

GPU Accelerated Nested Sampling

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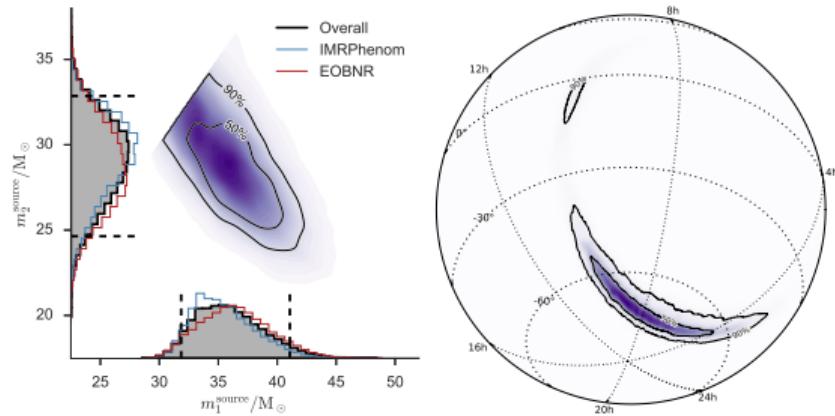
A Case Study in Astrostatistics

The Challenge: GW170817

- ▶ **Gravitational wave detected:** Binary neutron star merger
- ▶ **Real-time parameter estimation:** 15+ dimensional space
- ▶ **Sky localization:** $\sim 30 \text{ deg}^2$ uncertainty
- ▶ **EM counterpart follow-up:** Telescopes need targets within seconds to minutes

Statistical Requirements

- ▶ **Parameter estimation:** Masses, spins, distance, sky position
- ▶ **Model comparison:** Signal vs noise, waveform models



The Broader Astrostatistics Context

- ▶ **High-dimensional:** $d \sim 10^2\text{--}10^3$
- ▶ **Multimodal:** Competing physical models
- ▶ **Expensive likelihoods:** Complex sims
- ▶ **Model selection critical:** Which physics?

The Bayesian Inference Challenge

Parameter Estimation $P(\theta|D, M)$

- ▶ Posterior: $\mathcal{P}(\theta|D) \propto \mathcal{L}(D|\theta)\pi(\theta)$
- ▶ Need samples from $\mathcal{P}(\theta|D)$
- ▶ Standard approach: MCMC methods
- ▶ Well-solved problem in many cases

Model Comparison $P(M|D)$

- ▶ $\mathcal{Z} = \mathcal{P}(D|M) = \int \mathcal{L}(D|\theta)\pi(\theta)d\theta$
- ▶ Evidence/marginal likelihood/Bayes factor
- ▶ **Much harder to compute**
- ▶ MCMC doesn't estimate \mathcal{Z} directly

Challenges for Modern Science

- ▶ **High dimensions:** $d \sim 10^2 - 10^3$
- ▶ **Natural, relevant multimodality:** Multiple acceptable answers need investigation
- ▶ **Computational cost:** Complex forward models
- ▶ **Model selection:** Which physics to include?

Key Insight:

Need methods that compute *both* posterior samples *and* evidence

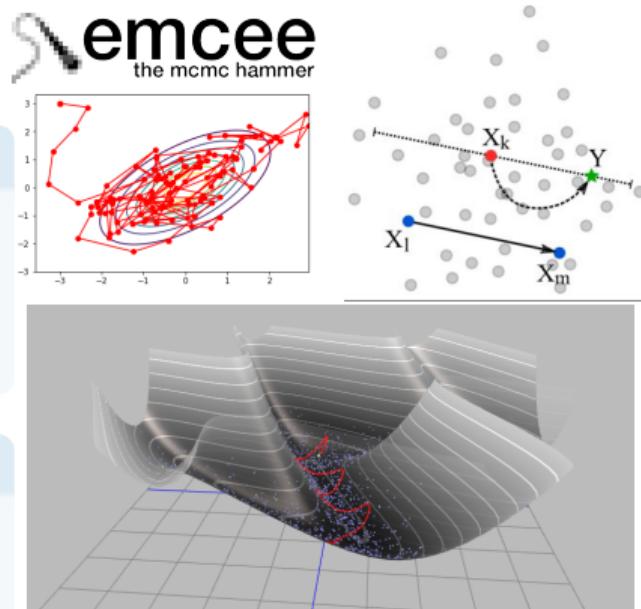
Sampling Methods for Bayesian Inference

Single-Chain MCMC

- ▶ **Metropolis-Hastings:** Simple, widely used (PyMC)
- ▶ **HMC/NUTS:** Gradient-based, efficient (Stan, BlackJAX)
- ▶ Fast for unimodal well-conditioned problems, no evidence

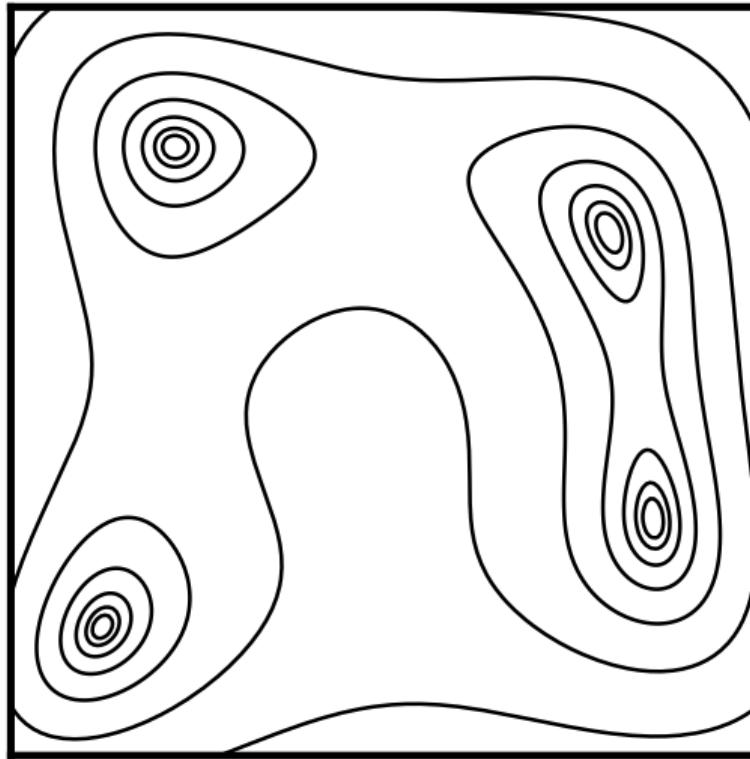
Ensemble Methods

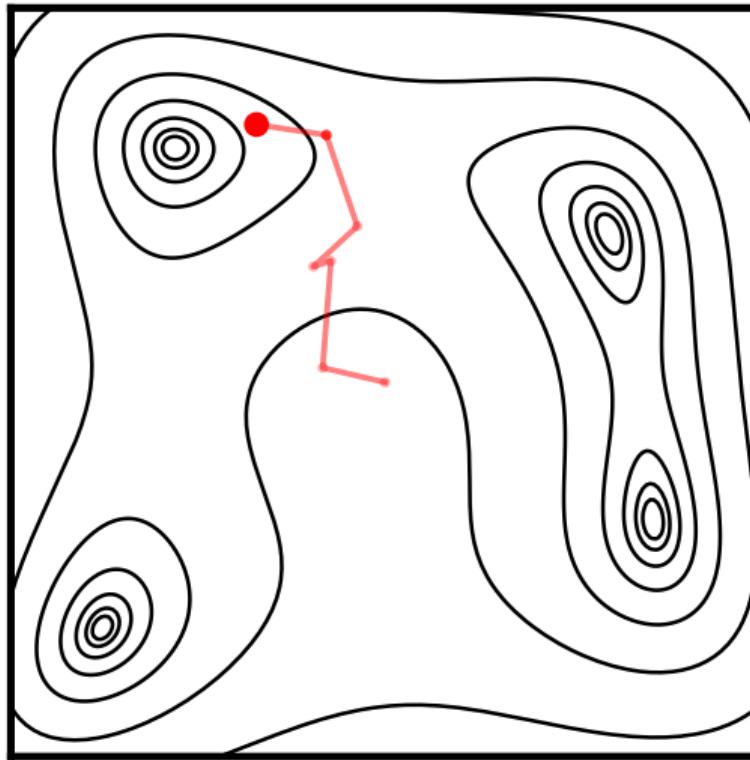
- ▶ **Affine-invariant:** emcee, zeus
- ▶ **Sequential Monte Carlo:** Tempering, annealing
- ▶ can struggle with multimodality, some estimate evidence

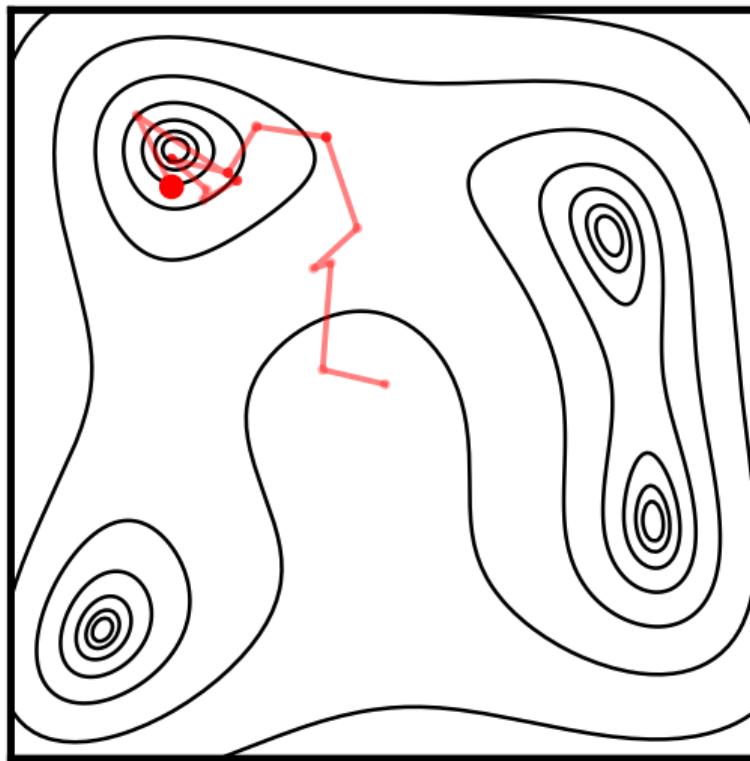


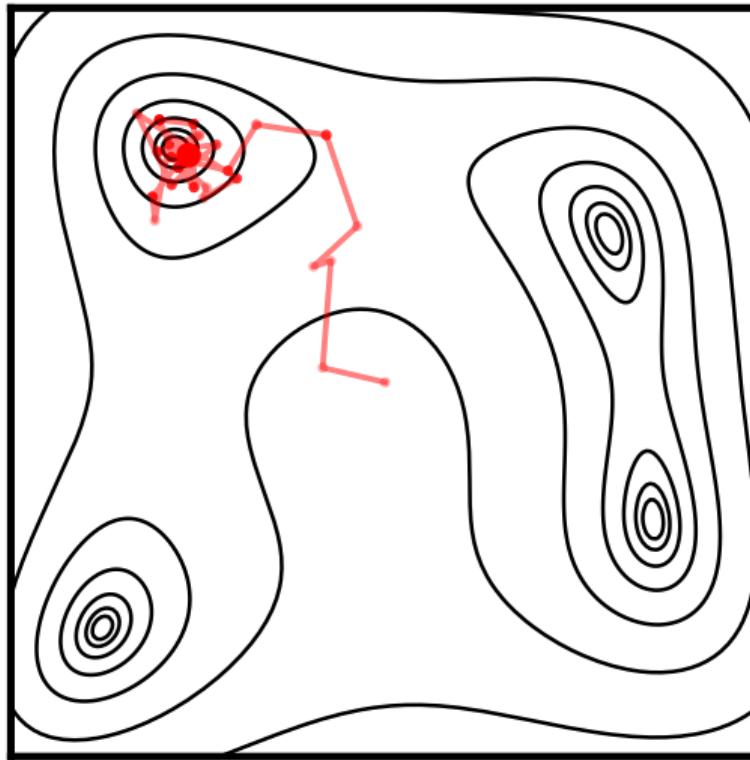
Nested sampling:

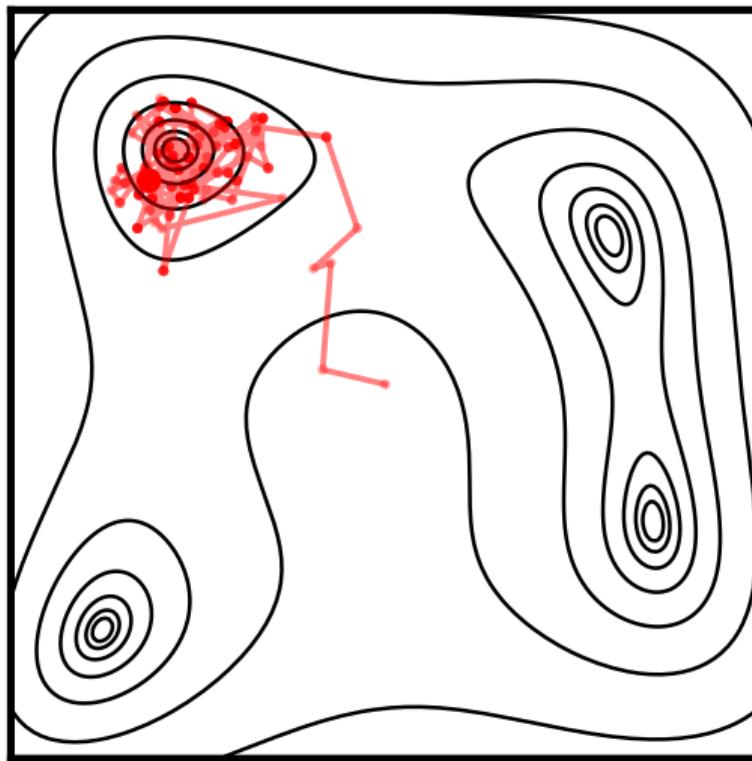
Unique in targeting evidence computation directly

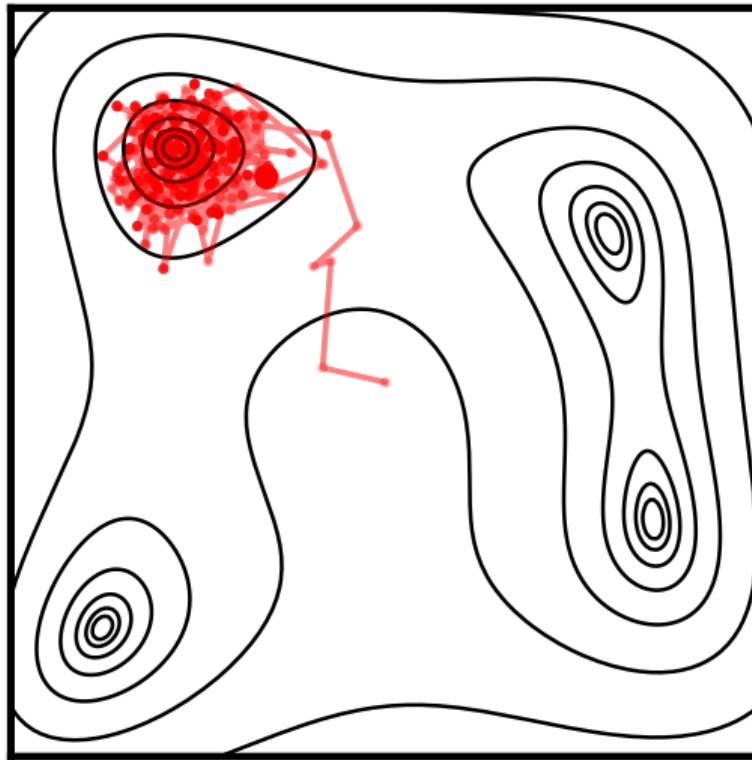




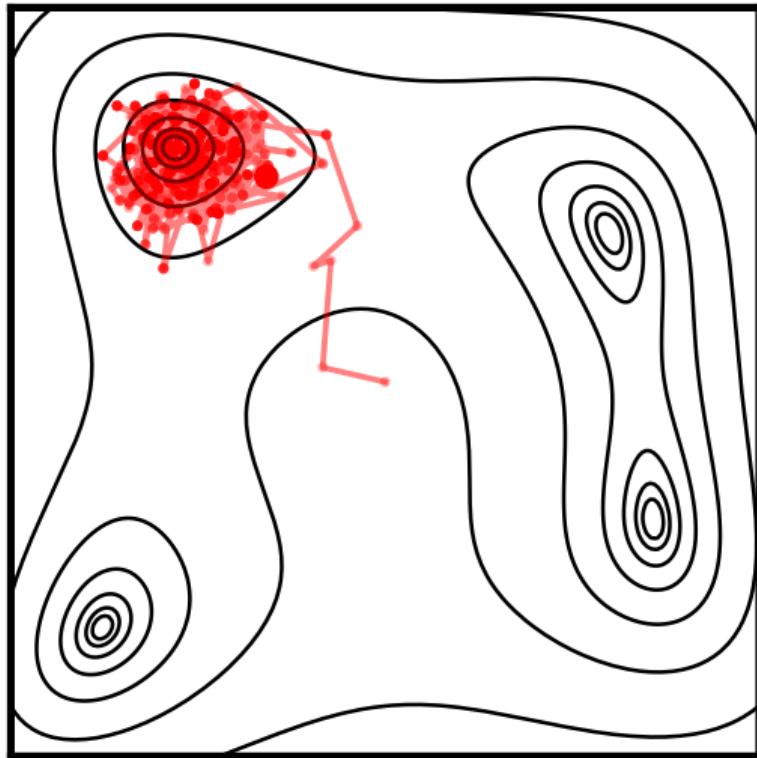




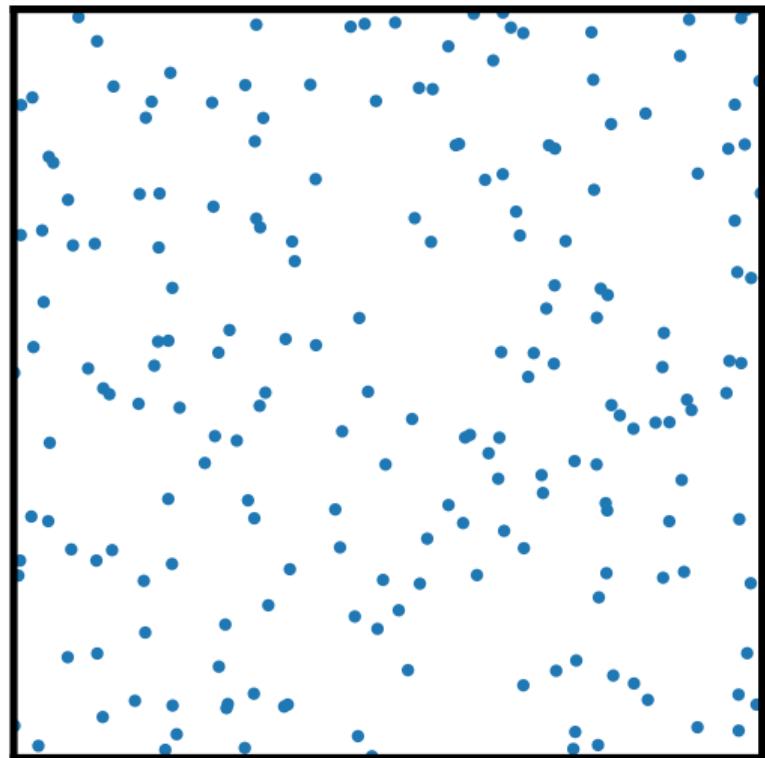




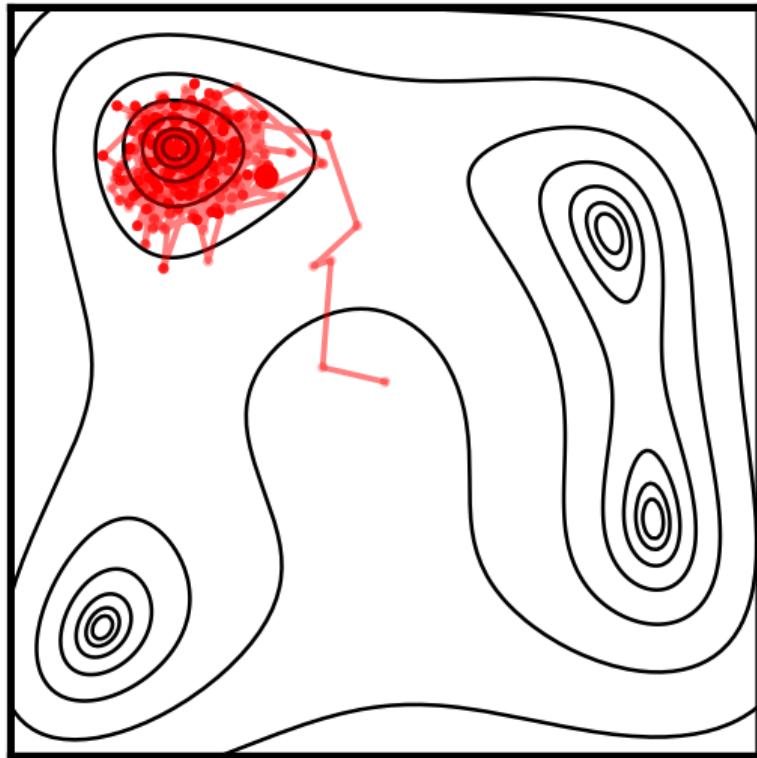
MCMC



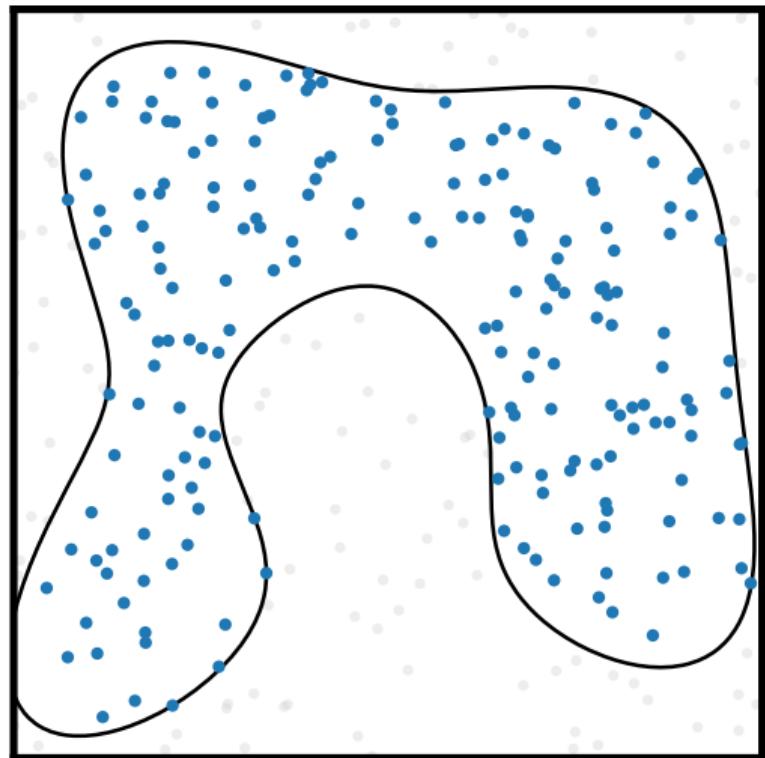
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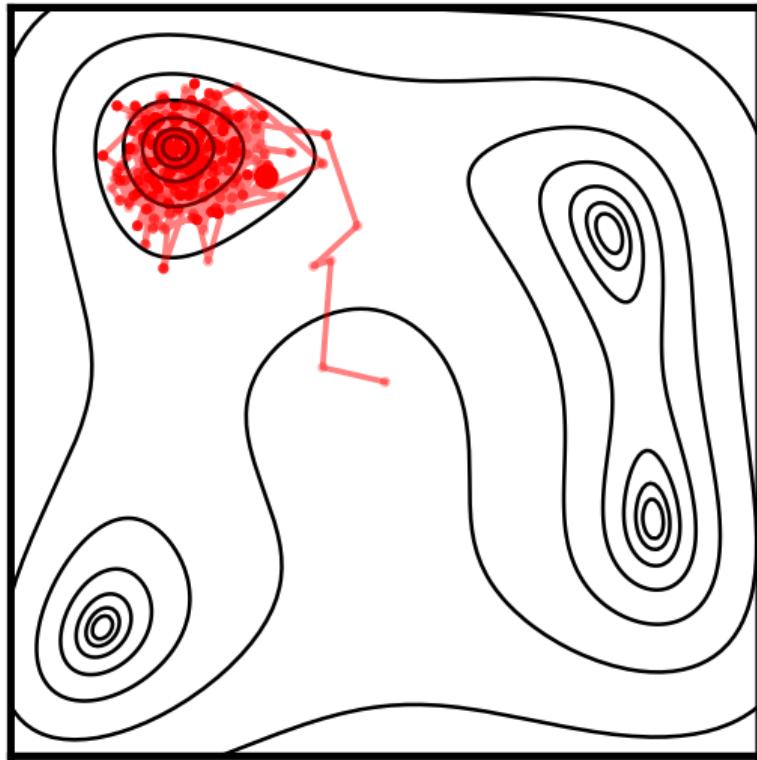
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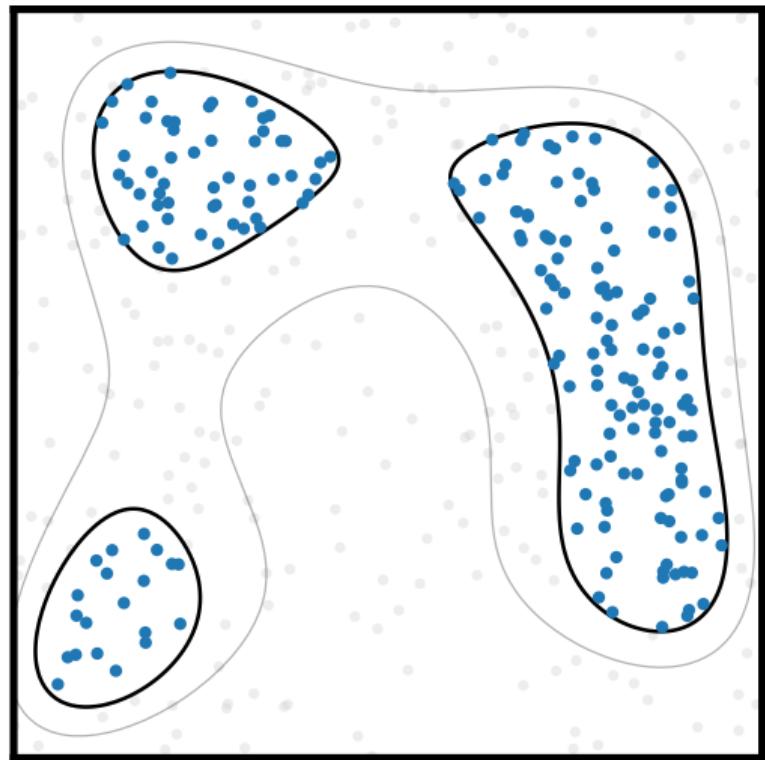
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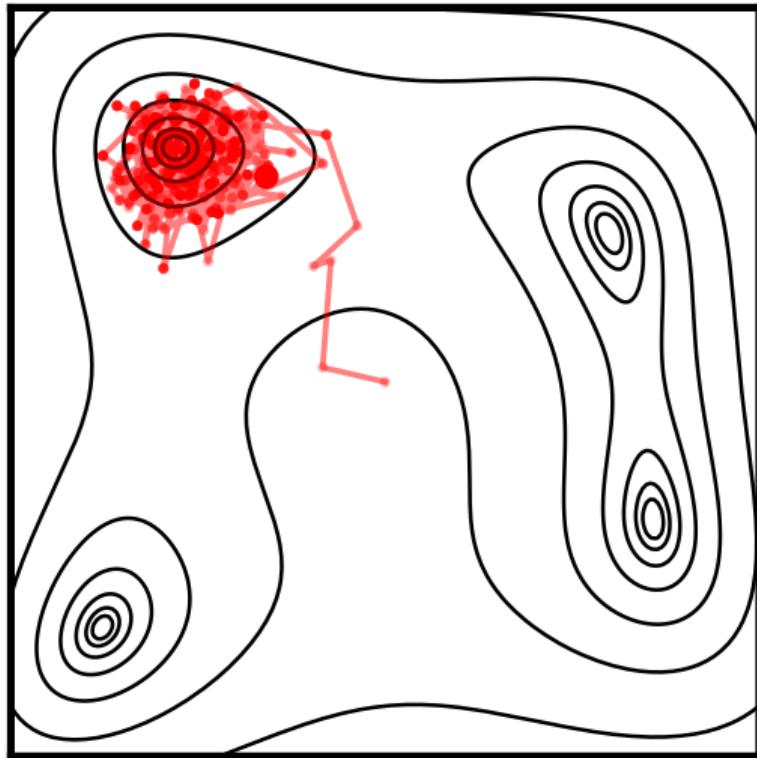
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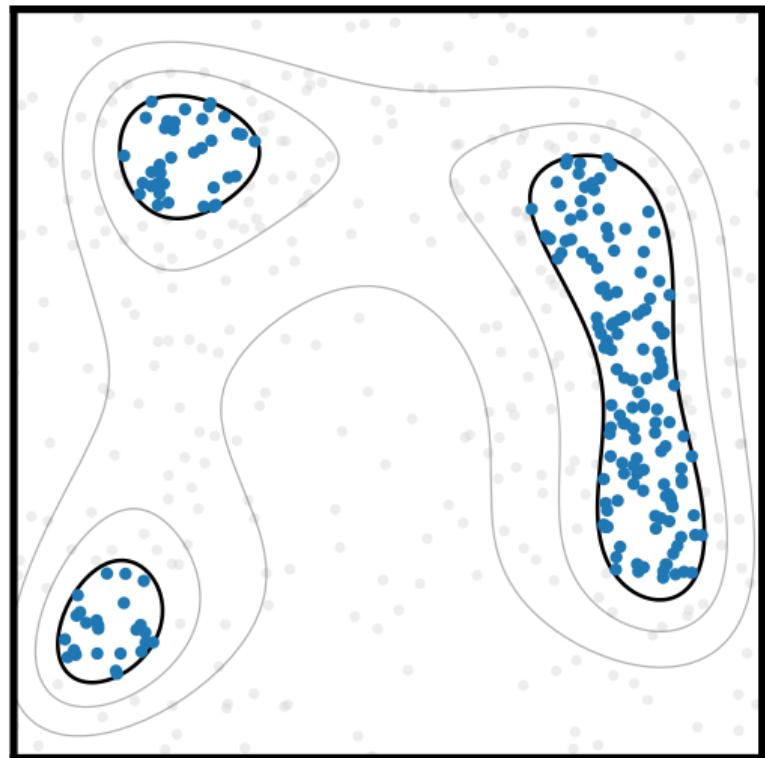
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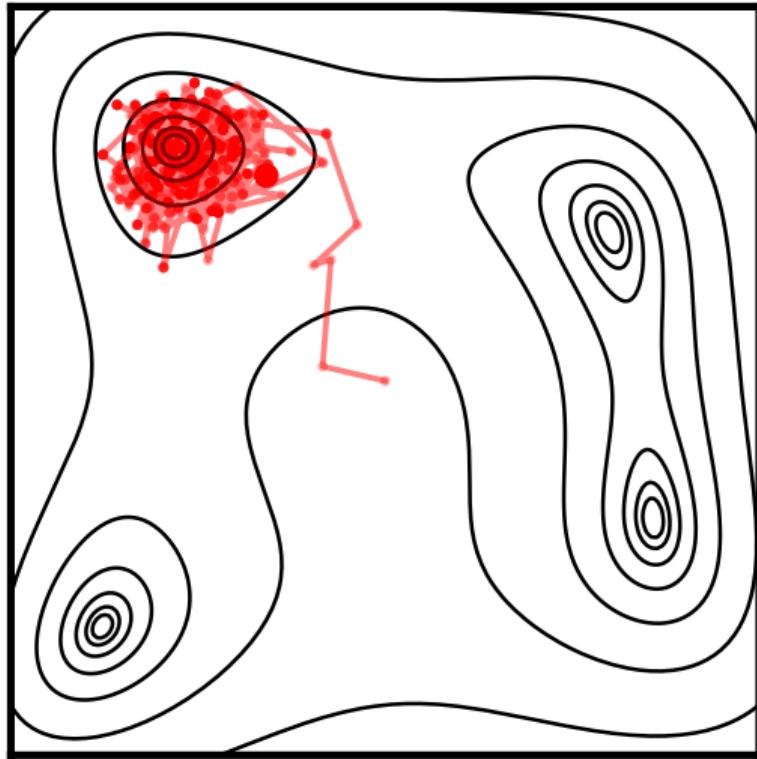
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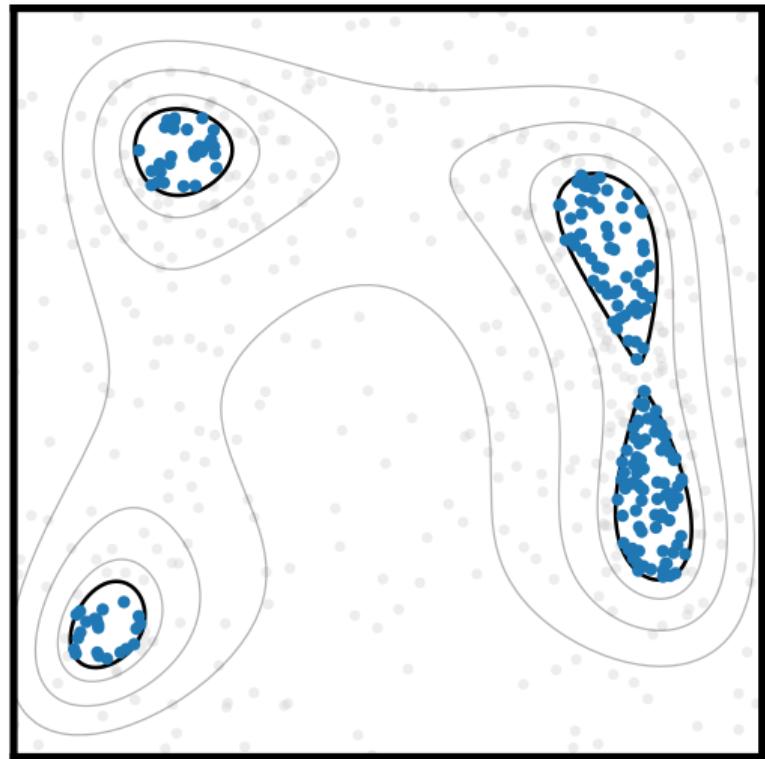
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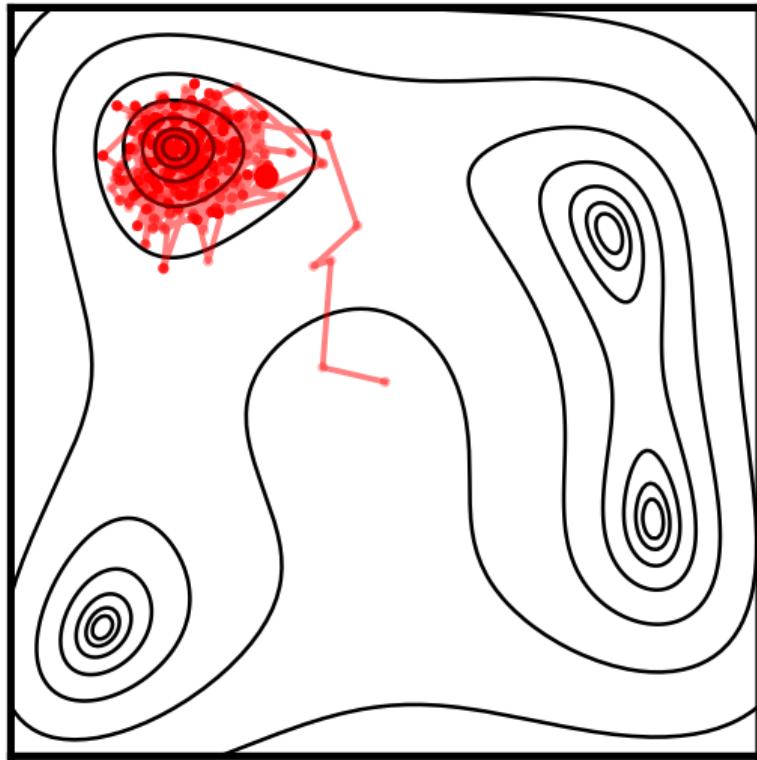
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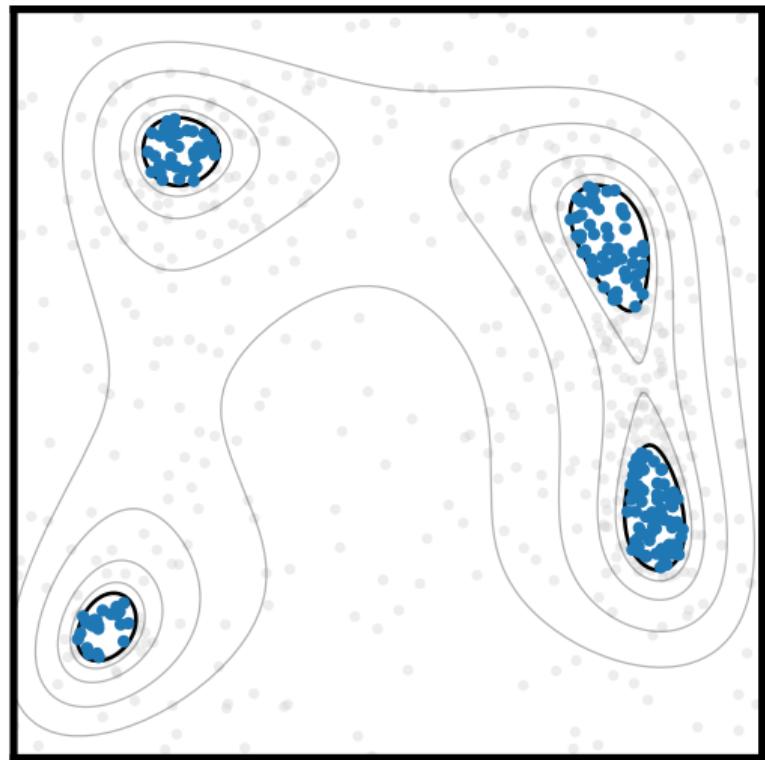
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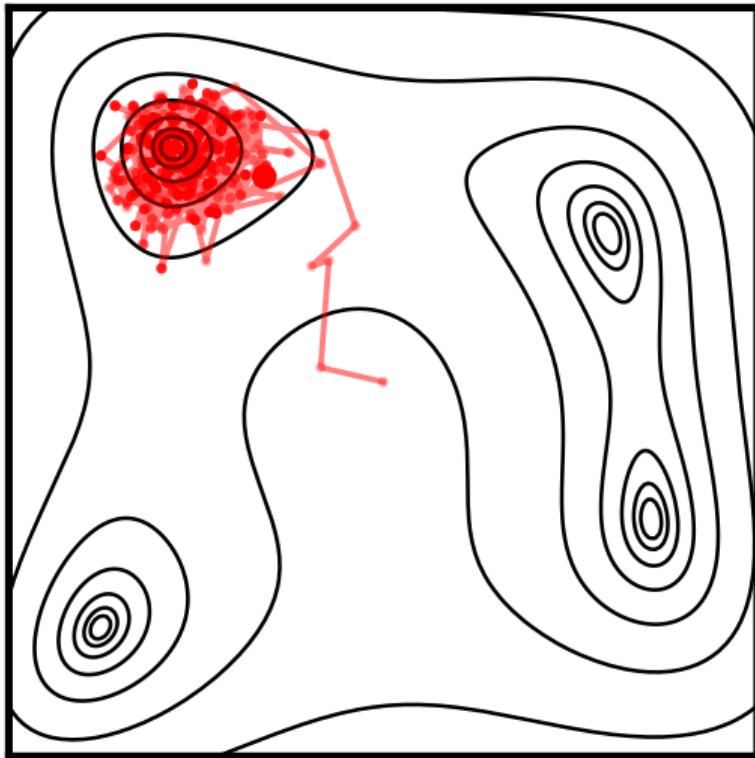
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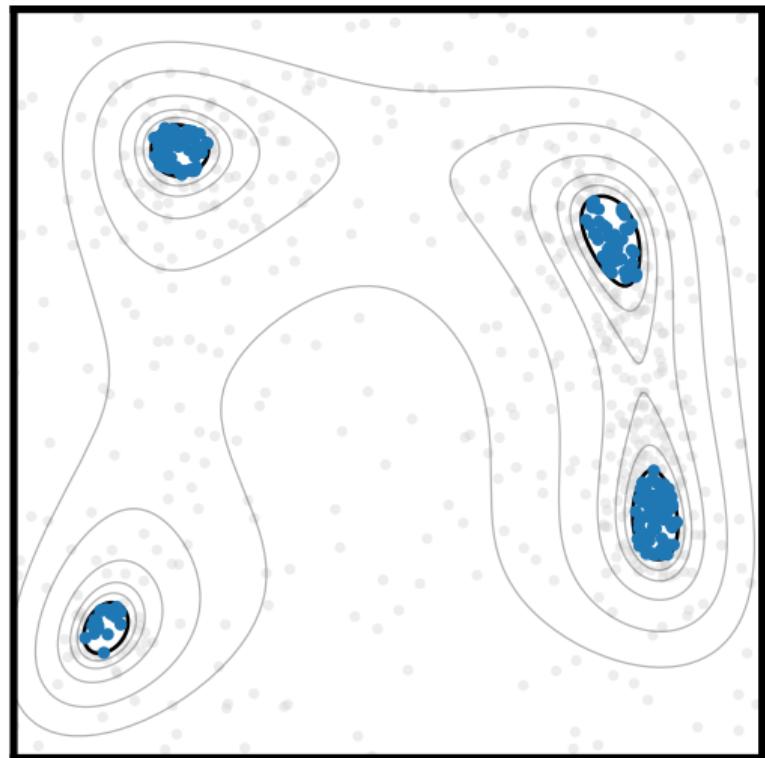
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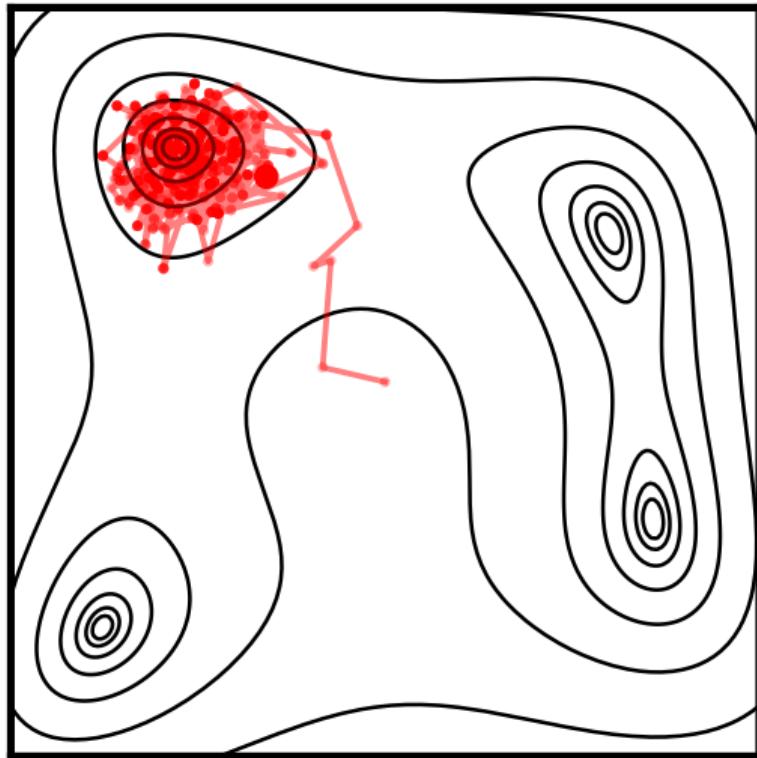
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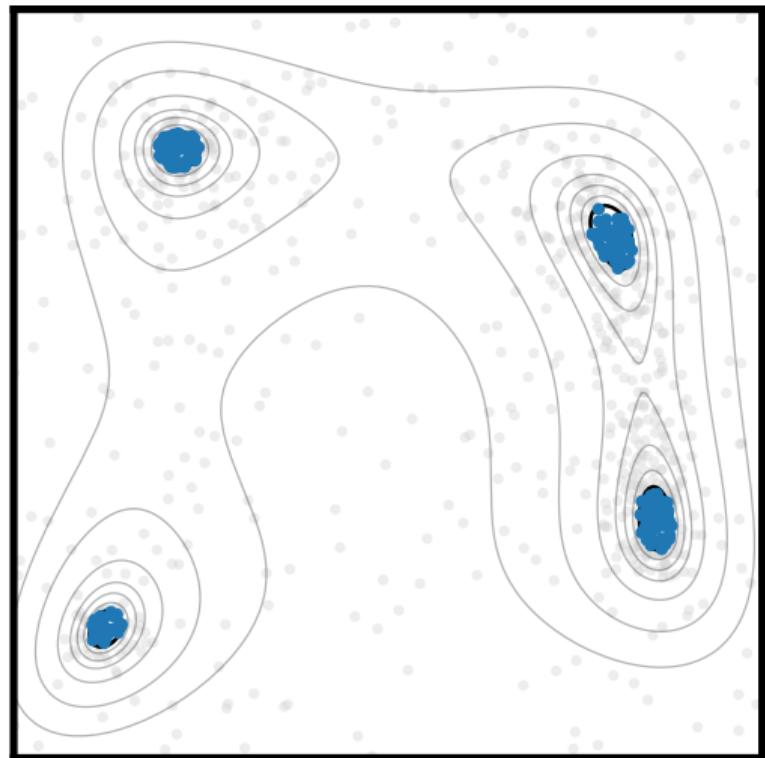
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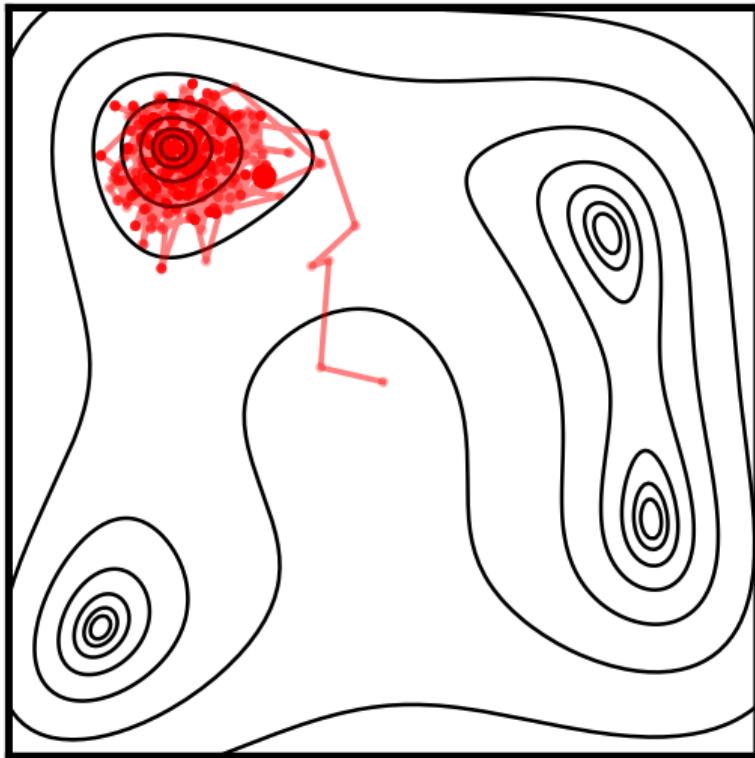
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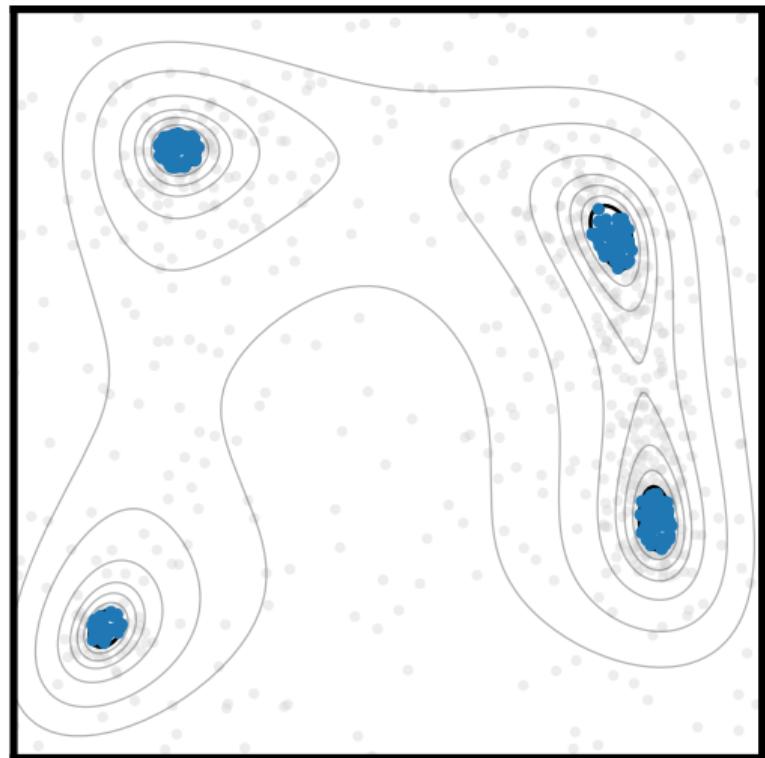
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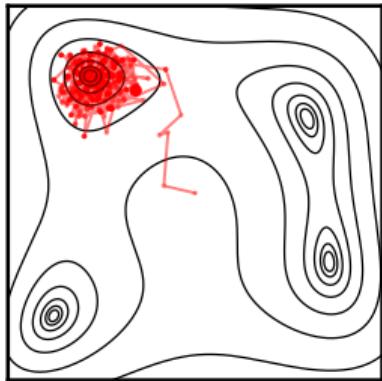


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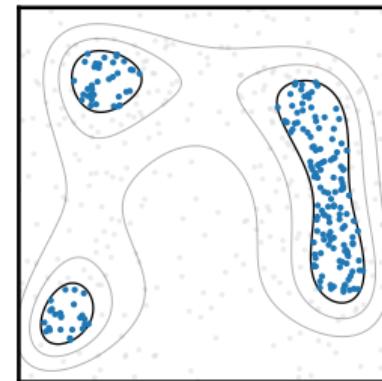
MCMC

- ▶ Single “walker”
- ▶ Explores posterior
- ▶ Fast, if proposal matrix is tuned
- ▶ Parameter estimation
- ▶ Channel capacity optimised for generating posterior samples



Nested sampling

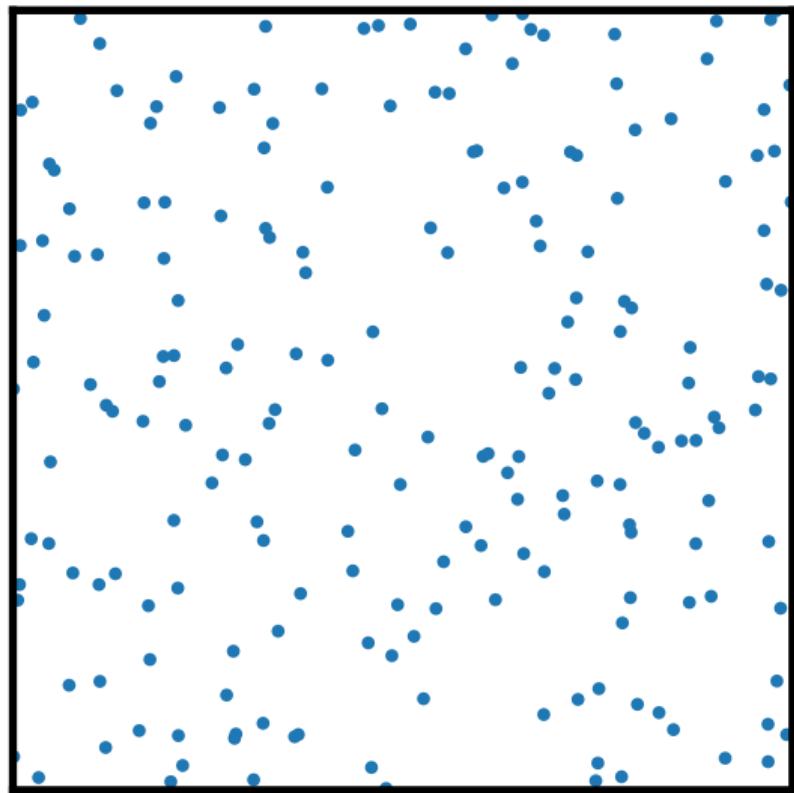
- ▶ Ensemble of “live points”
- ▶ Scans from prior to peak of likelihood
- ▶ Slower, no tuning required
- ▶ Parameter estimation, model comparison
- ▶ Channel capacity optimised for computing partition function



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

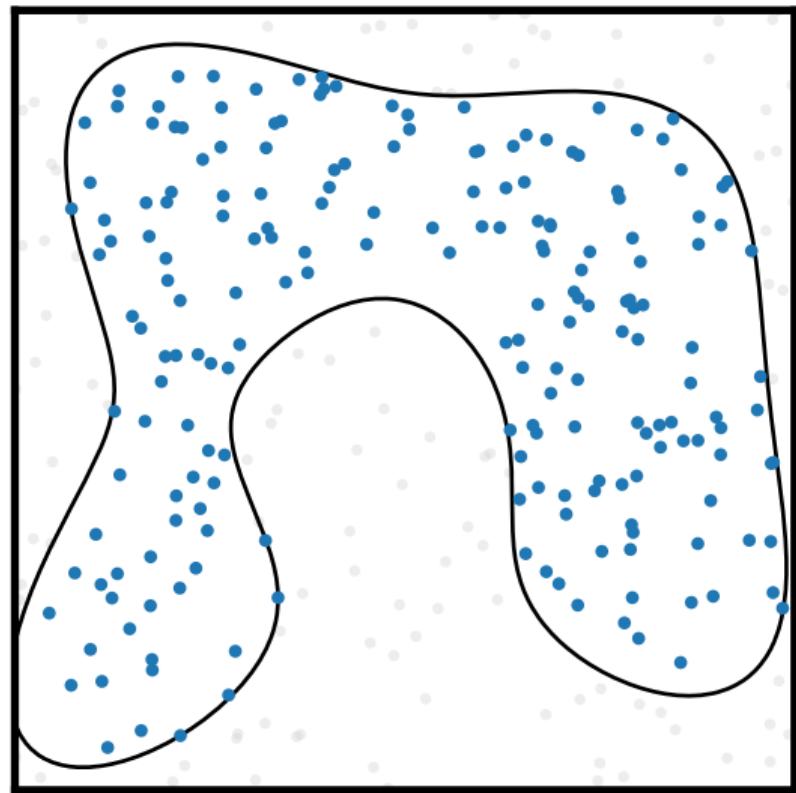
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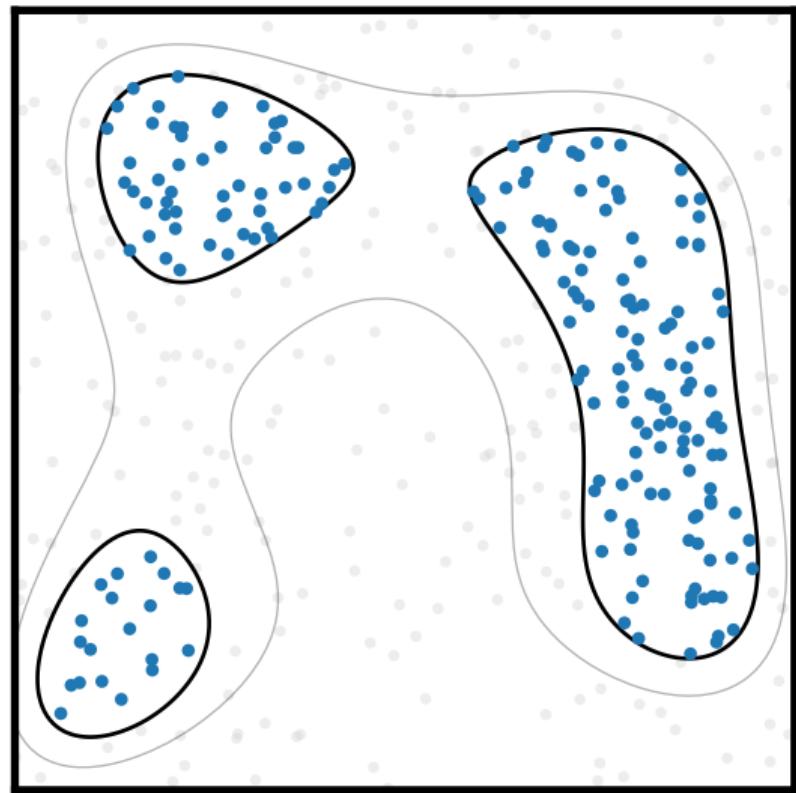
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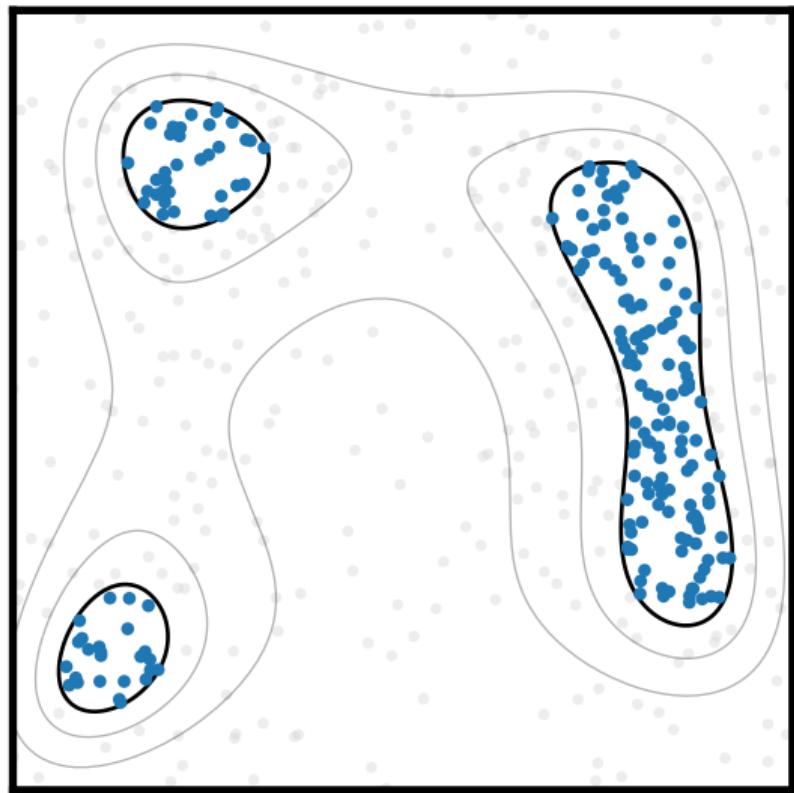
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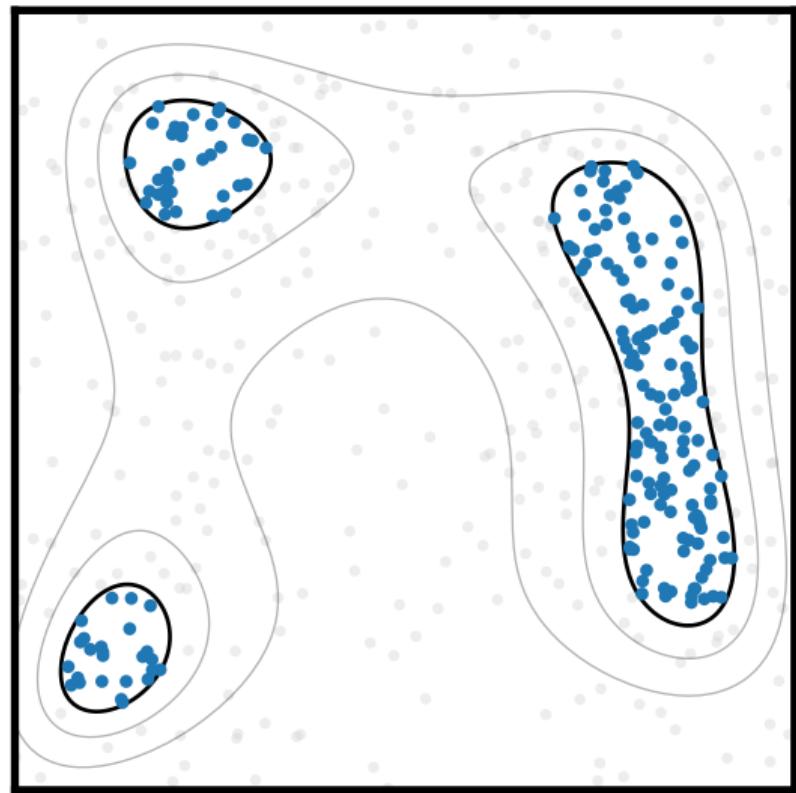
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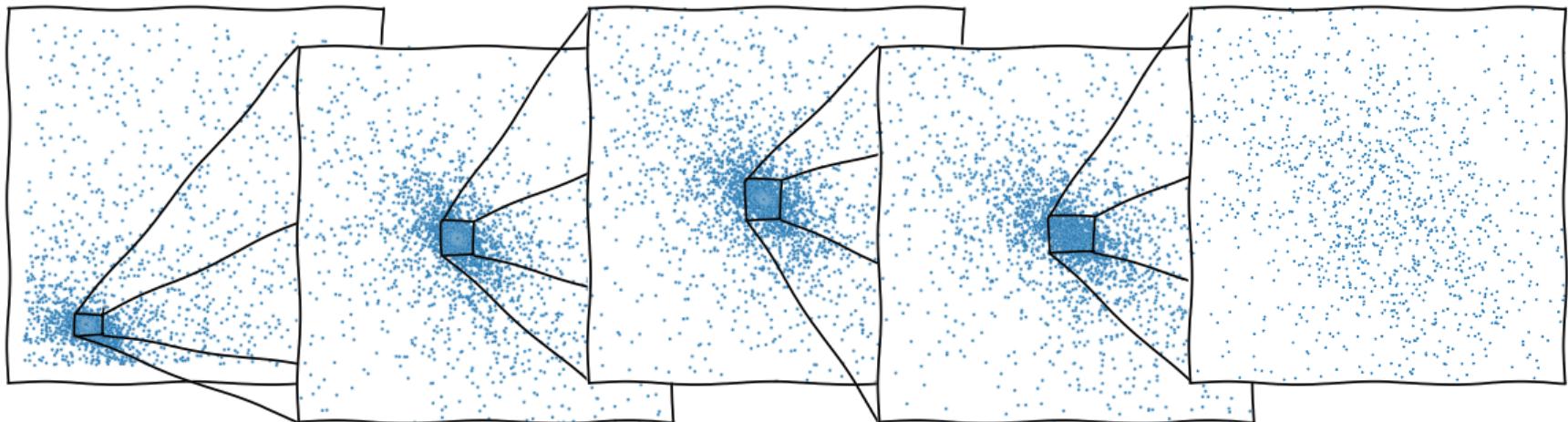
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- ▶ At each iteration, the contours contract by $\sim \frac{1}{n} \pm \frac{1}{n}$ of their volume.
- ▶ This is an exponential contraction, so

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



The nested sampling meta-algorithm: dead points



- ▶ At the end, left with a set of discarded “dead points”.
- ▶ Dead points have a unique scale-invariant distribution $\propto \frac{dV}{V}$.
- ▶ Each dead point gets a **posterior weight**: $w_i = \mathcal{L}_i \Delta V_i$

Key Output

- ▶ **Posterior samples** θ_i , weight $w_i = \mathcal{L}_i \Delta V_i$
- ▶ **Evidence** $\mathcal{Z} = \sum_i w_i$

Nested Sampling as Partition Function Calculator $\log \mathcal{Z}(\beta)$

The Key Insight

- ▶ Nested sampling directly estimates the **density of states**:

$$g(\mathcal{L}) = \int \delta(\mathcal{L}(\theta) - \mathcal{L}) \pi(\theta) d\theta$$

- ▶ This is the **partition function** at inverse temperature β :

$$\mathcal{Z}(\beta) = \int g(\mathcal{L}) \mathcal{L}^\beta d\mathcal{L}$$

- ▶ Evidence is special case: $\mathcal{Z} = \mathcal{Z}(\beta = 1)$
- ▶ **In practice:** $\mathcal{Z}(\beta) \approx \sum_i \mathcal{L}_i^\beta \Delta V_i$

Statistical Physics Connection

- ▶ **Canonical ensemble:** $p(\theta|\beta) \propto \mathcal{L}(\theta)^\beta \pi(\theta)$
- ▶ **Free energy:** $\beta F = -\log \mathcal{Z}$
- ▶ **Internal energy:** $U = -\frac{\partial \log \mathcal{Z}}{\partial \beta}$
- ▶ **Heat capacity:** $C = \frac{\partial U}{\partial \beta}$

Nested sampling provides the fundamental thermodynamic quantities
for any probabilistic model

Why GPUs? The Future of High-Performance Computing

GPU Advantages (Often Confused!)

- ▶ **Massive Parallelization:**
 - ▶ 1000s of cores vs 10s on CPU
 - ▶ Perfect for ensemble algorithms
 - ▶ Vectorization across particles/chains
 - ▶ Independent likelihood evaluations
- ▶ **Automatic Differentiation:**
 - ▶ GPU-accelerated gradients “for free”
 - ▶ JAX/PyTorch ecosystem make this possible
 - ▶ Essential for modern optimization

The HPC Reality

- ▶ Future HPC is GPU dominated:
- ▶ Legacy CPU codes becoming obsolete

Apples-to-Apples comparison

- ▶ Quantifying GPU advantage
 - ▶ GPUs 40× more expensive to rent
 - ▶ GPUs 100× rarer in HPC allocations
- ▶ Sometimes you don't care about walltime.

Why BlackJAX? Unified GPU Framework for Bayesian Inference

The Fragmentation Problem

- ▶ **Scattered ecosystem:** MultiNest, PolyChord, dynesty, UltraNest, nautilus, nessai, ...

BlackJAX Solution

- ▶ **Community JAX codebase**
- ▶ **Fair benchmarking** with identical GPU infrastructure
- ▶ **Composable algorithms** with shared components
- ▶ **Modern ML ecosystem integration**

Algorithm-Hardware Matching

- ▶ **Ensemble methods \leftrightarrow GPU parallelization:**
 - ▶ Nested sampling: 100-1000 live points
 - ▶ SMC: 1000s of particles
 - ▶ Embarrassingly parallel operations
- ▶ **Scientific problems are compute-bound:**
 - ▶ Unlike ultra-large DL models
 - ▶ GPU memory rarely limiting
 - ▶ Perfect match for vectorization

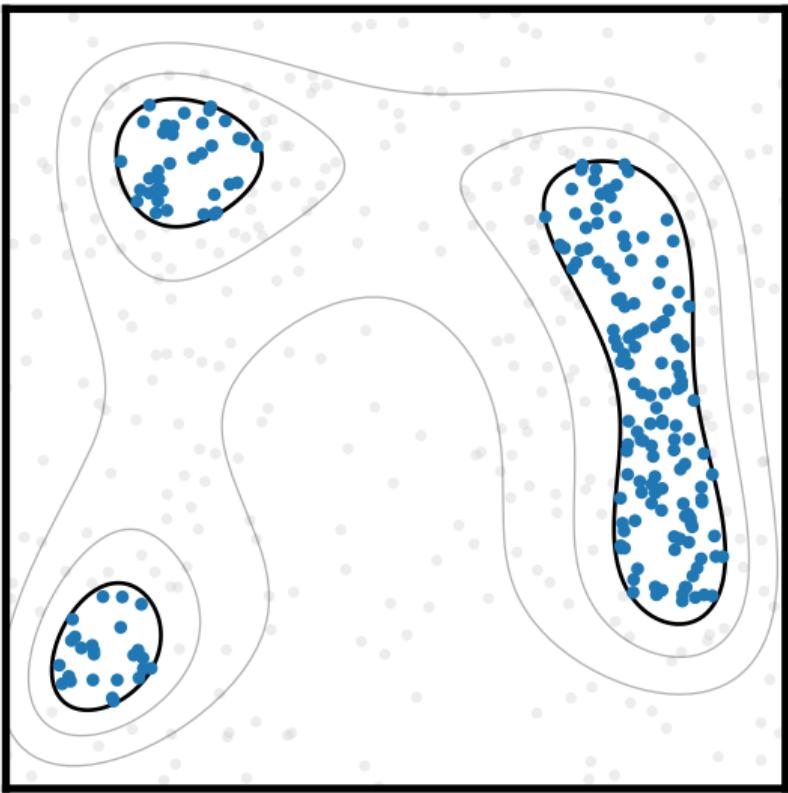


Nested Sampling Meta-Algorithm

- ▶ **Framework is kernel-agnostic:**
 - ▶ Original: Metropolis Hastings (Skilling 2006)
 - ▶ MultiNest: rejection ellipsoids
 - ▶ PolyChord: slice sampling
 - ▶ nessai/nautilus: ML techniques

Our Choice: Slice Sampling

- ▶ **First scalable generic solution** in BlackJAX
- ▶ **No tuning required** (unlike MCMC proposal matrices)
- ▶ **Robust across dimensions & problem types**



GW150914 Binary Black Hole Merger

Metha Prathaban

PhD



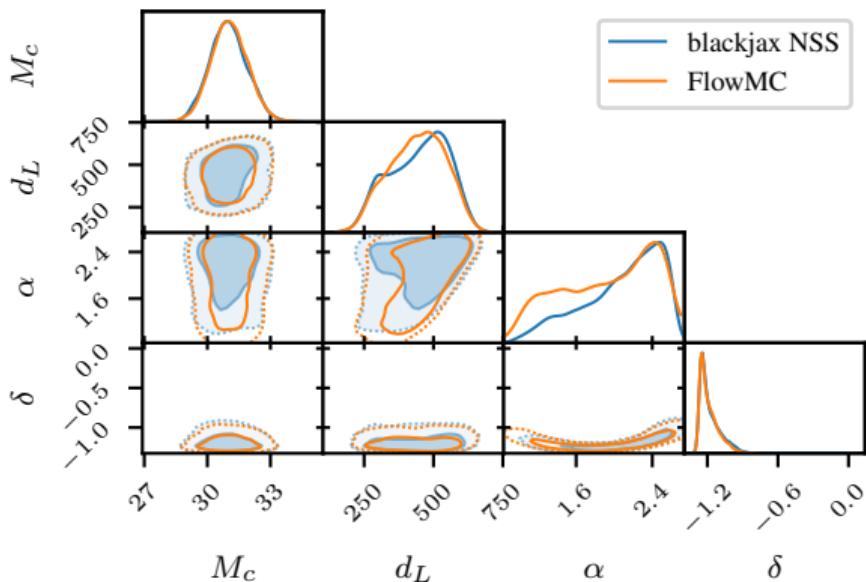
Performance on Real Data

- ▶ **BlackJAX GPU-NS:** 207 seconds (1 GPU)
- ▶ **FlowMC (GPU MCMC):** 742 seconds (1 GPU)
- ▶ **Bilby/Dynesty:** 2 hours (400 CPUs)

**Orders of magnitude speedup over CPU
Comparable to other GPU-native methods**

Key Achievement

- ▶ Nested sampling now competitive on GPUs
- ▶ Direct evidence computation included



Good agreement between BlackJAX
and FlowMC posteriors



CMB Power Spectrum (6 params)

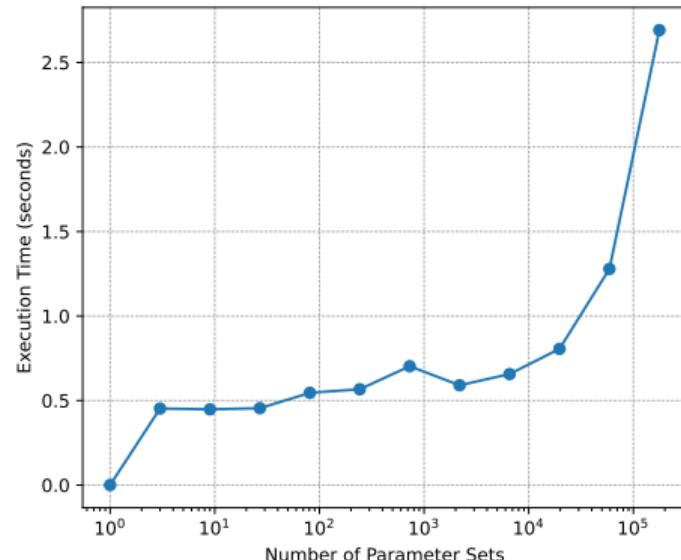
- ▶ PolyChord (CPU): 1 hour
- ▶ BlackJAX (GPU): 12 seconds

300× speedup

Cosmic Shear (37 params)

- ▶ PolyChord (48 CPUs): 8 months
- ▶ NUTS (12 A100 GPUs): 2 days
- ▶ BlackJAX (1 A100 GPU): 4.5 hours

>1000× speedup vs CPU
10× speedup vs existing GPU
approach[2405.12965]





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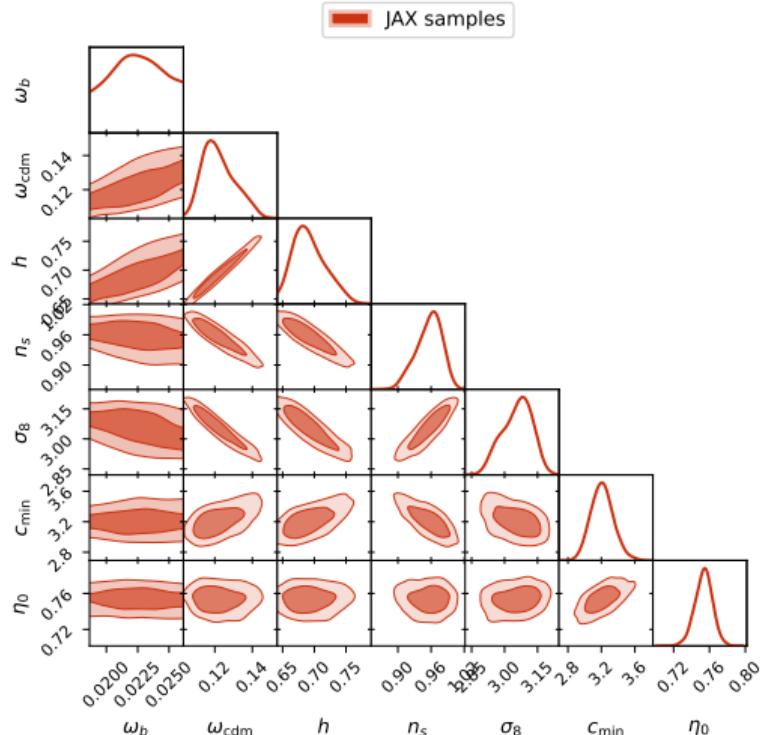
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The Real AI Revolution: LLMs as the Missing Piece

LLMs: The GPU Code Translator

- ▶ Automated translation: Fortran/C++ → JAX/PyTorch
- ▶ Bridges the gap between legacy science and modern hardware

The 80/20 Rule of Scientific Work

- ▶ **80% “boring” tasks:** forms, papers, grants, reviews, grading, code writing...
- ▶ **20% hard thinking:** Novel insights, experimental design, theory
- ▶ **AI’s biggest impact:** Automating the 80%, not the 20%

Beyond Scientific Analysis

- ▶ **Common focus:** Using LLMs for analysis
- ▶ **Real transformation:** Automating workflow
- ▶ **Already happening:**
 - ▶ Grant writing assistance
 - ▶ Paper drafting and review
 - ▶ Code generation and debugging
 - ▶ Literature review automation

The Productivity Explosion

- ▶ **Quality control:** Becomes the limiting factor
- ▶ **Focus shift:** writing → critical thinking

Resources

- ▶ **Installation:** pip install git+https://github.com/handley-lab/blackjax
- ▶ **Documentation:** handley-lab.co.uk/nested-sampling-book

BlackJAX Implementation

- ▶ **BlackJAX:** [\[github:handley-lab/blackjax\]](https://github.com/handley-lab/blackjax)
- ▶ **Nested sampling:** In PR to
[\[github:blackjax-devs/blackjax\] #755](https://github.com/blackjax-devs/blackjax/pull/755)

Theory & Background

- ▶ **Review papers:** [\[2205.15570\]](#),
[\[2101.09675\]](#)
- ▶ **Original paper:** [\[Skilling \(2006\)\]](#)

Workshop & Learning

- ▶ **GPU Nested Sampling Workshop:** github.com/handley-lab/workshop
- ▶ **Interactive tutorials:** JAX, BlackJAX, GPU acceleration

Conclusions



github.com/handley-lab/group

- ▶ **Nested sampling is widely used** across physical sciences for parameter estimation and model comparison
- ▶ **BlackJAX provides GPU-native implementation** with $10\times\text{--}100\times$ speedups
- ▶ **JAX ecosystem integration** enables modern scientific workflows
- ▶ **Real applications** from gravitational waves to cosmology benefit immediately
- ▶ **The future is GPU-accelerated** scientific computing with AI integration