

Cohere Research Talk: Massively Parallel Inference & Bayesian Evals

Sam Bowyer

10 November 2025

Outline

- 1 About Me
- 2 Alan: Massively Parallel Probabilistic Programming
- 3 Bayesian Evals: Uncertainty Quantification for LLM Evals

About Me

- Fourth (final) year PhD student at Bristol's Compass CDT (Computational Statistics and Data Science).

About Me

- Fourth (final) year PhD student at Bristol's Compass CDT (Computational Statistics and Data Science).
- Based in the School of Maths, but supervised by Laurence Aitchison (CS/Engineering Maths), Mengyue Yang (Engineering Maths), and Song Liu (Maths).

About Me

- Fourth (final) year PhD student at Bristol's Compass CDT (Computational Statistics and Data Science).
- Based in the School of Maths, but supervised by Laurence Aitchison (CS/Engineering Maths), Mengyue Yang (Engineering Maths), and Song Liu (Maths).
- Currently working on discrete diffusion models (training an ‘auxilliary’ model with VI to suggest the order in which to decode tokens).

About Me

- Fourth (final) year PhD student at Bristol's Compass CDT (Computational Statistics and Data Science).
- Based in the School of Maths, but supervised by Laurence Aitchison (CS/Engineering Maths), Mengyue Yang (Engineering Maths), and Song Liu (Maths).
- Currently working on discrete diffusion models (training an ‘auxilliary’ model with VI to suggest the order in which to decode tokens).
- Two projects I'll be talking about today: Alan (massively parallel probabilistic programming) & Bayesian Evals.

Alan: A Massively Parallel Probabilistic Programming Language



Work done with Laurence Aitchison and Thomas Heap over the first two years of my PhD.

Alan: A Massively Parallel Probabilistic Programming Language



Work done with Laurence Aitchison and Thomas Heap over the first two years of my PhD.

- Dual goals:

Alan: A Massively Parallel Probabilistic Programming Language



Work done with Laurence Aitchison and Thomas Heap over the first two years of my PhD.

- Dual goals:
 - Develop ‘massively parallel’ Bayesian inference algorithms: fast, accurate, and scalable; designed for GPU acceleration.

Alan: A Massively Parallel Probabilistic Programming Language



Work done with Laurence Aitchison and Thomas Heap over the first two years of my PhD.

- Dual goals:

- Develop ‘massively parallel’ Bayesian inference algorithms: fast, accurate, and scalable; designed for GPU acceleration.
- Implement these algorithms in a probabilistic programming language in pytorch (`alan`), allowing users to specify general probabilistic models.

Regular Bayesian Inference

- **Bayesian inference:** Prior $P(z)$ and likelihood $P(x|z)$ for latent variables z and data x .

$$P(z|x) = \frac{P(x|z)P(z)}{\int_{\mathcal{Z}} P(x, z') dz'}$$

Regular Bayesian Inference

- **Bayesian inference:** Prior $P(z)$ and likelihood $P(x|z)$ for latent variables z and data x .

$$P(z|x) = \frac{P(x|z)P(z)}{\int_{\mathcal{Z}} P(x, z') dz'}$$

- **Importance sampling:**

Regular Bayesian Inference

- **Bayesian inference:** Prior $P(z)$ and likelihood $P(x|z)$ for latent variables z and data x .

$$P(z|x) = \frac{P(x|z)P(z)}{\int_{\mathcal{Z}} P(x, z') dz'}$$

- **Importance sampling:**

- ① Sample K latent variables from a proposal distribution Q (usually IID):

$$z = (z^1, \dots, z^K) \sim Q(z).$$

Regular Bayesian Inference

- **Bayesian inference:** Prior $P(z)$ and likelihood $P(x|z)$ for latent variables z and data x .

$$P(z|x) = \frac{P(x|z)P(z)}{\int_{\mathcal{Z}} P(x, z') dz'}$$

- **Importance sampling:**

① Sample K latent variables from a proposal distribution Q (usually IID):

$$z = (z^1, \dots, z^K) \sim Q(z).$$

② Compute importance weights:

$$r_k(z) = \frac{P(x, z^k)}{Q(z^k)}.$$

Regular Bayesian Inference

- **Bayesian inference:** Prior $P(z)$ and likelihood $P(x|z)$ for latent variables z and data x .

$$P(z|x) = \frac{P(x|z)P(z)}{\int_{\mathcal{Z}} P(x, z') dz'}$$

- **Importance sampling:**

- ① Sample K latent variables from a proposal distribution Q (usually IID):

$$z = (z^1, \dots, z^K) \sim Q(z).$$

- ② Compute importance weights:

$$r_k(z) = \frac{P(x, z^k)}{Q(z^k)}.$$

- ③ Approximate the normalising constant using the 'global' estimator:

$$\mathcal{P}_{\text{global}}(z) = \frac{1}{K} \sum_{k=1}^K r_k(z) \quad \text{such that} \quad \mathbb{E}_{z \sim Q}[\mathcal{P}_{\text{global}}(z)] = P(x).$$

Limitations of Importance Sampling (IS)

- Global IS scales poorly with the number of latent variables, n .

Limitations of Importance Sampling (IS)

- Global IS scales poorly with the number of latent variables, n .
 - E.g. n is the dimension of z if all latent variables are scalar.

Limitations of Importance Sampling (IS)

- Global IS scales poorly with the number of latent variables, n .
 - E.g. n is the dimension of z if all latent variables are scalar.
- Chatterjee & Diaconis (2018) show that as n increases, the number of samples, K , must increase with $O(e^{D_{KL}(P(z|x)||Q(z))}) \approx O(e^n)$. (This is a lot!)

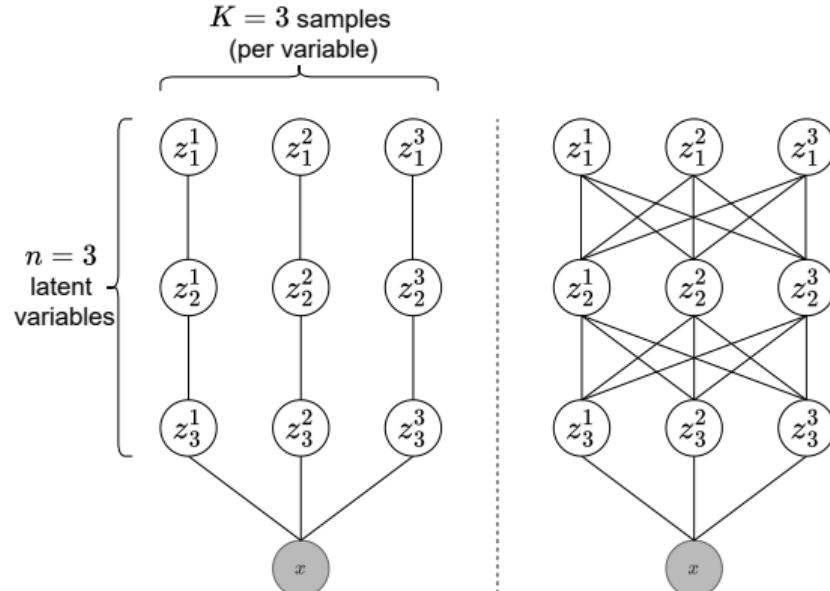
Limitations of Importance Sampling (IS)

- Global IS scales poorly with the number of latent variables, n .
 - E.g. n is the dimension of z if all latent variables are scalar.
- Chatterjee & Diaconis (2018) show that as n increases, the number of samples, K , must increase with $O(e^{D_{KL}(P(z|x)||Q(z))}) \approx O(e^n)$. (This is a lot!)
- Solution: **Massively Parallel Importance Sampling (MP-IS)**

Limitations of Importance Sampling (IS)

- Global IS scales poorly with the number of latent variables, n .
 - E.g. n is the dimension of z if all latent variables are scalar.
- Chatterjee & Diaconis (2018) show that as n increases, the number of samples, K , must increase with $O(e^{D_{KL}(P(z|x)||Q(z))}) \approx O(e^n)$. (This is a lot!)
- Solution: **Massively Parallel Importance Sampling (MP-IS)**
 - Reason about all K^N possible joint samples at once.

Massively Parallel Importance Sampling (MP-IS)

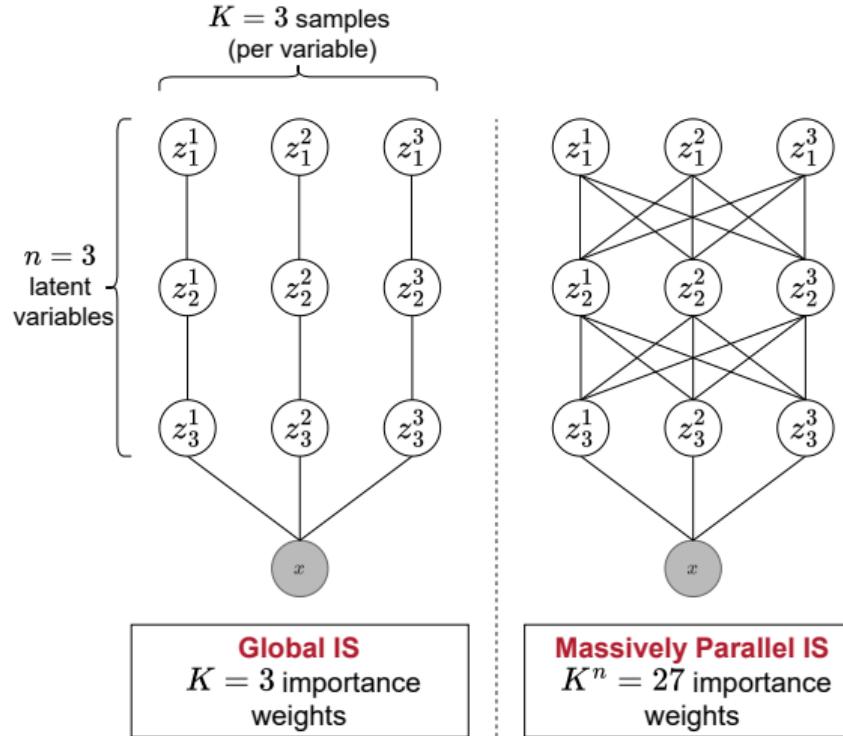


Global IS
 $K = 3$ importance weights

Massively Parallel IS
 $K^n = 27$ importance weights

- Suppose each latent sample $z^k = (z_1^k, \dots, z_n^k) \sim Q(z)$ is comprised of n variables.

Massively Parallel Importance Sampling (MP-IS)

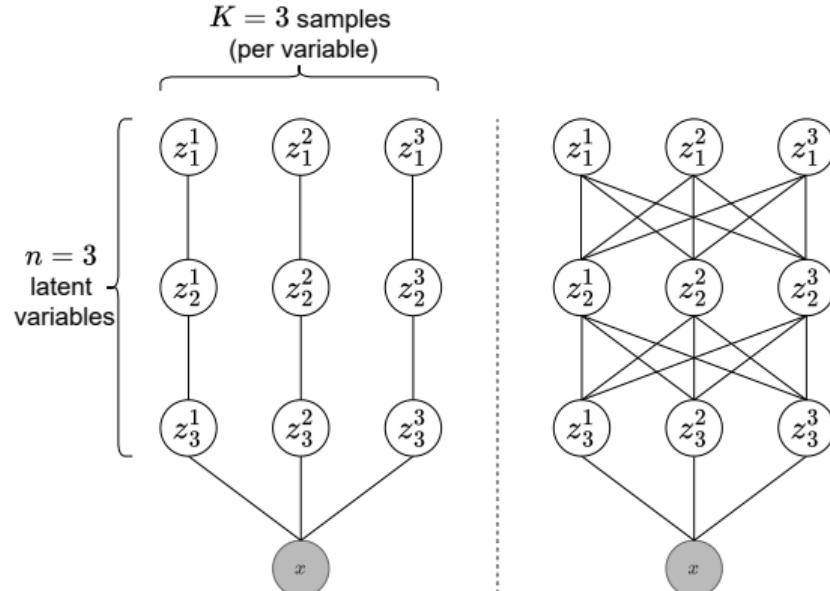


- Suppose each latent sample $z^k = (z_1^k, \dots, z_n^k) \sim Q(z)$ is comprised of n variables.
- We can construct K^n different samples from the full joint space

$$(z_1^{k_1}, \dots, z_n^{k_n}) \in \mathcal{Z}$$

where $\mathbf{k} = (k_1, \dots, k_n) \in [K]^n$ is the indexing vector for each latent variable.

Massively Parallel Importance Sampling (MP-IS)



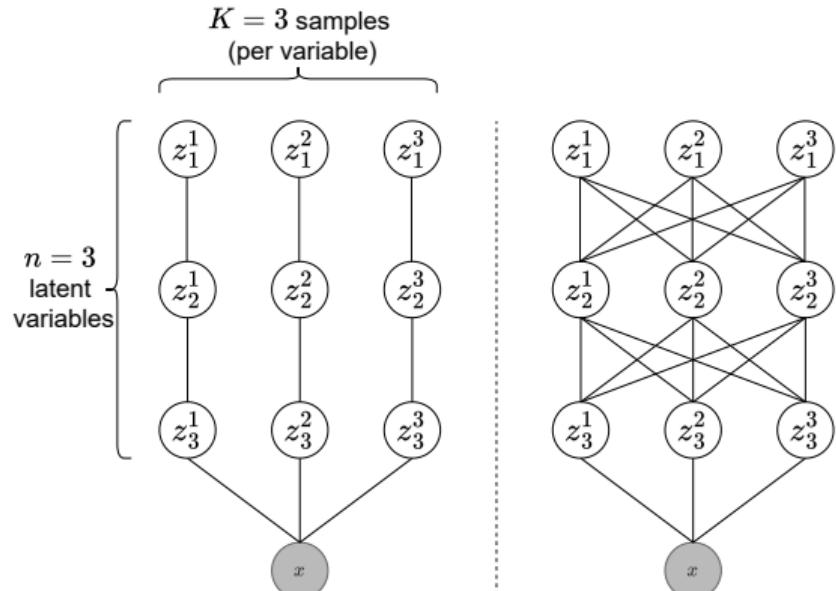
Global IS
 $K = 3$ importance
weights

Massively Parallel IS
 $K^n = 27$ importance
weights

- Rather than using the global IS estimator

$$\mathcal{P}_{\text{global}}(z) = \frac{1}{K} \sum_{k=1}^K \frac{P(x, z^k)}{Q(z^k)}.$$

Massively Parallel Importance Sampling (MP-IS)



Global IS
 $K = 3$ importance weights

Massively Parallel IS
 $K^n = 27$ importance weights

- Rather than using the global IS estimator

$$\mathcal{P}_{\text{global}}(z) = \frac{1}{K} \sum_{k=1}^K \frac{P(x, z^k)}{Q(z^k)}.$$

- ...we can use the MP-IS estimator

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^{\mathbf{k}})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}.$$

(Which is still unbiased.)

MP-IS: Some Complications...

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^{\mathbf{k}})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}.$$

- We have to be careful about how we define Q_{MP} over the space of all K^n joint samples.

MP-IS: Some Complications...

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^{\mathbf{k}})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}.$$

- We have to be careful about how we define Q_{MP} over the space of all K^n joint samples.
- We can use a hierarchical model:

$$Q_{\text{MP}}(z, \mathbf{k}) = \prod_{i=1}^n Q_{\text{MP}}(z_i^{k_i} | z_j \text{ for } j \in \text{qa}(i)),$$

where $\text{qa}(i)$ is the set of indices of parents of z_i in the proposal model.

MP-IS: Some Complications...

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^{\mathbf{k}})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}.$$

- We have to be careful about how we define Q_{MP} over the space of all K^n joint samples.
- We can use a hierarchical model:

$$Q_{\text{MP}}(z, \mathbf{k}) = \prod_{i=1}^n Q_{\text{MP}}(z_i^{k_i} | z_j \text{ for } j \in \text{qa}(i)),$$

where $\text{qa}(i)$ is the set of indices of parents of z_i in the proposal model.

- If variable z_i has a parent samples $z_j = (z_j^1, \dots, z_j^K) \sim Q(z_j)$, then we can sample $z_i^{k_i}$ from $Q(z_i^{k_i} | z_j^{\pi(k_i)})$ for a (uniformly) random permutation π of $[K]$.

MP-IS: Some More Complications...

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^\mathbf{k})}{Q_{\text{MP}}(z^\mathbf{k}, \mathbf{k})} = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} r_\mathbf{k}(z).$$

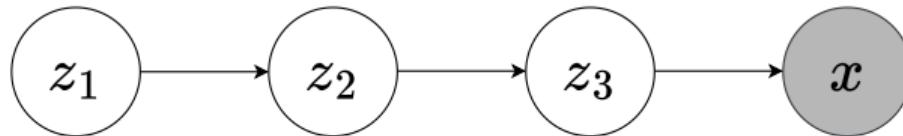
- At first glance, this thing doesn't look all that nice to compute...

MP-IS: Some More Complications...

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{P(x, z^\mathbf{k})}{Q_{\text{MP}}(z^\mathbf{k}, \mathbf{k})} = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} r_\mathbf{k}(z).$$

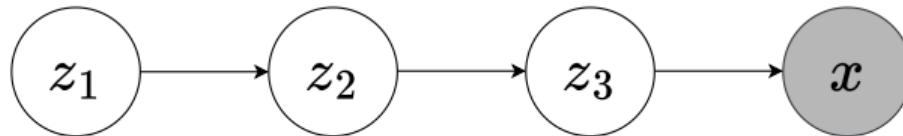
- At first glance, this thing doesn't look all that nice to compute...
- But we can exploit the conditional independencies in the model to render it tractable.

MP-IS: Some More Complications...



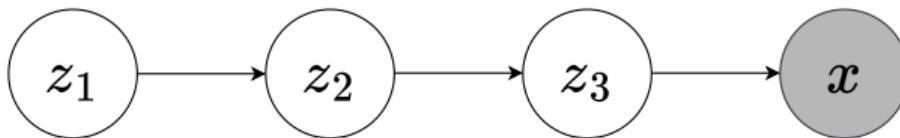
- E.g. with the model from before with $n = 3$, $P(x, z) = P(z_1)P(z_2|z_1)P(z_3|z_2)P(x|z_3)$, we can move the sums inside the product and get a bunch of tensor products:

MP-IS: Some More Complications...



- E.g. with the model from before with $n = 3$, $P(x, z) = P(z_1)P(z_2|z_1)P(z_3|z_2)P(x|z_3)$, we can move the sums inside the product and get a bunch of tensor products:

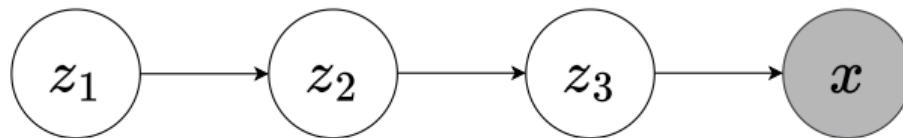
MP-IS: Some More Complications...



- E.g. with the model from before with $n = 3$, $P(x, z) = P(z_1)P(z_2|z_1)P(z_3|z_2)P(x|z_3)$, we can move the sums inside the product and get a bunch of tensor products:

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^3} \sum_{k_1 \in [K]} \sum_{k_2 \in [K]} \sum_{k_3 \in [K]} \frac{P(z_1^{k_1})P(z_2^{k_2}|z_1^{k_1})P(z_3^{k_3}|z_2^{k_2})P(x|z_3^{k_3})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}$$

MP-IS: Some More Complications...



- E.g. with the model from before with $n = 3$, $P(x, z) = P(z_1)P(z_2|z_1)P(z_3|z_2)P(x|z_3)$, we can move the sums inside the product and get a bunch of tensor products:

$$\mathcal{P}_{\text{MP}}(z) = \frac{1}{K^3} \sum_{k_1 \in [K]} \sum_{k_2 \in [K]} \sum_{k_3 \in [K]} \frac{P(z_1^{k_1})P(z_2^{k_2}|z_1^{k_1})P(z_3^{k_3}|z_2^{k_2})P(x|z_3^{k_3})}{Q_{\text{MP}}(z^{\mathbf{k}}, \mathbf{k})}$$

$$= \frac{1}{K^3} \underbrace{\sum_{k_1 \in [K]} \frac{P(z_1^{k_1})}{Q_{\text{MP}}(z_1^{k_1}, k_1)}}_{\text{Vector of size } K} \underbrace{\sum_{k_2 \in [K]} \frac{P(z_2^{k_2}|z_1^{k_1})}{Q_{\text{MP}}(z_2^{k_2}, \mathbf{k}_{1:2})}}_{\text{Matrix of size } K \times K} \underbrace{\sum_{k_3 \in [K]} \frac{P(z_3^{k_3}|z_2^{k_2})}{Q_{\text{MP}}(z_3^{k_3}, \mathbf{k}_{2:3})}}_{\text{Matrix of size } K \times K} \underbrace{\frac{P(x|z_3^{k_3})}{Q_{\text{MP}}(x|z_3^{k_3}, k_3)}}_{\text{Vector of size } K}$$

Can we hide these complications from the user?

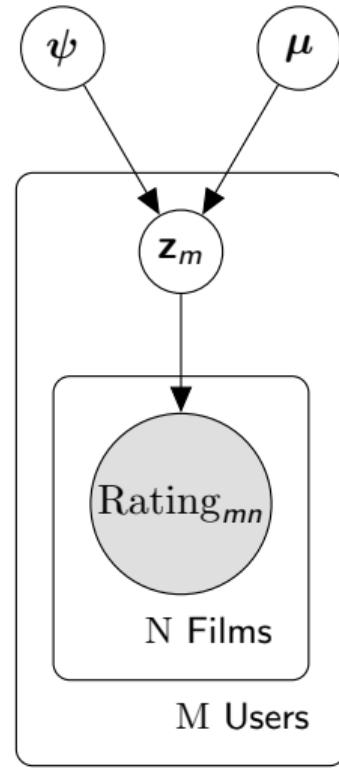
- Yes! We do this with `alan`.

Can we hide these complications from the user?

- Yes! We do this with `alan`.
- User specifies the model with `P` and `Q` as pytorch modules, and we handle the massively parallel inference for them.

Alan: A Probabilistic Programming Language

```
1  from alan import Normal, Bernoulli, Plate, BoundPlate, OptParam, Data, Problem
2  import torch as t
3
4  # Set up the model
5  d_z = 10
6
7  P = Plate(
8      mu_z = Normal(t.zeros((d_z,)), t.ones((d_z,))),
9      psi_z = Normal(t.zeros((d_z,)), t.ones((d_z,))),
10     plate_1 = Plate(
11         z = Normal("mu_z", lambda psi_z: psi_z.exp()),
12         plate_2 = Plate(
13             obs = Bernoulli(logits = lambda z, x: z @ x),
14         )
15     ),
16 )
17
18 Q = Plate(
19     mu_z = Normal(OptParam(t.zeros((d_z,))), OptParam(t.zeros((d_z,)), transformation=t.exp)),
20     psi_z = Normal(OptParam(t.zeros((d_z,))), OptParam(t.zeros((d_z,)), transformation=t.exp)),
21     plate_1 = Plate(
22         z = Normal(OptParam(t.zeros((d_z,))), OptParam(t.zeros((d_z,)), transformation=t.exp)),
23         plate_2 = Plate(
24             obs = Data()
25         )
26     ),
27 )
28
29 P = BoundPlate(P, platesizes={'plate_1': num_users, 'plate_2': num_movies}, inputs = {'x': x})
30 Q = BoundPlate(Q, platesizes={'plate_1': num_users, 'plate_2': num_movies}, inputs = {'x': x})
31
32 prob = Problem(P, Q)
```



- Using $\mathcal{P}_{\text{MP}}(z)$, we can do variational inference (VI) by maximising the ELBO:

$$\log P(x) \geq \mathcal{L}_{\text{MP}}(\theta) = \mathbb{E}_{z \sim Q_{\text{MP}}(\theta)}[\log \mathcal{P}_{\text{MP}}(z)]$$

MP-VI

- Using $\mathcal{P}_{\text{MP}}(z)$, we can do variational inference (VI) by maximising the ELBO:

$$\log P(x) \geq \mathcal{L}_{\text{MP}}(\theta) = \mathbb{E}_{z \sim Q_{\text{MP}}(\theta)} [\log \mathcal{P}_{\text{MP}}(z)]$$

- Aitchison (2019) showed that MP-VI is a tighter bound than the global VI objective (IWAE):

$$\log P(x) \geq \mathcal{L}_{\text{global}}(\theta) = \mathbb{E}_{z \sim Q_{\theta}} [\log \mathcal{P}_{\text{global}}(z)]$$

MP-VI

- Using $\mathcal{P}_{\text{MP}}(z)$, we can do variational inference (VI) by maximising the ELBO:

$$\log P(x) \geq \mathcal{L}_{\text{MP}}(\theta) = \mathbb{E}_{z \sim Q_{\text{MP}}(\theta)} [\log \mathcal{P}_{\text{MP}}(z)]$$

- Aitchison (2019) showed that MP-VI is a tighter bound than the global VI objective (IWAE):

$$\log P(x) \geq \mathcal{L}_{\text{global}}(\theta) = \mathbb{E}_{z \sim Q_{\theta}} [\log \mathcal{P}_{\text{global}}(z)]$$

MP-VI

- Using $\mathcal{P}_{\text{MP}}(z)$, we can do variational inference (VI) by maximising the ELBO:

$$\log P(x) \geq \mathcal{L}_{\text{MP}}(\theta) = \mathbb{E}_{z \sim Q_{\text{MP}}(\theta)} [\log \mathcal{P}_{\text{MP}}(z)]$$

- Aitchison (2019) showed that MP-VI is a tighter bound than the global VI objective (IWAE):

$$\log P(x) \geq \mathcal{L}_{\text{global}}(\theta) = \mathbb{E}_{z \sim Q_{\theta}} [\log \mathcal{P}_{\text{global}}(z)]$$

```
29 P = BoundPlate(P, platesizes={'plate_1': num_users, 'plate_2': num_movies}, inputs = {'x': x})
30 Q = BoundPlate(Q, platesizes={'plate_1': num_users, 'plate_2': num_movies}, inputs = {'x': x})
31
32 prob = Problem(P, Q)
33 opt = t.optim.Adam(prob.Q.parameters(), lr=lr)
34
35 # Train Q with VI
36 for i in range(num_iterations):
37     opt.zero_grad()
38     elbo = prob.sample(K=K).elbo_vi()
39     elbo.backward()
40     opt.step()
```

MP Algorithms

- We showed that we can obtain unbiased posterior moment estimates efficiently using autodiff (Bowyer et al. (2024)).

$$m_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{r_{\mathbf{k}}(z)}{\mathcal{P}_{\text{MP}}(z)} m(z^{\mathbf{k}})$$

MP Algorithms

- We showed that we can obtain unbiased posterior moment estimates efficiently using autodiff (Bowyer et al. (2024)).

$$m_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{r_{\mathbf{k}}(z)}{\mathcal{P}_{\text{MP}}(z)} m(z^{\mathbf{k}})$$

- We define a modified marginal likelihood estimator with an auxiliary variable $J \in \mathbb{R}$:

$$\mathcal{P}_{\text{MP}}^{\text{exp}}(z, J) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} r_{\mathbf{k}}(z) \exp(J m(z^{\mathbf{k}}))$$

MP Algorithms

- We showed that we can obtain unbiased posterior moment estimates efficiently using autodiff (Bowyer et al. (2024)).

$$m_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{r_{\mathbf{k}}(z)}{\mathcal{P}_{\text{MP}}(z)} m(z^{\mathbf{k}})$$

- We define a modified marginal likelihood estimator with an auxiliary variable $J \in \mathbb{R}$:

$$\mathcal{P}_{\text{MP}}^{\text{exp}}(z, J) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} r_{\mathbf{k}}(z) \exp(J m(z^{\mathbf{k}}))$$

- Then differentiating with respect to J and setting $J = 0$ we get:

$$\left. \frac{\partial}{\partial J} \right|_{J=0} \log \mathcal{P}_{\text{MP}}^{\text{exp}}(z, J) = m_{\text{MP}}(z)$$

MP Algorithms

- We showed that we can obtain unbiased posterior moment estimates efficiently using autodiff (Bowyer et al. (2024)).

$$m_{\text{MP}}(z) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} \frac{r_{\mathbf{k}}(z)}{\mathcal{P}_{\text{MP}}(z)} m(z^{\mathbf{k}})$$

- We define a modified marginal likelihood estimator with an auxiliary variable $J \in \mathbb{R}$:

$$\mathcal{P}_{\text{MP}}^{\text{exp}}(z, J) = \frac{1}{K^n} \sum_{\mathbf{k} \in [K]^n} r_{\mathbf{k}}(z) \exp(J m(z^{\mathbf{k}}))$$

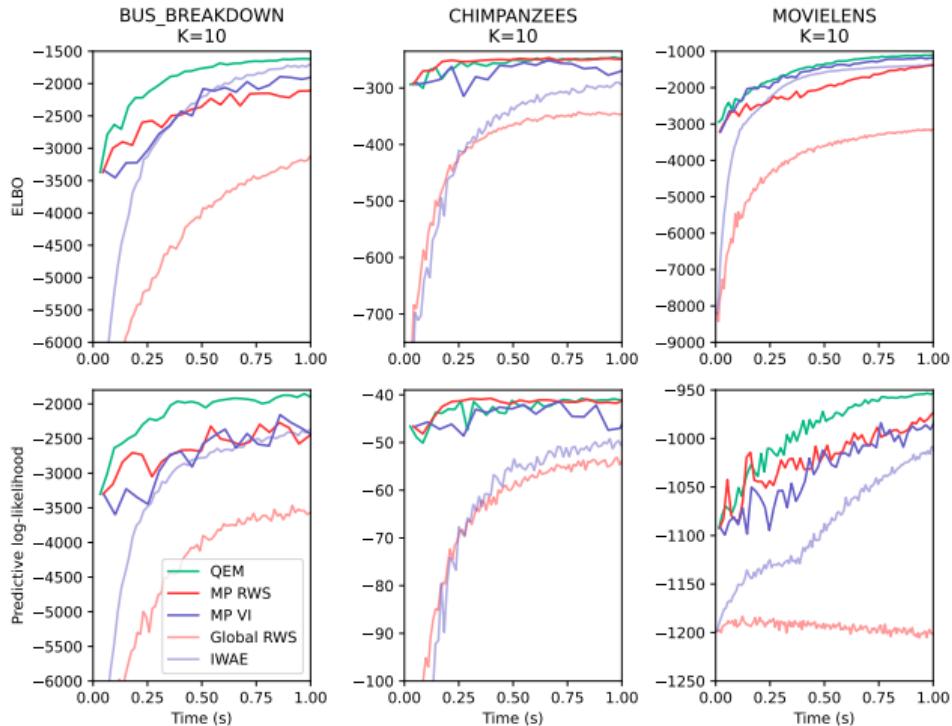
- Then differentiating with respect to J and setting $J = 0$ we get:

$$\left. \frac{\partial}{\partial J} \right|_{J=0} \log \mathcal{P}_{\text{MP}}^{\text{exp}}(z, J) = m_{\text{MP}}(z)$$

- Through a similar argument, we can set J to be vector- or tensor-valued based on K and the shape of z , allowing us to compute marginal likelihoods and importance samples too.

QEM: An Adaptive Importance Sampling Algorithm

- **QEM:** use these posterior moment estimates to iteratively update the approximate posterior Q_{MP} in an EM-like algorithm for adaptive importance sampling (Heap et al. (2025)).



Conclusions

- This project was a great (if, at times, complicated) way to learn about Bayesian inference and numerical and probabilistic programming.

Conclusions

- This project was a great (if, at times, complicated) way to learn about Bayesian inference and numerical and probabilistic programming.
- The results were pretty promising, but there are some drawbacks to massively parallel methods:

Conclusions

- This project was a great (if, at times, complicated) way to learn about Bayesian inference and numerical and probabilistic programming.
- The results were pretty promising, but there are some drawbacks to massively parallel methods:
 - The algorithms are complex to implement (hence wrapping them in a PPL).

Conclusions

- This project was a great (if, at times, complicated) way to learn about Bayesian inference and numerical and probabilistic programming.
- The results were pretty promising, but there are some drawbacks to massively parallel methods:
 - The algorithms are complex to implement (hence wrapping them in a PPL).
 - Not all models have lots of conditional independencies to exploit.

Conclusions

- This project was a great (if, at times, complicated) way to learn about Bayesian inference and numerical and probabilistic programming.
- The results were pretty promising, but there are some drawbacks to massively parallel methods:
 - The algorithms are complex to implement (hence wrapping them in a PPL).
 - Not all models have lots of conditional independencies to exploit.
 - Although it's slower and harder to tune, HMC is often hard to beat in terms of quality of inference.

Bayesian Evals: Uncertainty Quantification for LLM Evals



Work done with Laurence Aitchison and Desi R. Ivanova.

- Two directions:

Bayesian Evals: Uncertainty Quantification for LLM Evals



Work done with Laurence Aitchison and Desi R. Ivanova.

- Two directions:
 - Improved UQ for evals with Bayesian methods.

Bayesian Evals: Uncertainty Quantification for LLM Evals



Work done with Laurence Aitchison and Desi R. Ivanova.

- Two directions:
 - Improved UQ for evals with Bayesian methods.
 - Interpretability of evals with Bayesian hierarchical modelling and SAE-like approaches.

Bayesian Evals: Uncertainty Quantification for LLM Evals



Work done with Laurence Aitchison and Desi R. Ivanova.

- Two directions:
 - Improved UQ for evals with Bayesian methods.
 - Interpretability of evals with Bayesian hierarchical modelling and SAE-like approaches.
- The former direction led to an ICML spotlight position paper.

Bayesian Evals: Uncertainty Quantification for LLM Evals



Work done with Laurence Aitchison and Desi R. Ivanova.

- Two directions:
 - Improved UQ for evals with Bayesian methods.
 - Interpretability of evals with Bayesian hierarchical modelling and SAE-like approaches.
- The former direction led to an ICML spotlight position paper.
- The latter fell by the wayside, but is something I'd like to come back to at some point.

Motivation

Central Limit Theorem (CLT)

If X_1, \dots, X_N are IID r.v.s with mean $\mu \in \mathbb{R}$ and finite variance σ^2 , then

$$\sqrt{N}(\hat{\mu} - \mu) \xrightarrow{d} \mathcal{N}(0, \sigma^2) \text{ as } N \rightarrow \infty,$$

where $\hat{\mu} = \frac{1}{N} \sum_{i=1}^N X_i$ is the sample mean.

Motivation

Central Limit Theorem (CLT)

If X_1, \dots, X_N are IID r.v.s with mean $\mu \in \mathbb{R}$ and finite variance σ^2 , then

$$\sqrt{N}(\hat{\mu} - \mu) \xrightarrow{d} \mathcal{N}(0, \sigma^2) \text{ as } N \rightarrow \infty,$$

where $\hat{\mu} = \frac{1}{N} \sum_{i=1}^N X_i$ is the sample mean.

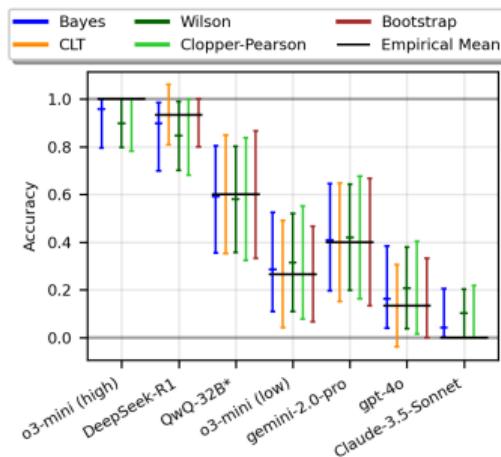
- In the case of binary data, the CLT-based confidence interval is:

$$\text{CI}_{1-\alpha}(\theta) = \bar{X} \pm z_{\alpha/2} \sqrt{\frac{\bar{X}(1 - \bar{X})}{N}}$$

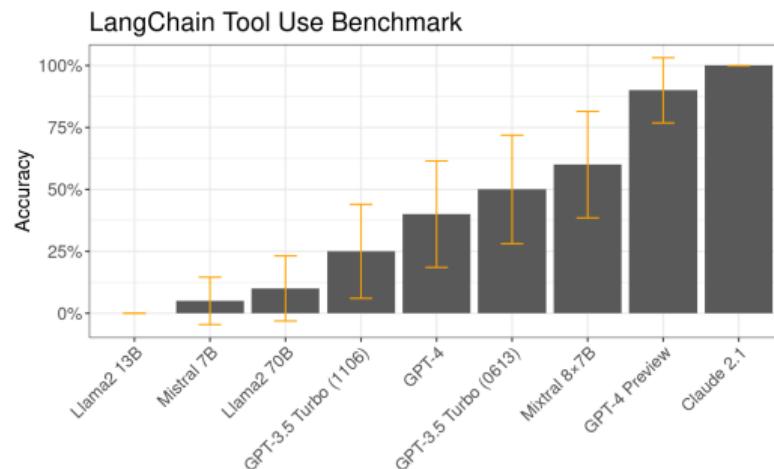
where $z_{\alpha/2}$ is the $100(1 - \alpha/2)$ -th percentile of $\mathcal{N}(0, 1)$.

Real-World Failures of the CLT

- If N is too small, CLT-based error bars can collapse to zero-width or extend past $[0, 1]$.



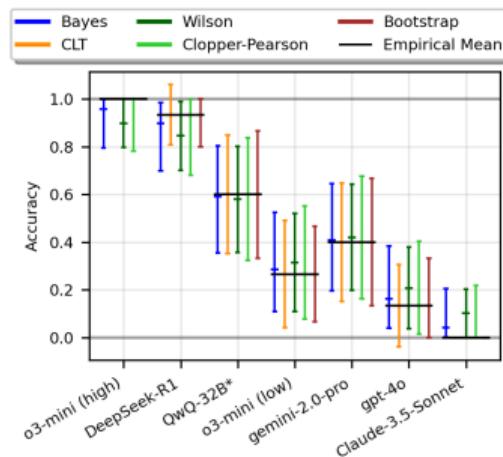
Math Arena's AIME II 2025 Benchmark
(N=15)



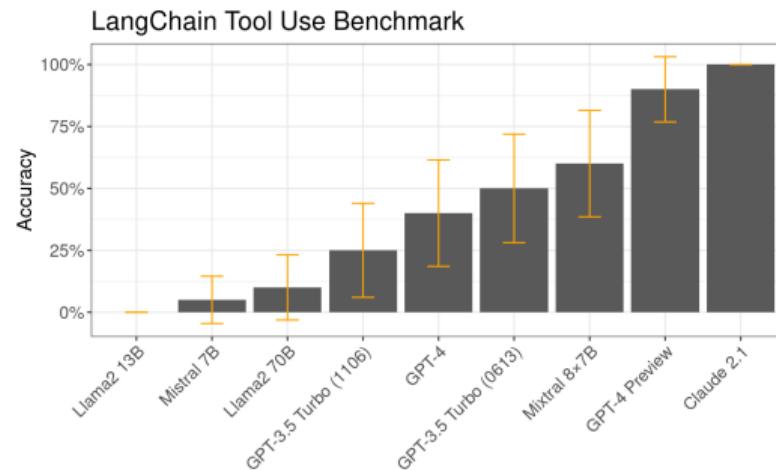
Langchain Typewriter Tool Use Benchmark
(N=20)

Real-World Failures of the CLT

- If N is too small, CLT-based error bars can collapse to zero-width or extend past $[0, 1]$.
- Smaller, more intricate, and expensive LLM benchmarks are becoming increasingly common, so we need to find alternatives for the few-data regime.



Math Arena's AIME II 2025 Benchmark
(N=15)



Langchain Typewriter Tool Use Benchmark
(N=20)

Bayesian Alternative: Beta-Binomial Model

- Treat the data as IID Bernoulli with a **uniform prior** on the parameter θ .

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1]$$

$$y_i \sim \text{Bernoulli}(\theta) \text{ for } i = 1, \dots, N$$

Bayesian Alternative: Beta-Binomial Model

- Treat the data as IID Bernoulli with a **uniform prior** on the parameter θ .

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1]$$

$$y_i \sim \text{Bernoulli}(\theta) \text{ for } i = 1, \dots, N$$

- Say y_i is correct if $y_i = 1$ and incorrect if $y_i = 0$.

Bayesian Alternative: Beta-Binomial Model

- Treat the data as IID Bernoulli with a **uniform prior** on the parameter θ .

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1]$$

$$y_i \sim \text{Bernoulli}(\theta) \text{ for } i = 1, \dots, N$$

- Say y_i is correct if $y_i = 1$ and incorrect if $y_i = 0$.
- Obtain quantile-based Bayesian **credible intervals** for θ from the closed form posterior.

$$p(\theta|y_{1:N}) = \text{Beta}\left(1 + \sum_{i=1}^N y_i, 1 + \sum_{i=1}^N (1 - y_i)\right)$$

Bayesian Alternative: Beta-Binomial Model

- Treat the data as IID Bernoulli with a **uniform prior** on the parameter θ .

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1]$$

$$y_i \sim \text{Bernoulli}(\theta) \text{ for } i = 1, \dots, N$$

- Say y_i is correct if $y_i = 1$ and incorrect if $y_i = 0$.
- Obtain quantile-based Bayesian **credible intervals** for θ from the closed form posterior.

$$p(\theta|y_{1:N}) = \text{Beta}\left(1 + \sum_{i=1}^N y_i, 1 + \sum_{i=1}^N (1 - y_i)\right)$$

Bayesian Alternative: Beta-Binomial Model

- Treat the data as IID Bernoulli with a **uniform prior** on the parameter θ .

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1]$$

$$y_i \sim \text{Bernoulli}(\theta) \text{ for } i = 1, \dots, N$$

- Say y_i is correct if $y_i = 1$ and incorrect if $y_i = 0$.
- Obtain quantile-based Bayesian **credible intervals** for θ from the closed form posterior.

$$p(\theta|y_{1:N}) = \text{Beta}\left(1 + \sum_{i=1}^N y_i, 1 + \sum_{i=1}^N (1 - y_i)\right)$$

Beta-Bernoulli Bayesian Credible Interval

```
1 posterior = scipy.stats.beta(1 + sum(y), 1 + N - sum(y))
2 bayes_ci  = posterior.interval(confidence=0.95)
```

Frequentist Alternatives

- Wilson score interval: Based on normal approximation to the binomial distribution.

Frequentist Alternatives

- Wilson score interval: Based on normal approximation to the binomial distribution.

Frequentist Alternatives

- **Wilson score interval:** Based on normal approximation to the binomial distribution.

$$\text{CI}_{1-\alpha, \text{Wilson}}(\theta) = \frac{\hat{\theta} + \frac{z_{\alpha/2}^2}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \pm \frac{\frac{z_{\alpha/2}}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \sqrt{4N\hat{\theta}(1 - \hat{\theta}) + z_{\alpha/2}^2}$$

- **Clopper-Pearson 'exact' interval:** A 'worst-case' approach; very conservative method guaranteed to never under-cover. $\text{CI}_{1-\alpha, \text{CP}}(\theta) = [\theta_{\text{lower}}, \theta_{\text{upper}}]$,

Frequentist Alternatives

- **Wilson score interval:** Based on normal approximation to the binomial distribution.

$$\text{CI}_{1-\alpha, \text{Wilson}}(\theta) = \frac{\hat{\theta} + \frac{z_{\alpha/2}^2}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \pm \frac{\frac{z_{\alpha/2}}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \sqrt{4N\hat{\theta}(1 - \hat{\theta}) + z_{\alpha/2}^2}$$

- **Clopper-Pearson 'exact' interval:** A 'worst-case' approach; very conservative method guaranteed to never under-cover. $\text{CI}_{1-\alpha, \text{CP}}(\theta) = [\theta_{\text{lower}}, \theta_{\text{upper}}]$,

Frequentist Alternatives

- **Wilson score interval:** Based on normal approximation to the binomial distribution.

$$\text{CI}_{1-\alpha, \text{Wilson}}(\theta) = \frac{\hat{\theta} + \frac{z_{\alpha/2}^2}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \pm \frac{\frac{z_{\alpha/2}}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \sqrt{4N\hat{\theta}(1 - \hat{\theta}) + z_{\alpha/2}^2}$$

- **Clopper-Pearson 'exact' interval:** A 'worst-case' approach; very conservative method guaranteed to never under-cover. $\text{CI}_{1-\alpha, \text{CP}}(\theta) = [\theta_{\text{lower}}, \theta_{\text{upper}}]$,

$$\theta_{\text{lower}} = B\left(\frac{\alpha}{2}, \sum_{i=1}^N y_i, 1 + \sum_{i=1}^N (1 - y_i)\right) \text{ and } \theta_{\text{upper}} = B\left(1 - \frac{\alpha}{2}, 1 + \sum_{i=1}^N y_i, \sum_{i=1}^N (1 - y_i)\right)$$

where $B(\alpha, a, b)$ is the α -th quantile of the $\text{Beta}(a, b)$ distribution.

Frequentist Alternatives

- **Wilson score interval:** Based on normal approximation to the binomial distribution.

$$\text{CI}_{1-\alpha, \text{Wilson}}(\theta) = \frac{\hat{\theta} + \frac{z_{\alpha/2}^2}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \pm \frac{\frac{z_{\alpha/2}}{2N}}{1 + \frac{z_{\alpha/2}^2}{N}} \sqrt{4N\hat{\theta}(1 - \hat{\theta}) + z_{\alpha/2}^2}$$

- **Clopper-Pearson 'exact' interval:** A 'worst-case' approach; very conservative method guaranteed to never under-cover. $\text{CI}_{1-\alpha, \text{CP}}(\theta) = [\theta_{\text{lower}}, \theta_{\text{upper}}]$,

$$\theta_{\text{lower}} = B\left(\frac{\alpha}{2}, \sum_{i=1}^N y_i, 1 + \sum_{i=1}^N (1 - y_i)\right) \text{ and } \theta_{\text{upper}} = B\left(1 - \frac{\alpha}{2}, 1 + \sum_{i=1}^N y_i, \sum_{i=1}^N (1 - y_i)\right)$$

where $B(\alpha, a, b)$ is the α -th quantile of the $\text{Beta}(a, b)$ distribution.

Wilson & Clopper-Pearson Confidence Interval

```
1 result = scipy.stats.binomtest(k=sum(y), n=N)
2 wilson_ci = result.proportion_ci("wilson", 0.95)
3 clop_ci   = result.proportion_ci("exact", 0.95)
```

Interval Comparison Simulations

We use synthetic eval data so that we **know** the true parameter θ .

- Draw $\theta \sim \text{Uniform}[0, 1]$.

Interval Comparison Simulations

We use synthetic eval data so that we **know** the true parameter θ .

- Draw $\theta \sim \text{Uniform}[0, 1]$.
- Draw $N \in \{3, 10, 30, 100\}$ IID Bernoulli datapoints with parameter θ .

Interval Comparison Simulations

We use synthetic eval data so that we **know** the true parameter θ .

- Draw $\theta \sim \text{Uniform}[0, 1]$.
- Draw $N \in \{3, 10, 30, 100\}$ IID Bernoulli datapoints with parameter θ .
- Construct intervals with various methods for various $1 - \alpha$ confidence levels.

Interval Comparison Simulations

We use synthetic eval data so that we **know** the true parameter θ .

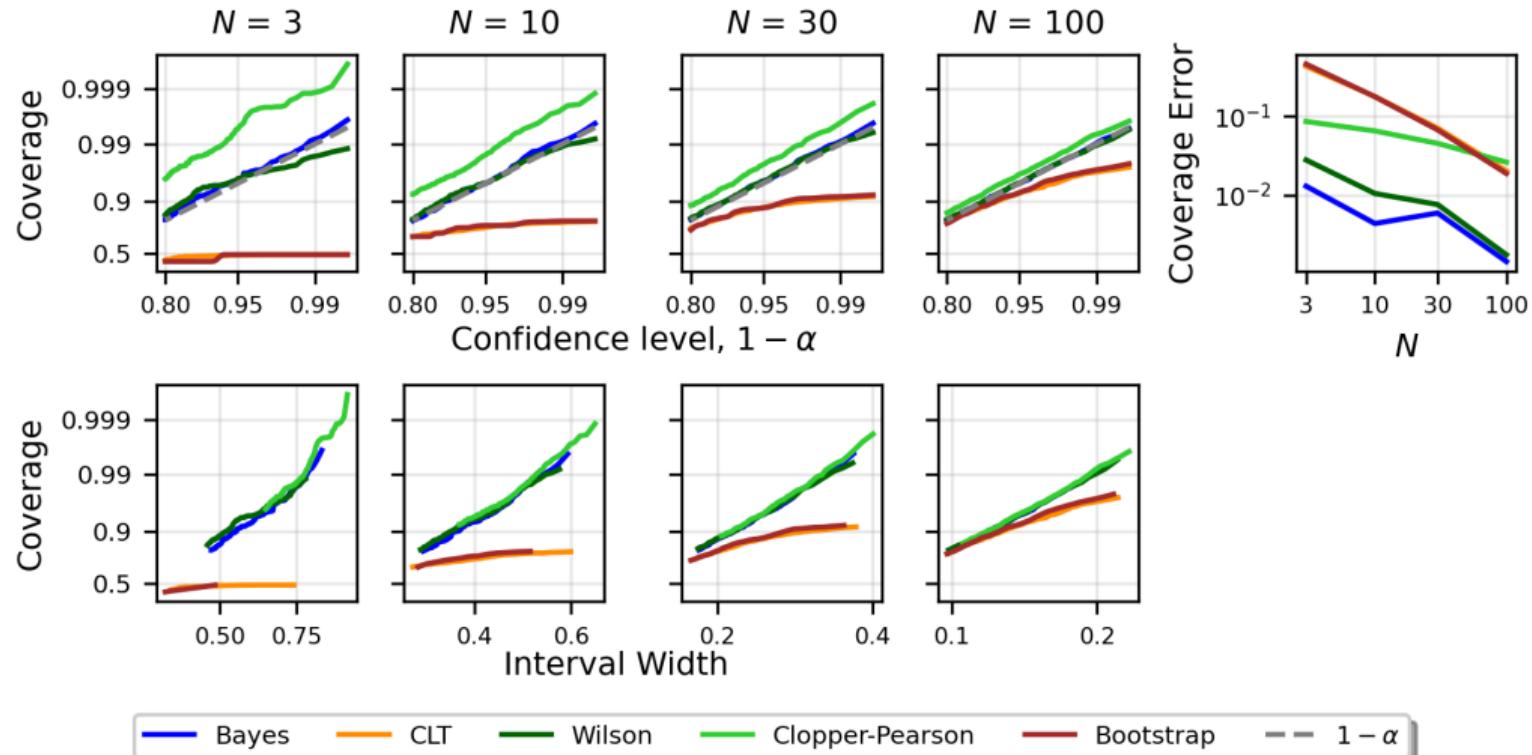
- Draw $\theta \sim \text{Uniform}[0, 1]$.
- Draw $N \in \{3, 10, 30, 100\}$ IID Bernoulli datapoints with parameter θ .
- Construct intervals with various methods for various $1 - \alpha$ confidence levels.
- Repeat many times and calculate the true coverage and width of the intervals.

Interval Comparison Simulations

We use synthetic eval data so that we **know** the true parameter θ .

- Draw $\theta \sim \text{Uniform}[0, 1]$.
- Draw $N \in \{3, 10, 30, 100\}$ IID Bernoulli datapoints with parameter θ .
- Construct intervals with various methods for various $1 - \alpha$ confidence levels.
- Repeat many times and calculate the true coverage and width of the intervals.
 - Coverage: What proportion of the time does a $1 - \alpha$ confidence-level interval **actually contain** the true parameter? (A frequentist metric, really.)

IID Questions Setting: Results



Other Eval Settings

- **Clustered Questions**

Other Eval Settings

- **Clustered Questions**

- We have T tasks, each with N_t IID questions, instead of N IID questions.

Other Eval Settings

- **Clustered Questions**
 - We have T tasks, each with N_t IID questions, instead of N IID questions.
- **Comparisons Between Two Models, θ_A and θ_B**

Other Eval Settings

- **Clustered Questions**

- We have T tasks, each with N_t IID questions, instead of N IID questions.

- **Comparisons Between Two Models, θ_A and θ_B**

- Independent Comparisons (using $N_A, N_B, \bar{y}_A, \bar{y}_B$ only).

Other Eval Settings

- **Clustered Questions**

- We have T tasks, each with N_t IID questions, instead of N IID questions.

- **Comparisons Between Two Models, θ_A and θ_B**

- Independent Comparisons (using $N_A, N_B, \bar{y}_A, \bar{y}_B$ only).
- Paired Comparisons (using $N_A = N_B, \{y_{A;i}\}_{i=1}^N, \{y_{B;i}\}_{i=1}^N$).

Other Eval Settings

- **Clustered Questions**
 - We have T tasks, each with N_t IID questions, instead of N IID questions.
- **Comparisons Between Two Models, θ_A and θ_B**
 - Independent Comparisons (using $N_A, N_B, \bar{y}_A, \bar{y}_B$ only).
 - Paired Comparisons (using $N_A = N_B, \{y_{A;i}\}_{i=1}^N, \{y_{B;i}\}_{i=1}^N$).
- **Metrics that aren't simple averages of binary results** (e.g. F1 score).

Other Eval Settings

- **Clustered Questions**
 - We have T tasks, each with N_t IID questions, instead of N IID questions.
- **Comparisons Between Two Models, θ_A and θ_B**
 - Independent Comparisons (using $N_A, N_B, \bar{y}_A, \bar{y}_B$ only).
 - Paired Comparisons (using $N_A = N_B, \{y_{A;i}\}_{i=1}^N, \{y_{B;i}\}_{i=1}^N$).
- **Metrics that aren't simple averages of binary results** (e.g. F1 score).
- **Prior Mismatch** (i.e. what if the uniform prior is incorrect, $\theta \not\sim \text{Uniform}[0, 1]$?).

Clustered Questions Setting: Frequentist Approach

- Instead of N IID questions, we have T tasks, each with N_t IID questions.

Clustered Questions Setting: Frequentist Approach

- Instead of N IID questions, we have T tasks, each with N_t IID questions.
- Some tasks are easier than others.

Clustered Questions Setting: Frequentist Approach

- Instead of N IID questions, we have T tasks, each with N_t IID questions.
- Some tasks are easier than others.
- Frequentist approach (Miller, 2024):

$$\text{CI}_{1-\alpha}(\theta) = \bar{X} \pm z_{\alpha/2} \text{SE}_{\text{Clustered}}$$

$$\text{SE}_{\text{Clustered}} = \sqrt{\text{SE}_{\text{CLT}}^2 + \frac{1}{N^2} \sum_{t=1}^T \sum_{i=1}^{N_t} \sum_{j \neq i} (y_{i,t} - \bar{y})(y_{j,t} - \bar{y})}$$

Clustered Questions Setting: A Bayesian Approach

- 'Dispersion' parameter d controls the range of difficulty across tasks,

$$d \sim \text{Gamma}(1, 1).$$

Clustered Questions Setting: A Bayesian Approach

- 'Dispersion' parameter d controls the range of difficulty across tasks,

$$d \sim \text{Gamma}(1, 1).$$

- θ is the mean difficulty of the questions across tasks,

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1].$$

Clustered Questions Setting: A Bayesian Approach

- 'Dispersion' parameter d controls the range of difficulty across tasks,

$$d \sim \text{Gamma}(1, 1).$$

- θ is the mean difficulty of the questions across tasks,

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1].$$

- θ_t is the difficulty of the questions in task t (we ensure that $\mathbb{E}[\theta_t] = \theta$),

$$\theta_t \sim \text{Beta}(d\theta, d(1 - \theta)).$$

Clustered Questions Setting: A Bayesian Approach

- 'Dispersion' parameter d controls the range of difficulty across tasks,

$$d \sim \text{Gamma}(1, 1).$$

- θ is the mean difficulty of the questions across tasks,

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1].$$

- θ_t is the difficulty of the questions in task t (we ensure that $\mathbb{E}[\theta_t] = \theta$),

$$\theta_t \sim \text{Beta}(d\theta, d(1 - \theta)).$$

- If d is small, then θ_t is close to θ for all tasks.

Clustered Questions Setting: A Bayesian Approach

- 'Dispersion' parameter d controls the range of difficulty across tasks,

$$d \sim \text{Gamma}(1, 1).$$

- θ is the mean difficulty of the questions across tasks,

$$\theta \sim \text{Beta}(1, 1) = \text{Uniform}[0, 1].$$

- θ_t is the difficulty of the questions in task t (we ensure that $\mathbb{E}[\theta_t] = \theta$),

$$\theta_t \sim \text{Beta}(d\theta, d(1 - \theta)).$$

- If d is small, then θ_t is close to θ for all tasks.
- If d is large, then θ_t is more variable across tasks.

Clustered Questions Setting: A Bayesian Approach

$$d \sim \text{Gamma}(1, 1), \quad \theta \sim \text{Beta}(1, 1), \quad \theta_t \sim \text{Beta}(d\theta, d(1 - \theta)), \quad y_{i,t} \sim \text{Bernoulli}(\theta_t)$$

Clustered Questions Setting: A Bayesian Approach

$$d \sim \text{Gamma}(1, 1), \quad \theta \sim \text{Beta}(1, 1), \quad \theta_t \sim \text{Beta}(d\theta, d(1 - \theta)), \quad y_{i,t} \sim \text{Bernoulli}(\theta_t)$$

- Can we integrate out the per-task difficulty parameters θ_t ?

Clustered Questions Setting: A Bayesian Approach

$$d \sim \text{Gamma}(1, 1), \quad \theta \sim \text{Beta}(1, 1), \quad \theta_t \sim \text{Beta}(d\theta, d(1 - \theta)), \quad y_{i,t} \sim \text{Bernoulli}(\theta_t)$$

- Can we integrate out the per-task difficulty parameters θ_t ?
- Yes! The number of successes per task is **Beta-Binomial** distributed:

$$\sum_{i=1}^{N_t} y_{i,t} = Y_t \sim \text{BetaBinomial}(N_t, d\theta, d(1 - \theta)).$$

Clustered Questions Setting: A Bayesian Approach

$$d \sim \text{Gamma}(1, 1), \quad \theta \sim \text{Beta}(1, 1), \quad \theta_t \sim \text{Beta}(d\theta, d(1 - \theta)), \quad y_{i,t} \sim \text{Bernoulli}(\theta_t)$$

- Can we integrate out the per-task difficulty parameters θ_t ?
- Yes! The number of successes per task is **Beta-Binomial** distributed:

$$\sum_{i=1}^{N_t} y_{i,t} = Y_t \sim \text{BetaBinomial}(N_t, d\theta, d(1 - \theta)).$$

- Get an **importance-weighted posterior** for θ : draw prior samples $\{(\theta^{(k)}, d^{(k)})\}_{k=1}^K$, then compute weights

$$w^{(k)} = \prod_{t=1}^T p(Y_t | \theta^{(k)}, d^{(k)}).$$

Clustered Questions Setting: A Bayesian Approach

$$d \sim \text{Gamma}(1, 1), \quad \theta \sim \text{Beta}(1, 1), \quad \theta_t \sim \text{Beta}(d\theta, d(1 - \theta)), \quad y_{i,t} \sim \text{Bernoulli}(\theta_t)$$

- Can we integrate out the per-task difficulty parameters θ_t ?
- Yes! The number of successes per task is **Beta-Binomial** distributed:

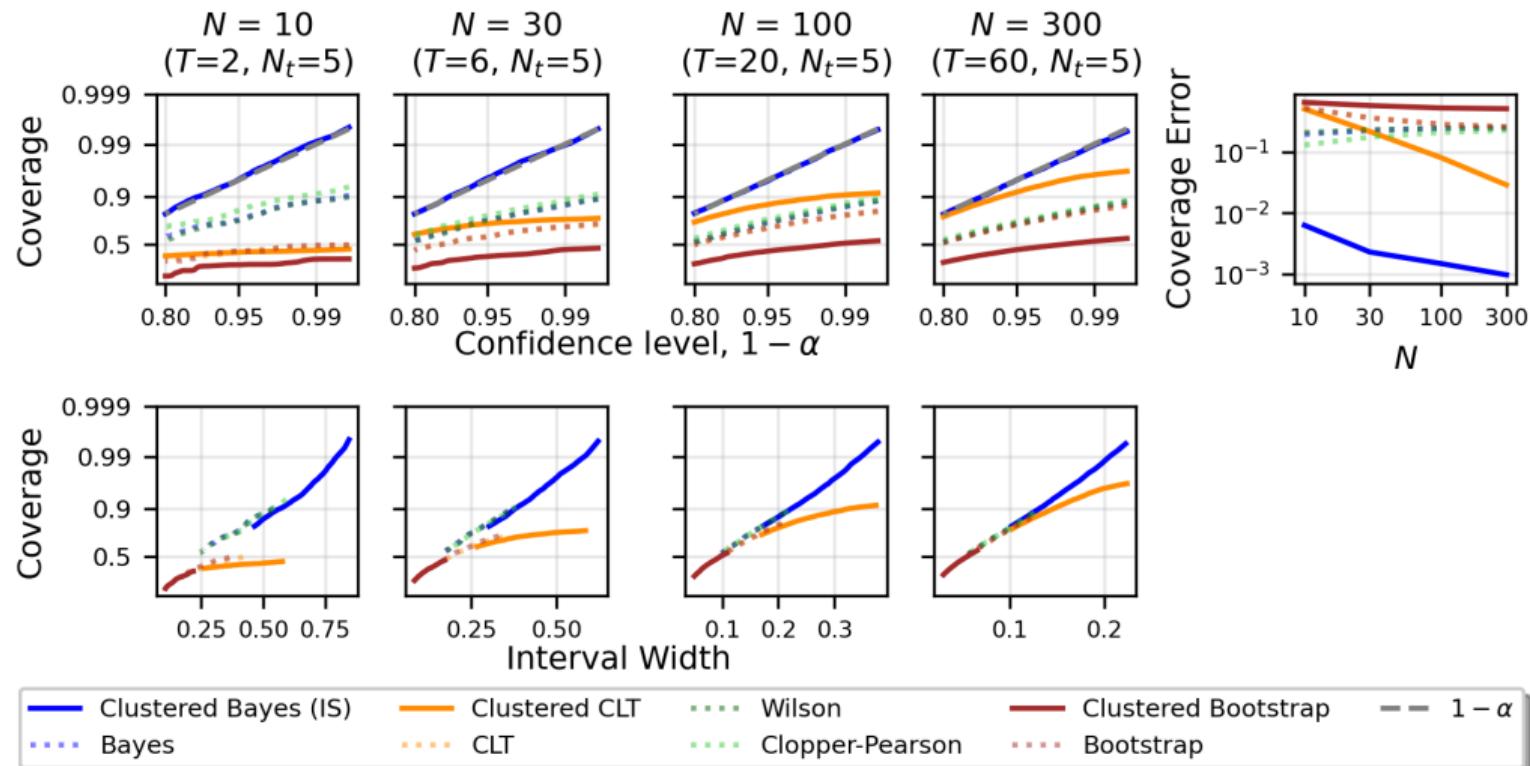
$$\sum_{i=1}^{N_t} y_{i,t} = Y_t \sim \text{BetaBinomial}(N_t, d\theta, d(1 - \theta)).$$

- Get an **importance-weighted posterior** for θ : draw prior samples $\{(\theta^{(k)}, d^{(k)})\}_{k=1}^K$, then compute weights

$$w^{(k)} = \prod_{t=1}^T p(Y_t | \theta^{(k)}, d^{(k)}).$$

- Compute quantile-based Bayesian credible intervals for θ .

Clustered Questions Setting: Results



Conclusion

Advice to practitioners:

- Use Bayesian Beta-Bernoulli or Wilson Score intervals.

Conclusion

Advice to practitioners:

- Use Bayesian Beta-Bernoulli or Wilson Score intervals.
- It's **simple** (use `scipy` or `bayes_evals`).

Conclusion

Advice to practitioners:

- Use Bayesian Beta-Bernoulli or Wilson Score intervals.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.

Conclusion

Advice to practitioners:

- Use **Bayesian Beta-Bernoulli** or **Wilson Score intervals**.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.
- It's still **cheap** for large N .

Conclusion

Advice to practitioners:

- Use **Bayesian Beta-Bernoulli** or **Wilson Score intervals**.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.
- It's still **cheap** for large N .

Conclusion

Advice to practitioners:

- Use **Bayesian Beta-Bernoulli** or **Wilson Score intervals**.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.
- It's still **cheap** for large N .

My takeaways from this project:

- The project really cemented my understanding of Bayesianism vs Frequentism in practice.

Conclusion

Advice to practitioners:

- Use **Bayesian Beta-Bernoulli** or **Wilson Score intervals**.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.
- It's still **cheap** for large N .

My takeaways from this project:

- The project really cemented my understanding of Bayesianism vs Frequentism in practice.
- There's a big communication gap between AI researchers and classical statisticians.

Conclusion

Advice to practitioners:

- Use **Bayesian Beta-Bernoulli** or **Wilson Score intervals**.
- It's **simple** (use `scipy` or `bayes_evals`).
- It's **safer** than CLT-based methods.
- It's still **cheap** for large N .

My takeaways from this project:

- The project really cemented my understanding of Bayesianism vs Frequentism in practice.
- There's a big communication gap between AI researchers and classical statisticians.
- UQ for evals is an incredibly rich space.

References I

-  Bowyer, Sam, Laurence Aitchison, and Desi R. Ivanova (Oct. 2025). “Position: Don’t Use the CLT in LLM Evals With Fewer Than a Few Hundred Datapoints”. en. In: *Proceedings of the 42nd International Conference on Machine Learning*. ISSN: 2640-3498. PMLR, pp. 81143–81184. URL: <https://proceedings.mlr.press/v267/bowyer25a.html> (visited on 11/09/2025).
-  Bowyer, Sam, Thomas Heap, and Laurence Aitchison (Sept. 2024). “Using Autodiff to Estimate Posterior Moments, Marginals and Samples”. en. In: *Proceedings of the Fortieth Conference on Uncertainty in Artificial Intelligence*. ISSN: 2640-3498. PMLR, pp. 394–417. URL: <https://proceedings.mlr.press/v244/bowyer24a.html> (visited on 11/09/2025).

References II

-  Chatterjee, Sourav and Persi Diaconis (Apr. 2018). “The sample size required in importance sampling”. en. In: *The Annals of Applied Probability* 28.2. ISSN: 1050-5164. DOI: 10.1214/17-AAP1326. URL: <https://projecteuclid.org/journals/annals-of-applied-probability/volume-28/issue-2/The-sample-size-required-in-importance-sampling/10.1214/17-AAP1326.full> (visited on 02/03/2023).
-  Heap, Thomas, Sam Bowyer, and Laurence Aitchison (July 2025). “Massively Parallel Expectation Maximization For Approximate Posteriors”. en. In: *Proceedings of the 7th Symposium on Advances in Approximate Bayesian Inference*. ISSN: 2640-3498. PMLR, pp. 25–66. URL: <https://proceedings.mlr.press/v289/heap25a.html> (visited on 11/09/2025).
-  Miller, Evan (Nov. 2024). *Adding Error Bars to Evals: A Statistical Approach to Language Model Evaluations*. en. arXiv:2411.00640 [stat]. DOI: 10.48550/arXiv.2411.00640. URL: <http://arxiv.org/abs/2411.00640> (visited on 12/17/2024).