GPU Accelerated Nested Sampling

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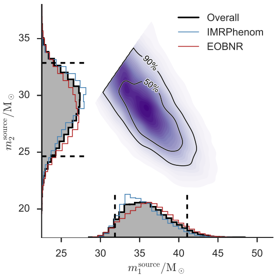
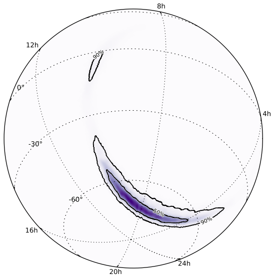
A Case Study in Astrostatistics

The Challenge: GW170817

- **Gravitational wave detected**: Binary neutron star merger
- **Real-time parameter estimation**: 15+ dimensional space
- **Sky localization**: ~ 30 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**: $d \sim 10^2$–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

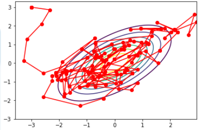
Single-Chain MCMC

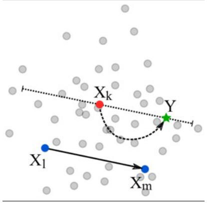
- **Metropolis-Hastings**: Simple, widely used (PyMC)
- **HMC/NUTS**: Gradient-based, efficient (Stan, BlackJAX)
- Fast for unimodal well-conditioned problems, no evidence

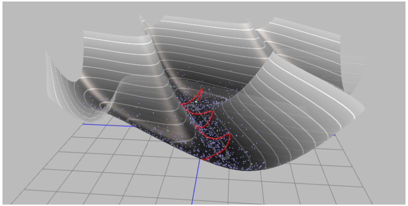
Ensemble Methods

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

emcee
the mcmc hammer

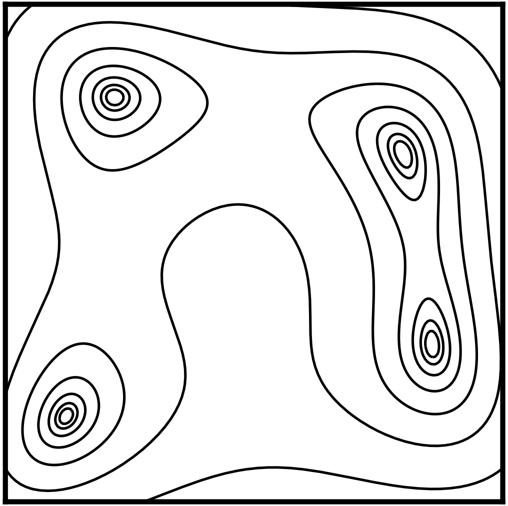






Nested sampling:
Unique in targeting evidence computation directly

MCMC



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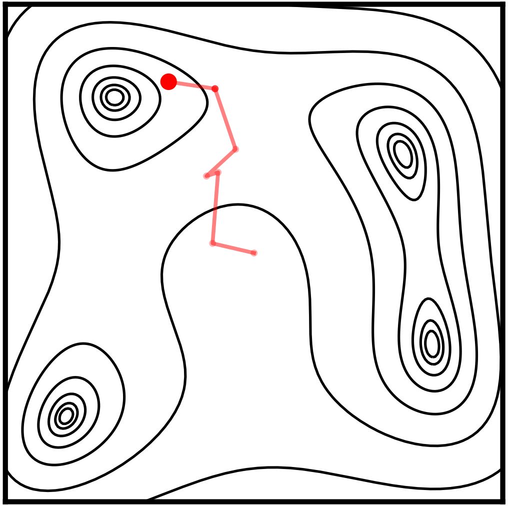

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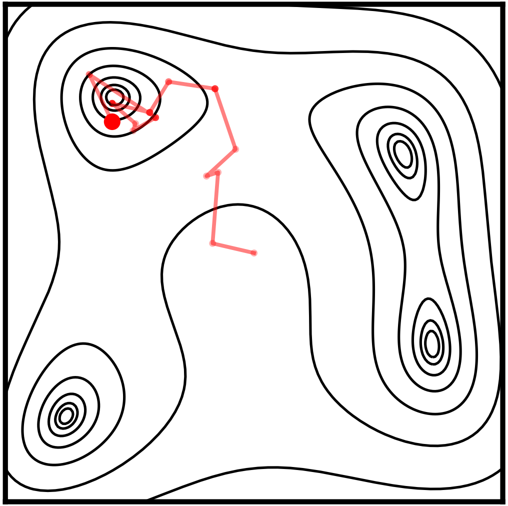

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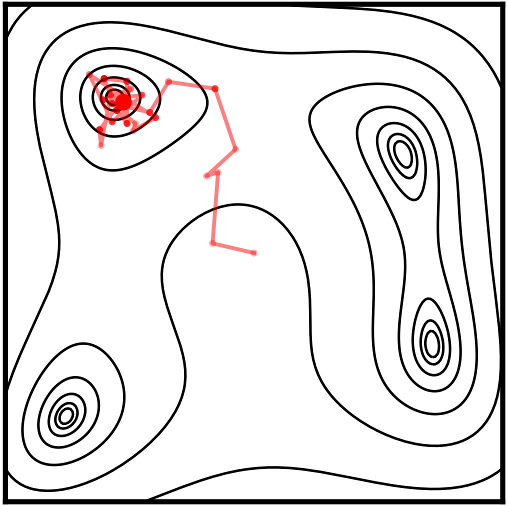

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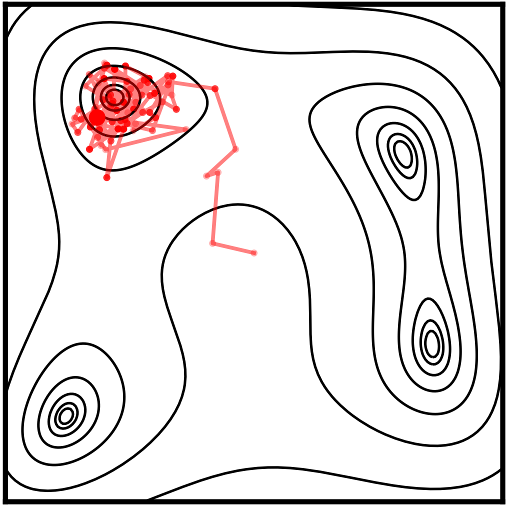

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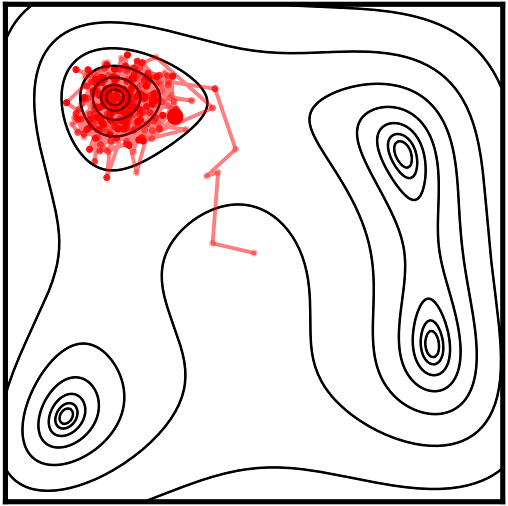

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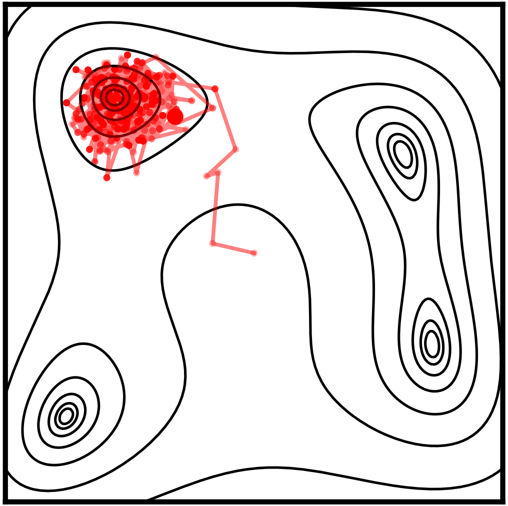

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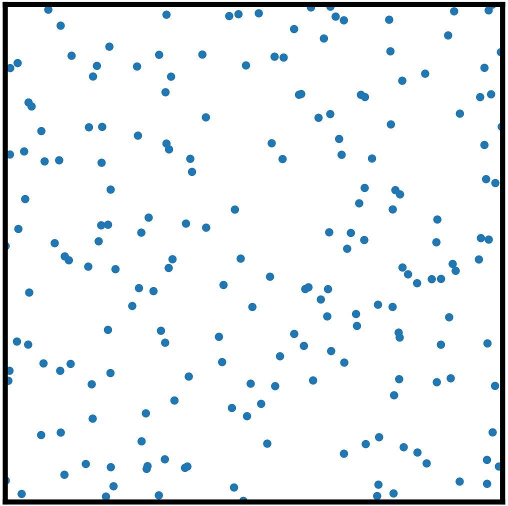

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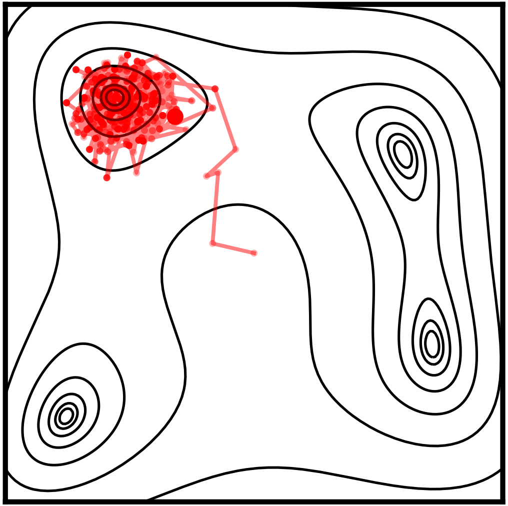

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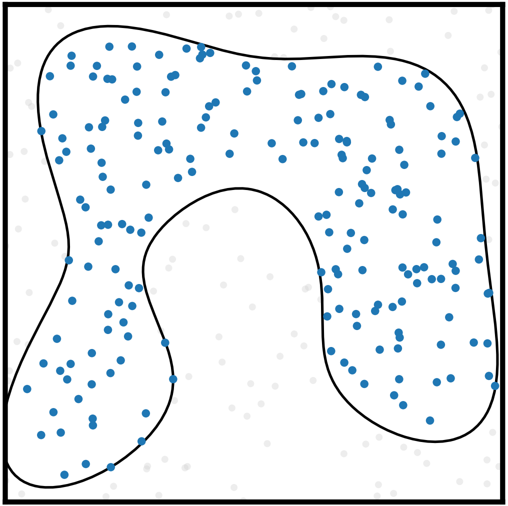

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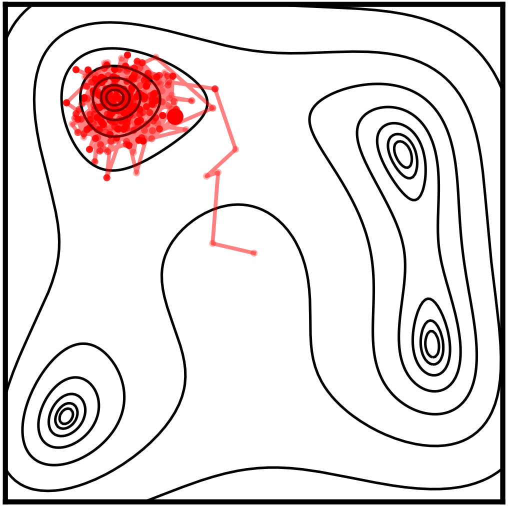

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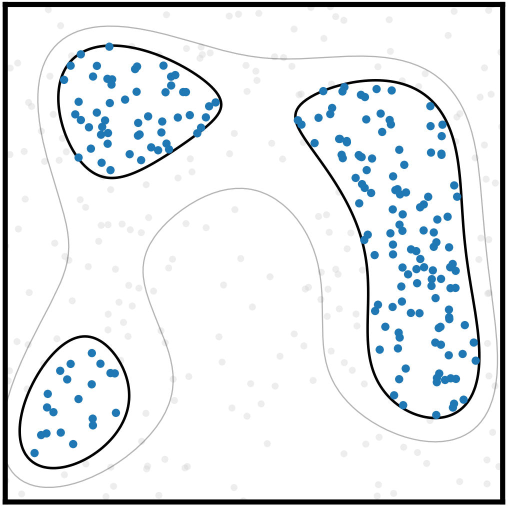

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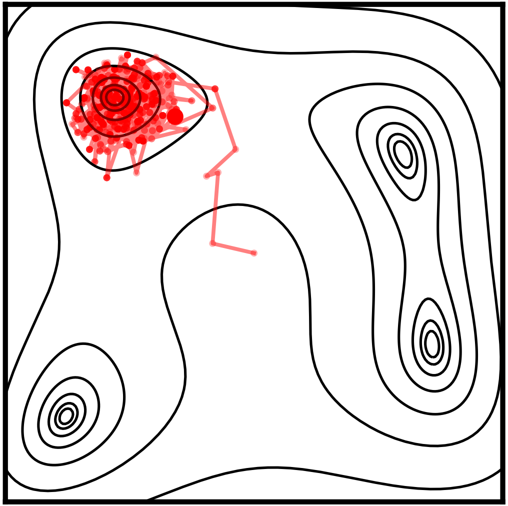

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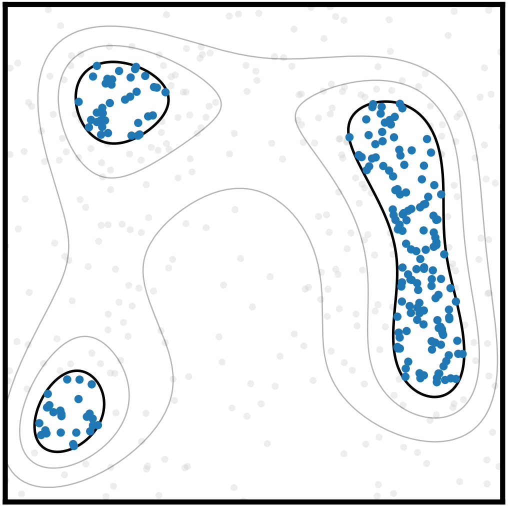

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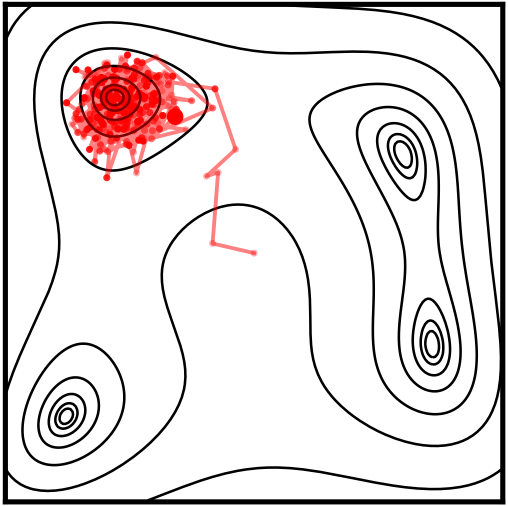

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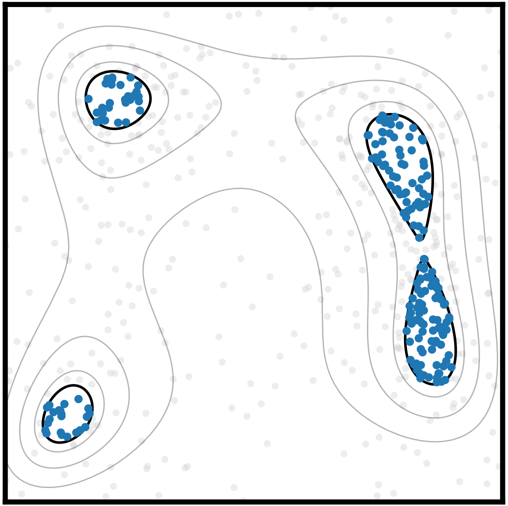

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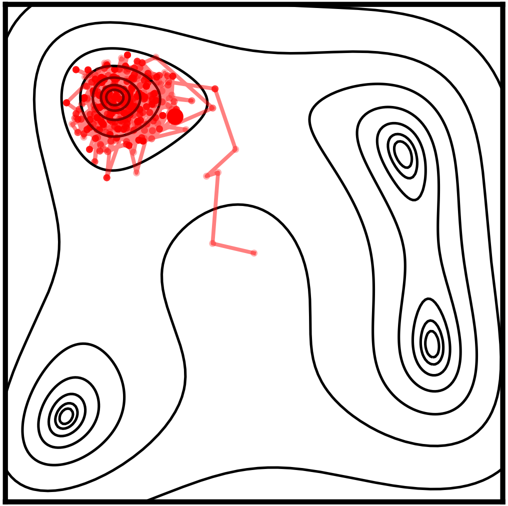

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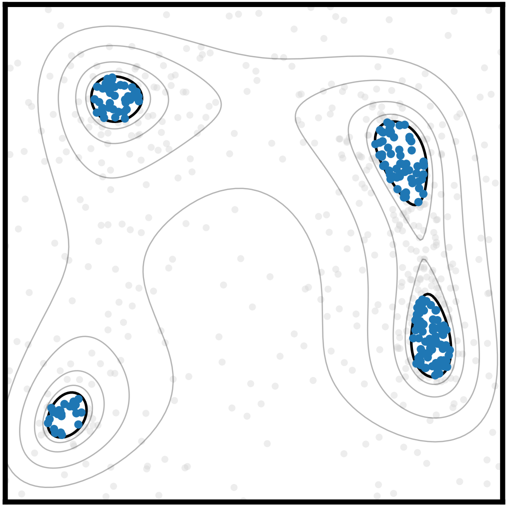

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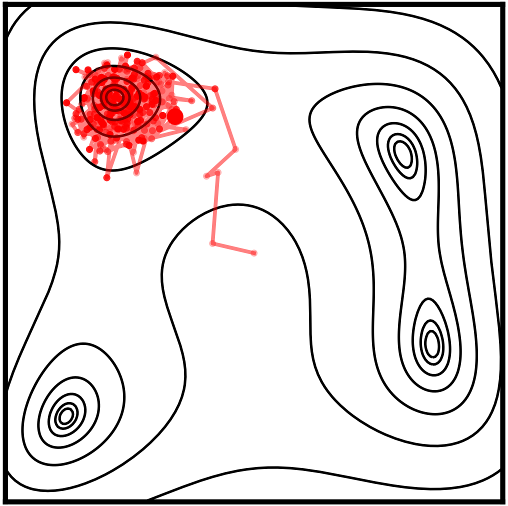

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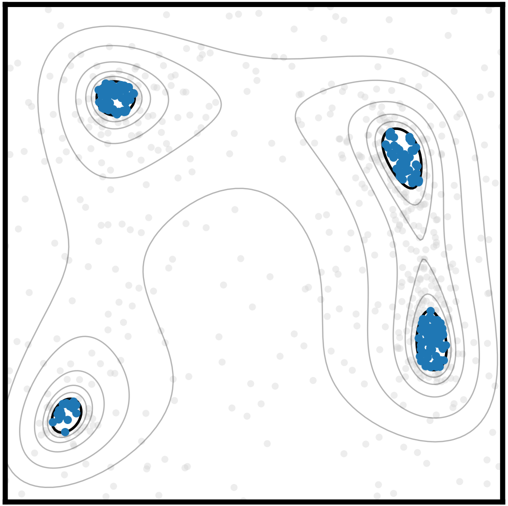

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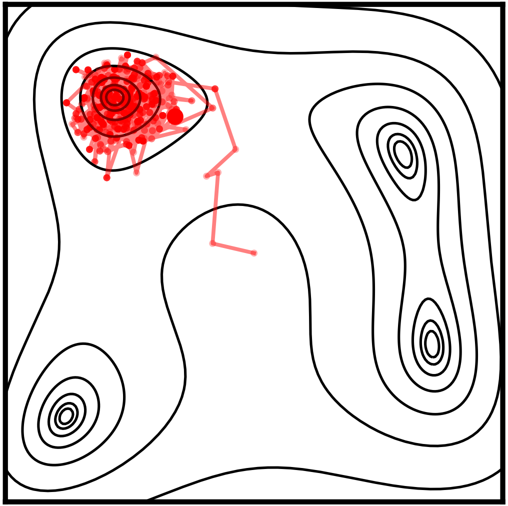

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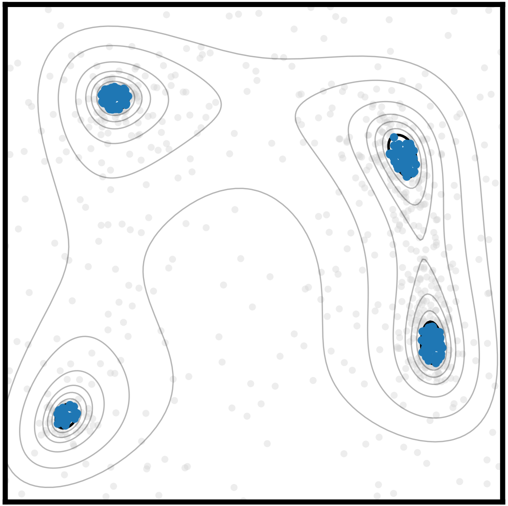

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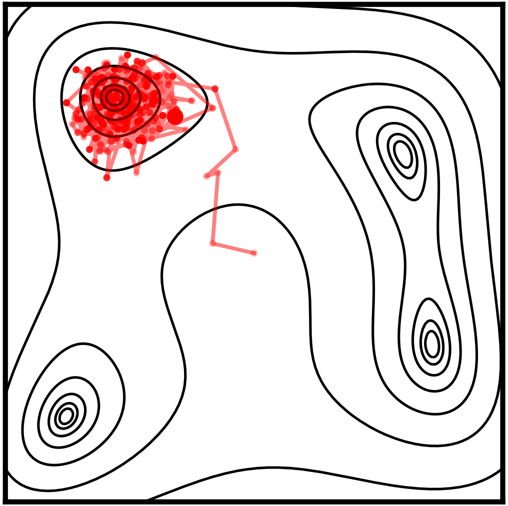

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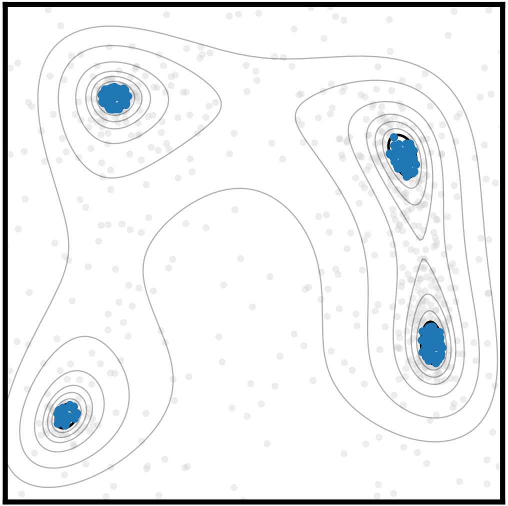
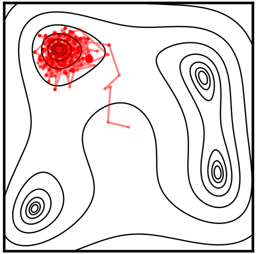


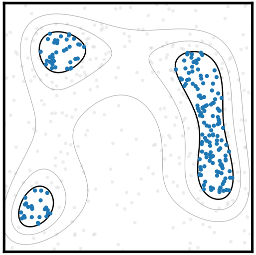
MCMC

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



Nested sampling

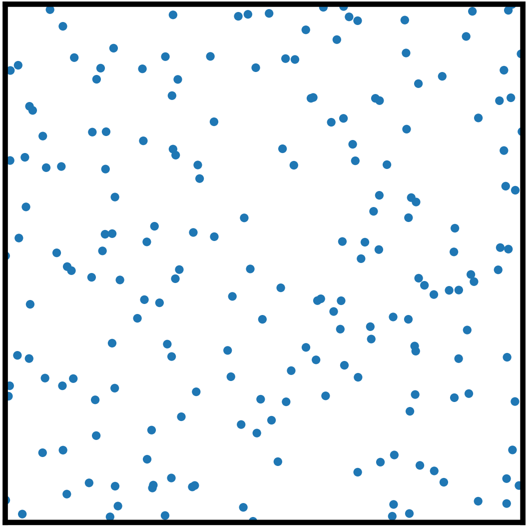
- Ensemble of "live points"
- Scans from prior to peak of likelihood
- Slower, no tuning required
- Parameter estimation, model comparison
- Channel capacity optimised for computing partition function



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

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



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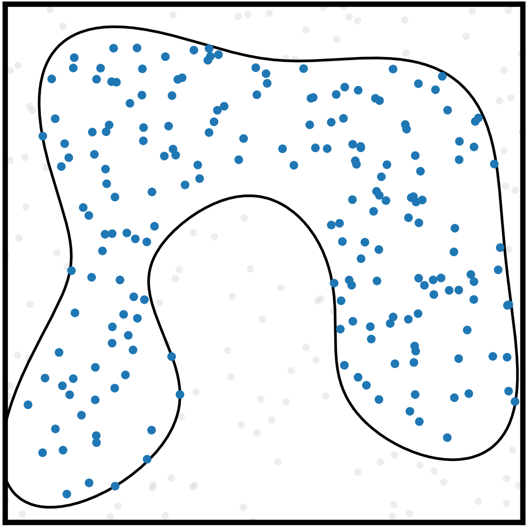

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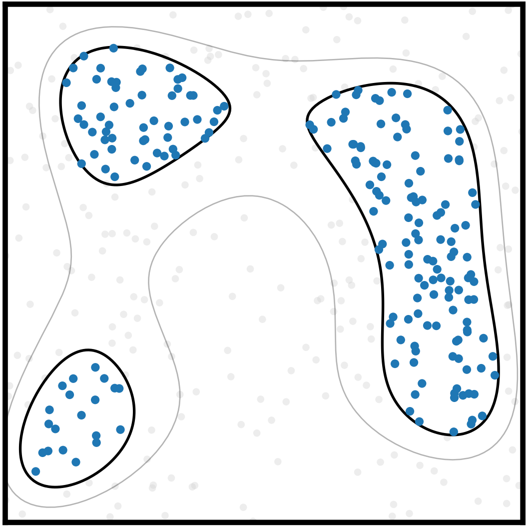

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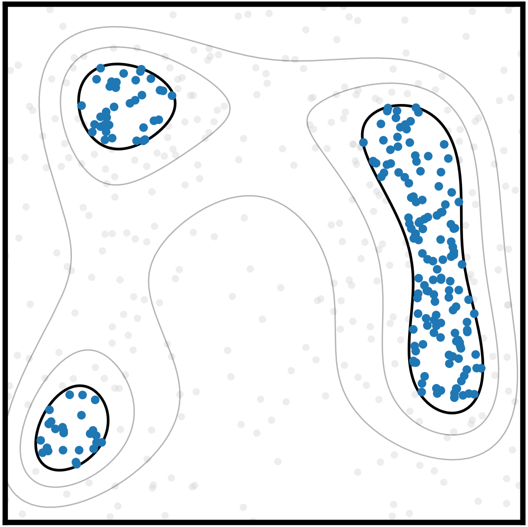

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- We can use this evolution to estimate volume *probabilistically*.
- At each iteration, the contours contract by $\sim \frac{1}{n} \pm \frac{1}{n}$ of their volume.
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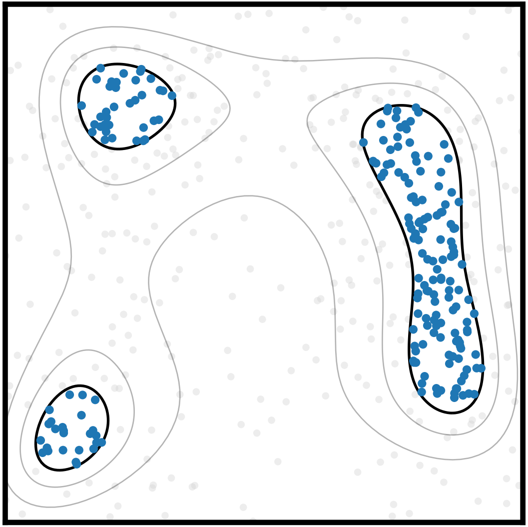
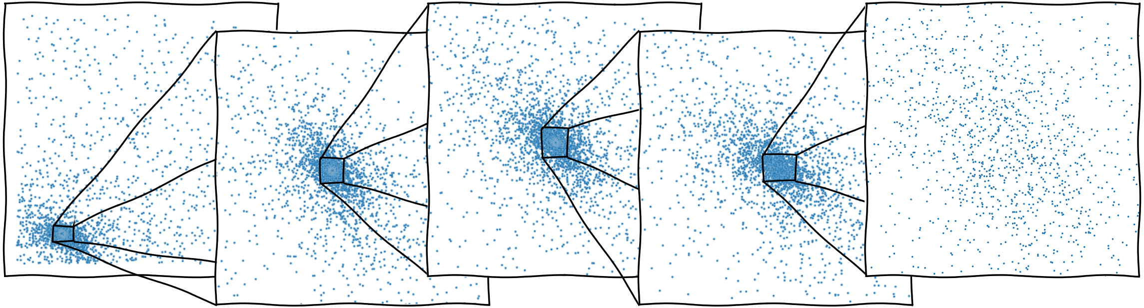
$$\int f(x) dV \approx \sum_i f(x_i) \Delta V_i, \qquad V_i = V_0 e^{-(i\pm\sqrt{i})/n}$$



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 $40\times$ more expensive to rent
  - GPUs $100\times$ 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

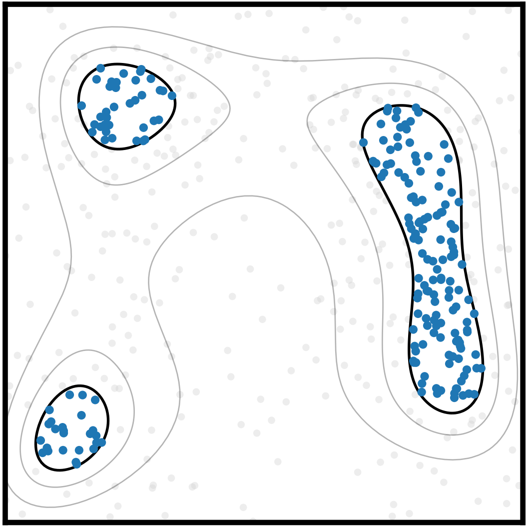
David Yallup
PDRA

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

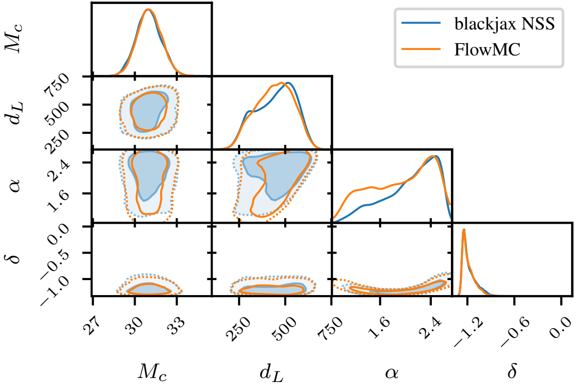
Performance on Real Data

- **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 & Cosmic Shear Analysis

Toby Lovick

PhD

CMB Power Spectrum (6 params)

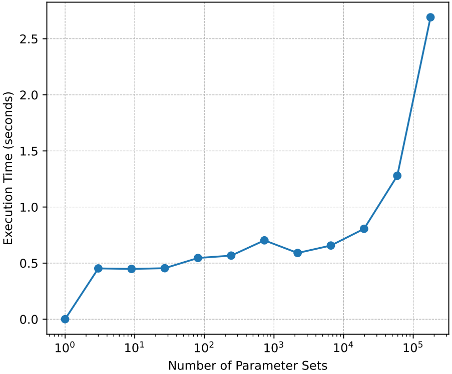
- **PolyChord (CPU)**: 1 hour
- **BlackJAX (GPU)**: 12 seconds

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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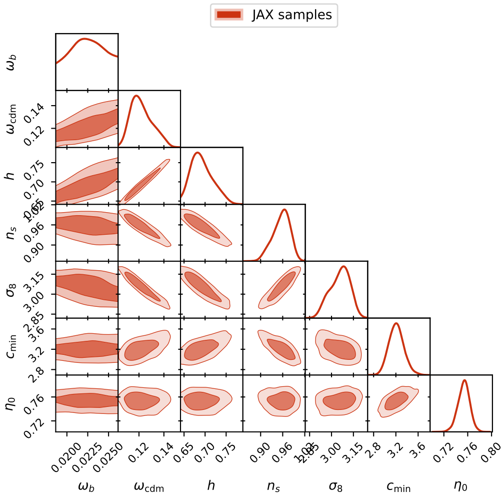


The Real AI Revolution: LLMs as the Missing Piece

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]
- **Nested sampling**: In PR to [github:blackjax-devs/blackjax] #755

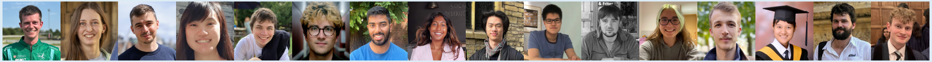
Theory & Background

- **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×-100× 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