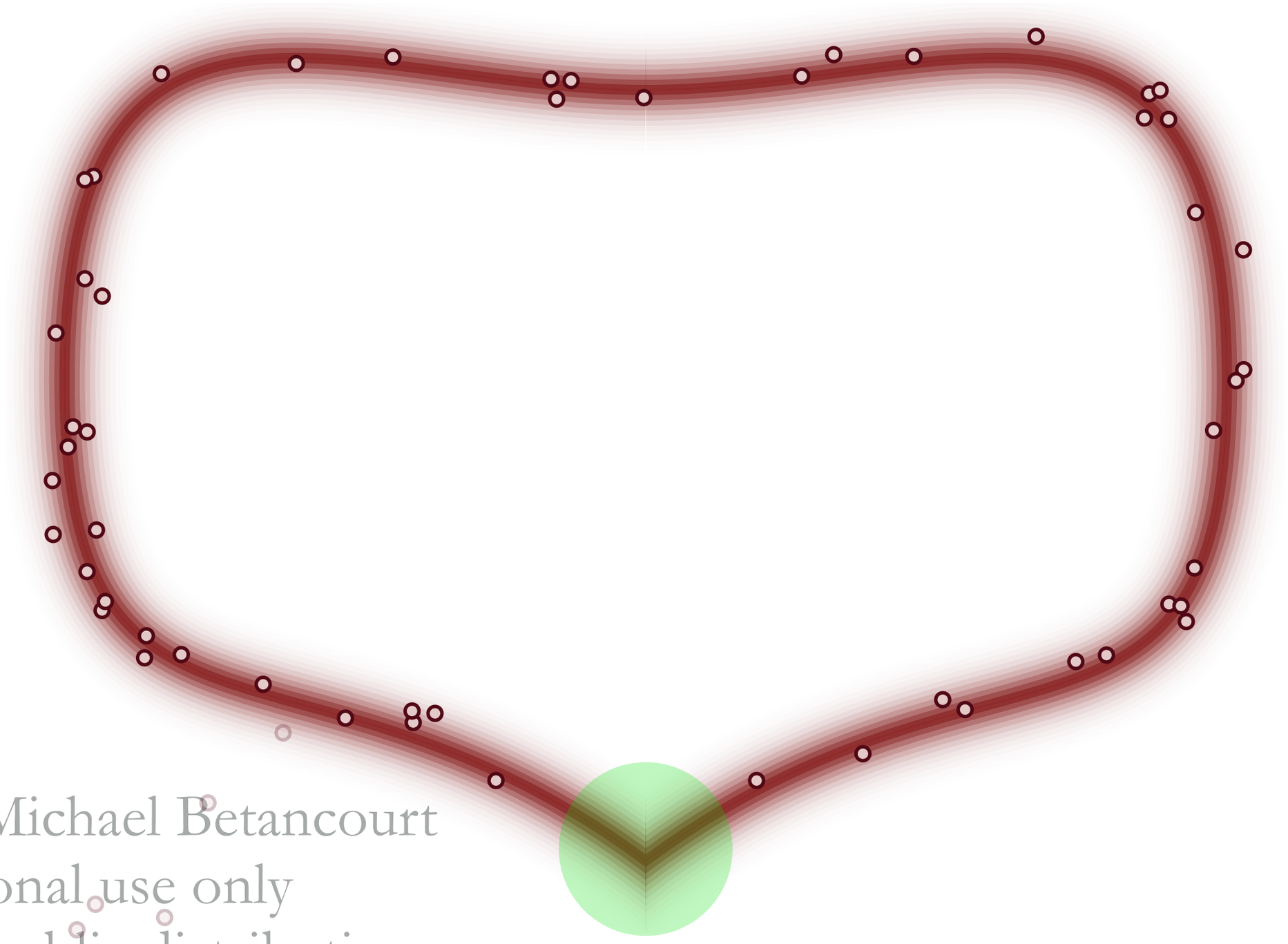

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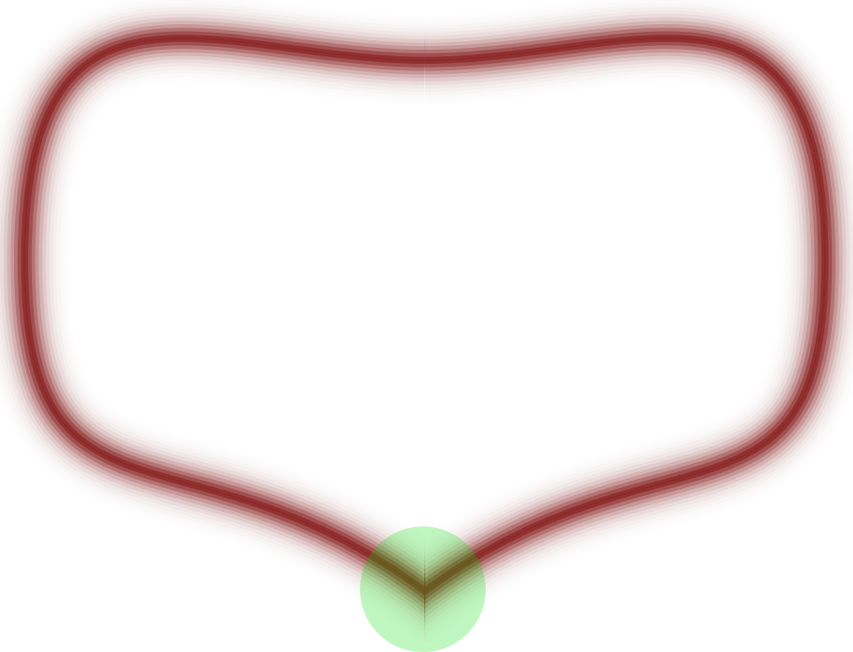

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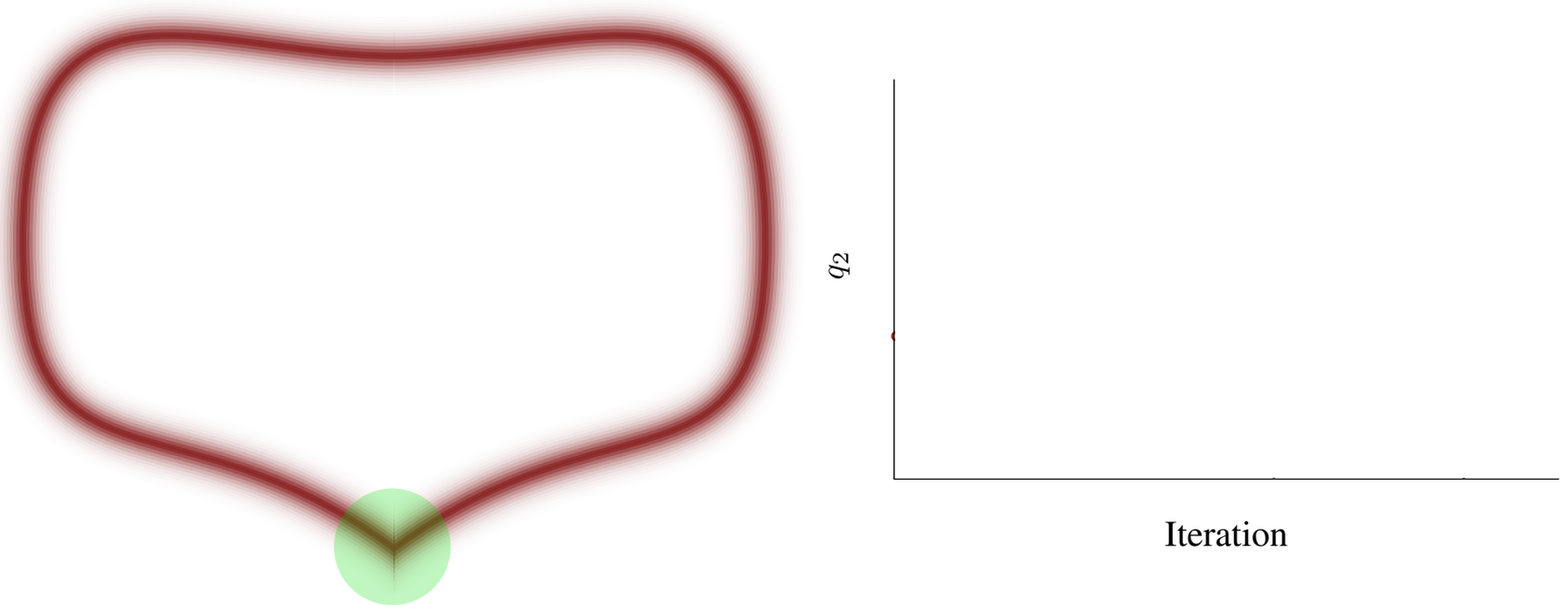

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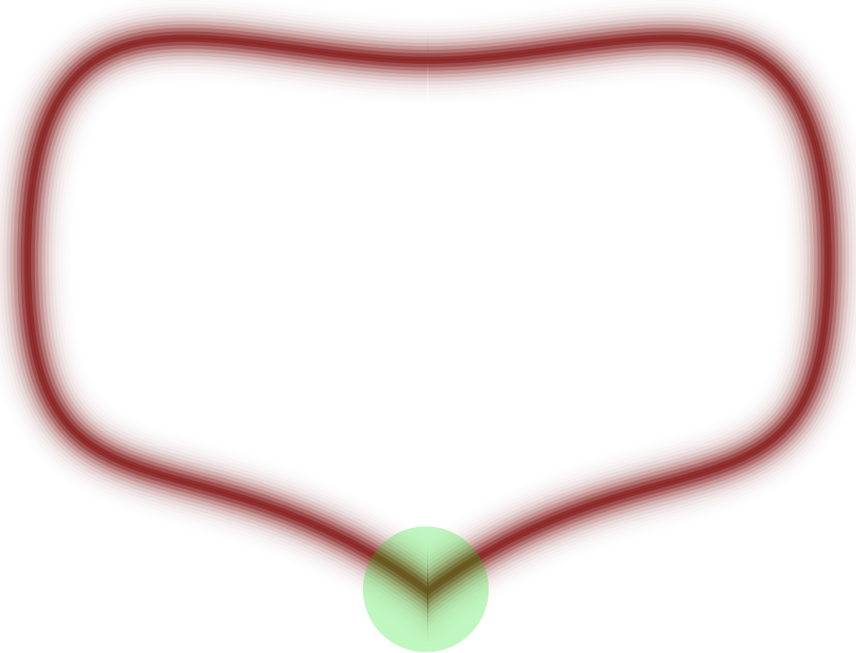

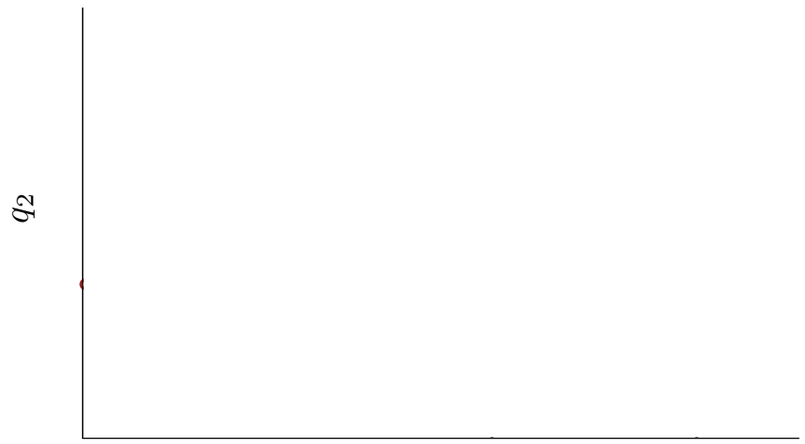

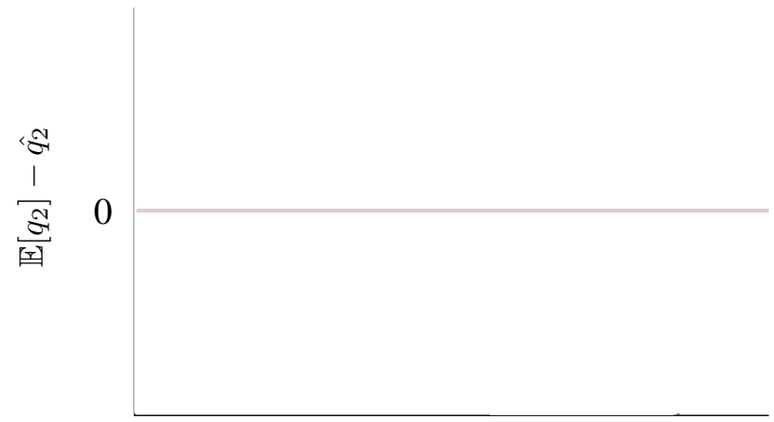

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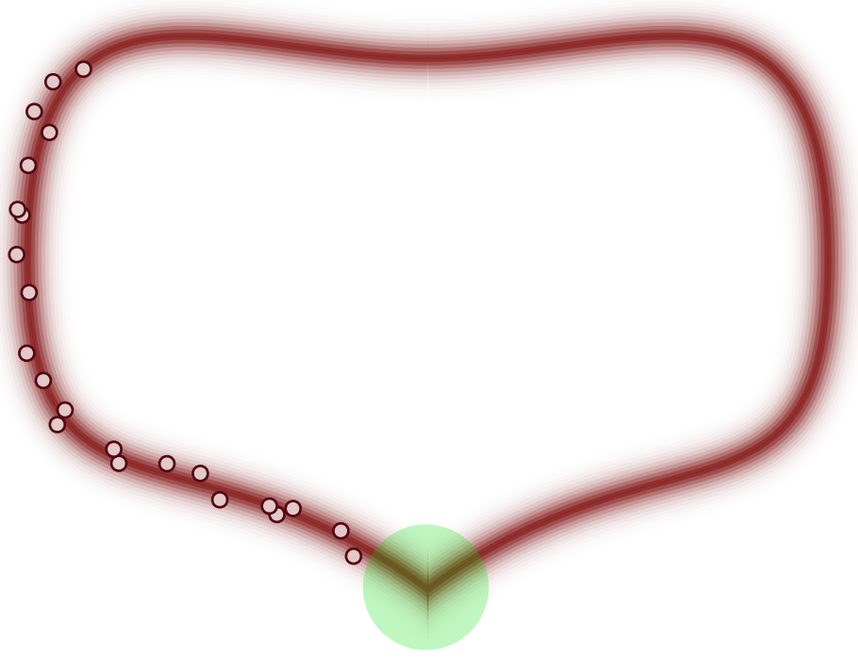

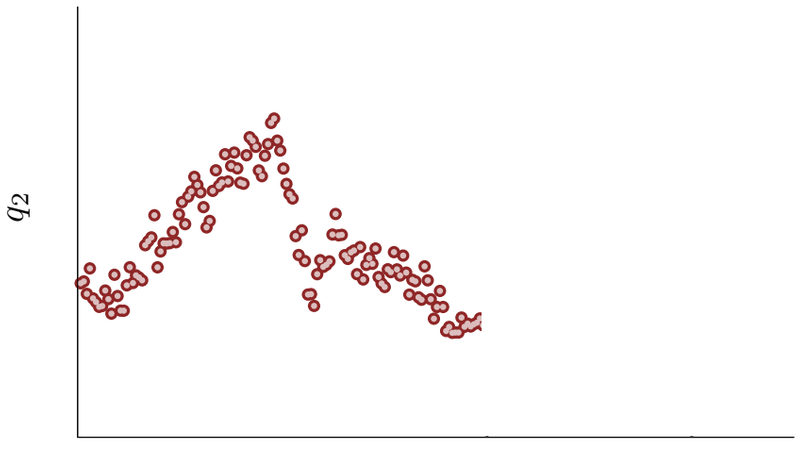

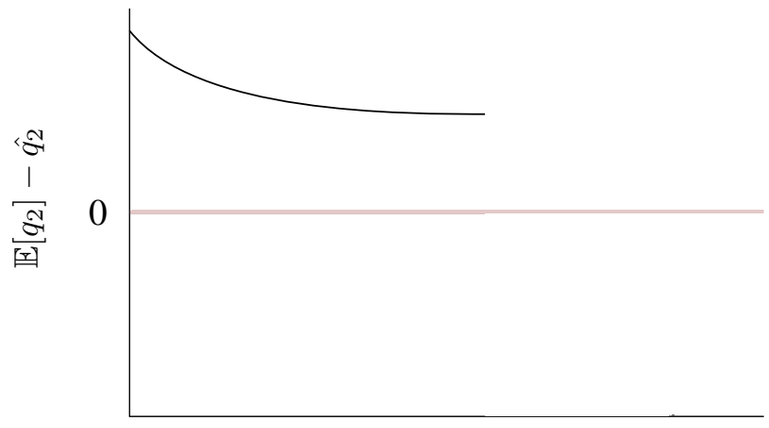

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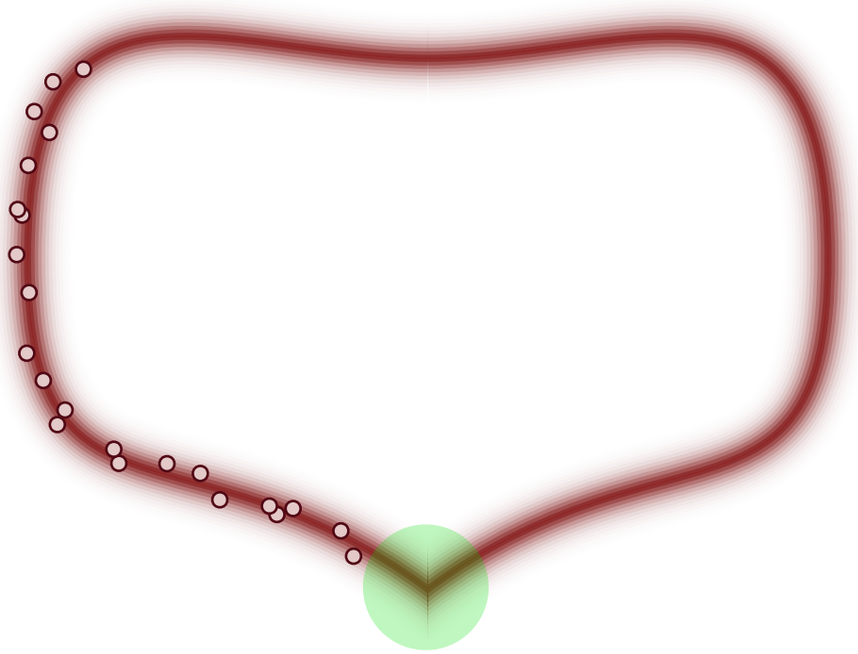

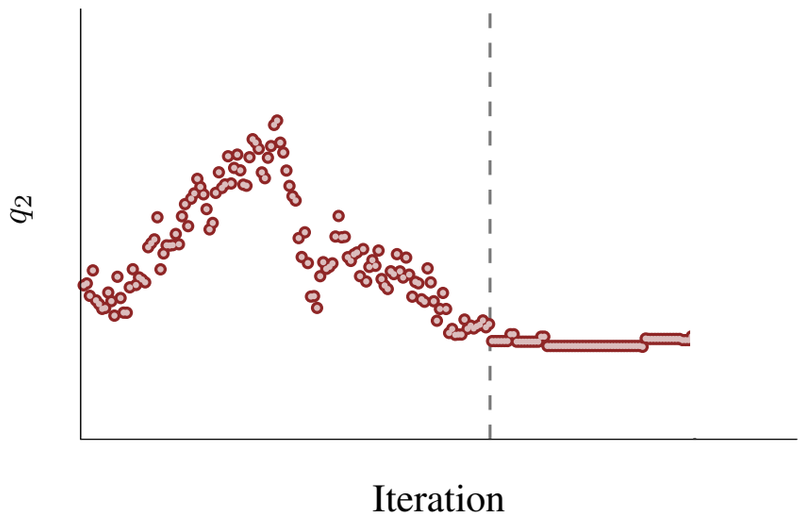

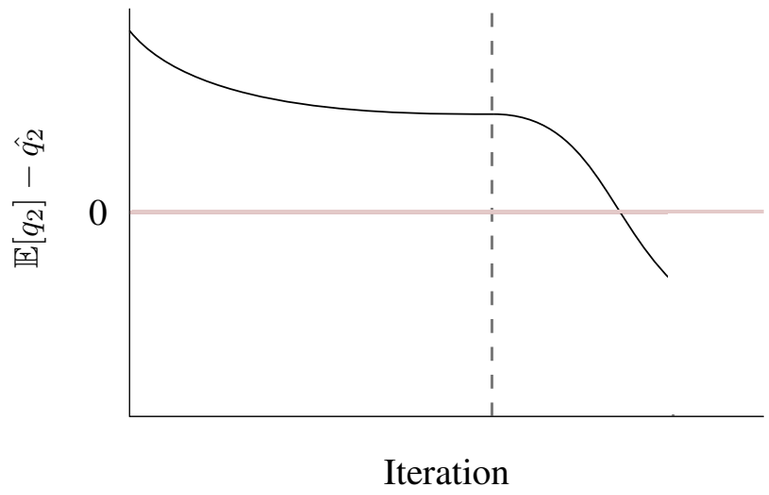

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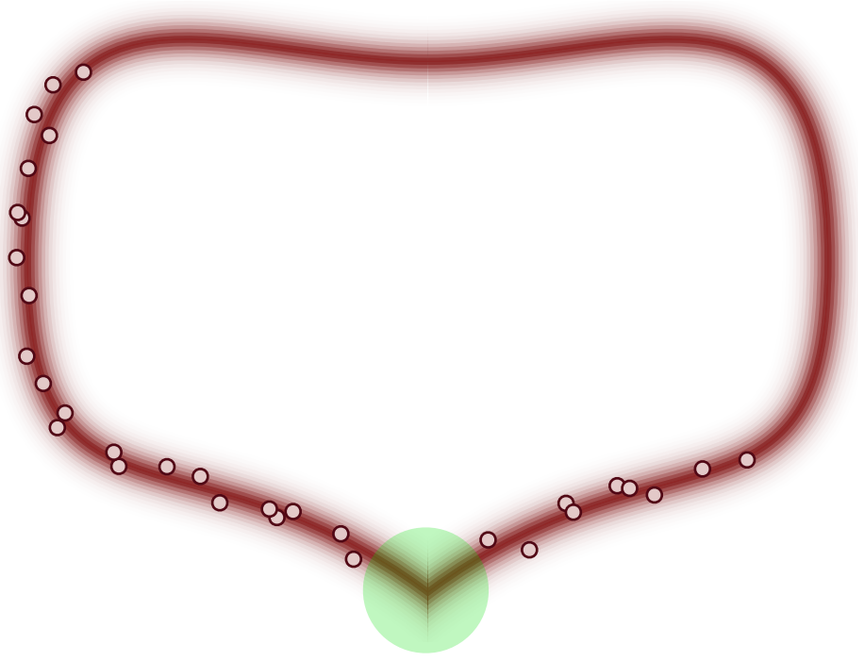

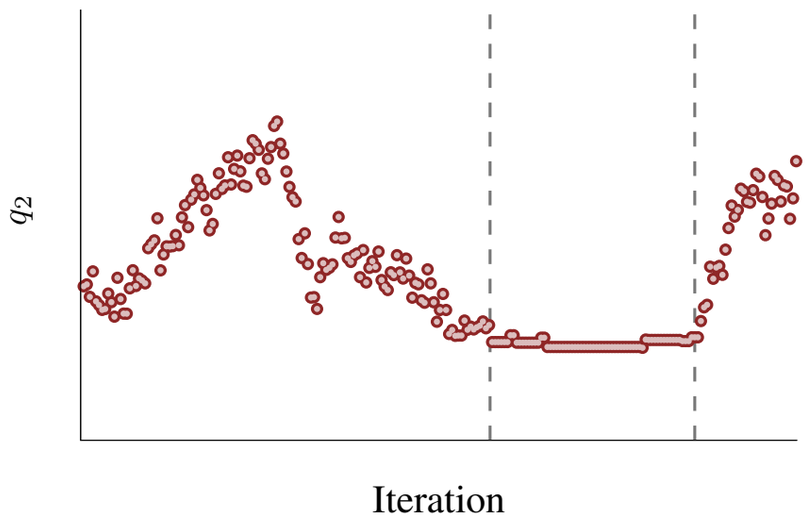

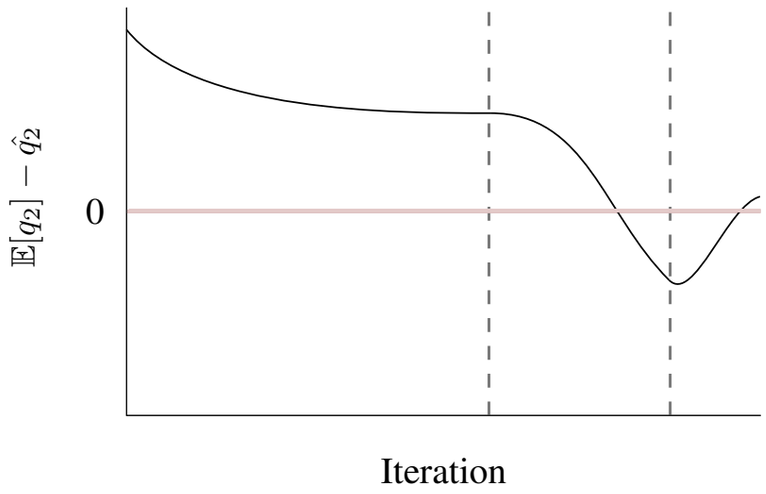

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$$||T^N \delta_{\theta_0} - \pi||$$

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$$||T^N \delta_{\theta_0} - \pi|| \leq f(\theta_0, N)$$

Geometric ergodicity occurs when the convergence proceeds *geometrically* with the number of transitions.

$$||T^N \delta_{\theta_0} - \pi||_{\mathrm{TV}} \leq C(\theta_0) \rho^N$$

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At least under the same circumstances as the Monte Carlo central limit theorem.

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$$\mathrm{ESS}[f] = \frac{N}{1 + 2\sum_{l=1}^{\infty} \rho_l[f]}$$

The more positive the autocorrelation sum the lower the effective sample size; the more negative the higher.

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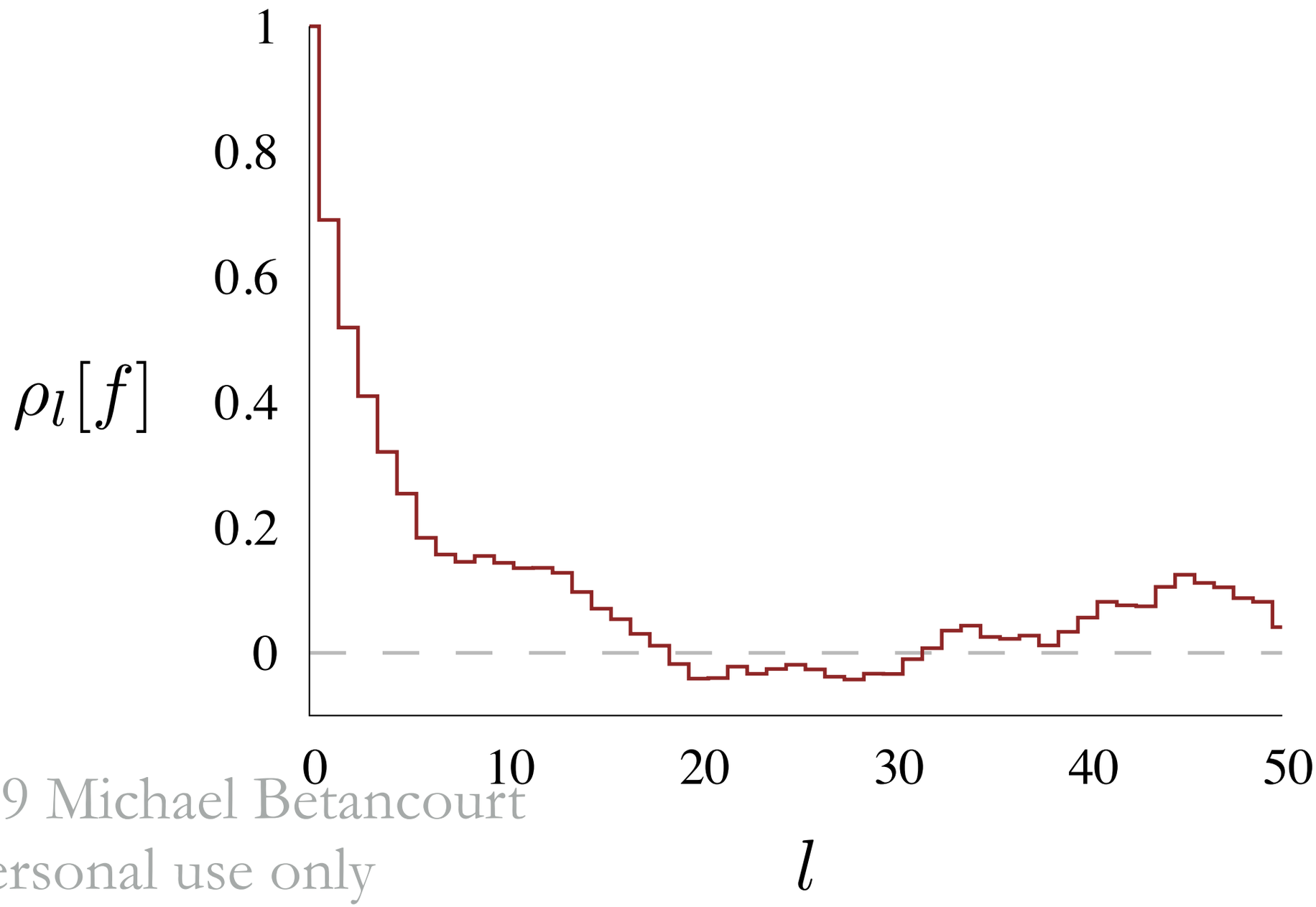

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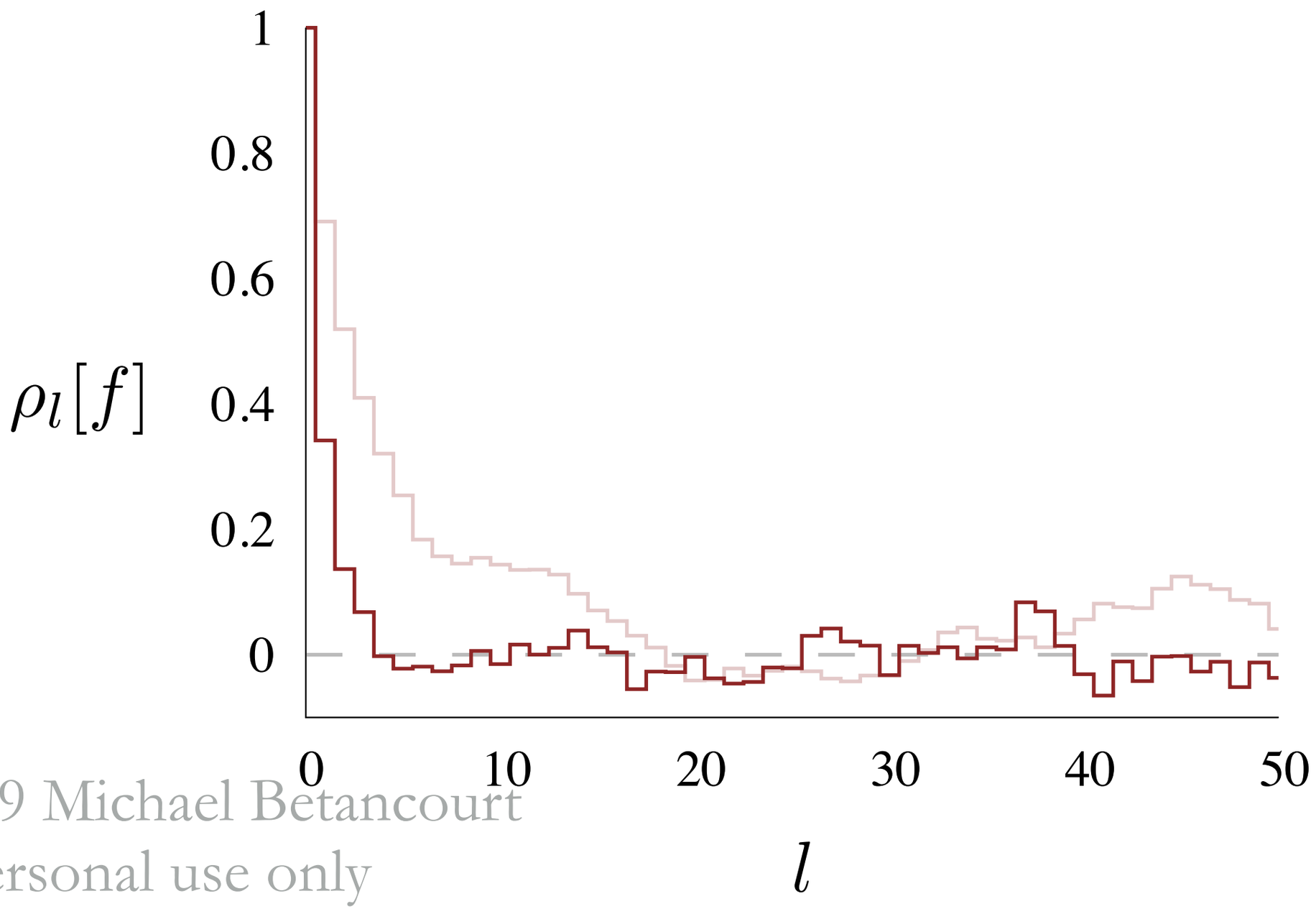

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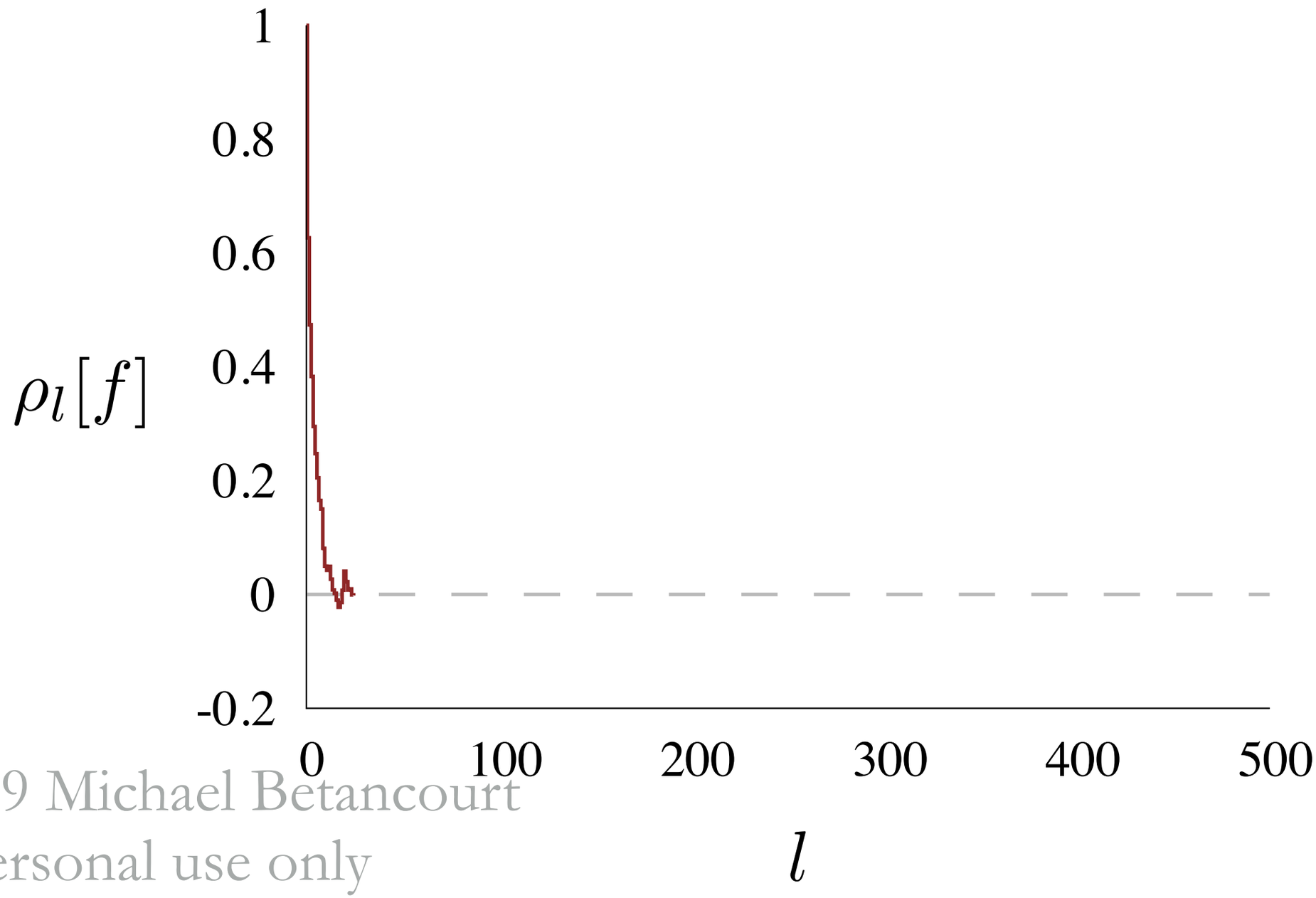
In order to accurately estimate autocorrelations we have to make sure that we run sufficiently long chains.



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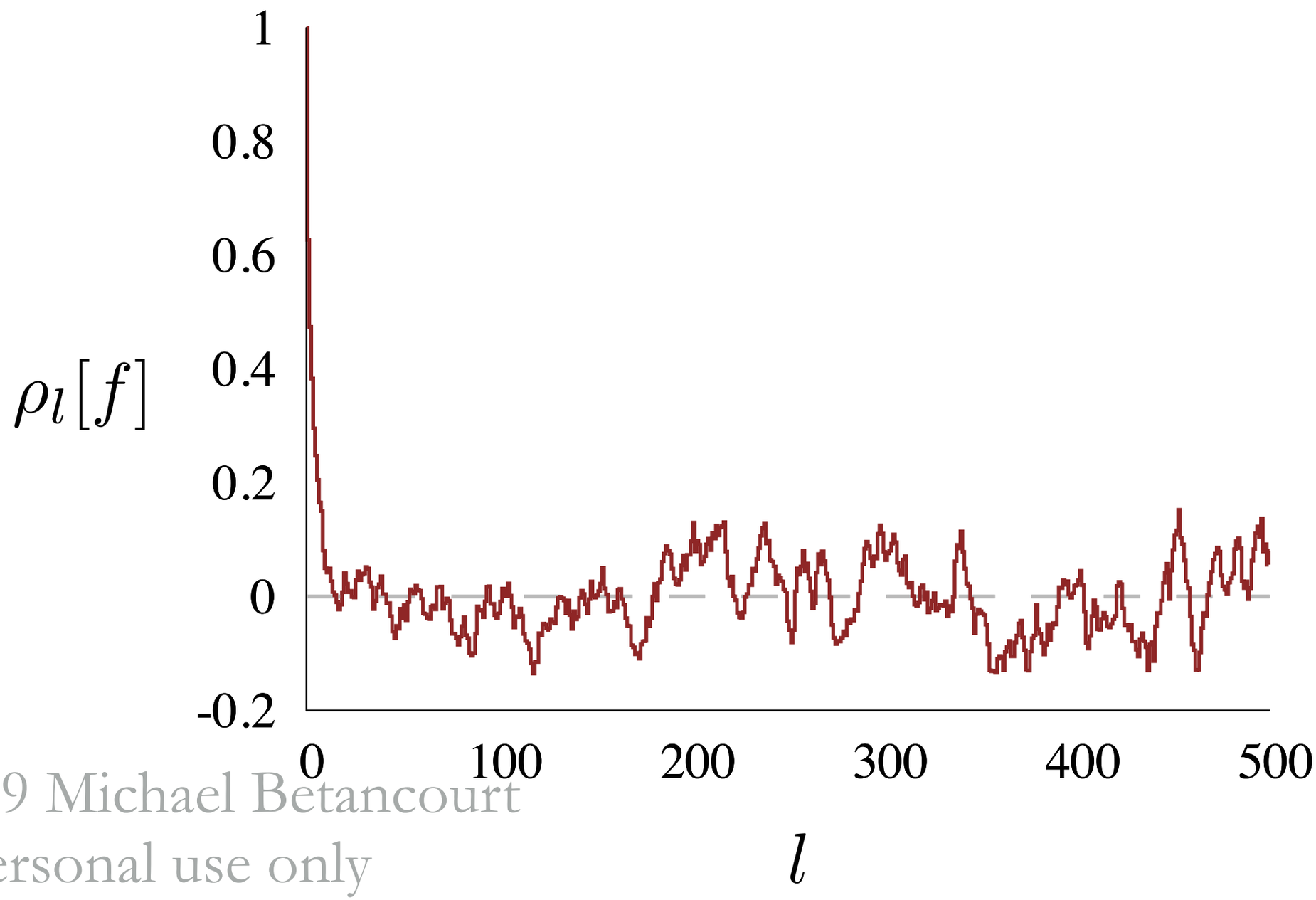

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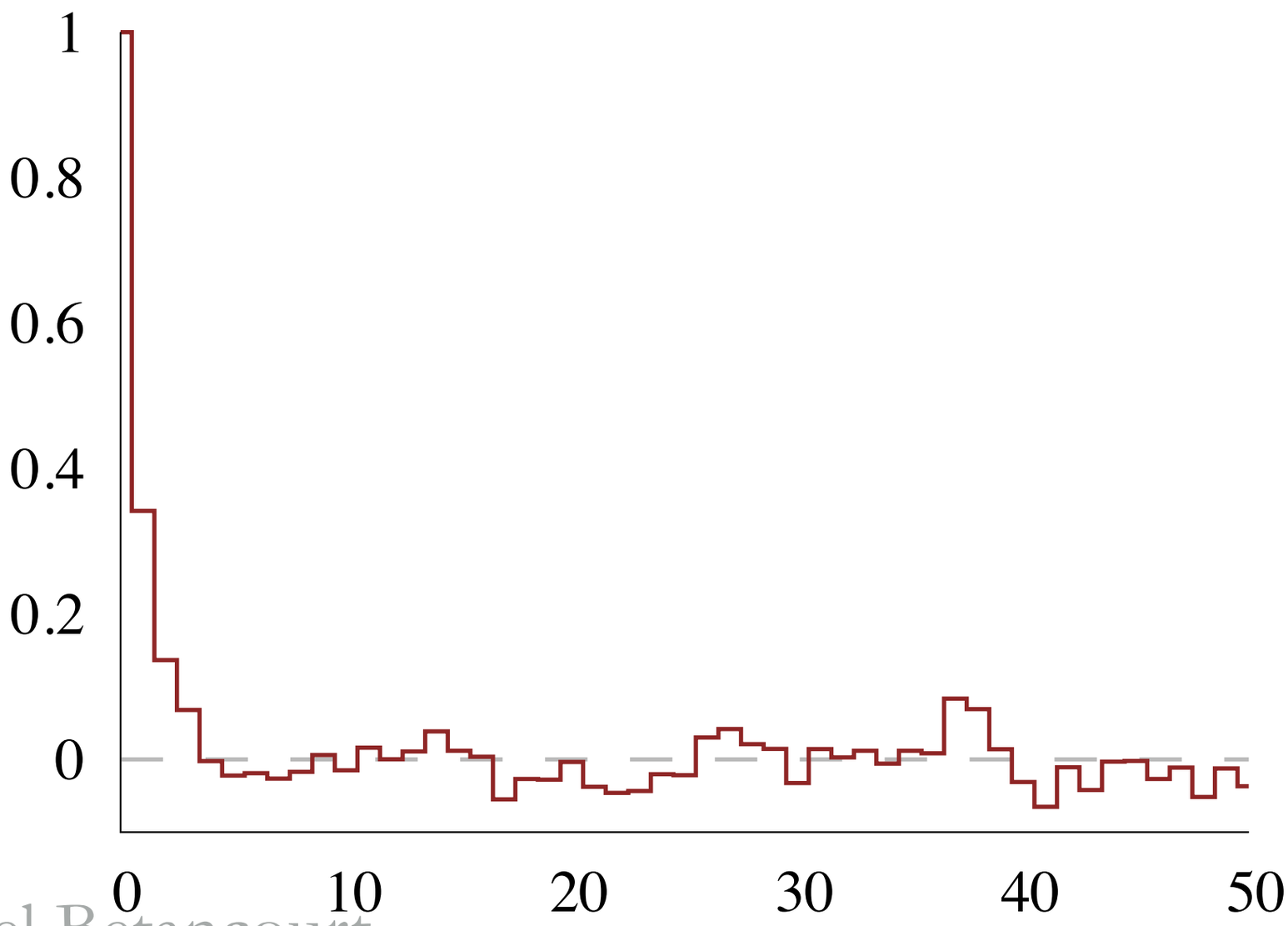

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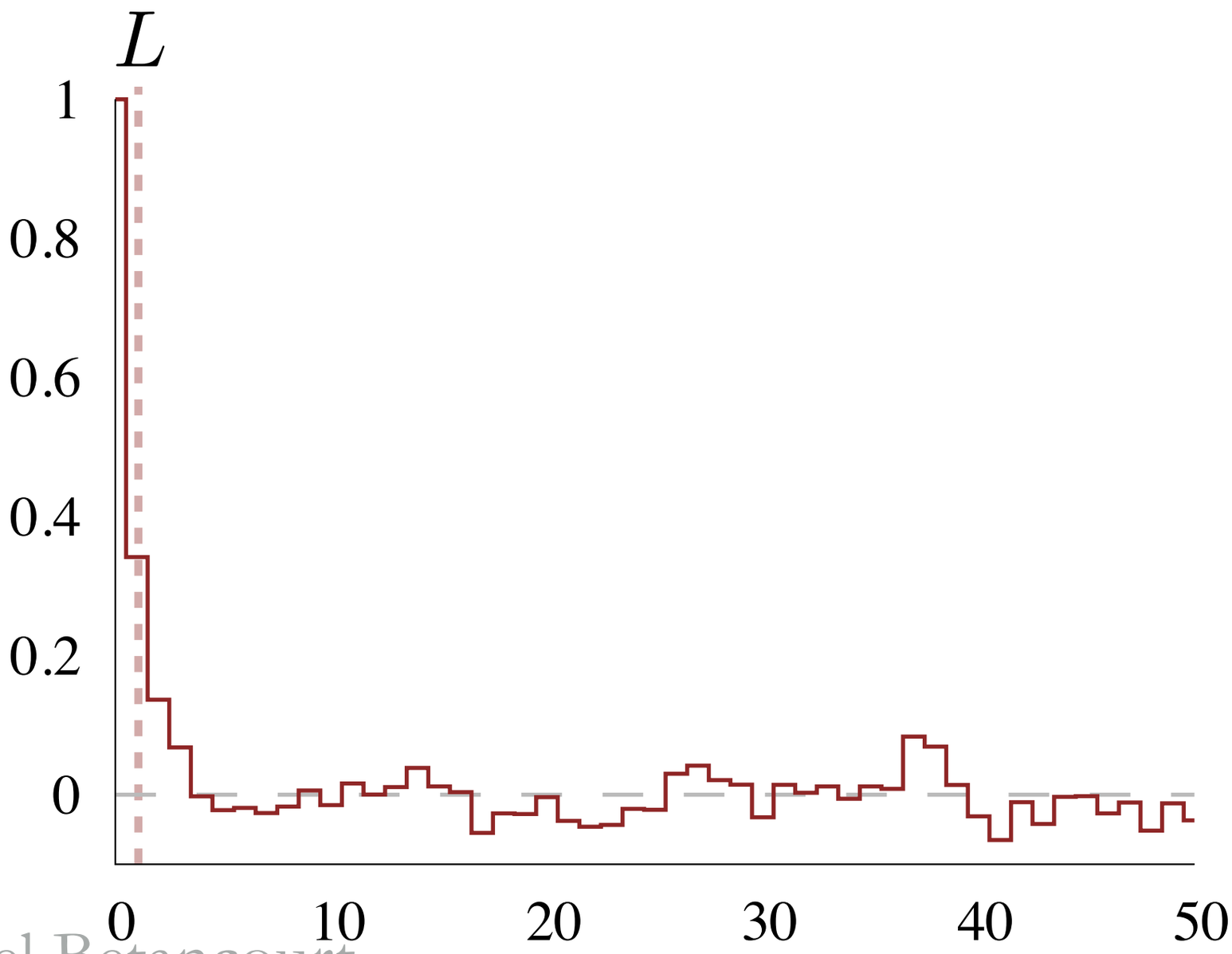

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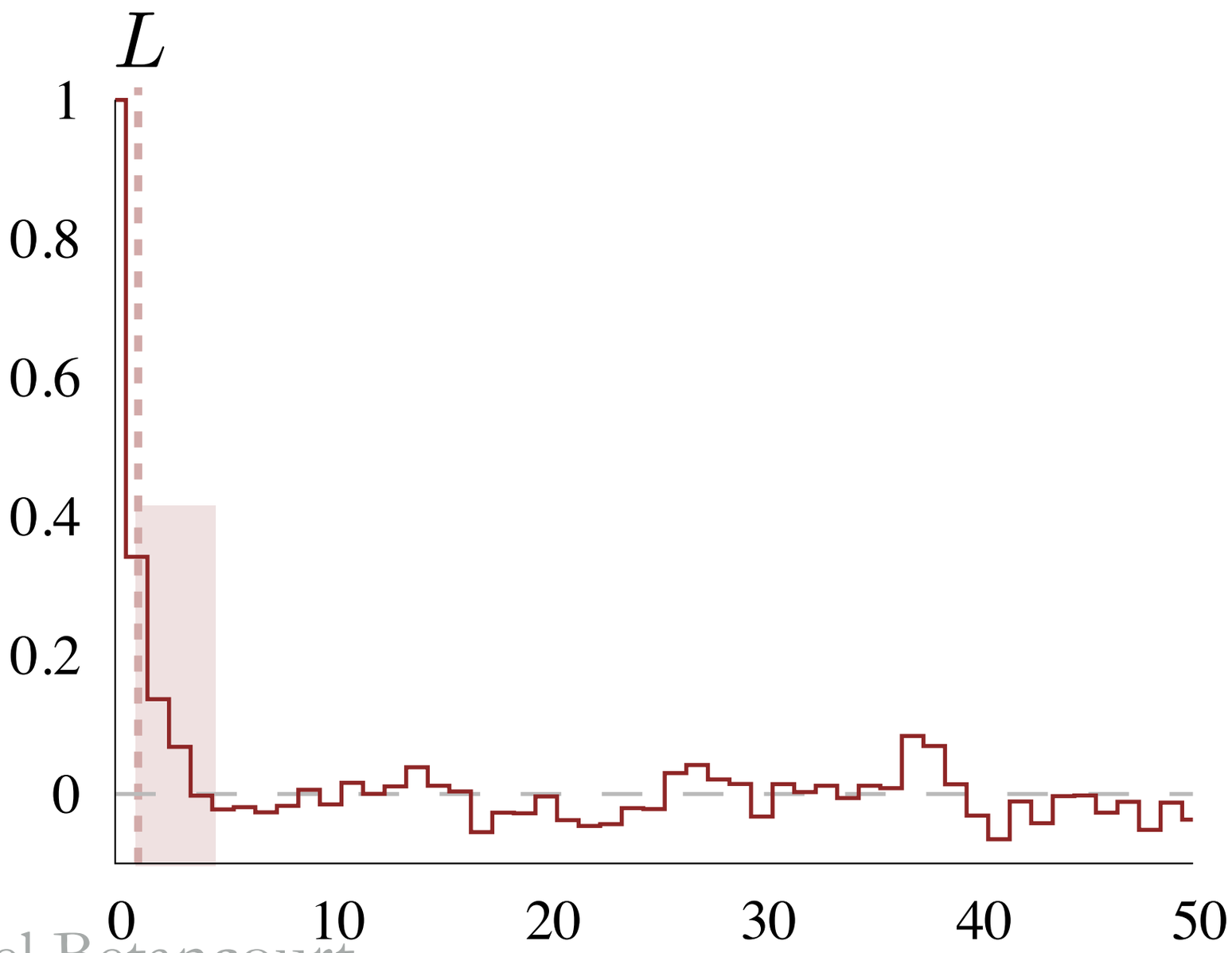

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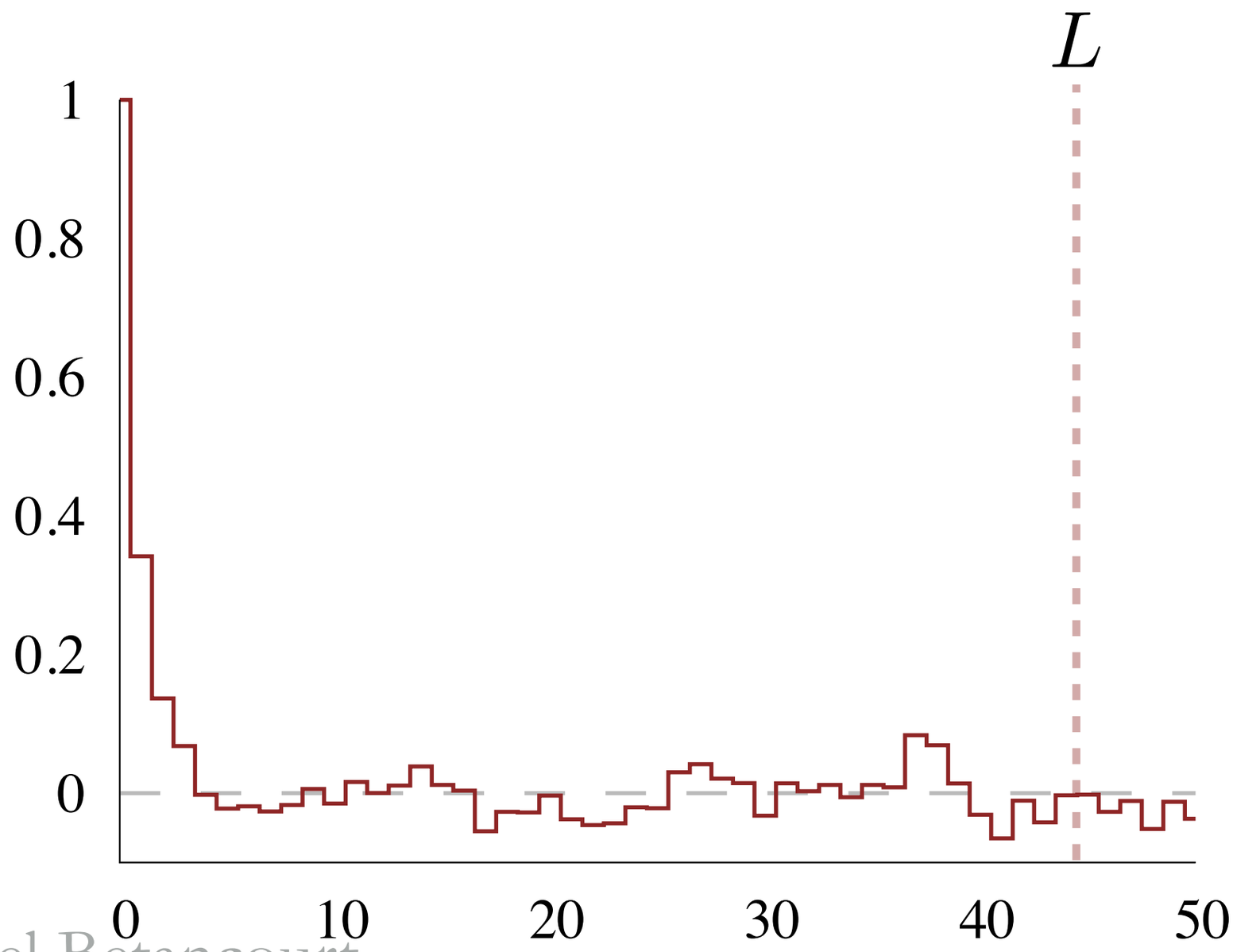

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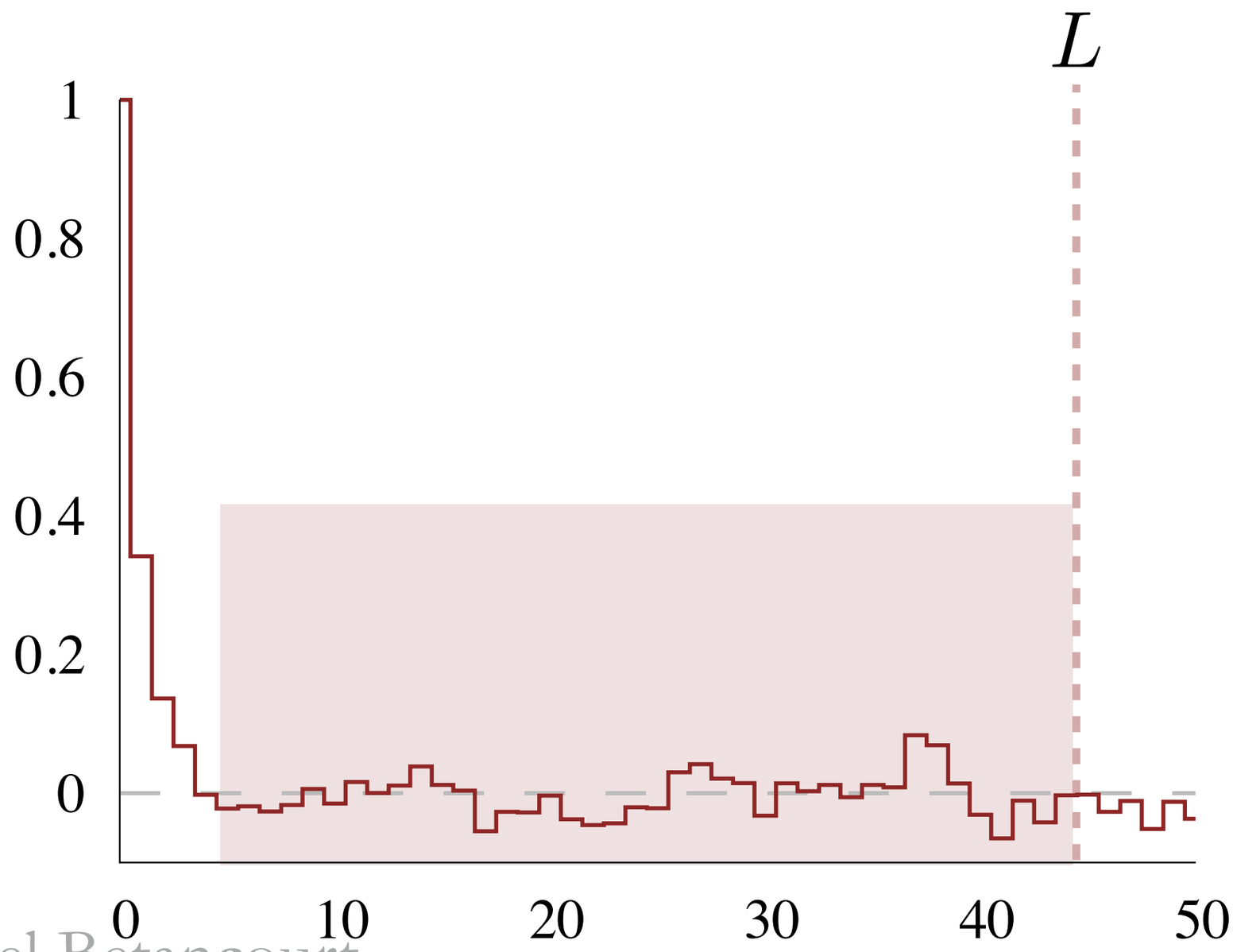

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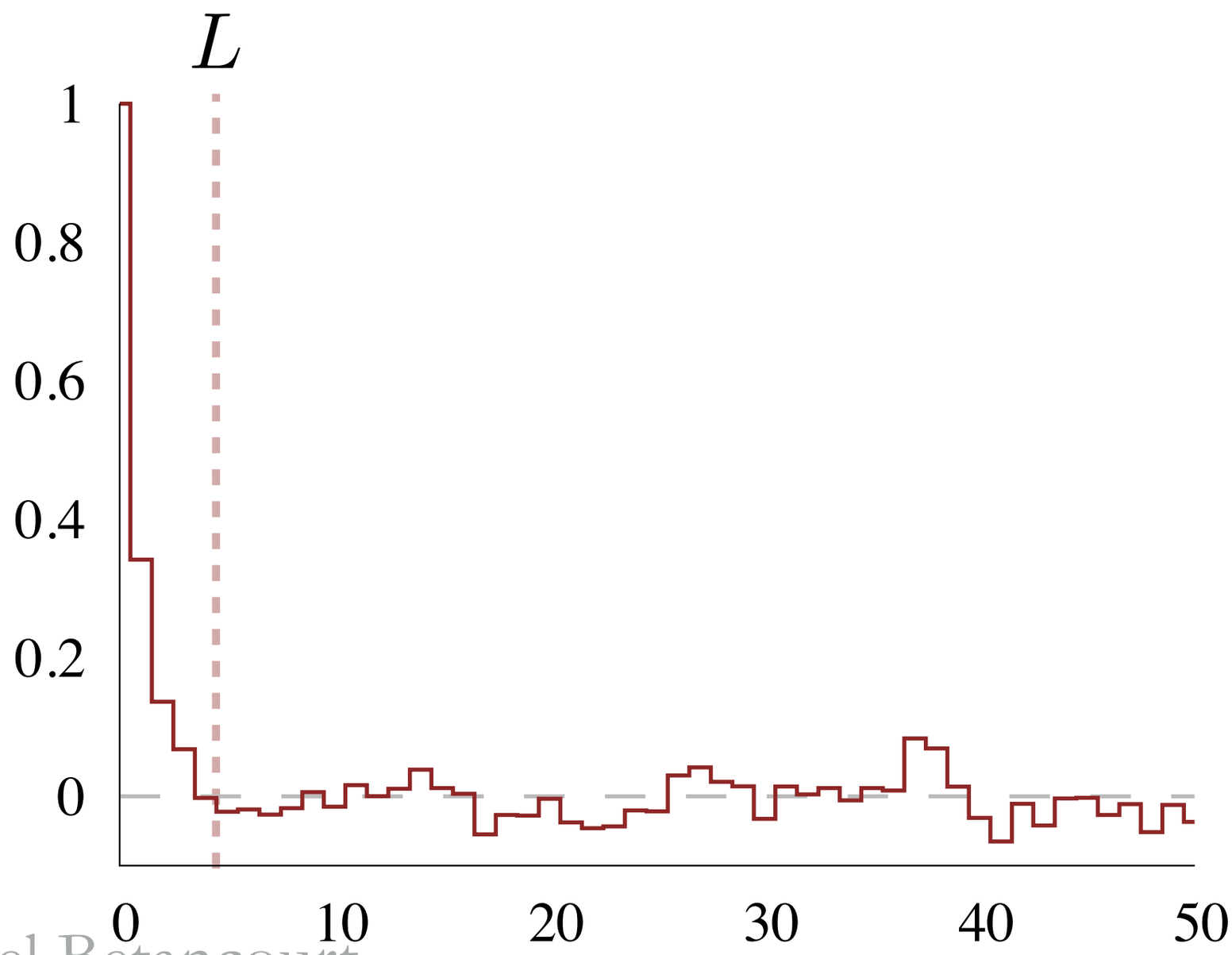

Once we've estimated the effective sample sizes we can estimate the standard errors of our MCMC estimators.

$$\hat{f} = \frac{1}{N} \sum_{n=1}^{N} f(\theta_i)$$

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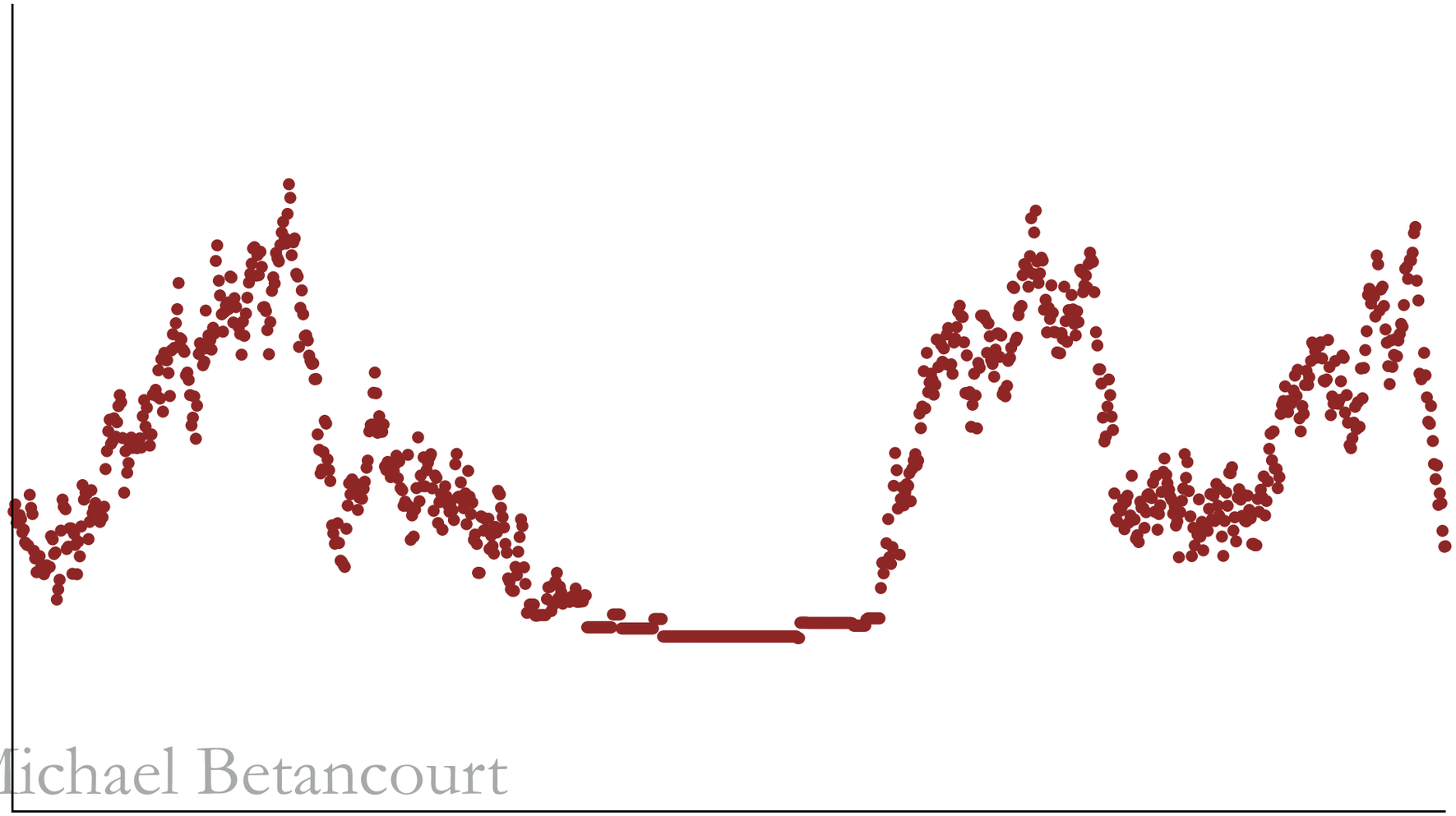
Diagnosing Inadequate Convergence



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Such an analysis, however, is impractically complex even in seemingly simple problems.

$$\pi_S(\theta \mid \tilde{y}) = \int \mathrm{d}\theta' \, \pi_S(\theta' \mid \tilde{y}) \, T(\theta \mid \theta')$$

If we have geometric ergodicity, however, then we can *estimate* convergence empirically.

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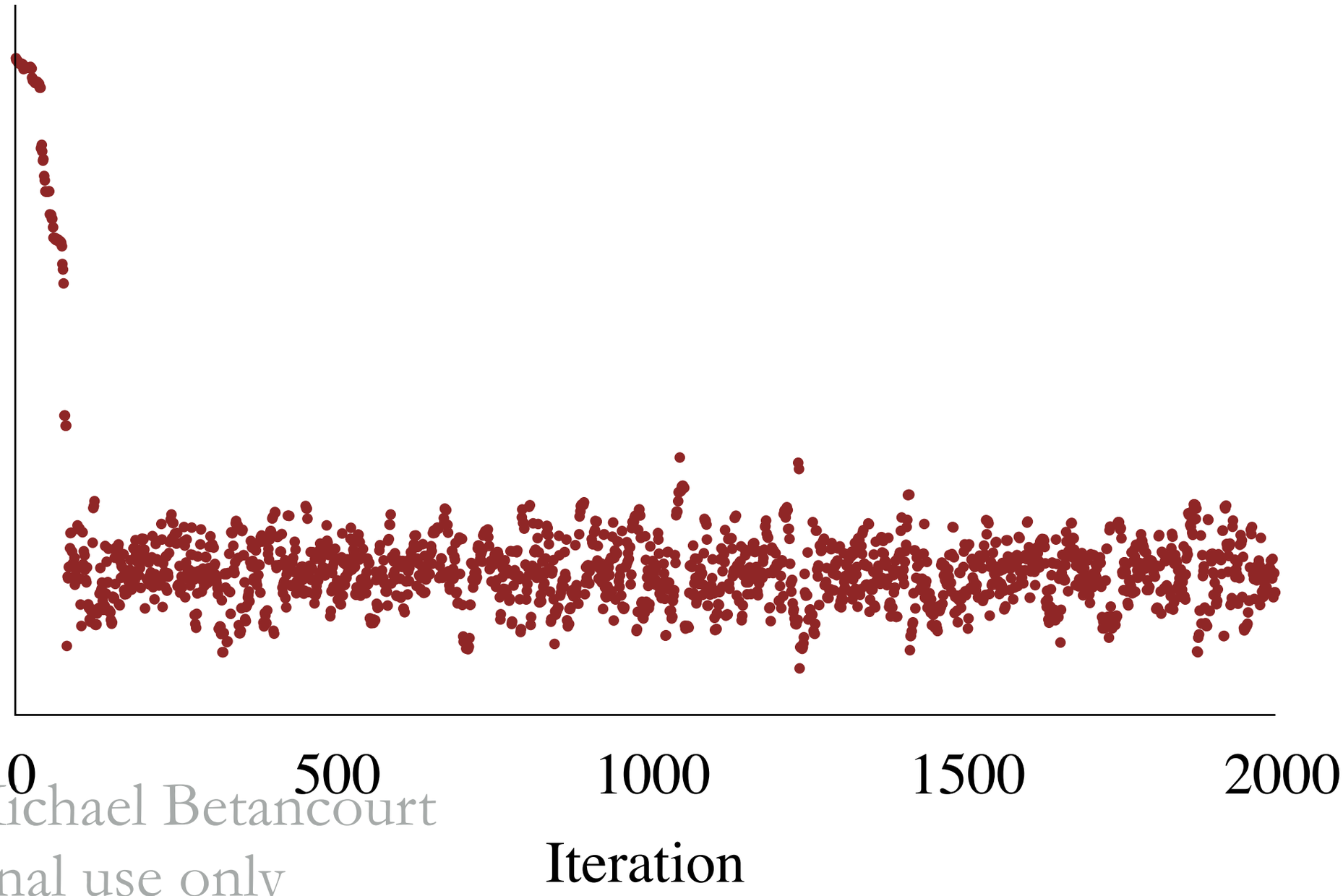
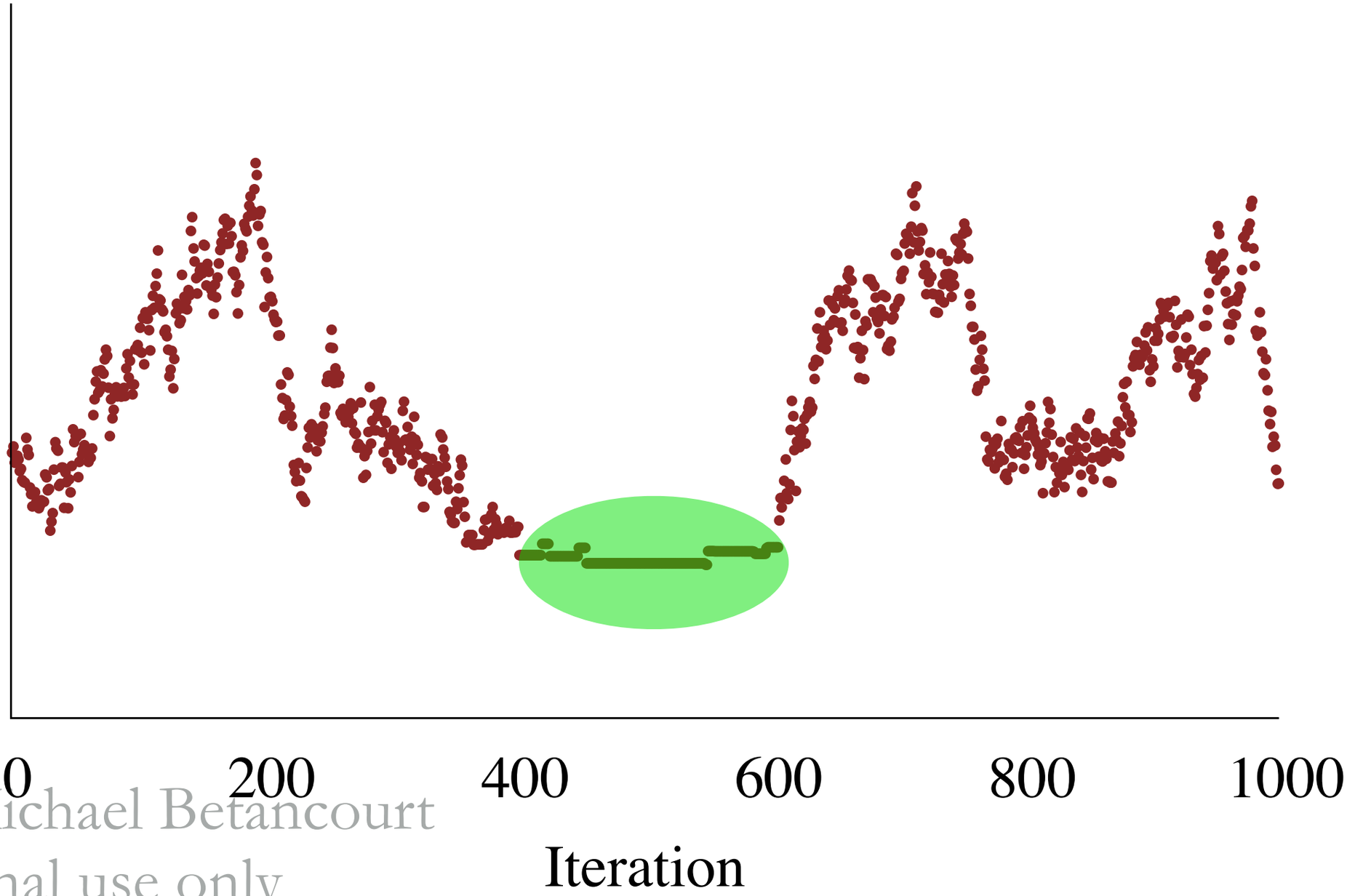
Often our best strategy is to empirically identify *obstructions* to geometric ergodicity.

$$\hat{f} \sim \mathcal{N}(\mathbb{E}[f], \text{MCMC-SE}[f])$$

Visual diagnostics from *trace plots* is one immediate option for identify obstructive behavior.



For example, we might identify regions of high curvature where Markov chain stick.



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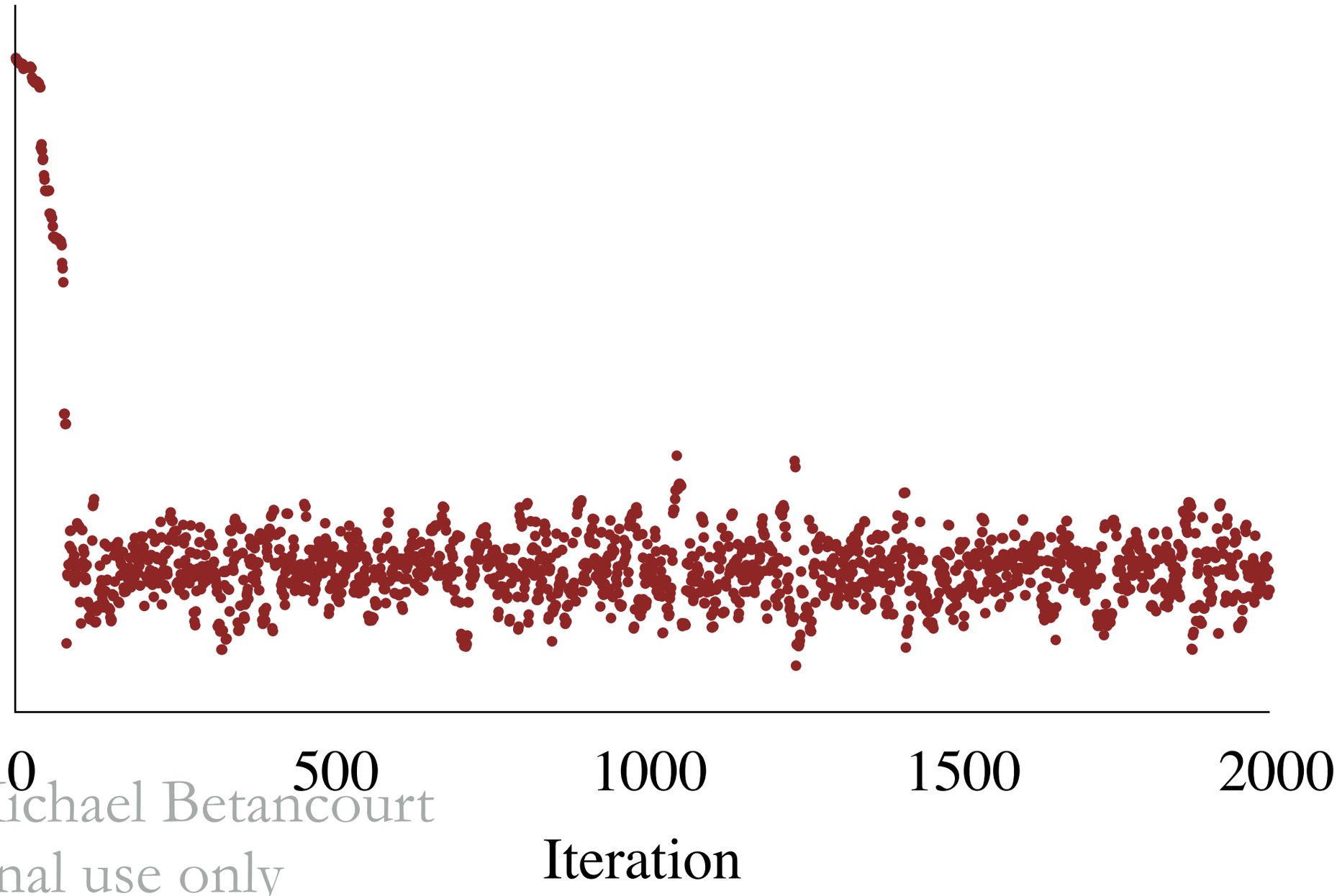

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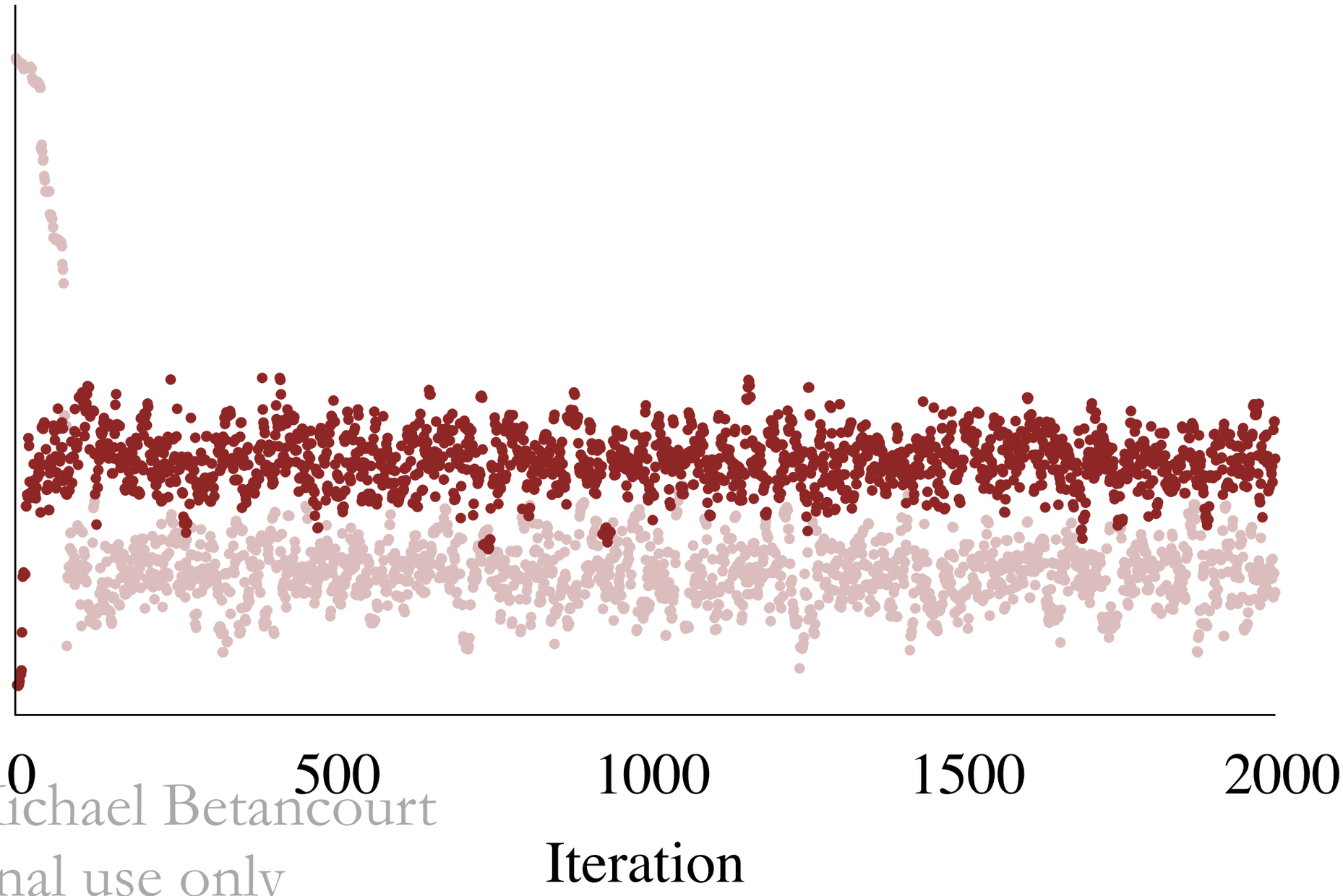

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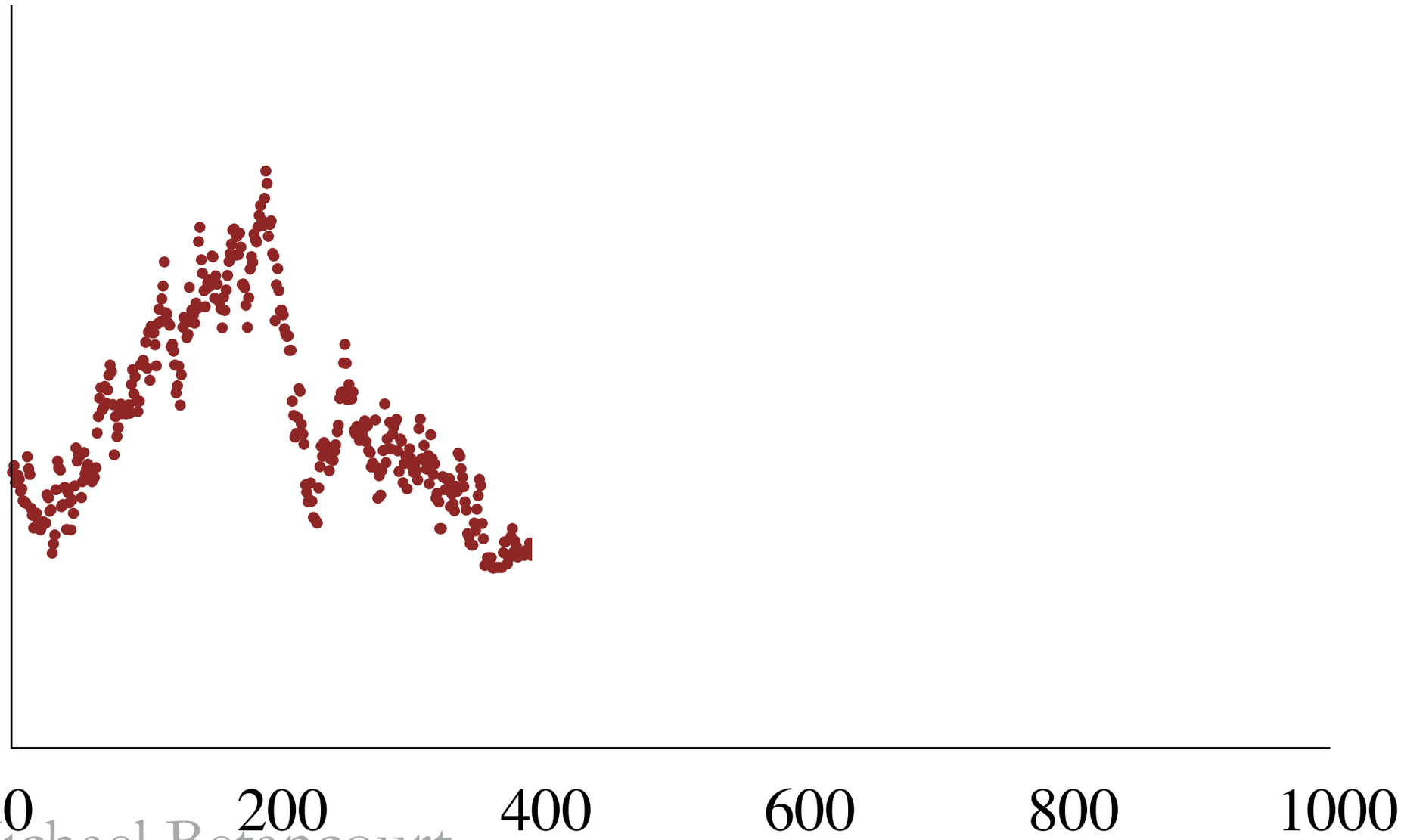

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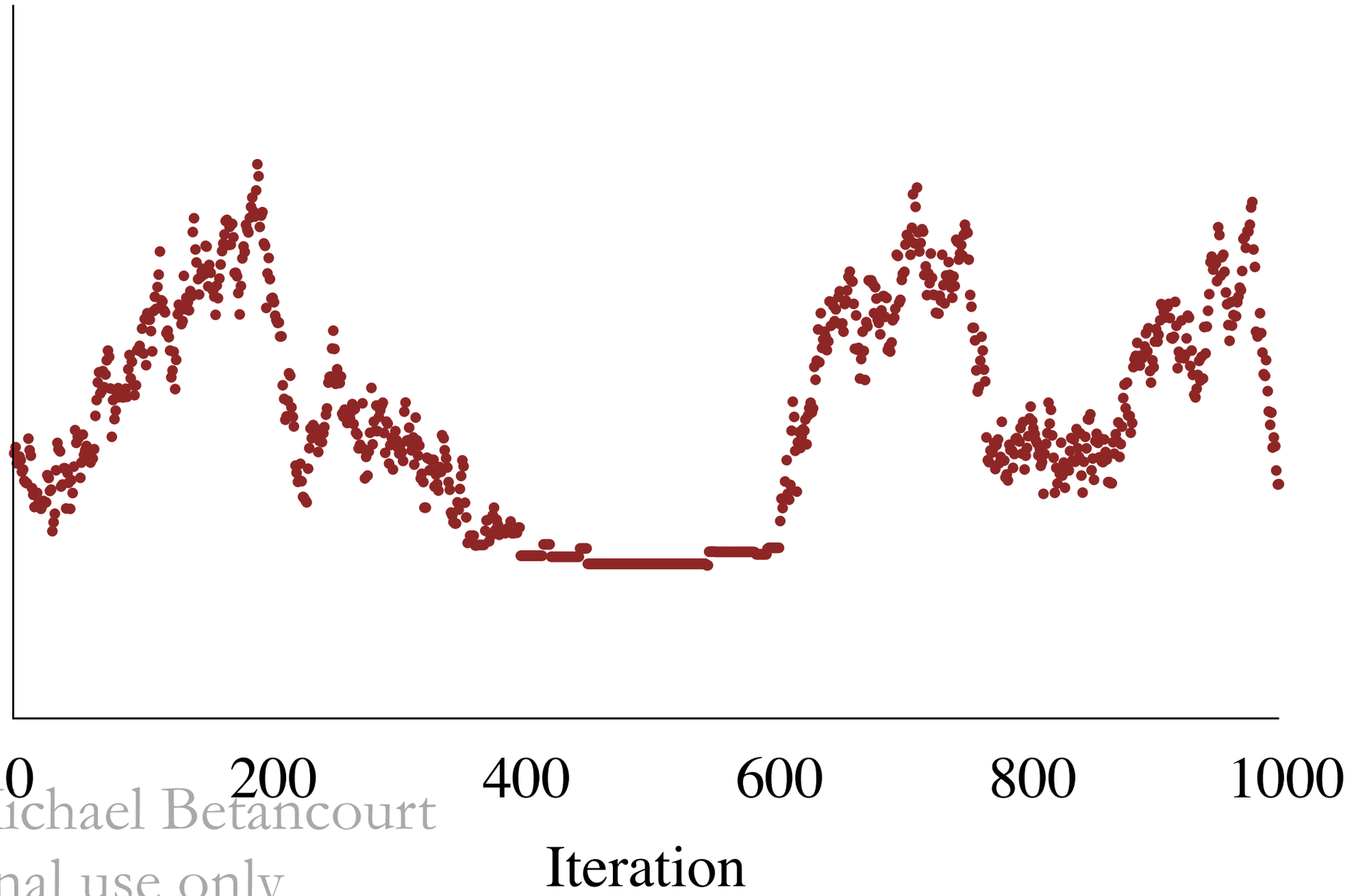
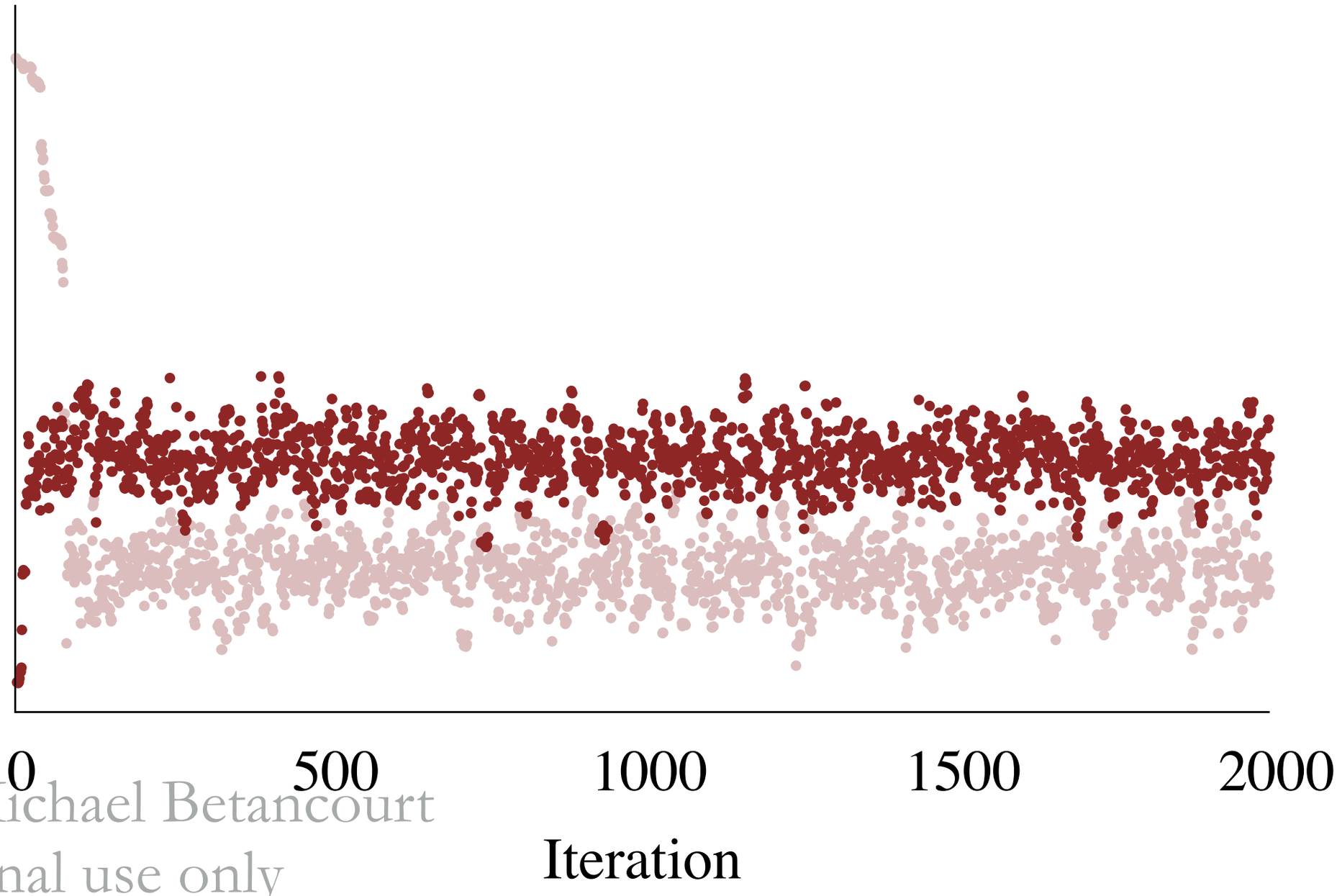


A more robust strategy runs *multiple* chains from *diffuse* initial states and compares the expectations to each other.



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$$\hat{R}[f] = \sqrt{\frac{N-1}{N} + \frac{1}{N} \frac{\hat{B}[f]}{\hat{W}[f]}}$$

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Improved Rhat

In practice one should first verify that there are no identifiable obstructions to geometric ergodicity.

```
Inference for Stan model: example_model
1 chains: each with iter=(1000); warmup=(0); thin=(1); 1000 iterations saved.

Warmup took (0.034) seconds, 0.034 seconds total
Sampling took (0.039) seconds, 0.039 seconds total
```

	Mean	MCSE	StdDev	5%	50%	95%	N_Eff	N_Eff/s	R_hat
lp__	5.0	5.7e-02	9.6e-01	3.1	5.2	5.9	287	7431	1.0
accept_stat__	0.93	2.7e-03	8.6e-02	0.76	0.96	1.0	1000	25869	1.0
stepsize__	0.78	3.1e-15	2.2e-15	0.78	0.78	0.78	0.50	13	1.0
treedepth__	2.0	2.0e-02	5.7e-01	1.0	2.0	3.0	778	20124	1.0
n_leapfrog__	3.4	5.8e-02	1.8e+00	1.0	3.0	7.0	950	24588	1.0
divergent__	0.00	0.0e+00	0.0e+00	0.00	0.00	0.00	1000	25869	1.0
theta	20	4.3e-02	1.0e+00	18	20	22	568	14697	1.0

If there are no diagnostic failures then we can proceed to computing MCMC estimators.

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And finally the MCMC estimator standard errors.

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Finally, we can construct an MCMC estimator of any pertinent function as well as an estimate of its error.

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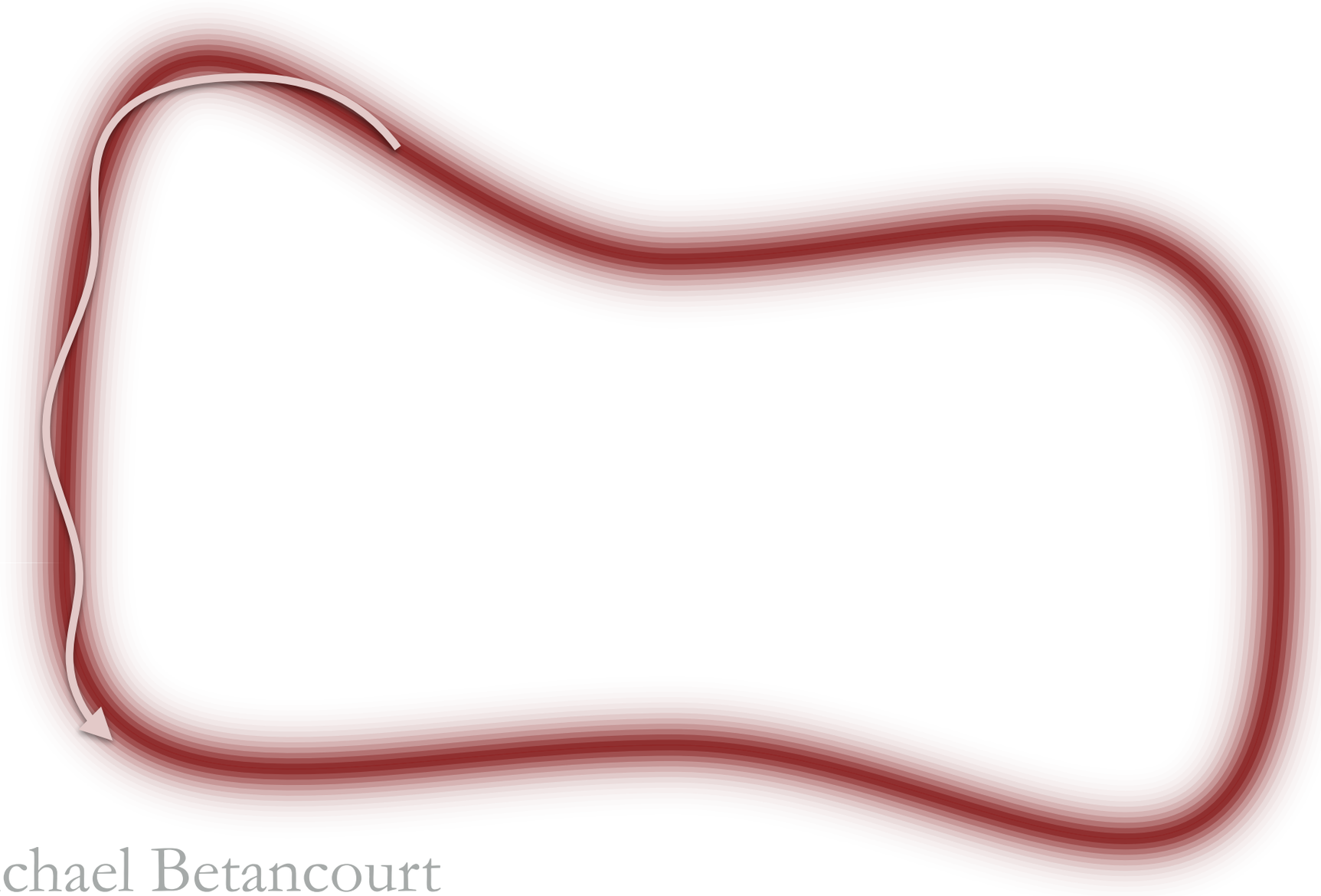
Hamiltonian Monte Carlo



The previous discussion presumed the existence of a Markov chain that targets our specific posterior.

$$\pi_S(\theta \mid \tilde{y}) = \int \mathrm{d}\theta' \, \pi_S(\theta' \mid \tilde{y}) \, T(\theta \mid \theta')$$

To simplify notation let's generalize from a posterior distribution to an arbitrary target distribution.

$$\pi(q) = \int \mathrm{d}q' \, \pi(q') \, T(q \mid q')$$

How exactly can we design a Markov transition that preserves a given target distribution?

$$\pi(q) = \int \mathrm{d}q' \, \pi(q') \, T(q \mid q')$$

One way to construct a chain is Random Walk Metropolis which explores the posterior with a "guided" diffusion.

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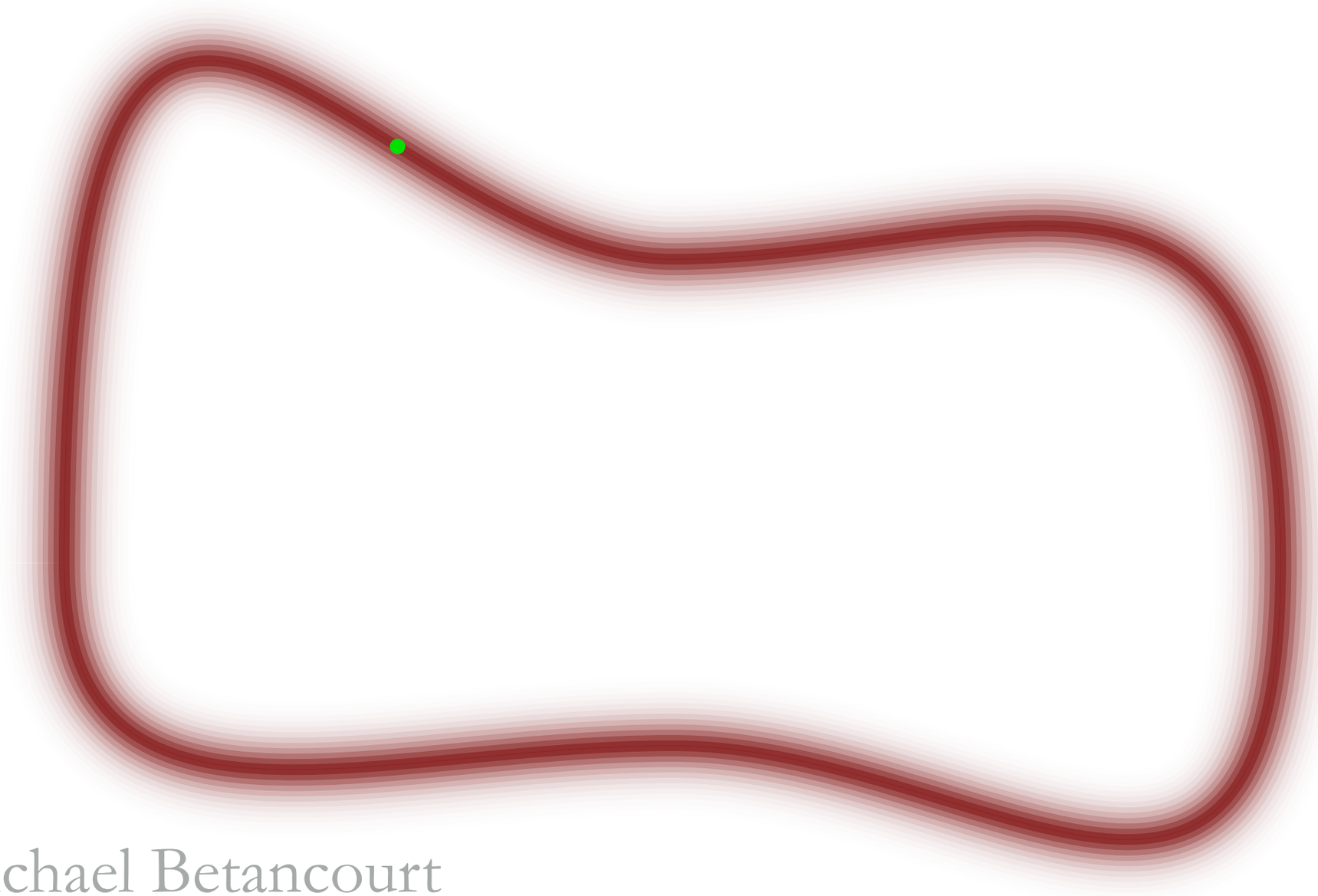

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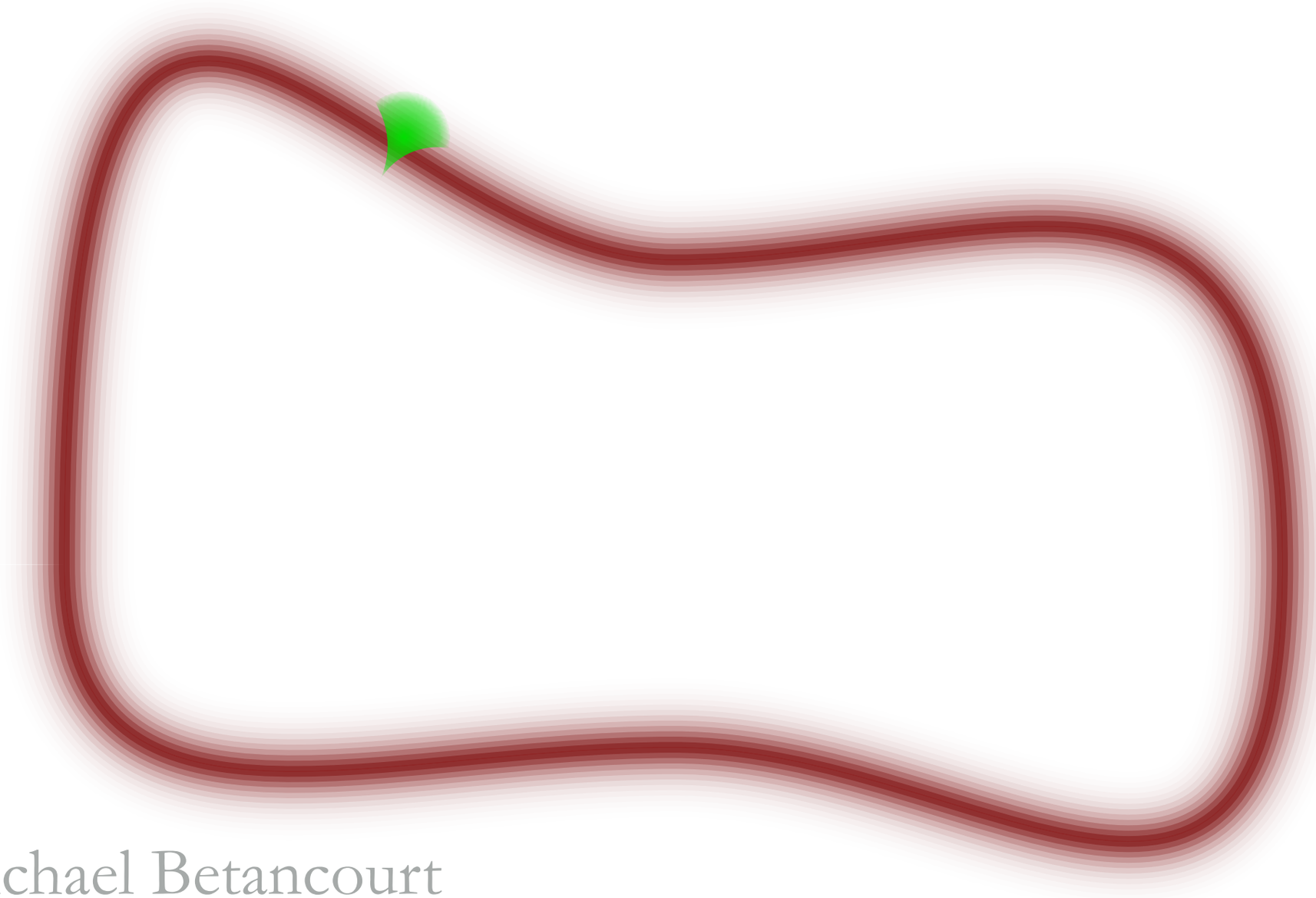

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