GPU-native nested sampling in BlackJAX

For simulation-based inference at scale

Will Handley
<wh260@cam.ac.uk>

Royal Society University Research Fellow
Institute of Astronomy, University of Cambridge
Kavli Institute for Cosmology, Cambridge
Gonville & Caius College
willhandley.co.uk/talks

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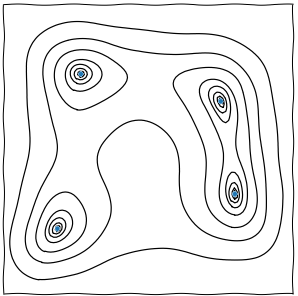
UNIVERSITY OF CAMBRIDGE


What is Nested Sampling?

- Nested sampling is a radical, multi-purpose numerical tool.
- Given a (scalar) function f with a vector of parameters θ, it can be used for:

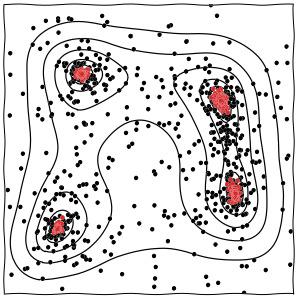
Optimisation

$$\theta_{\max} = \max_{\theta} f(\theta)$$



Exploration

draw/sample $\theta \sim f$

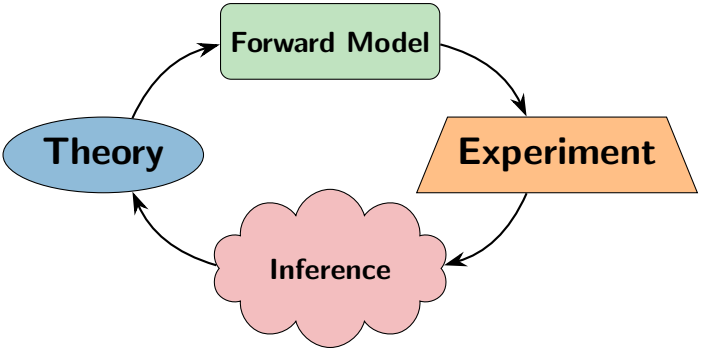


Integration

$$\int f(\theta) dV$$

Why nested sampling for SBI?

- Other than NPE, all SBI methods (NLE, NRE, NJE etc) need a sampler
- Most existing samplers are limited:
  - **Legacy implementations**: MultiNest, PolyChord (Fortran)
  - **Slow Python codes**: dynesty, ultranest, nautilus
- BlackJAX solution:
  - GPU-native implementation
  - Open source & community-driven
  - Dissociated from original authors



The GPU imperative

- The future is GPU, whether we like it or not:
  - All future HPC heavily weighted toward GPUs
  - Driven by machine learning adoption
- JAX does two *separate* things:
  1. **Automatic differentiation**
  2. **Just-in-time compilation** for GPUs
- People often conflate these - they are separate and glorious!
- Alternative tools (harmonic, floz) get strength from GPU, not sampling method

GPU ecosystem growth

CMB	`cosmopower`, `candl`
SNe	`BayesSN`
GW	`ripple`, `jim`
EP	`ExoJAX`

[github:JAXtronomy]

BlackJAX nested sampling

David Yallup
PDRA

- Very recent development (December 2024!)
- GPU-native nested slice sampler
- Modern alternative to MultiNest/PolyChord
- Slice sampling with adaptive live point allocation
- Compatible with existing BlackJAX ecosystem

Learn more

- Theory: `handley-lab.co.uk/nested-sampling-book`
- Implementation: David Yallup's PDRA work
- Workshop: Hands-on tutorial today

Installation

```
pip install git+https://github.com/handley-lab/blackjax
```

AI-enabled research workflows

- Modern scientific computing benefits from AI integration:
  - GPU-accelerated inference
  - Neural networks in SBI methods
  - Automatic differentiation for sampling
- But the real coming disruption is from using AI to do day-to-day scientific tasks.
  - I wrote this talk with AI assistance [claude code]. This morning.
  - I have written and been awarded several grants that were majority written by AI.
  - My most recent papers are drafted with AI.

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Workshop goals

- Today we'll explore:
  1. Running nested sampling with BlackJAX
  2. Visualization with Anesthetic
  3. Performance comparison: nested sampling vs AIES
  4. Integration with your JAX workflows
- Hands-on notebook environment
- Google Colab compatible
- Build on Viraj's JAX/SciML workshop

Links

- BlackJAX: [github:handley-lab/blackjax]
- Anesthetic: `anesthetic.readthedocs.io`
- Workshop materials: [github:handley-lab]

Performance promise

Compare BlackJAX nested sampling performance with traditional tools and see the GPU advantage firsthand!

Conclusions
[github:handley-lab]

- **Nested sampling is essential** for most SBI methods (except NPE)
- **BlackJAX** provides GPU-native, community-driven implementation
- **JAX's dual power**: autodiff + JIT compilation for unprecedented performance
- **The future is GPU-accelerated** scientific computing with AI integration

Integration in Physics

- Integration is a fundamental concept in physics, statistics and data science:

Partition functions

$$Z(\beta) = \int e^{-\beta H(q,p)} dq dp$$

Path integrals

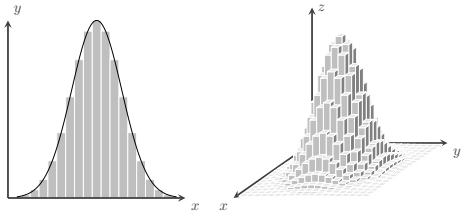
$$\Psi = \int e^{iS} \mathcal{D}x$$

Bayesian marginals

$$\mathcal{Z}(D) = \int \mathcal{L}(D|\theta)\pi(\theta) d\theta$$

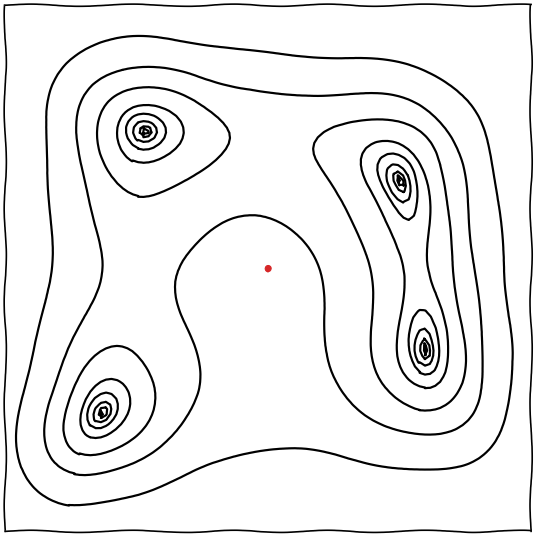
- Need numerical tools if analytic solution unavailable.
- High-dimensional numerical integration is hard.
- Riemannian strategy estimates volumes geometrically:

$$\int f(x) d^n x \approx \sum_i f(x_i) \Delta V_i \sim \mathcal{O}(e^n)$$



- Curse of dimensionality $\Rightarrow$ exponential scaling.

MCMC



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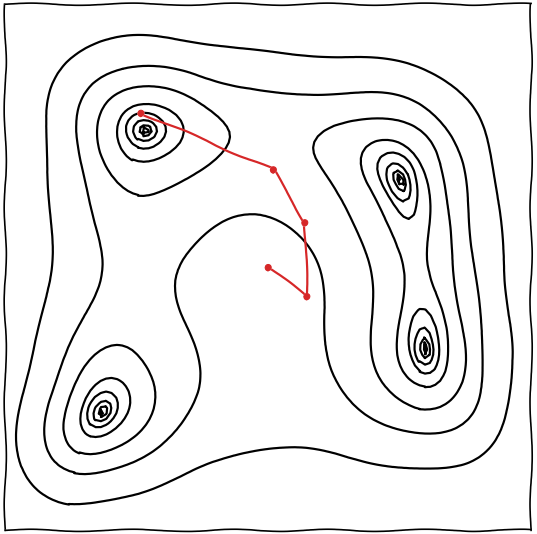

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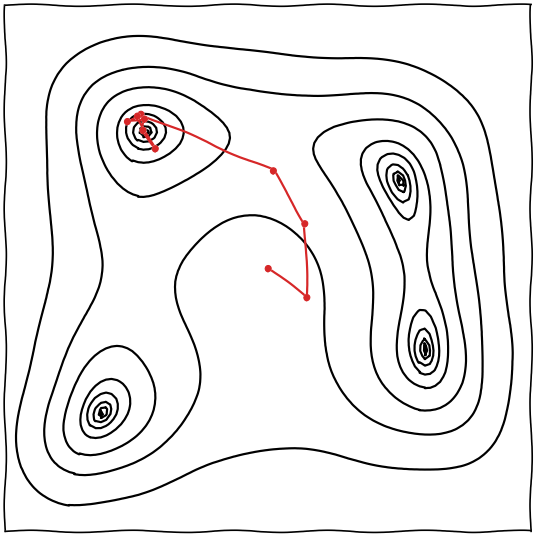

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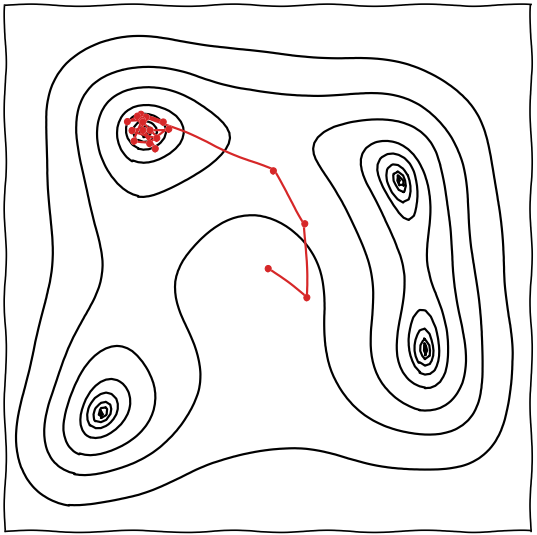

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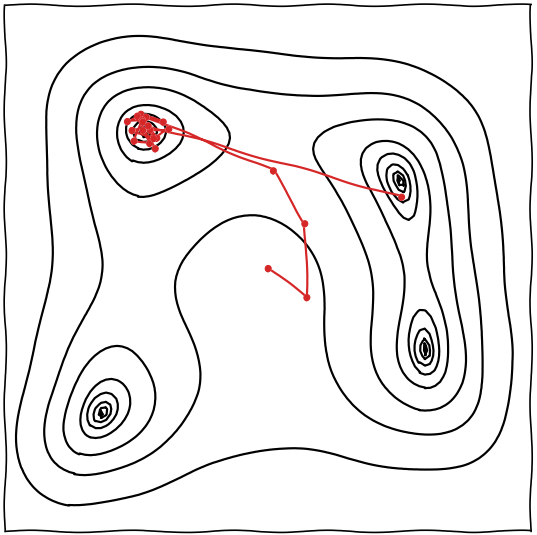

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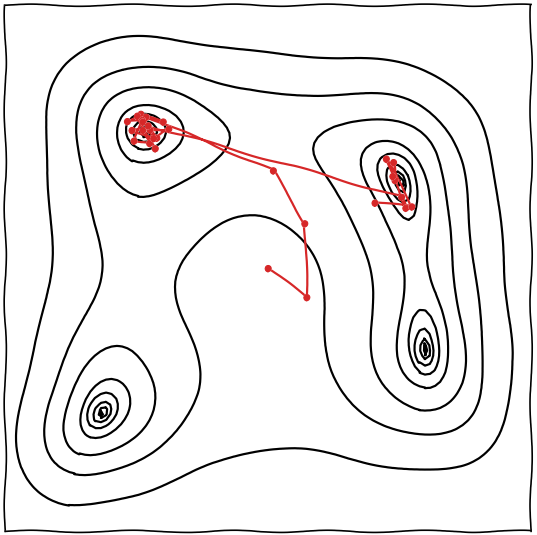

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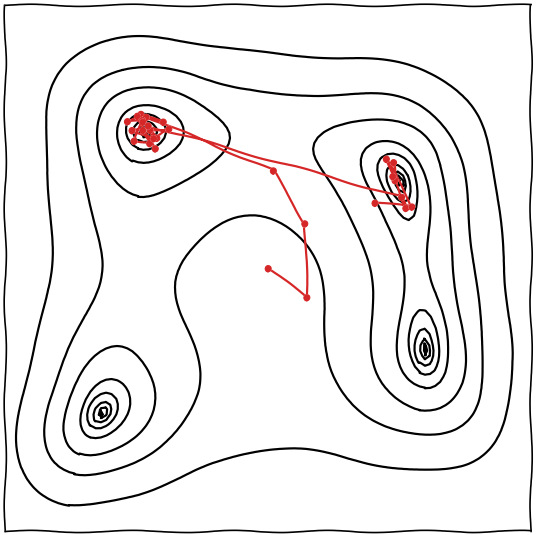

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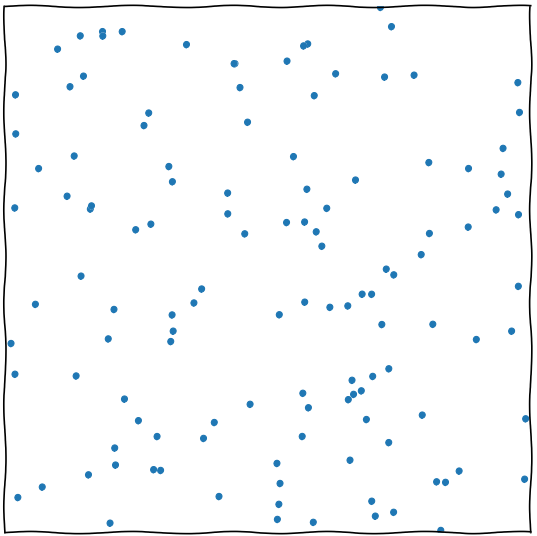

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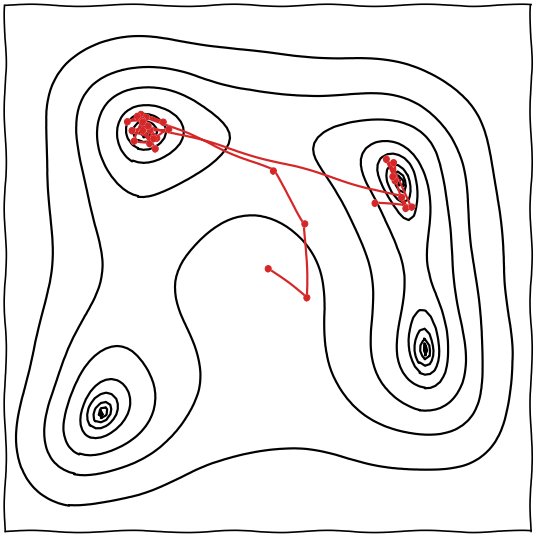

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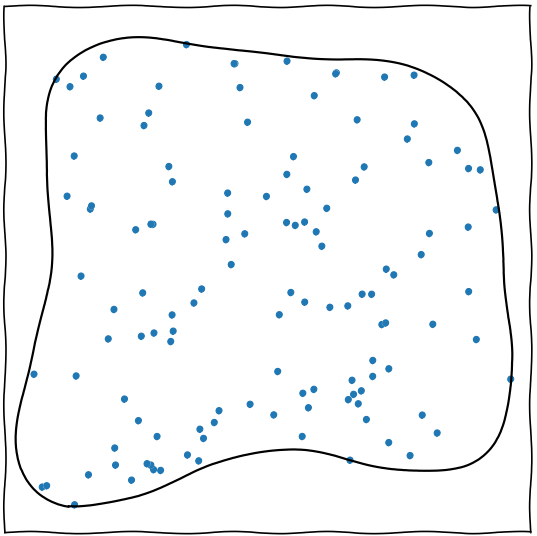

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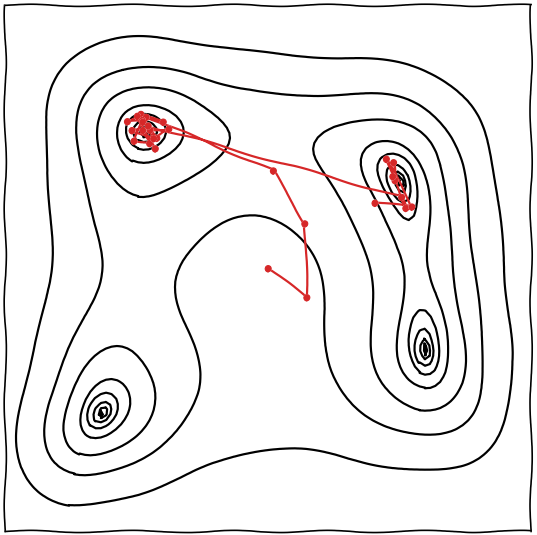

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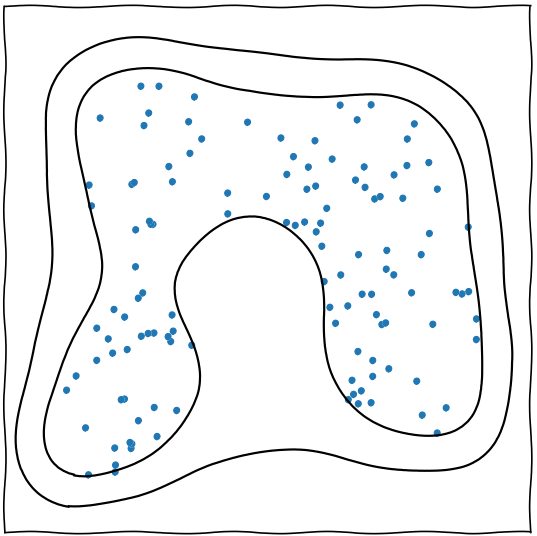

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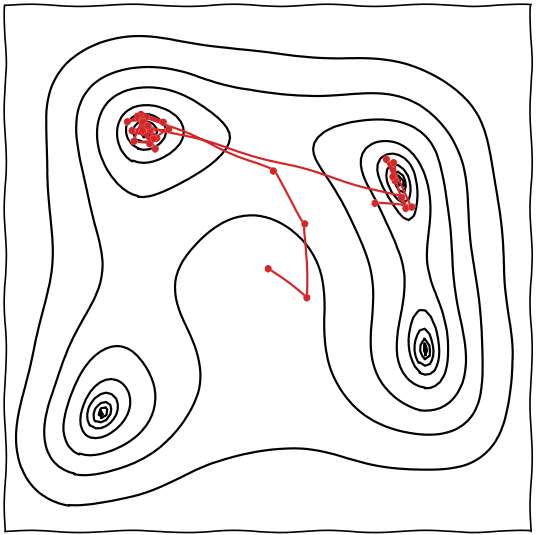

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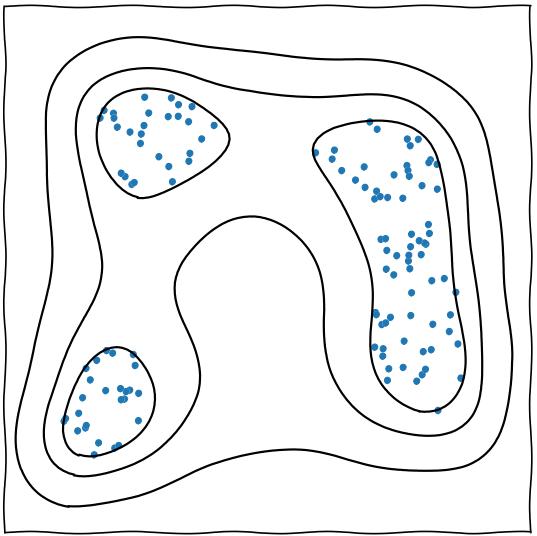

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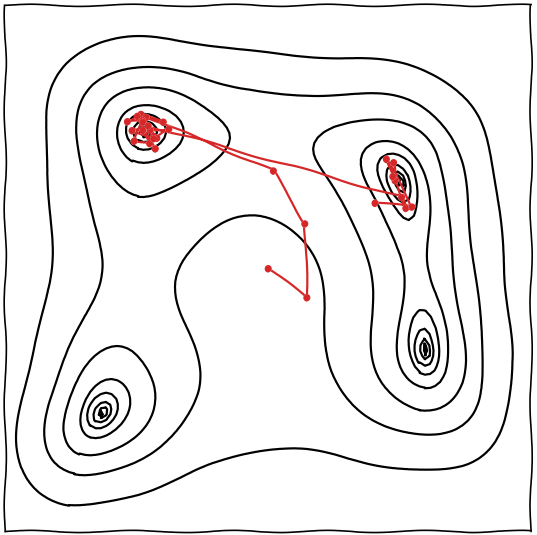

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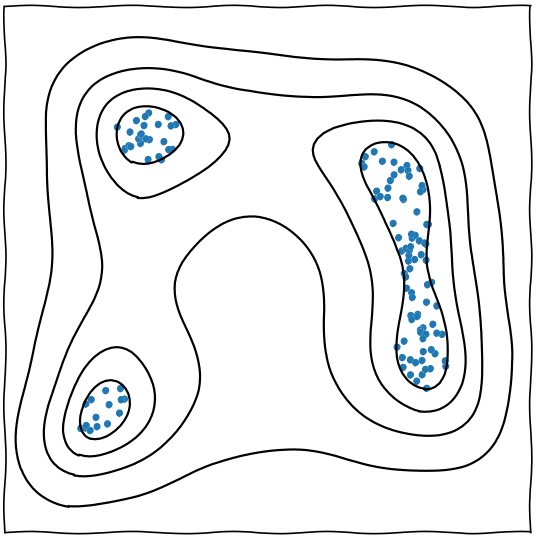

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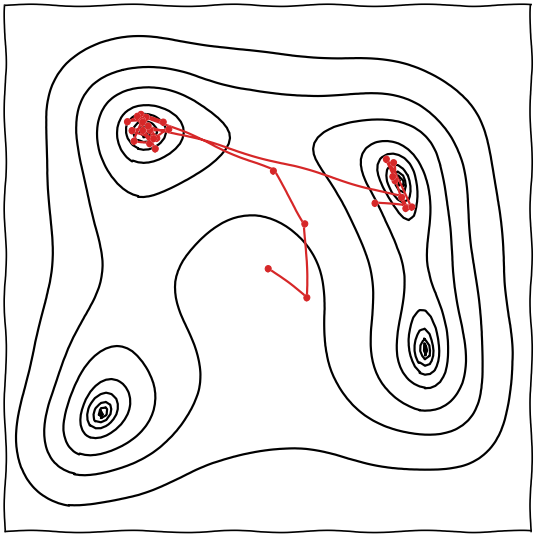

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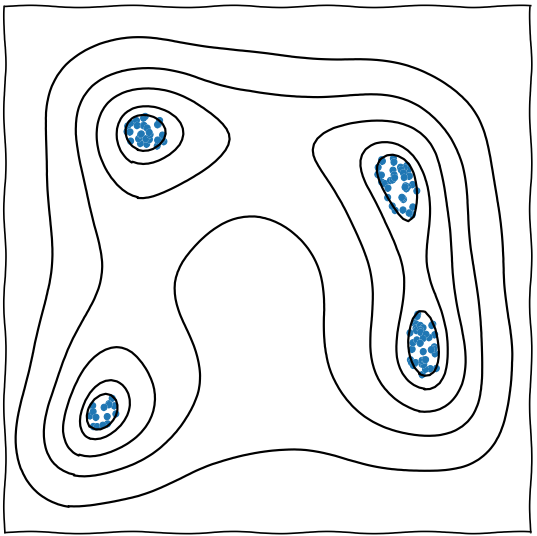

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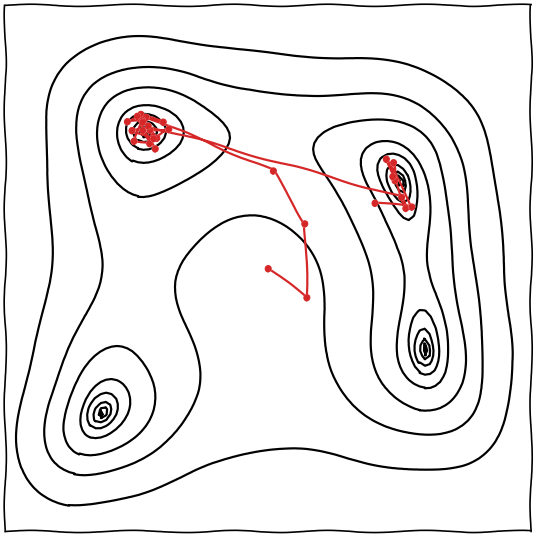

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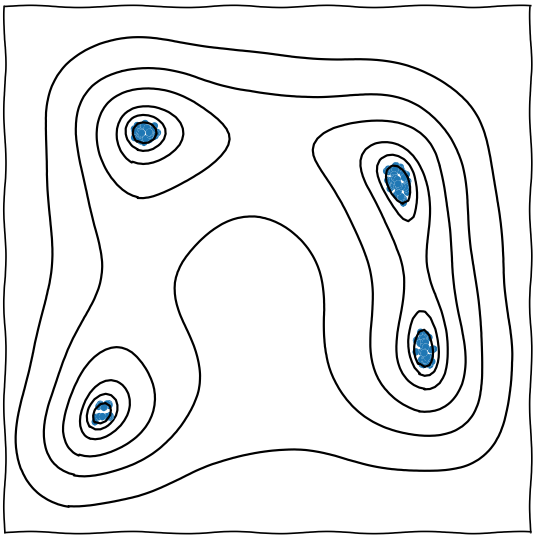

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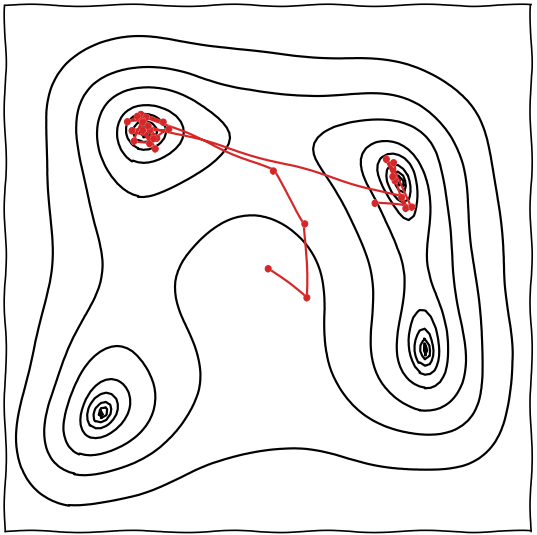

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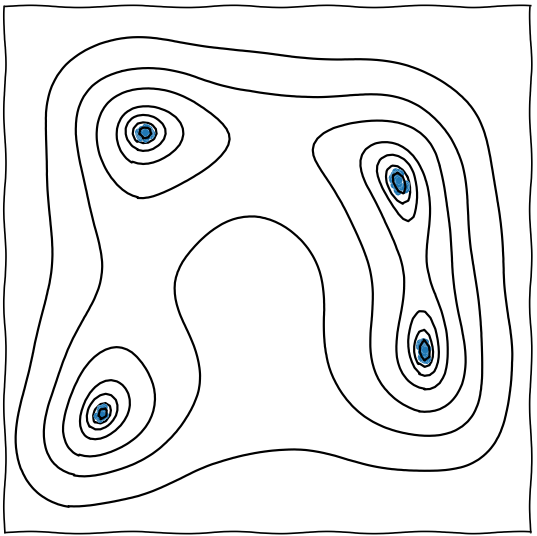

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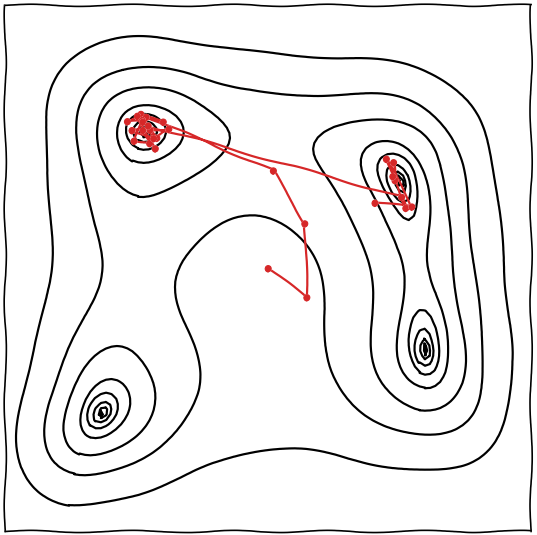

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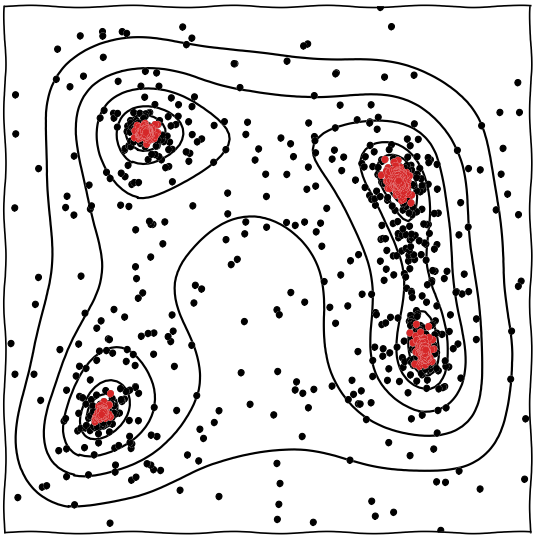
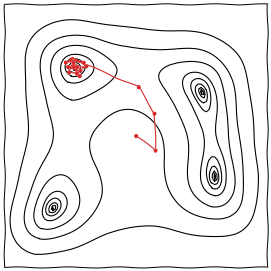


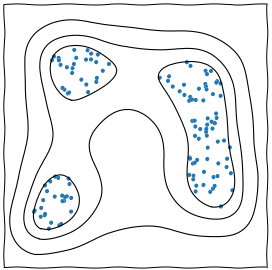
MCMC

- Single "walker"
- Explores posterior
- Fast, if proposal matrix is tuned
- Parameter estimation, suspiciousness calculation
- Channel capacity optimised for generating posterior samples



Nested sampling

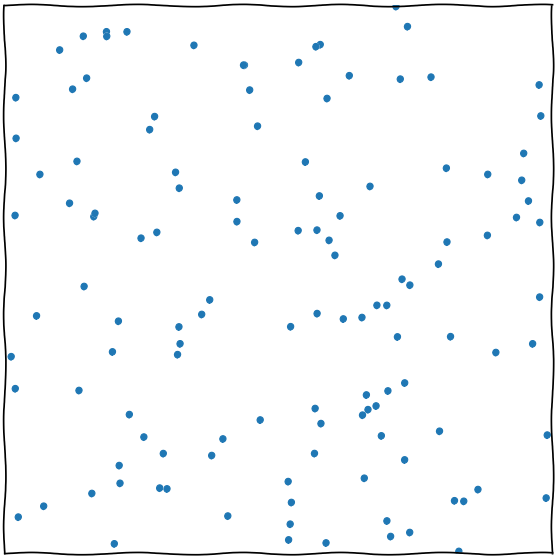
- Ensemble of "live points"
- Scans from prior to peak of likelihood
- Slower, no tuning required
- Parameter estimation, model comparison, tension quantification
- Channel capacity optimised for computing partition function



The nested sampling meta-algorithm: live points

- Start with n random samples over the space.
- Delete outermost sample, and replace with a new random one at higher integrand value.
- The "live points" steadily contract around the peak(s) of the function.
- We can use this evolution to estimate volume *probabilistically*.
- At each iteration, the contours contract by $\sim \frac{1}{n}$ of their volume.
- This is an exponential contraction, so

$$\int f(x)dV \approx \sum_i f(x_i)\Delta V_i, \quad V_i = V_0 e^{-i/n}$$



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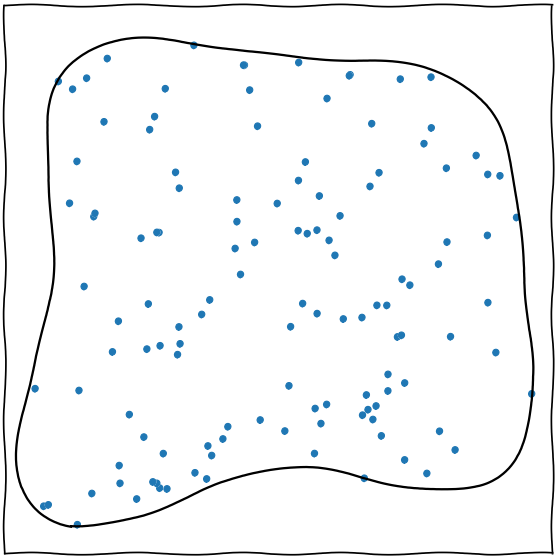

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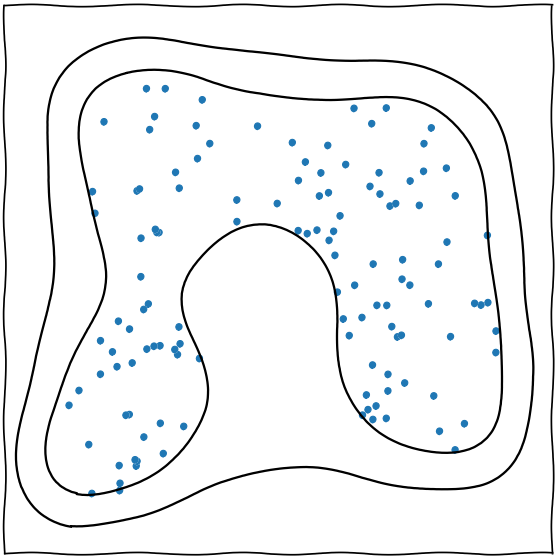

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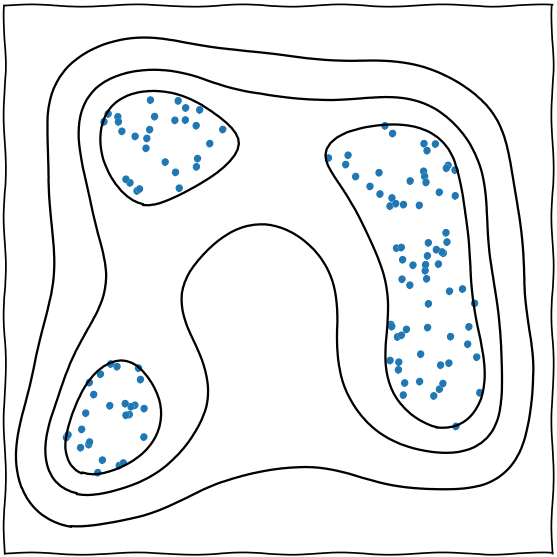

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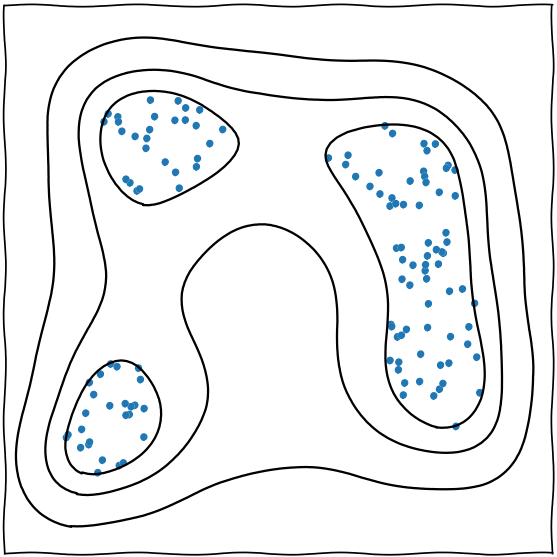

Types of nested sampler

- Broadly, most nested samplers can be split into how they create new live points.
- i.e. how they sample from the hard likelihood constraint $\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$.

Rejection samplers

- e.g. `MultiNest`, `UltraNest`.
- Constructs bounding region and draws many invalid points until $\mathcal{L}(\theta) > \mathcal{L}_*$.
- Efficient in low dimensions, exponentially inefficient $\sim \mathcal{O}(e^{d/d_0})$ in high $d > d_0 \sim 10$.

Chain-based samplers

- e.g. `PolyChord`, `ProxNest`.
- Run Markov chain starting at a live point, generating many valid (correlated) points.
- Linear $\sim \mathcal{O}(d)$ penalty in decorrelating new live point from the original seed point.

- Nested samplers usually come with:
  - *resolution* parameter n_{live} (which improve results as $\sim \mathcal{O}(n_{\text{live}}^{-1/2})$).
  - set of *reliability* parameters, which don't improve results if set arbitrarily high, but introduce systematic errors if set too low.
  - e.g. `Multinest` efficiency `eff` or `PolyChord` chain length n_{repeats}.