

# The scaling frontier of nested sampling

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1<sup>st</sup> July 2024



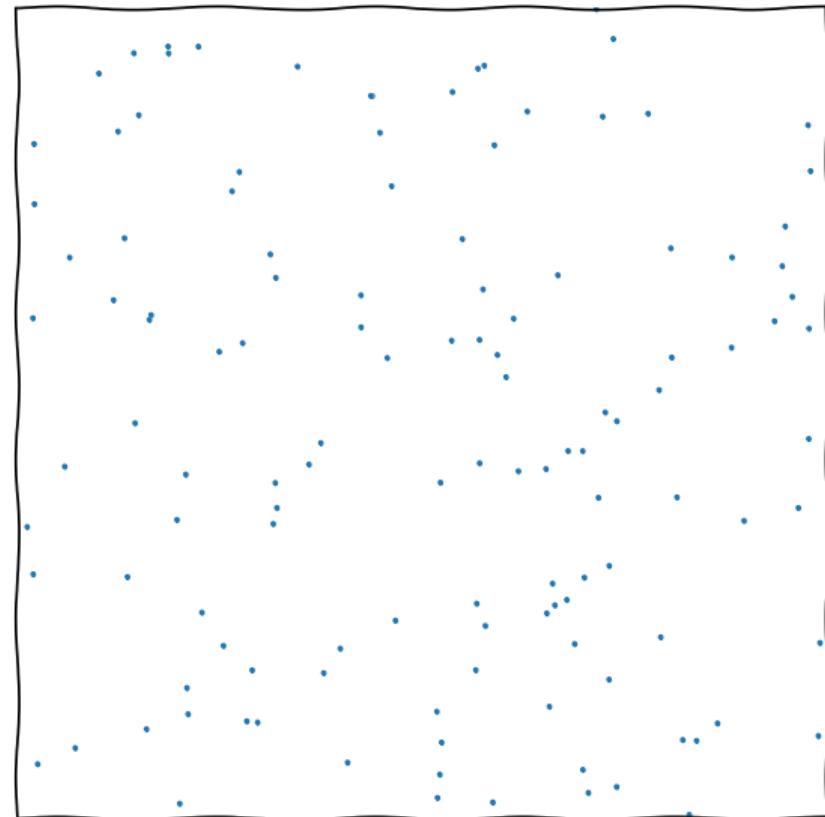
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## Recap: the nested sampling meta-algorithm

- ▶ Start with  $n_{\text{live}}$  random prior samples  $\theta \sim \pi$ .
- ▶ Delete lowest likelihood sample, and replace with a new one at higher 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  $\sim \frac{1}{n_{\text{live}}}$  of their volume.
- ▶ This is an exponential contraction, so

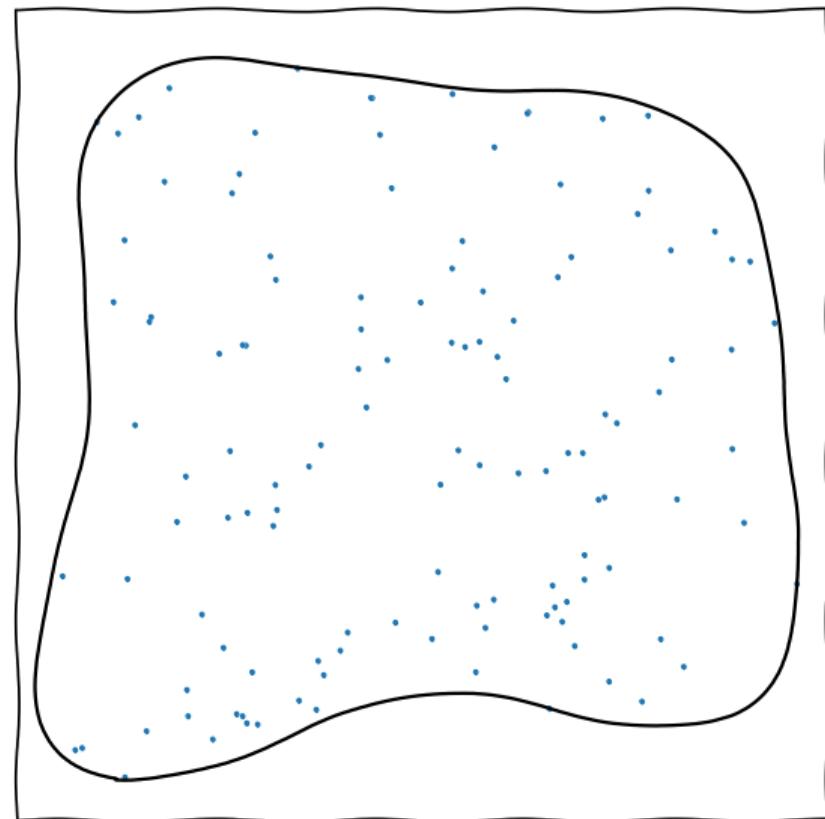
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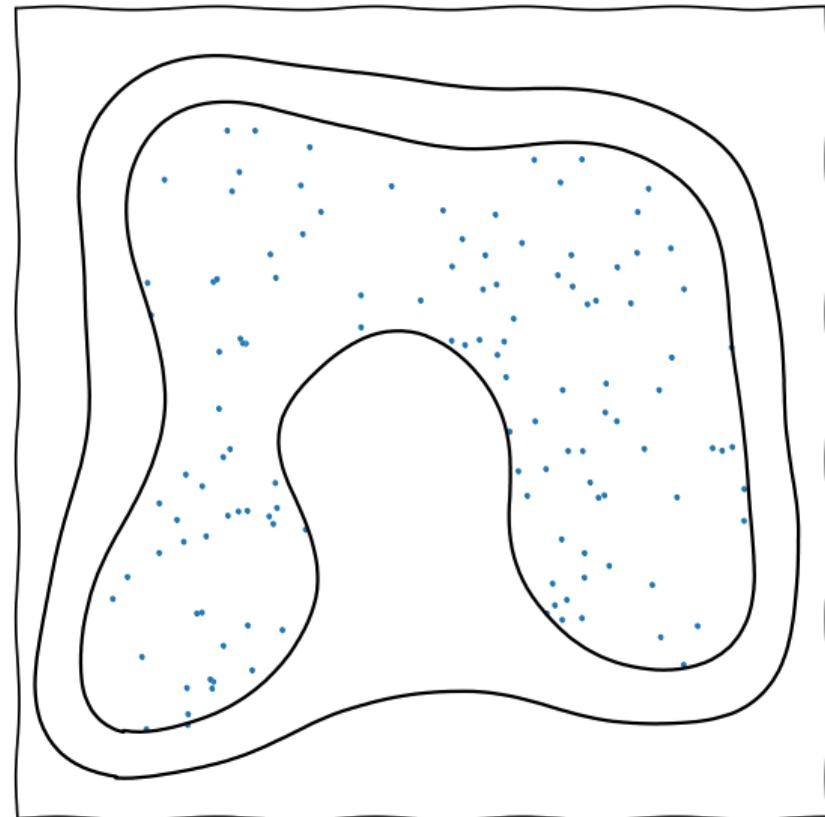
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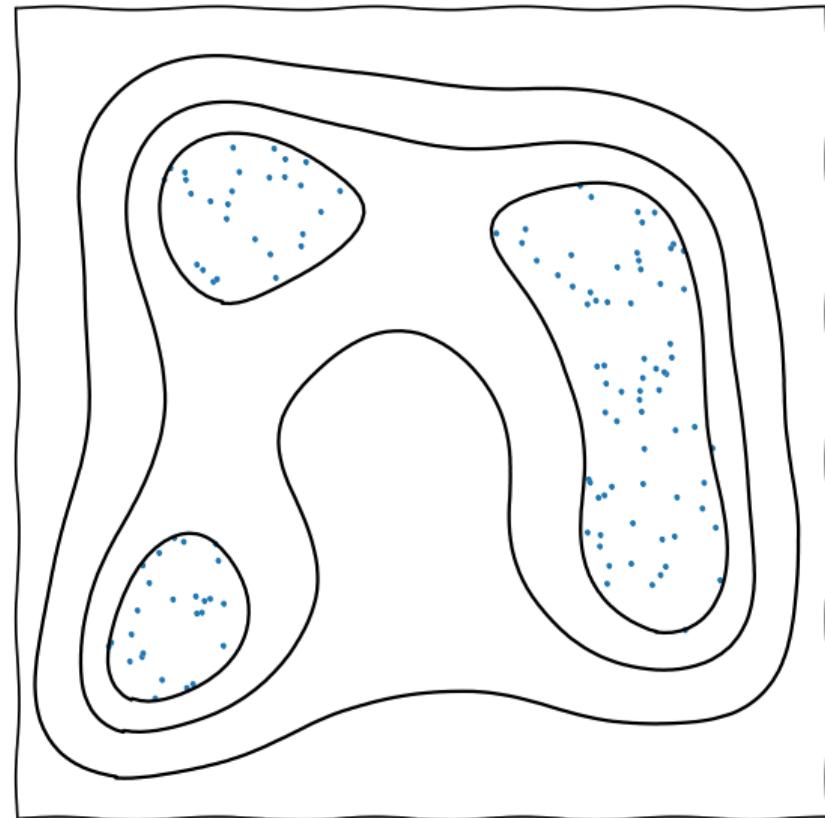
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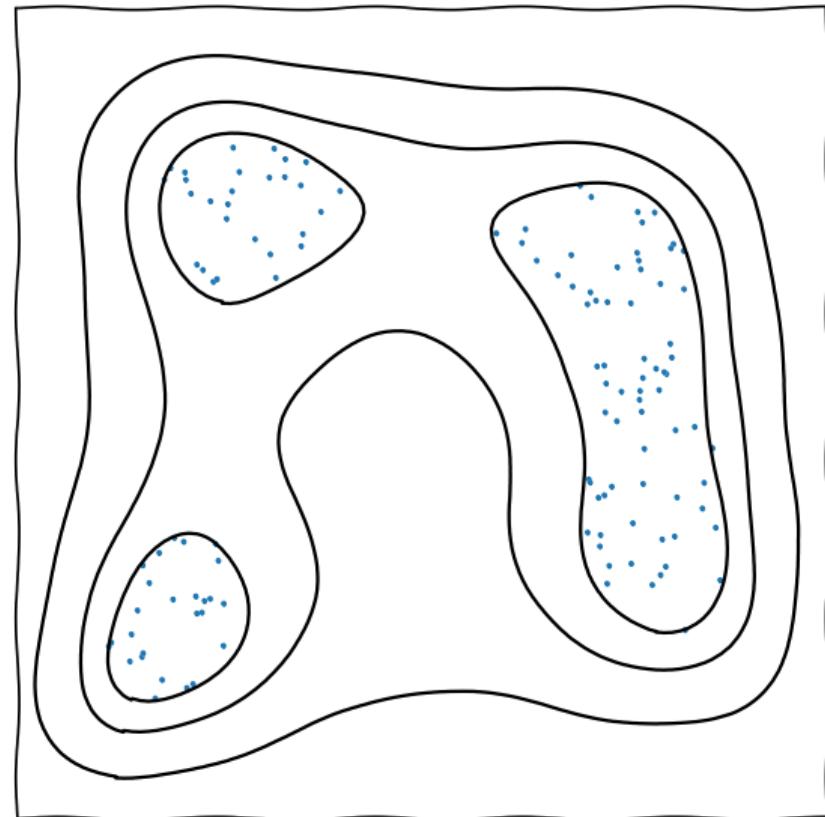
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$$\mathcal{Z} = \int \mathcal{L} \pi d\theta \approx \sum_{i \in \text{dead}} \mathcal{L}_i \Delta X_i, \quad X_i = e^{-(i \pm \sqrt{i})/n_{\text{live}}}$$



# Kullback Leibler divergence (or entropy $H$ or, information gain)

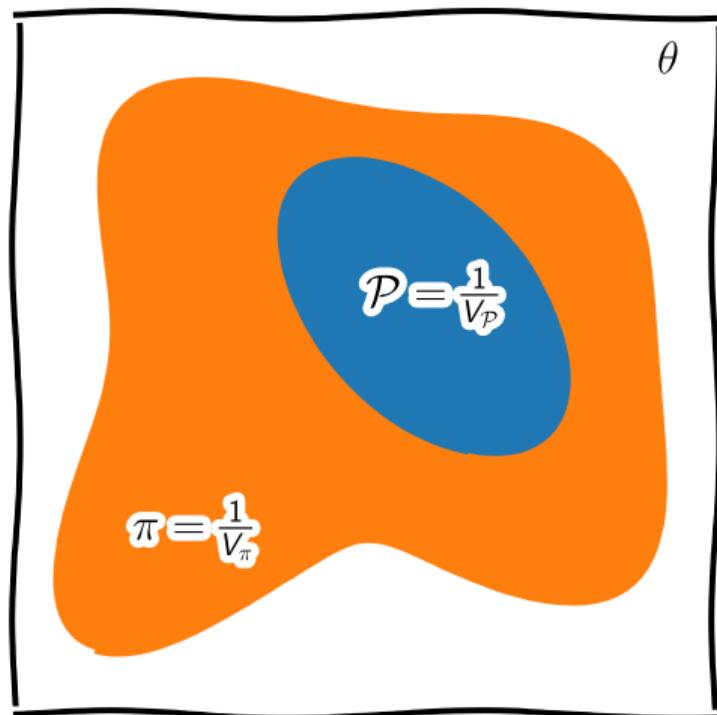
- The KL divergence between prior  $\pi$  and posterior  $\mathcal{P}$  is defined as:

$$\mathcal{D}_{\text{KL}} = \left\langle \log \frac{\mathcal{P}}{\pi} \right\rangle_{\mathcal{P}} = \int \mathcal{P}(\theta) \log \frac{\mathcal{P}(\theta)}{\pi(\theta)} d\theta.$$

- Whilst not a distance,  $\mathcal{D} = 0$  when  $\mathcal{P} = \pi$ .
- Occurs in the context of machine learning as an objective function for training functions.
- In Bayesian inference it can be understood as a log-ratio of “volumes”:

$$\mathcal{D}_{\text{KL}} \approx \log \frac{V_{\pi}}{V_{\mathcal{P}}}.$$

(this is exact for top-hat distributions).

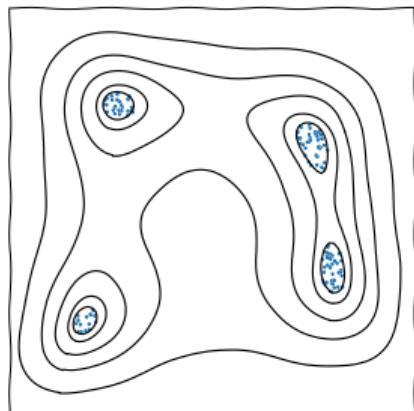
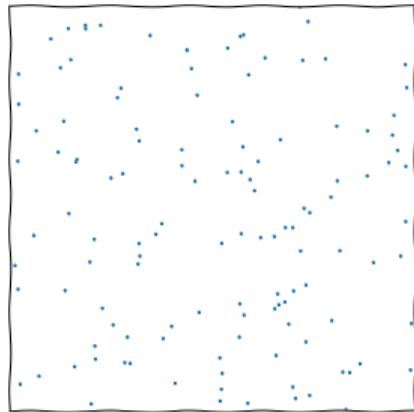


# How fast in nested sampling?



$$T = T_{\mathcal{L}} \times \underbrace{n_{\text{live}} \times \mathcal{D}_{\text{KL}}}_{n_{\mathcal{L}}} \times f_{\text{sampler}},$$

- ▶ NS compresses the volume  $X$  of the live points from prior  $X = 1$  to posterior  $X = e^{-\mathcal{D}_{\text{KL}}}$ .
- ▶ It does this exponentially so at iteration  $i$ ,  $X_i = e^{-i/n_{\text{live}}}$
- ▶ Need  $e^{-n_{\text{dead}}/n_{\text{live}}} \sim e^{-\mathcal{D}_{\text{KL}}} \Rightarrow n_{\text{dead}} \sim n_{\text{live}} \times \mathcal{D}_{\text{KL}}$ .
- ▶ It takes a  $f_{\text{sampler}}$  likelihood evaluations to generate a new live point, so  $n_{\mathcal{L}} = n_{\text{dead}} \times f_{\text{sampler}}$
- ▶ It takes  $T_{\mathcal{L}}$  seconds to call the likelihood, so  $T = T_{\mathcal{L}} \times n_{\mathcal{L}}$



Further reading [2312.00294]

aeons: approximating the end of nested sampling, (Zixiao Hu et al)

# How accurate is nested sampling?

Lukas Hergt



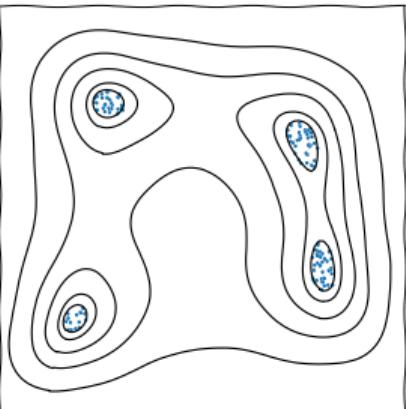
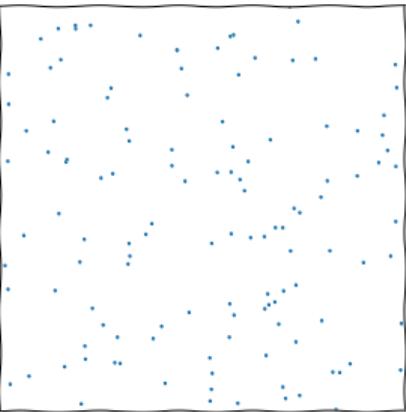
PhD 2020

$$\sigma(\log \mathcal{Z}) \approx \sqrt{\mathcal{D}_{\text{KL}} / n_{\text{live}}}$$

- ▶ From the Occam's razor equation [2102.11511]:

$$\log \mathcal{Z} = \langle \log \mathcal{L} \rangle_{\mathcal{P}} - \mathcal{D}_{\text{KL}}$$

- ▶ The dominant error is in the estimation of compression  $\mathcal{D}_{\text{KL}}$
- ▶ At each iteration, compress by  $\exp(-\frac{1}{n_{\text{live}}} \pm \frac{1}{n_{\text{live}}})$
- ▶ After  $n_{\text{dead}}$  iterations, compressed by  $e^{-\frac{n_{\text{dead}}}{n_{\text{live}}} \pm \frac{\sqrt{n_{\text{dead}}}}{n_{\text{live}}}} = e^{-\mathcal{D}_{\text{KL}}}$
- ▶ As before  $n_{\text{dead}} \sim n_{\text{live}} \times \mathcal{D}_{\text{KL}}$
- ▶  $\sigma(\log \mathcal{Z}) = \sigma(\mathcal{D}_{\text{KL}}) = \frac{\sqrt{n_{\text{dead}}}}{n_{\text{live}}} = \sqrt{\frac{\mathcal{D}_{\text{KL}}}{n_{\text{live}}}}$



# The scaling frontier of nested sampling

## How fast in nested sampling?

$$T = T_{\mathcal{L}} \times n_{\text{live}} \times \mathcal{D}_{\text{KL}} \times f_{\text{sampler}}$$

## How accurate is nested sampling?

$$\sigma(\log \mathcal{Z}) \approx \sqrt{\mathcal{D}_{\text{KL}} / n_{\text{live}}}$$

in  $d$  dimensional parameter space:

$T_{\mathcal{L}}$ : likelihood eval time

$\sim \mathcal{O}(d)$

- ▶ Algorithmically improving  $f_{\text{sampler}}$  is only a fraction of the story!

$n_{\text{live}}$ : number of live points

$\sim \mathcal{O}(d)$

- ▶  $\mathcal{D}_{\text{KL}}$  appears twice, so improvements here are quadratically important.

$\mathcal{D}_{\text{KL}}$ : KL divergence from prior to

posterior  $\approx \log V_{\pi} / V_{\mathcal{P}}$   $\sim \mathcal{O}(d)$

- ▶ Gradients give you  $d$  more information.

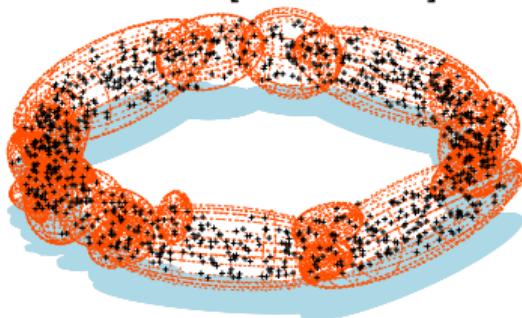
$f_{\text{sampler}}$ : efficiency of point generation

region  $\sim \mathcal{O}(e^{d/d_0})$  or path  $\sim \mathcal{O}(d)$

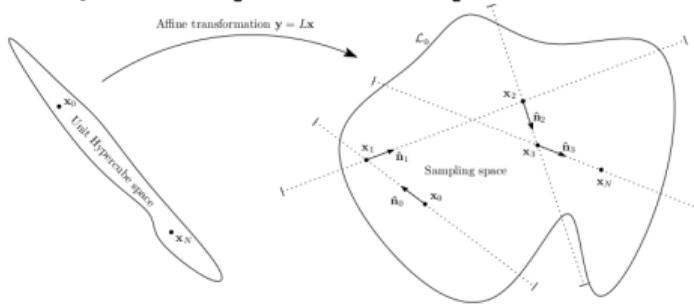
- ▶  $T \sim \mathcal{O}(d^4)$  whilst polynomial is far from ideal! – Let's unpack the caveats.

# $f_{\text{sampler}}$ : live-point generation efficiency

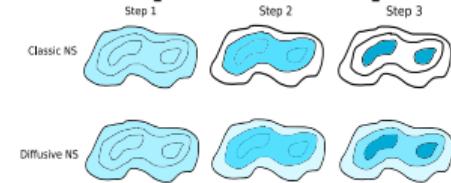
MultiNest [0809.3437]



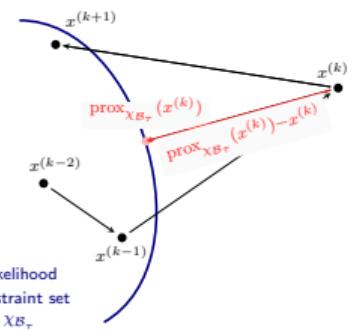
PolyChord [1506.00171]



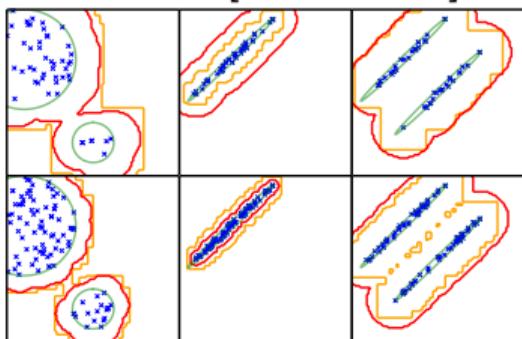
DNest [1606.03757]



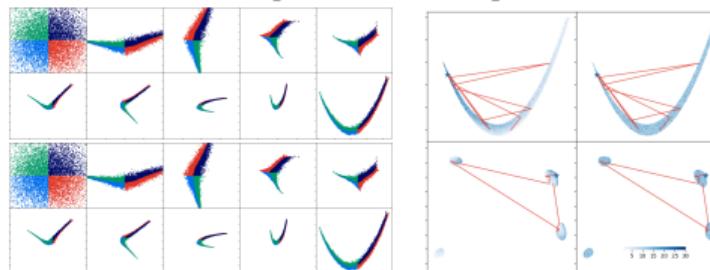
ProxNest [2106.03646]



UltraNest [2101.09604]



NeuralNest [1903.10860]



nessai [2102.11056]

nora [2305.19267]

jaxnest [2012.15286],

[willhandley.co.uk/talks](http://willhandley.co.uk/talks)

nautilus [2306.16923]

<wh260@cam.ac.uk>

dynesty [1904.02180]

nested\_fit [1611.10189]

pymatnext [0906.3544]

# $f_{\text{sampler}}$ : live-point generation efficiency

- ▶ 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  $d > d_0 \sim 10$ .
- ▶ for high dimensions, state of the art is linear
- ▶ Recent innovations in UltraNest allow self-tuning of efficiency for rejection sampling

## 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.

## Frontier

Can chain-based NS self-tune chain length to be sub-linear at run time?

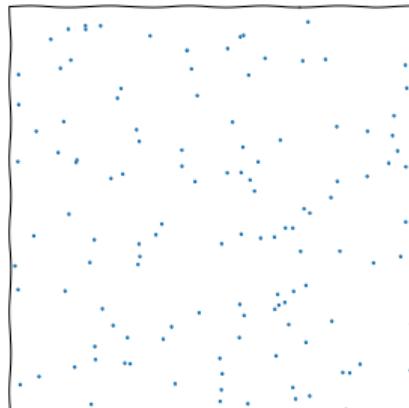
## $n_{\text{live}}$ : the number of live points

There are two reasons one might increase the number of live points:

### Multimodality

At each iteration, if a mode has a basin of attraction  $< 1/n_{\text{live}}$  of the space you are more likely than not to miss it

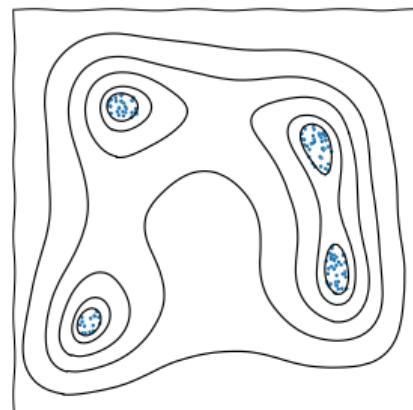
- ▶ No reason to expect multimodality to have anything so simple as linear scaling with dimension.



### Accuracy

$$\text{Evidence error } \sigma(\log \mathcal{Z}) = \sqrt{\mathcal{D}_{\text{KL}} / n_{\text{live}}}$$

- ▶ So if  $\mathcal{D}_{\text{KL}} \sim \mathcal{O}(d)$ , then to maintain the same quality of inference have to scale  $n_{\text{live}}$  at the same rate.



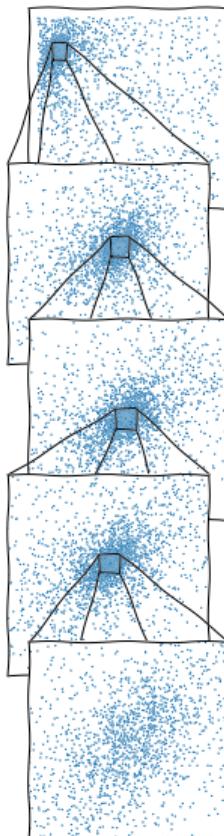
### Frontier

Can we make this “mode missing” argument more quantitative?

# $T_{\mathcal{L}}$ : the time to evaluate the likelihood

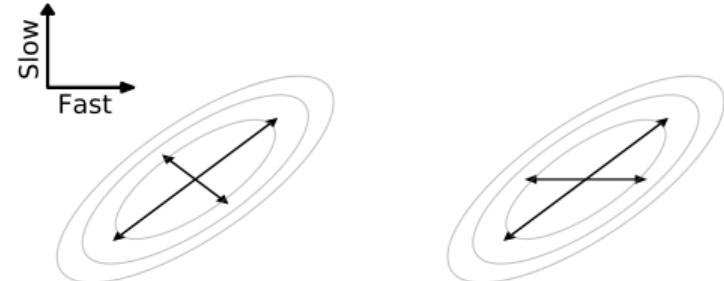
## Acceleration/emulation

- ▶ Increasing emphasis of using machine learning/AI emulators to accelerate slow components of pipelines
- ▶ Nested sampling dead points are good at training emulators of likelihoods, due to their nose-to-tail sampling (Brewer's "Dead measure")
- ▶ BAMBI [1110.2997] does this at run-time to accelerate nested sampling



## Fast-slow hierarchies

- ▶ Success in cosmology where some parameters take longer than others
- ▶ reduces  $T_{\mathcal{L}} \sim \mathcal{O}(d_{\text{slow}})$ .



## Frontier

Can fast-slow hierarchies be better automated within algorithms?

## Frontier

Is BAMBI the best we can do?

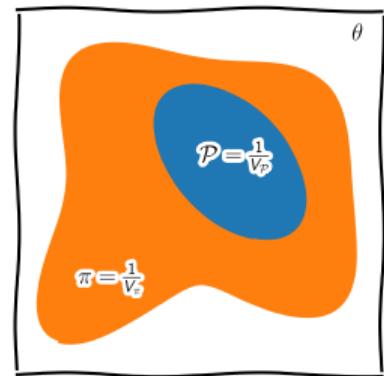
# $\mathcal{D}_{\text{KL}}$ : The Kullback Leibler divergence

- ▶ Naively  $\mathcal{D}_{\text{KL}} \sim \mathcal{O}(d)$ , since if you have  $d$  *useful* parameters, you would expect to need to compress each of them, so each contribute linearly to the volume contribution
- ▶ From the Occam's razor equation however:

$$\log \mathcal{Z} = \langle \log \mathcal{L} \rangle_{\mathcal{P}} - \mathcal{D}_{\text{KL}}$$

a large  $\mathcal{D}_{\text{KL}}$  means a “bad” model

- ▶ Methods which explore models weighted by their evidence won't spend as much time in high  $\mathcal{D}_{\text{KL}}$  regions [1506.09024].
- ▶ There's also an intuition of the KL being “information”, so increasing the number of parameters shouldn't extract more content.
- ▶ The KL divergence is a property of the model, so one would initially consider this to be something that the user has no control over...



$$\mathcal{D}_{\text{KL}} = \log \frac{V_{\pi}}{V_{\mathcal{P}}}$$

$$\mathcal{D}_{\text{KL}} = \left\langle \log \frac{\mathcal{P}}{\pi} \right\rangle_{\mathcal{P}}$$

# Posterior repartitioning

Aleksandr Petrosyan

MSci 2021



- ▶ Almost all sampling algorithms (MH, HMC, SMC) are only sensitive to the product of likelihood and prior  $\mathcal{L} \times \pi$ .
- ▶ In practice this manifests as many codes implementing “prior terms” in the likelihood (or visa-versa) with no ill effect
- ▶ Nested sampling is unusual, in that one “samples from the prior  $\pi$ , subject to a hard constraint  $\mathcal{L} > \mathcal{L}_*$ .”:

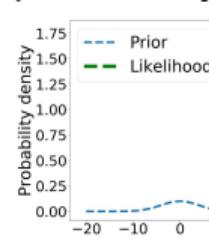
$$\{\theta \sim \pi : \mathcal{L}(\theta) > \mathcal{L}_*\}$$

- ▶ This separates the prior from the likelihood at an algorithmic level.

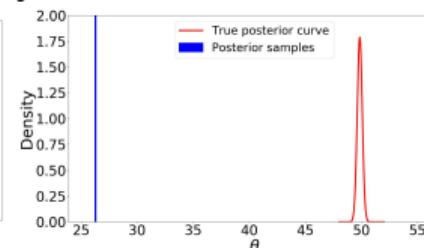
- ▶ One can therefore repartition the likelihood and prior  $(\mathcal{L}, \pi) \rightarrow (\tilde{\mathcal{L}}, \tilde{\pi})$ , providing

$$\mathcal{L} \times \pi = \tilde{\mathcal{L}} \times \tilde{\pi}$$

- ▶ This moves pieces between likelihood and prior that you have analytic control over.



(a) unrepresentative prior,  $\theta_* = 50$



(b) estimated posterior by MultiNest,  $\theta_* = 50$

- ▶ Chen, Feroz & Hobson [1908.04655] invented this to deal with misspecified priors

# Posterior repartitioning for acceleration

Metha Prathaban

PhD



## Key idea

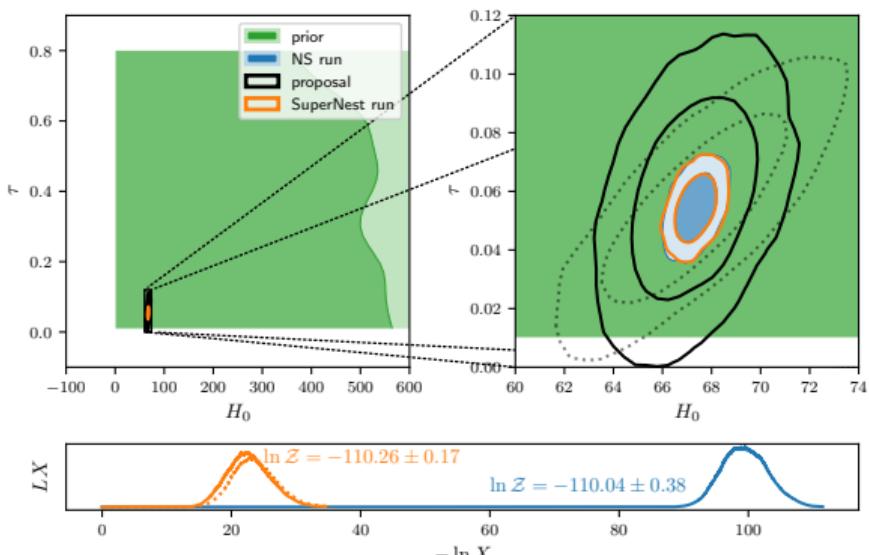
Whilst posteriors and evidences are invariant to repartitioning  $\mathcal{L} \rightarrow \tilde{\mathcal{L}}$ , the KL divergence is not.

- For constant “run quality”  $\sigma$ ,

$$T = T_{\mathcal{L}} \times n_{\text{live}} \times \mathcal{D}_{\text{KL}} \times f_{\text{sampler}}, \quad \sigma \approx \sqrt{\mathcal{D}_{\text{KL}} / n_{\text{live}}}$$
$$\Rightarrow T = T_{\mathcal{L}} \times \sigma \times \mathcal{D}_{\text{KL}}^2 \times f_{\text{sampler}}$$

so if you can reduce the KL divergence, then quadratic gains to be made

- SuperNest [2212.01760]
- Ongoing work with Metha Prathaban & Harry Bevis.



## Frontier

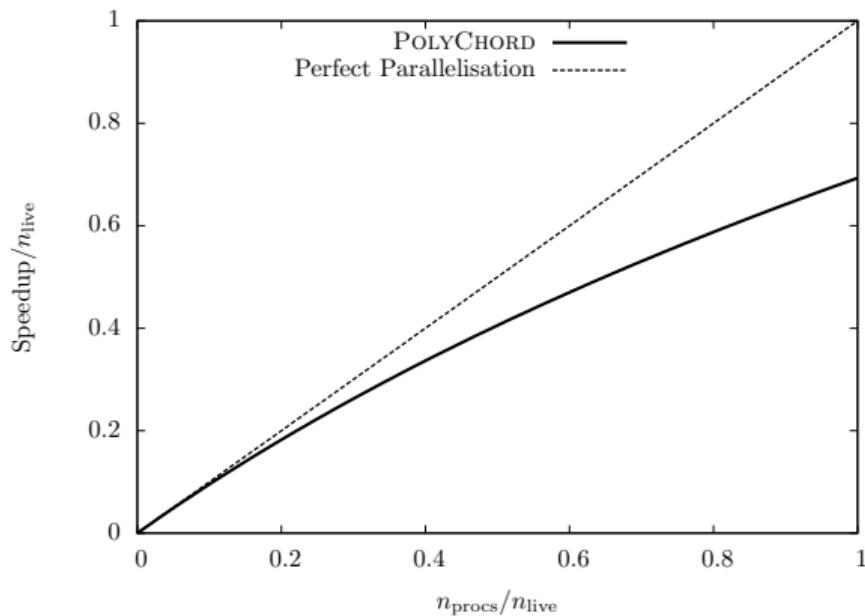
Can we use posterior repartitioning to quadratically reduce the run time of nested sampling?

# Parallelisation

- ▶ Nested sampling is well-suited to parallelisation, up to the number of live points, in contrast with MH/HMC
- ▶ I've known people run nested sampling on 10,000 CPUs
- ▶ This is in addition to any existing parallelisation in the likelihood
- ▶ Dynamic nested sampling very useful here adding machinery for throwing away multiple points [1704.03459]

## Frontier

Are there any other parallelisation strategies, e.g. clustering/divide & conquer?



# Nested sampling with gradients

Namu Kroupa

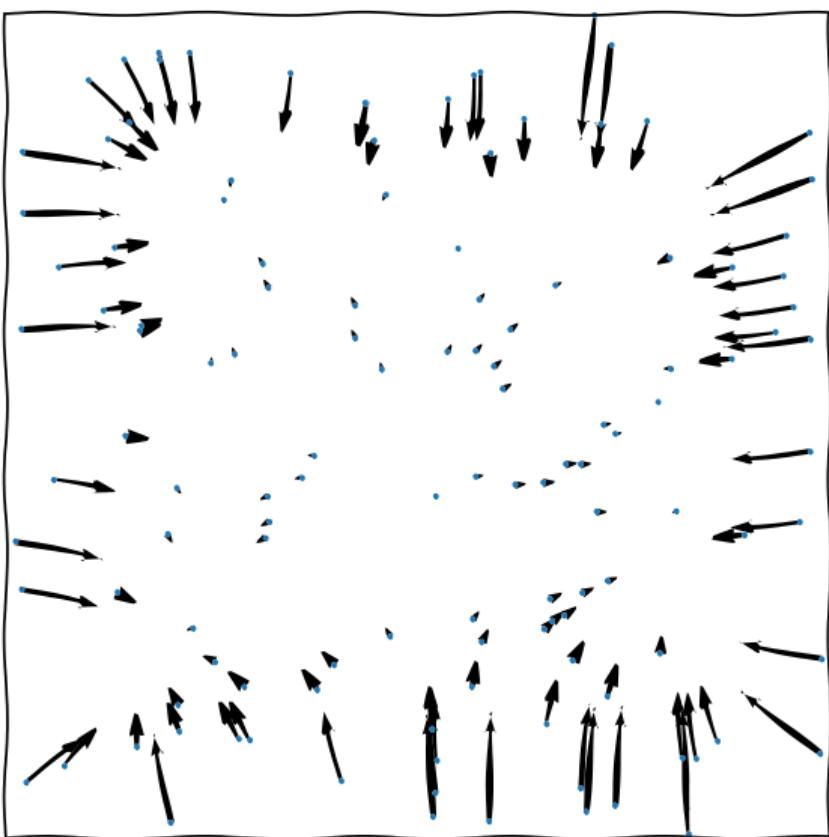


PhD (with Gábor Csányi)

- ▶ In principle, gradients give you  $\sim \mathcal{O}(d)$  pieces of information to help with exploration
- ▶ With modern automatic differentiation codes (JAX, PyTorch, TensorFlow, Enzyme ...) these now come “for free”.
- ▶ However nested sampling has unique challenges, so plugging in default (e.g. HMC/Langevin) algorithms does not work

## Frontier

Can you come up with a nested sampling strategy that uses gradients and scales pass  $d \sim \mathcal{O}(100)$ ?



# Nested sampling with gradients

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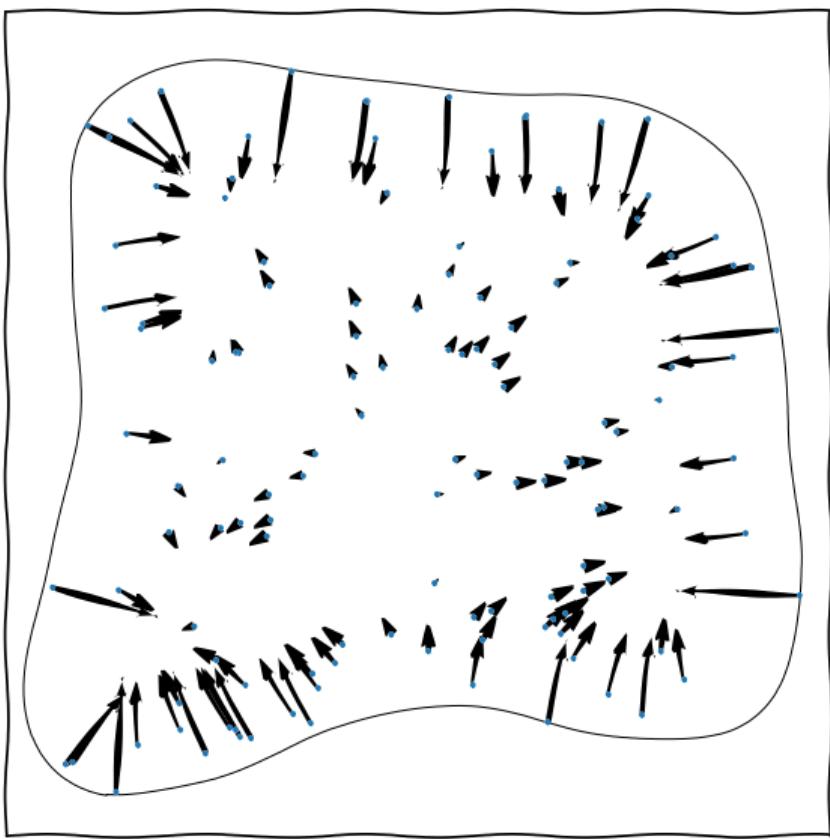
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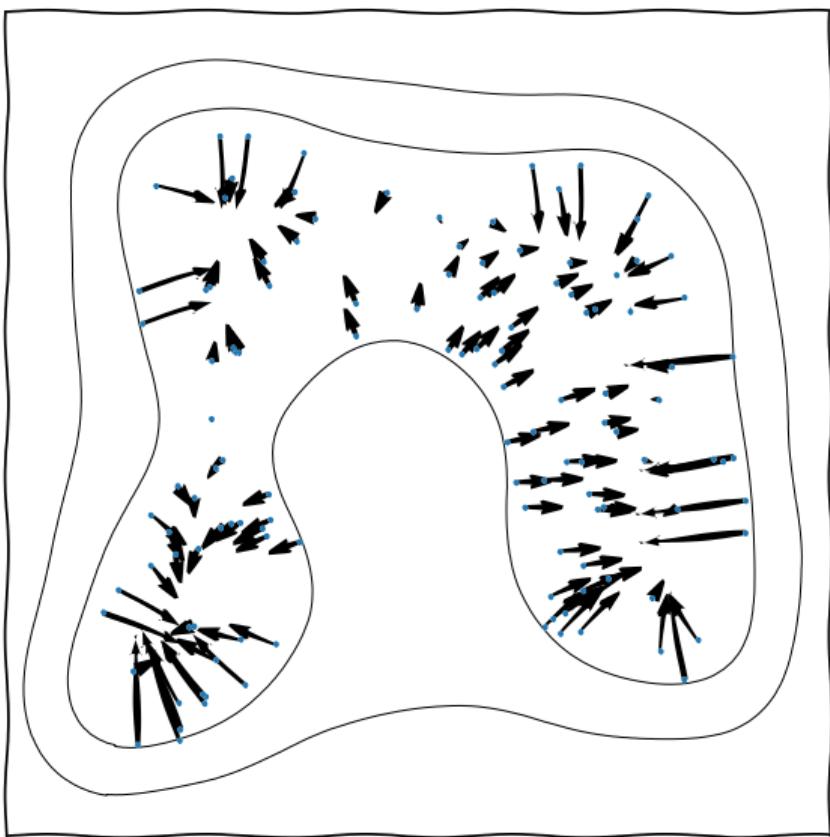
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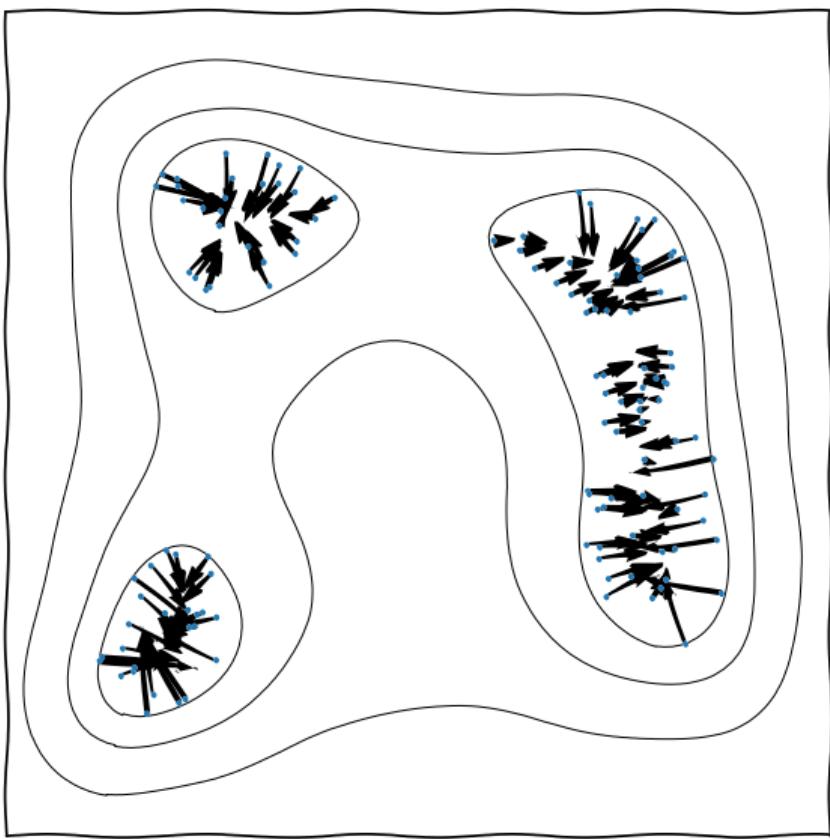
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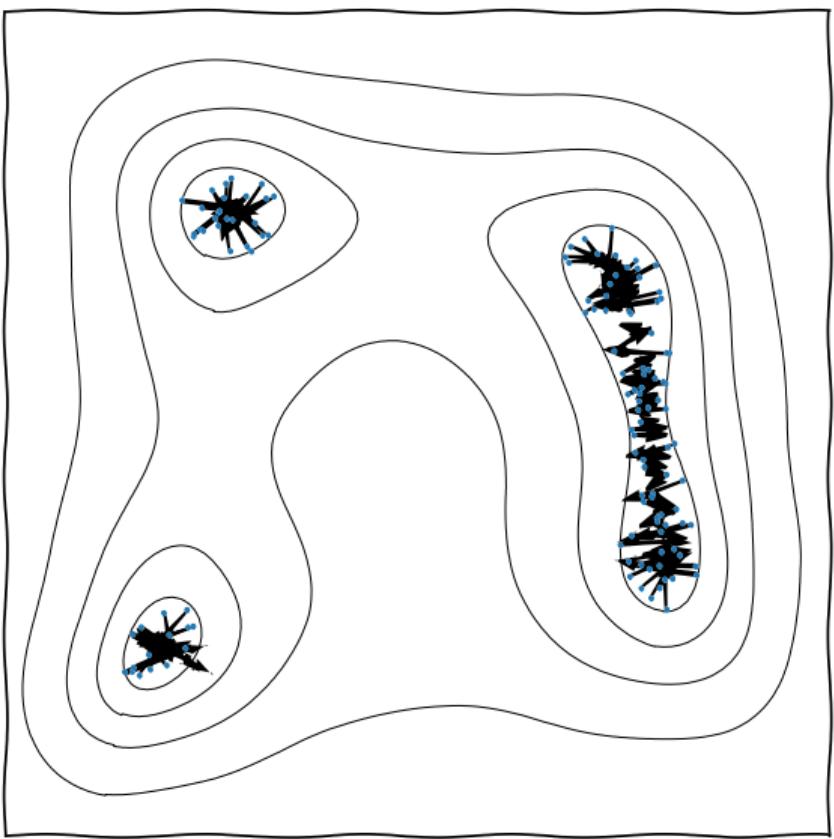
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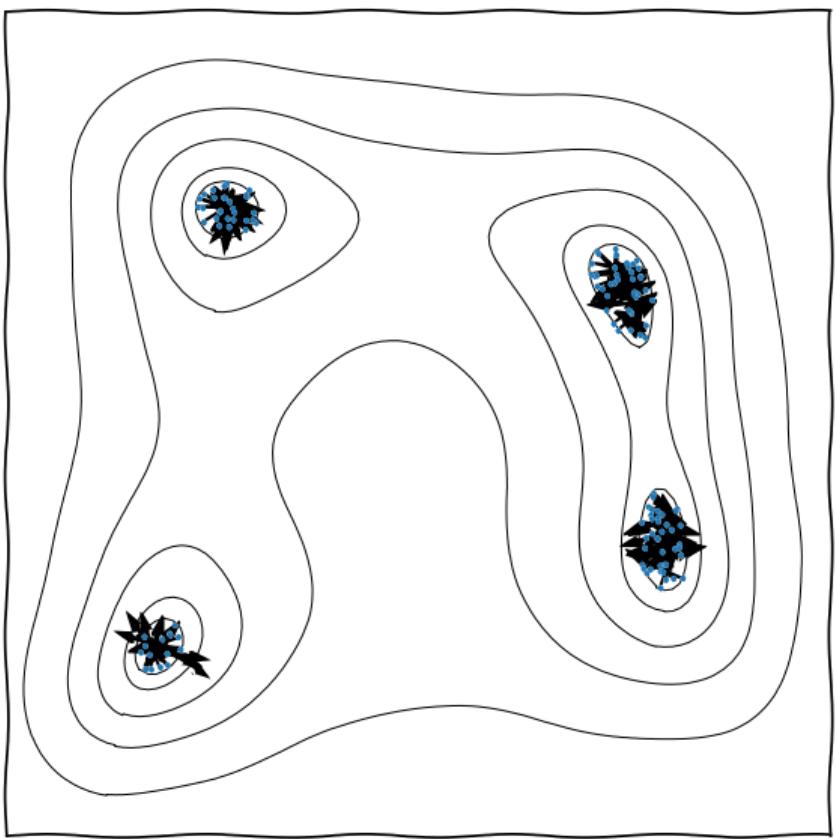
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Betancourt Hamiltonian constrained nested sampling [[1005.0157](#)].

Feroz Galilean Nested Sampling [[1312.5638](#)].

Skilling Galilean and Hamiltonian Monte Carlo [[doi:10.3390/proceedings2019033019](#)]

Speagle Incorporated into dynesty [[1904.02180](#)].

Habeck Habeck Demonic nested sampling – uses thermodynamic analogy to soften the hard boundary with a Maxwell daemon [[doi:10.1063/1.4905971](#)].

Baldock Total Enthalpy HMC, incorporating momenta in a more HMC like way, but specialised to materials science [[1710.11085](#)].

Cai ProxNest for high-dimensional convex imaging problems [[2106.03646](#)].

Lemos Updated existing HMC/Galilean nested sampling to use differentiable programming (jax/torch) ICML 2024 [[2312.03911](#)]

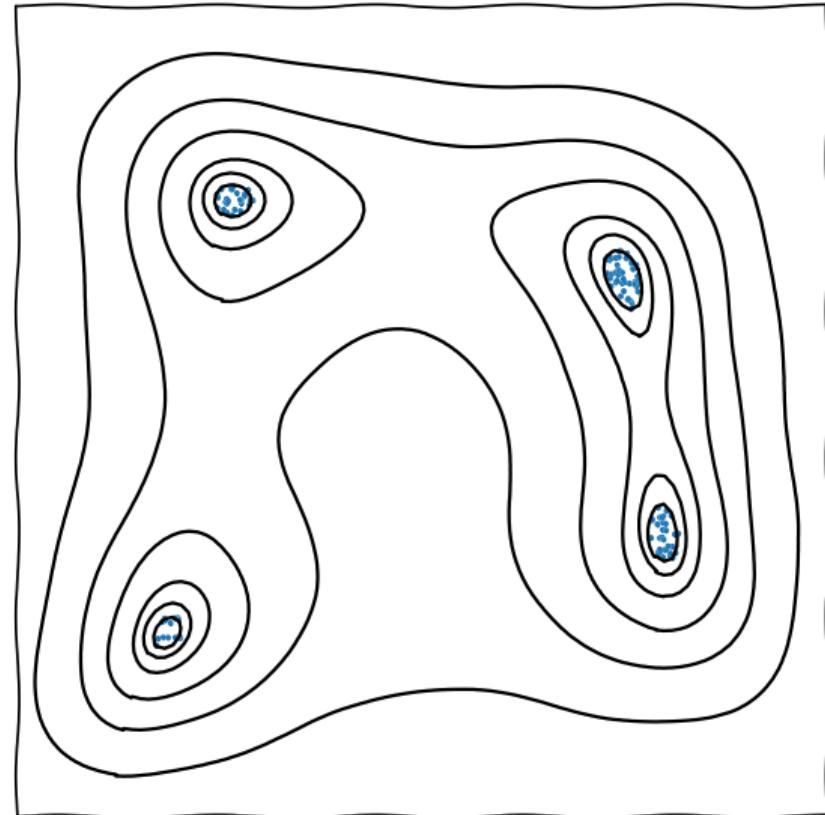
- ▶ See also 2023 MIAPbP talk “Gradients and nested sampling: The present state of the art”
- ▶ Come talk to me afterwards for further detail on what I’m working on with Namu Kroupa.

# Reversible nested sampling

- ▶ One could in principle reverse the direction of travel, and move outward from a peak.
- ▶ Need to know the initial volume  $X_{\text{start}} \neq 1$
- ▶ e.g. if a Laplace estimation were good enough at the peak.
- ▶ The same trick in normal nested sampling would reduce volume estimation error and hence improve scaling.

## Frontier

- ▶ Can you come up with a reversible nested sampling algorithm?
- ▶ Can you reduce the volume estimation error by clamping the end point?

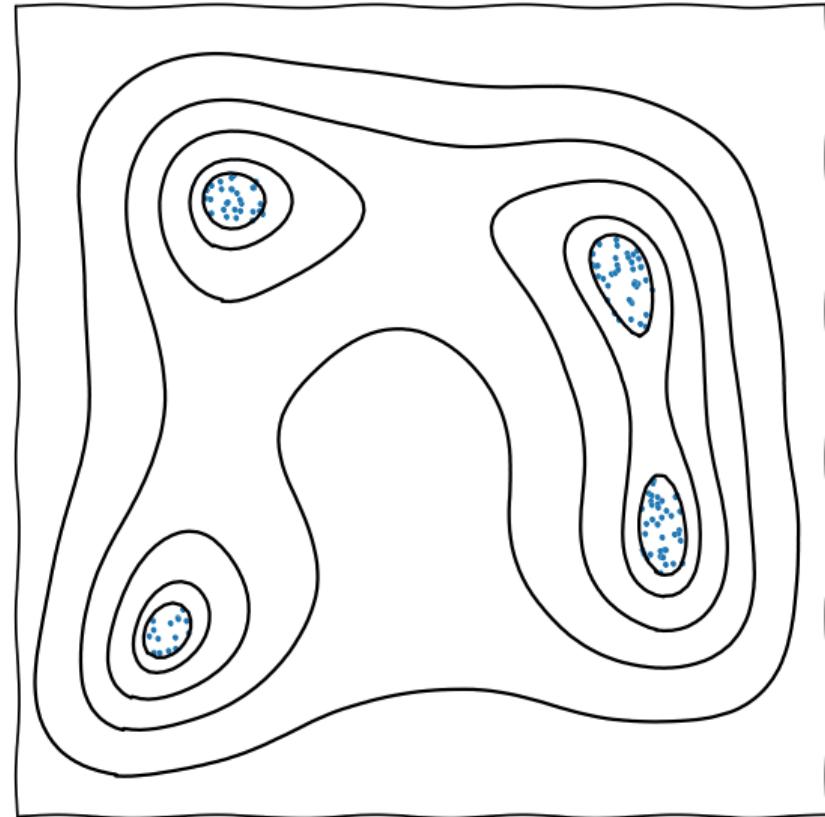


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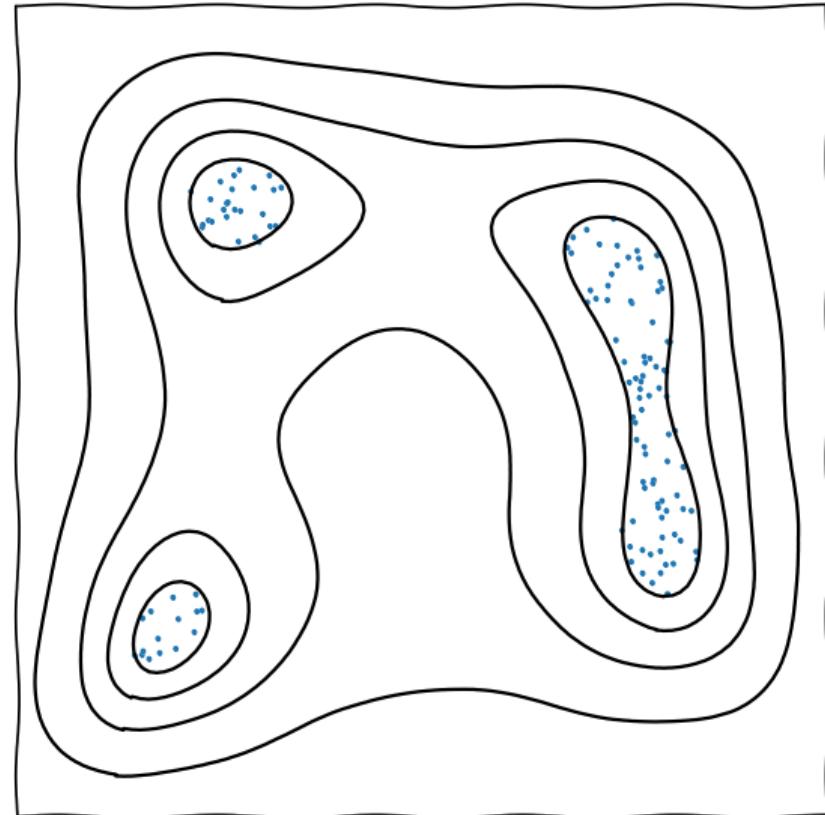


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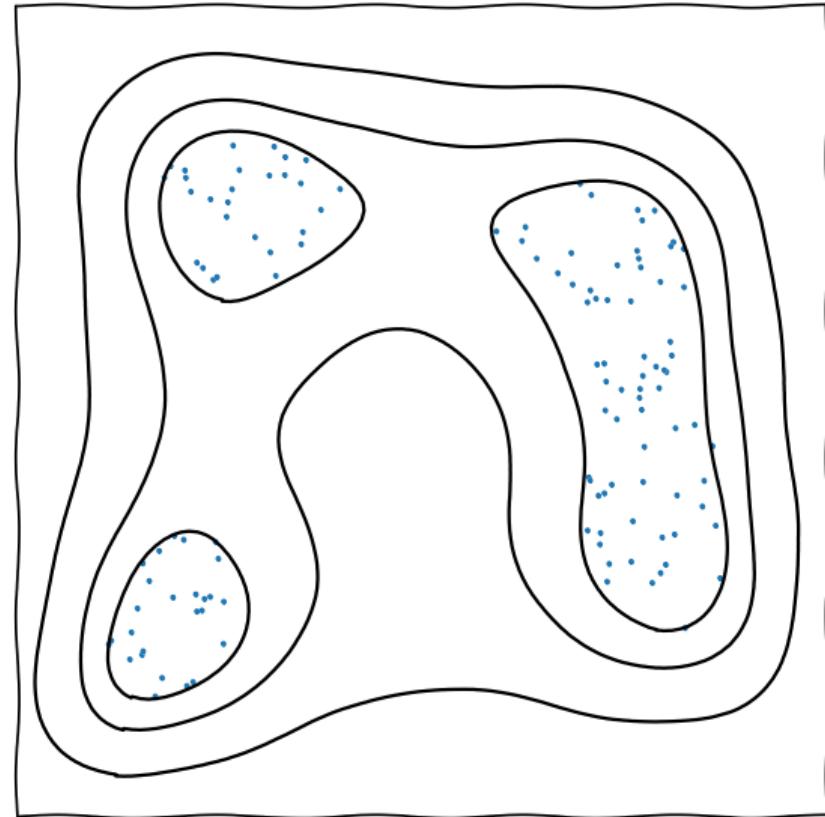


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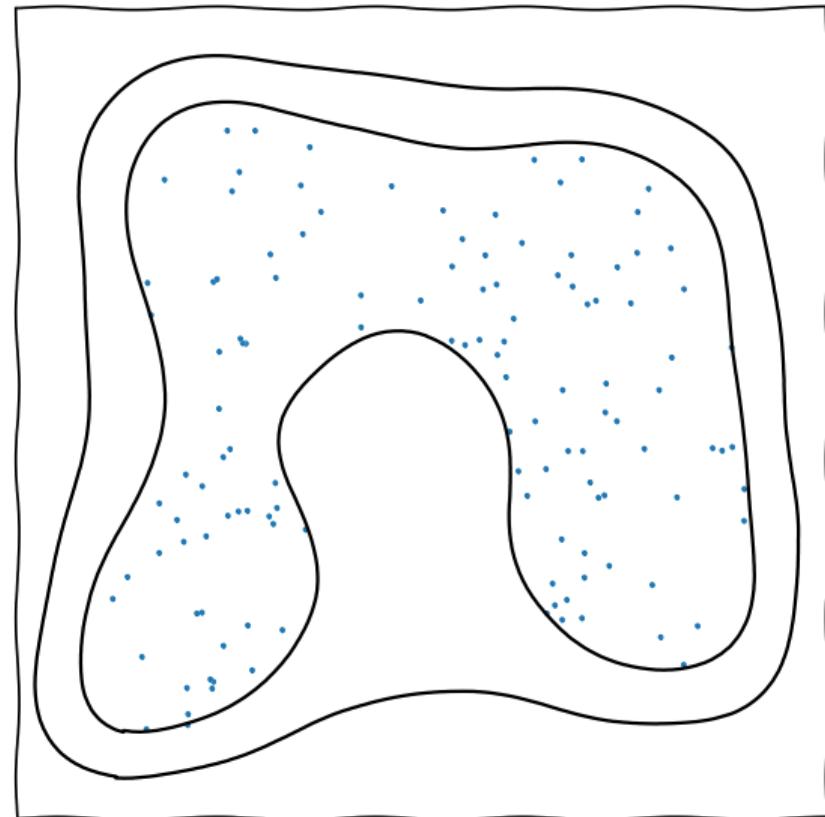


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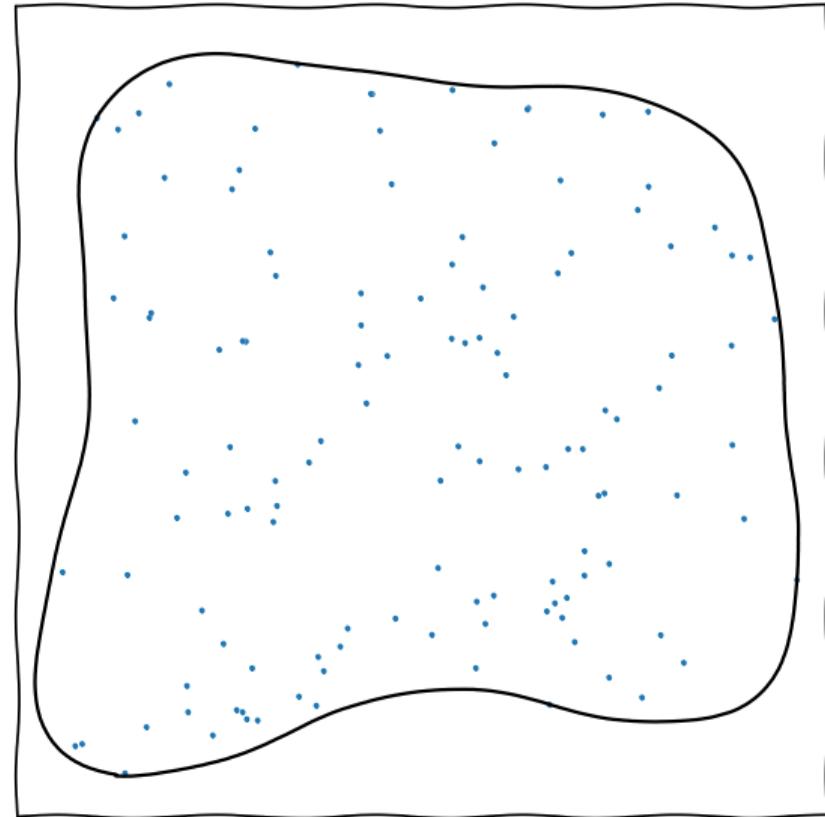


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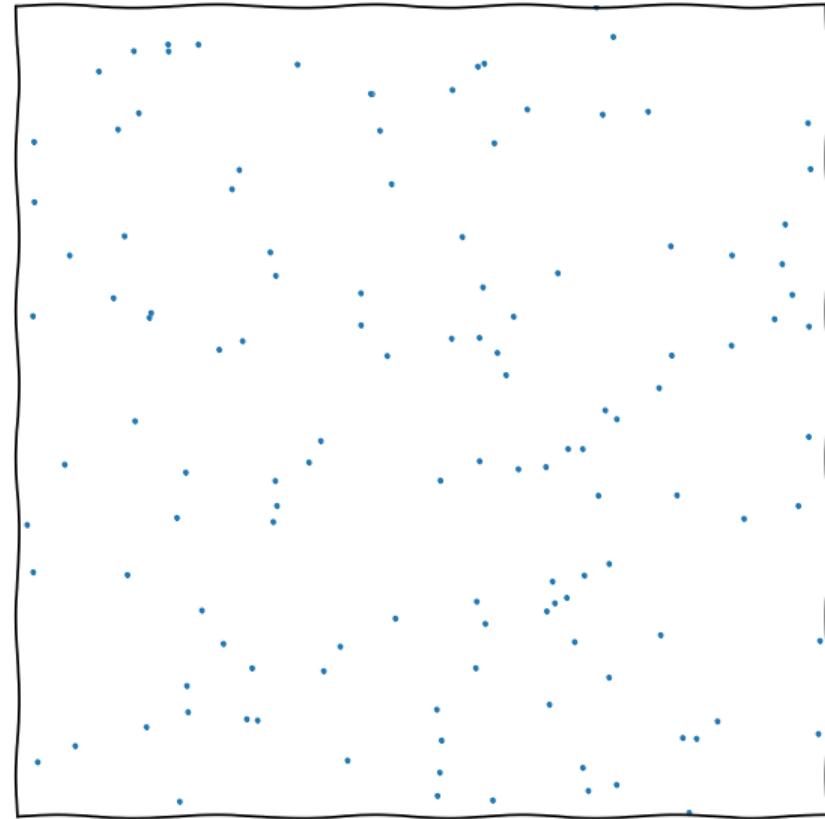


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# Conclusions

[github.com/handley-lab](https://github.com/handley-lab)



## How fast in nested sampling?

$$T = T_{\text{L}} \times n_{\text{live}} \times \mathcal{D}_{\text{KL}} \times f_{\text{sampler}}$$

## How accurate is nested sampling?

$$\sigma(\log \mathcal{Z}) \approx \sqrt{\mathcal{D}_{\text{KL}} / n_{\text{live}}}$$

- ▶ Technical Review paper: Buchner [2101.09675]
- ▶ Nature Review paper: [2205.15570]
- ▶ aeons [2312.00294]
- ▶ SuperNest [2212.01760]

# Probabalistic volume estimation

- ▶ Key idea in NS: estimating volumes probabilistically

$$\frac{V_{\text{after}}}{V_{\text{before}}} \approx \frac{n_{\text{in}}}{n_{\text{out}} + n_{\text{in}}}$$

- ▶ This is the **only** way to calculate volume in high dimensions  $d > 3$ .
  - ▶ Geometry is exponentially inefficient.
- ▶ This estimation process does not depend on geometry, topology or dimensionality
- ▶ Basis of all Monte-Carlo integration
- ▶ Nested Sampling uniquely uses a nested framework to couple together MC integrals in a robust, scalable manner.

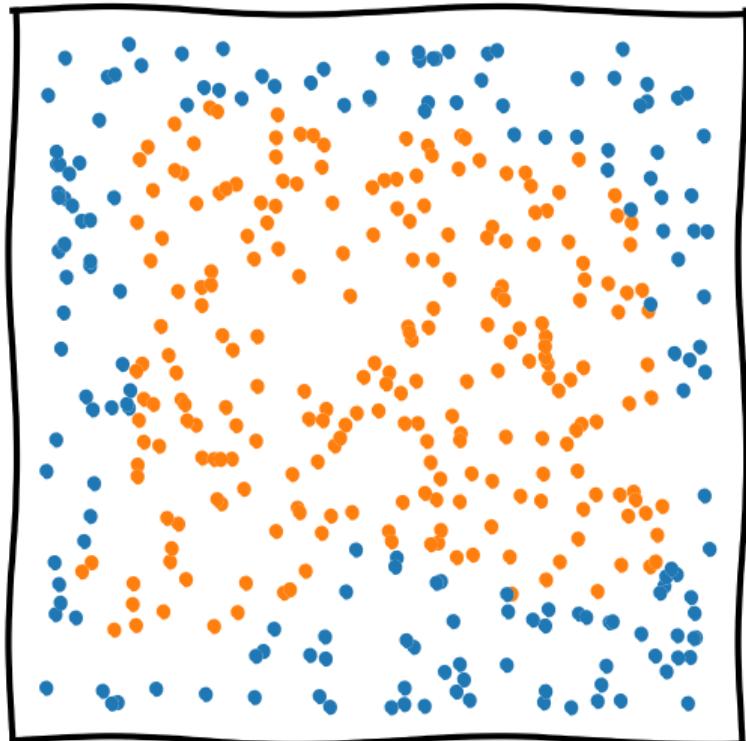


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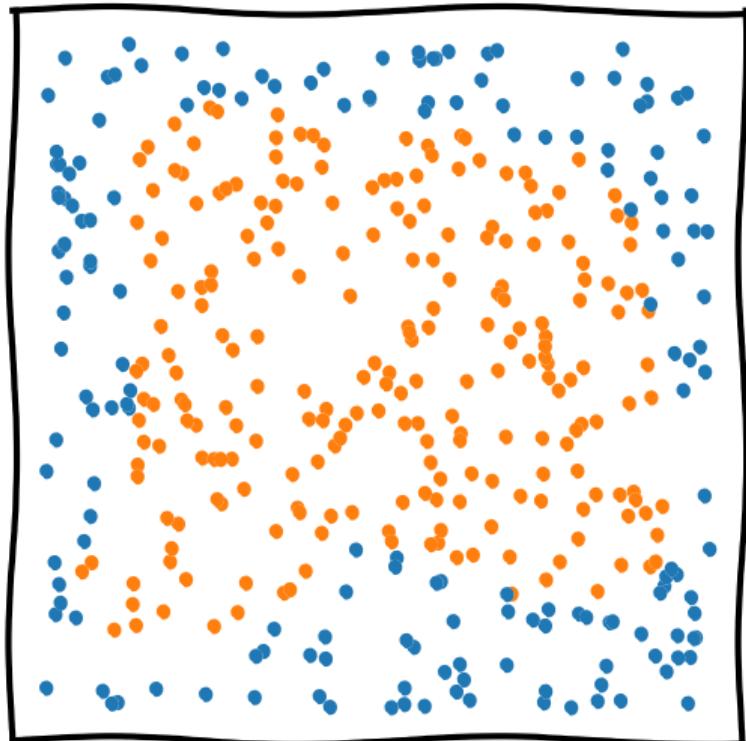


# Probabalistic volume estimation

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# Probabalistic volume estimation

- ▶ Key idea in NS: estimating volumes probabilistically

$$\frac{V_{\text{after}}}{V_{\text{before}}} \sim \frac{n_{\text{in}} + 1}{n_{\text{out}} + n_{\text{in}} + 2} \pm \sqrt{\frac{(n_{\text{in}}+1)(n_{\text{out}}+1)}{(n_{\text{out}}+n_{\text{in}}+2)^2(n_{\text{out}}+n_{\text{in}}+3)}}$$

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