


# Nested sampling for next generation gravitational-wave inference

Metha Prathaban


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# About Me

- 3rd year PhD student in Will Handley's group
- Handley group works on Bayesian statistical inference and artificial intelligence methodologies, with a focus on analyzing complex datasets from next-generation surveys to explore a wide range of physics questions related to dark matter, dark energy, and the early Universe.
- My work on Bayesian numerical method development in context of GWs

## The Handley group!

+ others!


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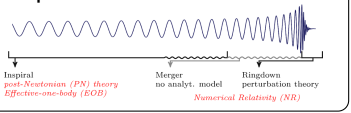
# Inverse problems in GW physics

**Forward problem**

model parameters
$\theta = \mathcal{M}, q, d_L, t_c \ldots$

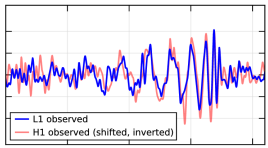
→ waveform model →

template for strain waveform




**Inverse problem**

observed signal strain
Livingston, Louisiana (L1)




← inference ←

model parameters, inferred
$\theta_{\text{est}}$

Given some model $\mathcal{M}$ and observed signal $\mathcal{D}$, Bayes' theorem enables us to relate the posterior probability of the set of parameters $\theta$ which generated the signal to the likelihood of the $\mathcal{D}$ given $\theta$ and the prior probability of $\theta$ given $\mathcal{M}$:

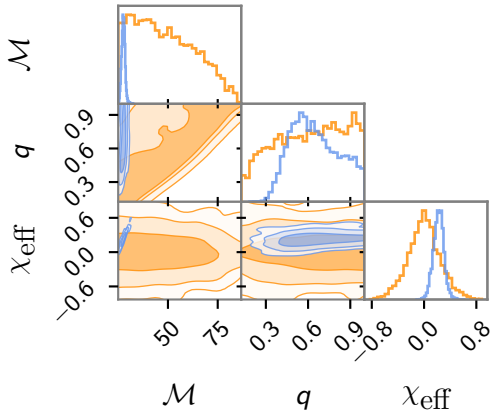
$$\mathcal{P}(\theta|D,\mathcal{M}) = \frac{P(D|\theta,\mathcal{M})P(\theta|\mathcal{M})}{P(D|\mathcal{M})} = \frac{\mathcal{L}(D|\theta)\pi(\theta)}{\mathcal{Z}} \tag{1}$$

The evidence, $\mathcal{Z}$, plays a key role in model comparison.

- Define prior, **sample** (unnormalized) posterior ($\mathcal{L}(\mathbf{d}|\theta) \times \pi(\theta)$).

Challenges:

- High-dimensional parameter spaces $\Rightarrow$ posterior occupies vanishingly small region of prior.
- Complex waveform models with high costs



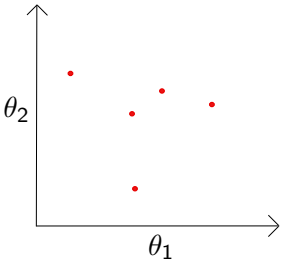
Goal is efficient exploration of parameter space, to do GW inference in feasible timescales.

Posterior samplers:

- Metropolis-Hastings
- Hamiltonian Monte-Carlo
- Ensemble samplers

None of these calculate the evidence, $\mathcal{Z}$ - crucial for Bayesian model comparison (e.g. testing for precession vs. no precession)!

Nested sampling first and foremost calculates evidence, $\mathcal{Z} = \int \mathcal{L}(\theta)\pi(\theta)d\theta$.

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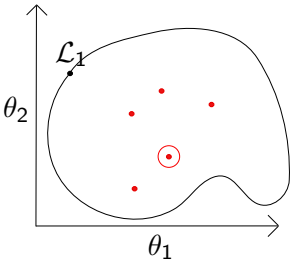


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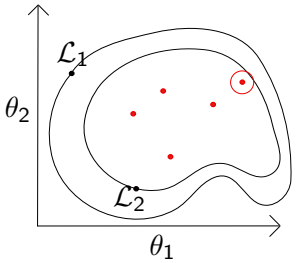


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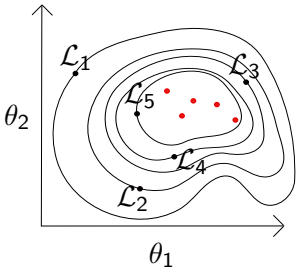


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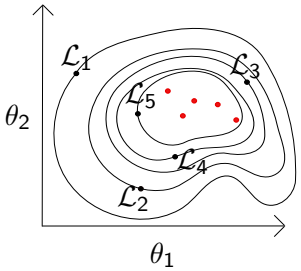


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- Evidence is calculated as weighted sum over deleted ('dead') points.

Time of convergence of NS: 2212.01760

likelihood evaluation time

$$T \propto T_{\mathcal{L}} \times f_{\text{sampler}} \times D_{\text{KL}} \times n_{\text{live}} \tag{2}$$

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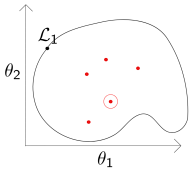
drawing new live point



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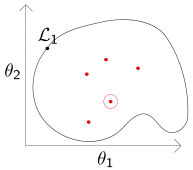
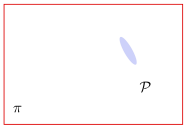
compression from prior to posterior ($\approx \ln \frac{V_\pi}{V_\mathcal{P}}$)

drawing new live point



# Current vs. future data

## LVK data so far

- Short-duration signals from compact binary coalescences (CBCs)
- End of O4a: $\approx 200$ confident detections
- Detection rate: $\approx 1$ every few days
  - Signals not overlapping
- BBH mergers last seconds, BNS mergers last minutes
- Computationally intensive to analyse, but doable with current pipelines.

## ET + CE

- Ten-fold improvement in sensitivity compared to 2G detectors
- Detection rate: $\approx 10^5 - 10^6$ BBH and $\approx 7 \times 10^4$ BNS mergers per year
- Wider frequency band $\Rightarrow$ more intermediate mass BHs
- Improved localization
- Significantly higher SNR
- Longer signal durations
  - Overlapping signals expected
- New GW sources


# Scaling of traditional methods

$$T_{\text{total}} \propto N_{\text{signals}} \times T_{\mathcal{L}} \times f_{\text{sampler}} \times D_{\text{KL}} \times n_{\text{live}} \tag{3}$$

higher sensitivity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**Billions to quadrillions of CPU core hours for 1 month of ET data...** 2412.02651

## Heterodyning

Exploits the smooth changes in GW waveforms near the maximum likelihood point. Assigns fiducial source parameter close to the true value and uses coarser frequency resolution.

## Reduced Order Quadrature

Approximates the waveform model as a linear combination of a small number of pre-trained bases evaluated at representative frequencies.

## Multibanding

Adjusts data resolution for gravitational wave signals across frequency bands, particularly during low-frequency early inspiral stage of CBCs.

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# ML for traditional methods

ROM, surrogates

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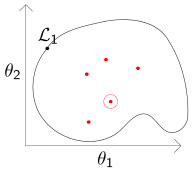
NESSAI







# ML for traditional methods

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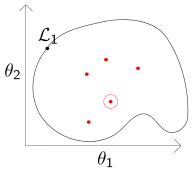
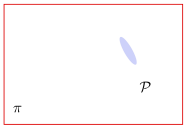
not as baked-in as you might think!

NESSAI



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focus of this section

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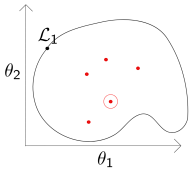
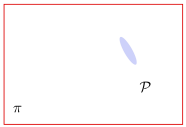







## Time of convergence of NS

$$T \propto T_{\mathcal{L}} \times f_{\text{sampler}} \times D_{\text{KL}} \times n_{\text{live}} \tag{5}$$

## Uncertainty in $\log \mathcal{Z}$

$$\sigma \propto \sqrt{D_{\text{KL}}/n_{\text{live}}} \tag{6}$$

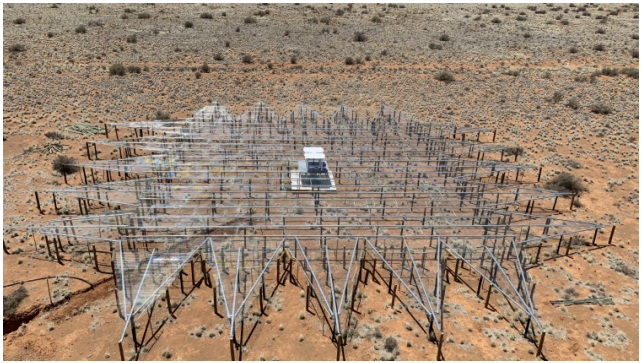
Precision-normalized runtime has quadratic dependence on KL divergence. 2212.01760







One way to do this (REACH):







# Reducing $D_{\mathrm{KL}}$

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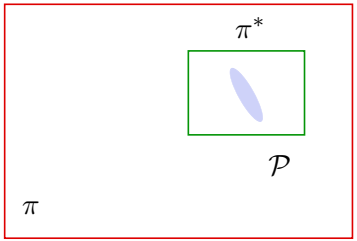


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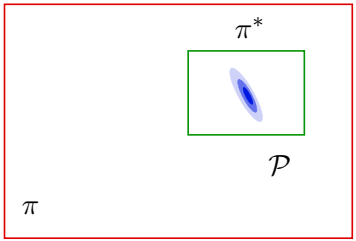


- Perform low resolution (low live points) run first to roughly identify where posterior lies.
- Then set off second, high resolution, run with **narrower** box prior (much quicker).
- Evidence has **changed** (since different prior), but easy to correct (multiply new evidence by $\frac{V_{\pi^*}}{V_\pi}$)






- Can iterate on this by using **normalizing flows** (NF) to learn the rough posterior.

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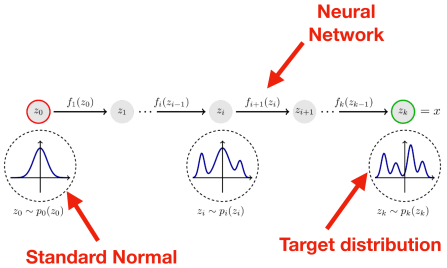
- NFs perform density estimation, by learning a series of invertible mappings from the standard normal distribution to the target (posterior).







# NF + PR

- Use **normalizing flows** (NF) to learn the rough posterior, and use this as our updated prior, $\pi^*$.
- In this case, can't do our trick of correcting the second evidence by volume ratio, $\frac{V_{\pi^*}}{V_\pi}$!
- Must rely on another technique to get around this!

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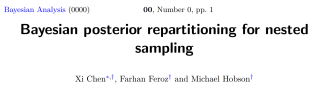
Posterior repartitioning (PR) can help us with this! (see e.g. 2212.01760)


Bayesian Analysis (0000) 00, Number 0, pp. 1

**Bayesian posterior repartitioning for nested sampling**

Xi Chen*,†, Farhan Feroz† and Michael Hobson†


Improving the efficiency and robustness of nested sampling using posterior repartitioning

Xi Chen · Michael Hobson · Saptarshi Das · Paul Gelderblom


Article

SuperNest: accelerated nested sampling applied to astrophysics and cosmology†

Aleksandr Petrosyan[1,2,3,*] & Will Handley[1,2,4,†]





# Posterior repartitioning (PR)

- Evidence and posterior only depend on product of $\mathcal{L}$ and $\pi$:

$$\mathcal{Z} = \int \mathcal{L}(\theta)\pi(\theta)d\theta \qquad (7) \qquad\qquad \mathcal{P}(\theta) = \frac{\mathcal{L}(\theta)\pi(\theta)}{\mathcal{Z}} \qquad (8)$$

We are free to redefine the likelihood and prior however we like - as long as the product is the same! arXiv:1908.04655

$$\tilde{\mathcal{Z}} = \int \tilde{\mathcal{L}}(\theta)\tilde{\pi}(\theta)d\theta = \int \mathcal{L}(\theta)\pi(\theta)d\theta = \mathcal{Z} \qquad (9)$$




# PR (cont.)

- Many sampling algorithms do not distinguish between $\mathcal{L}$ and $\pi$ at the algorithmic level.
- e.g. Metropolis-Hastings acceptance ratio only depends on the **joint distribution**, $\mathcal{L}(\theta)\pi(\theta)$.
- Nested sampling does distinguish between prior and likelihood at the algorithmic level, by 'sampling from the prior $\pi$, subject to the hard likelihood constraint, $\mathcal{L}$'.

- $\mathcal{Z}$ and $\mathcal{P}$ will not change if we repartition $\mathcal{L}$ and $\pi$, **but $\mathcal{D}_{\mathsf{KL}}$ will**.





# PR-NS w/ NFs

$$\pi(\theta) \longrightarrow \mathrm{NF}(\theta)$$





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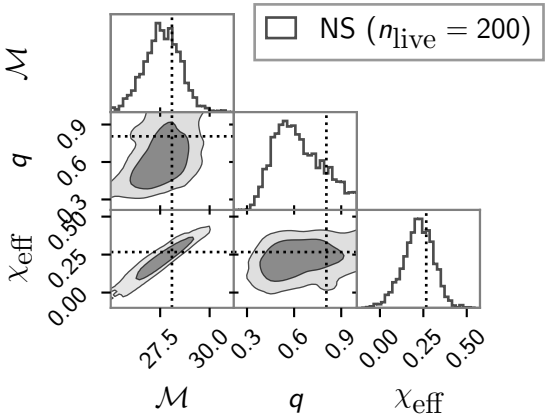
$$\mathcal{D}_{\mathrm{KL}} \approx \log \frac{V_{\mathrm{NF}}}{V_{\mathcal{P}}}$$





# Demo on simulated example

- Perform low resolution run on simulated data.







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- Perform low resolution run on simulated data.
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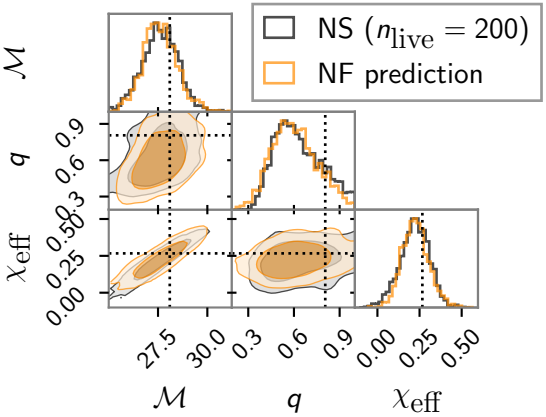





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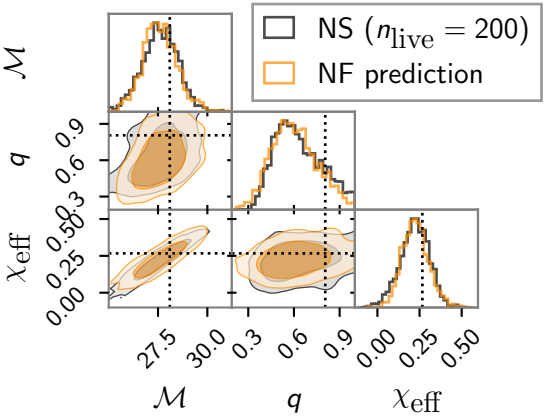





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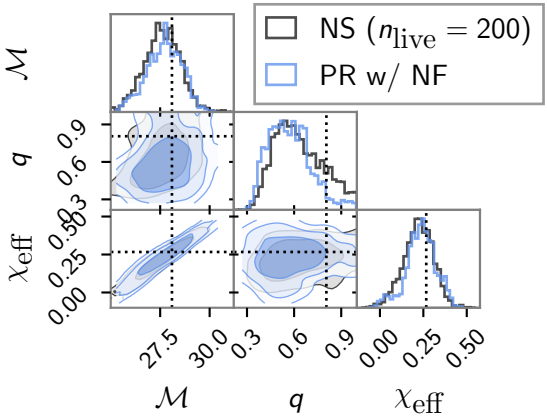





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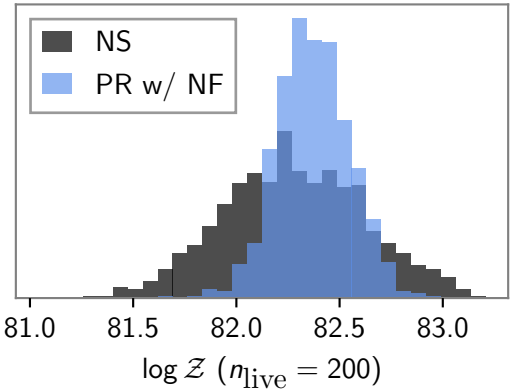
- Train NF on the weighted samples.
- Use this as 'repartitioned prior' for new high resolution run (using PR to also update likelihood accordingly to same evidences and posteriors out).




Same answer as doing a full resolution pass of NS, but 7x faster (precision-normalized).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# CPUs & GPUs in Scientific Computing

- **CPUs (Central Processing Units):**
  - Optimized for a wide range of tasks.
  - Equipped with a limited number of powerful cores.
  - Excel at sequential, complex calculations and intricate decision-making.
  - Ideal for tasks featuring non-uniform workloads and conditional branching.

- **GPUs (Graphics Processing Units):**
  - Architectured with thousands of smaller, efficient cores.
  - Tailored for massive parallel arithmetic operations.
  - Best suited for repetitive, data-parallel tasks.
  - Increasingly used in scientific computing.




# Advantages of GPUs for GW inference

- **Likelihood Evaluation:**
  - Frequency bins are independent, so waveforms can be evaluated across many bins in parallel.
  - On Nvidia A100 GPU, we can evaluate the waveform model $\approx O(10^9)$ times in a second for different frequencies or source parameters [2302.05333].
- **Sampling:**
  - Multiple chains can be executed in parallel.
  - For NS, if using a slice sampler, can run many slicing operations at once.

Parallel processing power of GPUs can speed up Bayesian inference by factor of thousands.





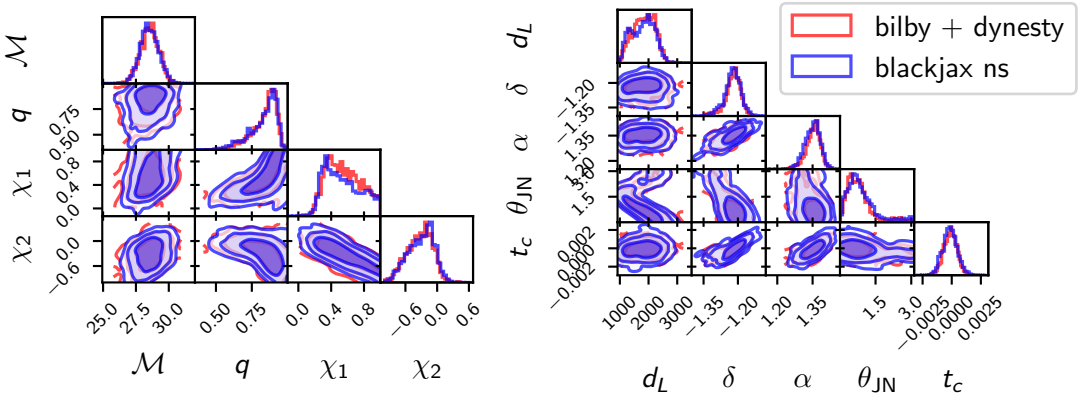

- RIPPLE: JAX implementation of models for GPU-accelerated waveform calls
- JIM uses RIPPLE + FLOWMC

- RIPPLE: JAX implementation of models for GPU-accelerated waveform calls
- JIM uses RIPPLE + FLOWMC

## BLACKJAX NS

- Nested sampling implementation in BLACKJAX, developed by David Yallup.
- 11 parameter nested sampling run on GW150914 in minutes

# Injection examples





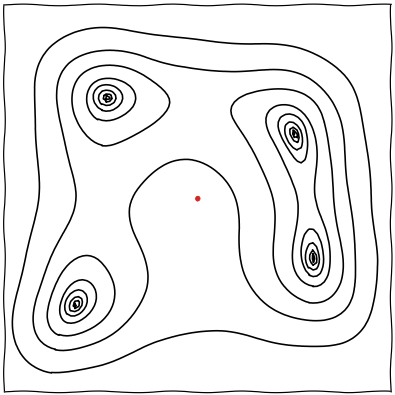

# Future of scientific computing

- **Shift in Hardware Paradigm:**
  - Scientific computing is increasingly relying on architectures that favor parallel operations.
  - Computing power will become heavily skewed towards GPUs.
- **Implications for Research:**
  - GPUs are becoming the norm in many areas, including astrophysics.
  - Adapting our algorithms to modern hardware is essential to keep pace with the cutting edge of computing power.
- **For GWs:**
  - Need to get more waveforms models onto GPUs!


# Conclusions

- 3G + LISA era presents significant challenges for data analysis
- Current standard inference methods, including traditional nested sampling, will not scale well
- ML-accelerated sampling and GPU-accelerated pipelines work towards addressing these challenges, and offer a complementary approach to SBI

## MCMC



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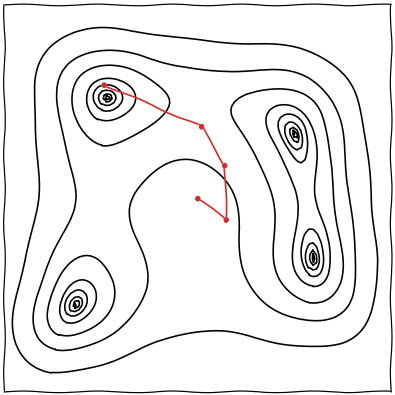

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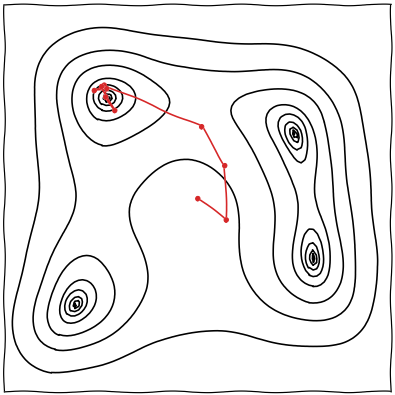

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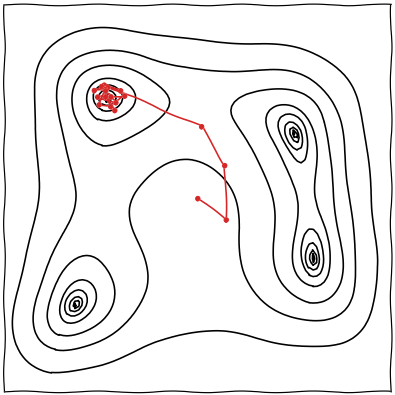

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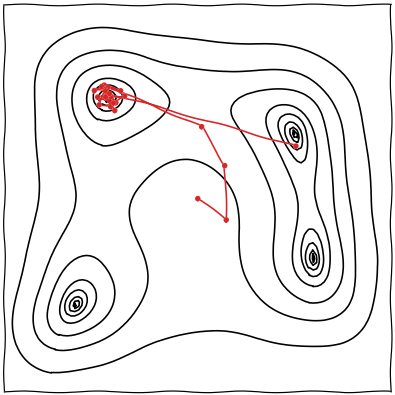

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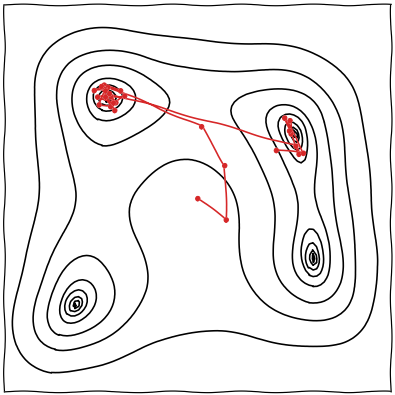

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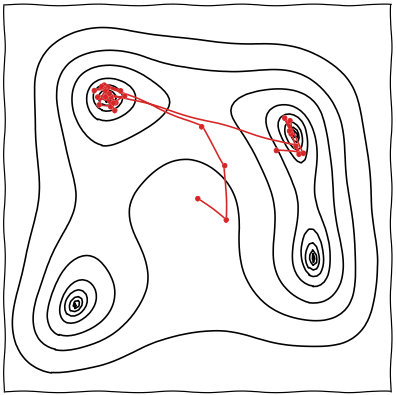

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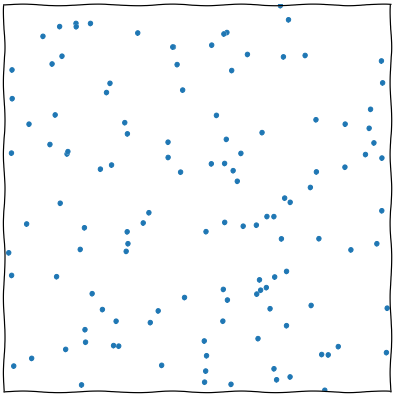

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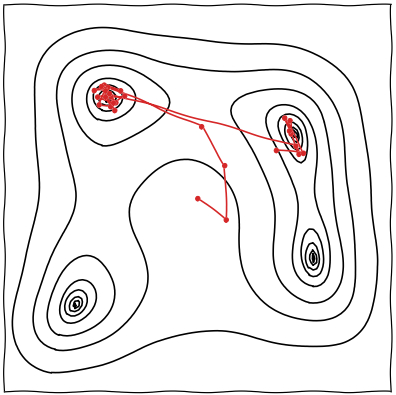

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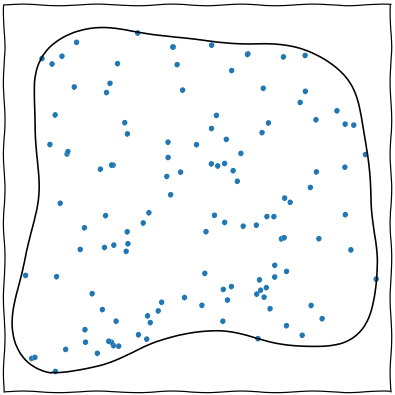

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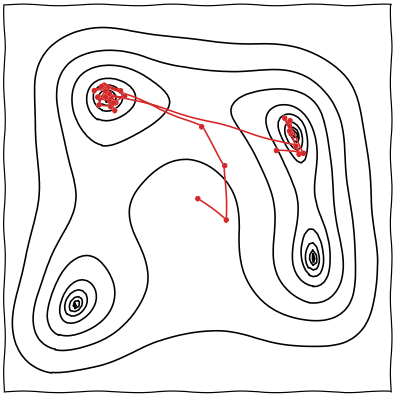

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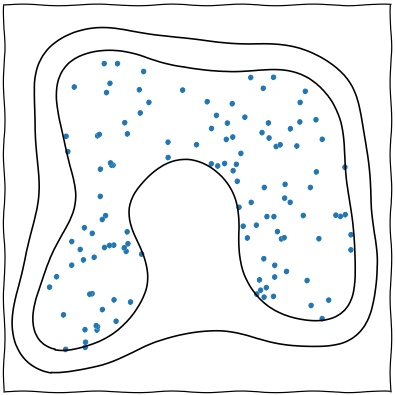

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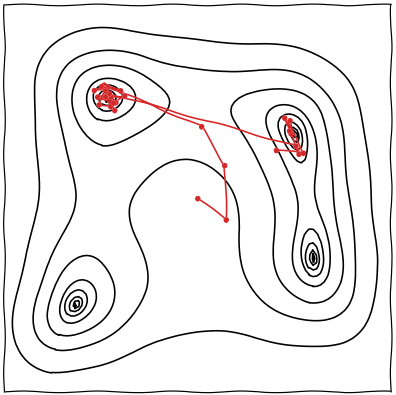

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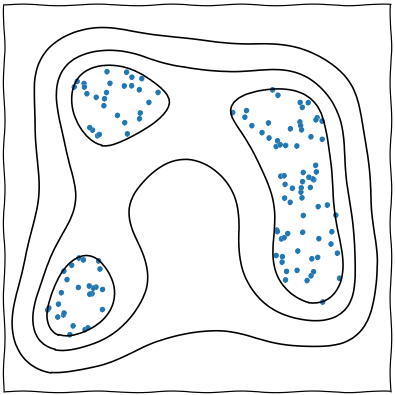

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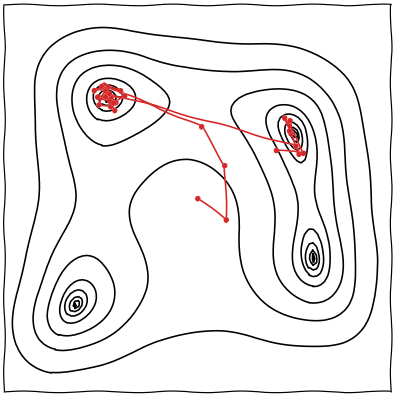

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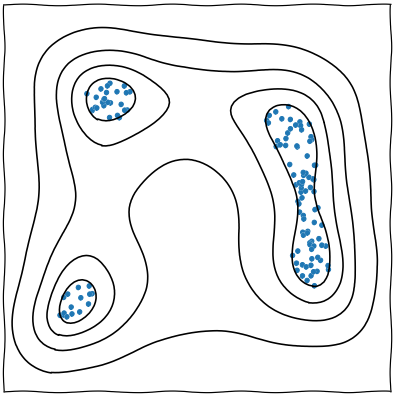

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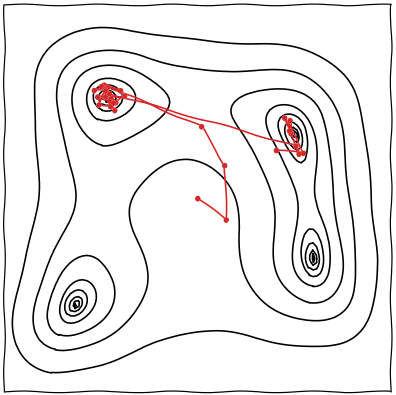

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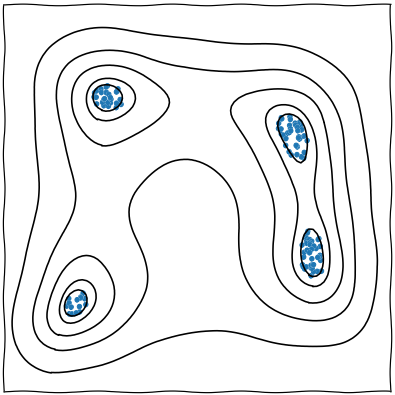

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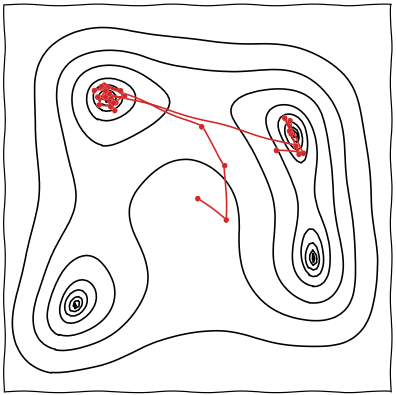

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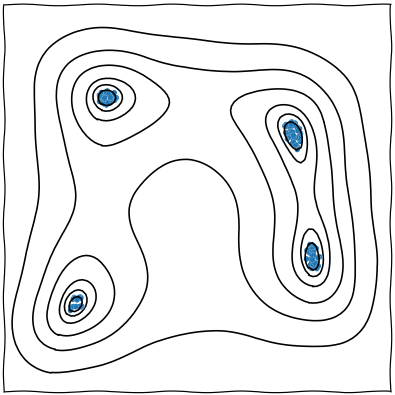

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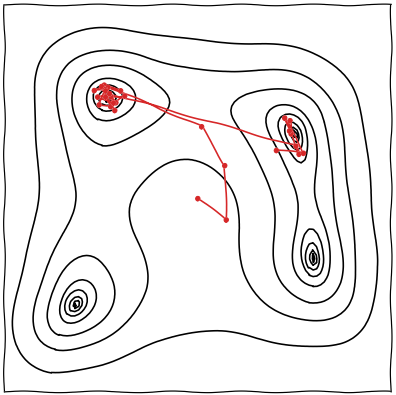

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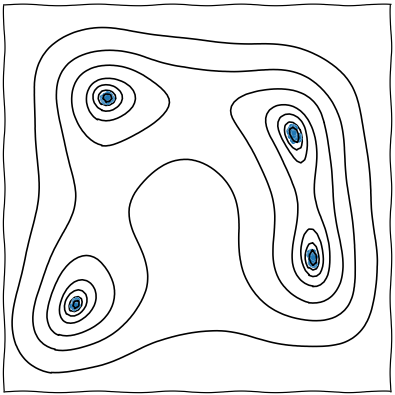

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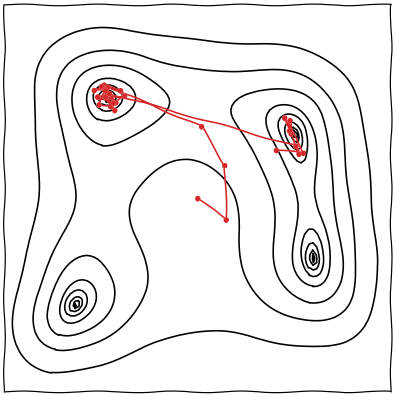

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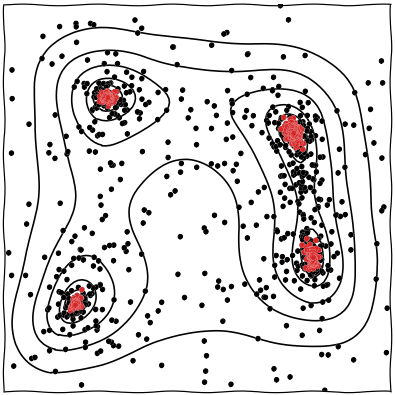

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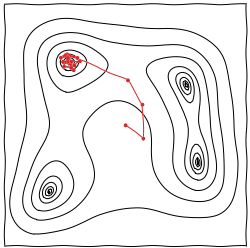

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