Robust inference and model selection using bagged posteriors

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Slides: http://jwmi.github.io/talks/Harvard2021.pdf
Preprint 1: https://arxiv.org/abs/1912.07104
Preprint 2: https://arxiv.org/abs/2007.14845

Outline

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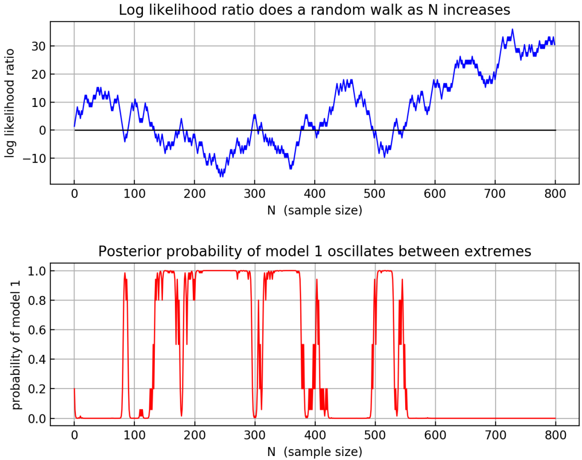
Motivation

- Standard Bayesian inference is known to be sensitive to model misspecification.
- This leads to unreliable uncertainty quantification and poor predictive performance.
- Several methods exist for robust Bayesian inference under misspecification.
- However, finding generally applicable and computationally feasible methods is a difficult challenge.

Toy Bernoulli example

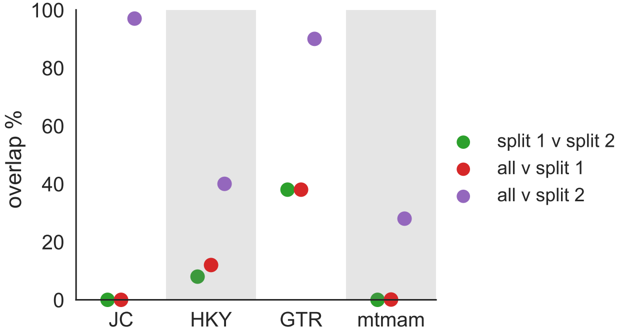
- Suppose $X_1, \ldots, X_N \sim \text{Bernoulli}(p)$ i.i.d.
- Consider the (yes, contrived!) situation in which we only consider two models: (1) $p = 0.2$ and (2) $p = 0.8$, but the true value is $p = 0.501$.



Example: Phylogenetic tree inference for whale species

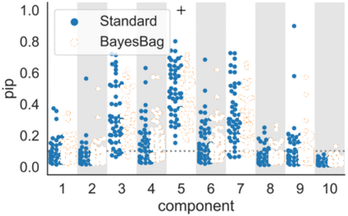
- This is not just a contrived issue – it frequently occurs in practice in phylogenetic inference.
  - Alfaro et al. (2003), Douady et al. (2003), Wilcox et al. (2002).
- Bayesian phylogenetic inference is very widely used, however, it often yields self-contradictory results due to misspecification.

Overlap between posteriors from two subsets of a whale genetics data set

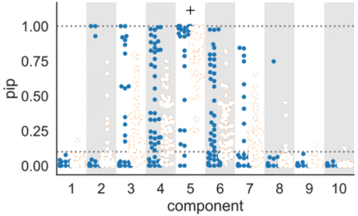


Example: Variable selection in linear regression

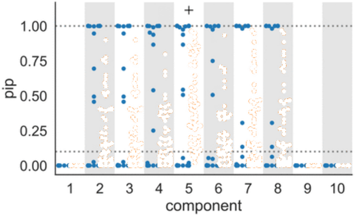
- Similarly, variable selection is unstable when there is misspecification.
- Posterior inclusion probabilities (pips) often flip-flop as N grows.



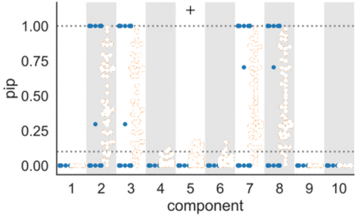
(a) $N = 5 \times 10^1$



(b) $N = 5 \times 10^2$



(c) $N = 5 \times 10^3$

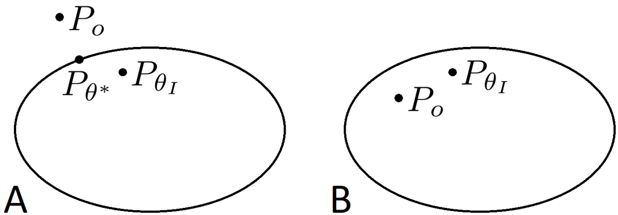


(d) $N = 5 \times 10^4$

Outline

What do we mean by misspecification? Two scenarios

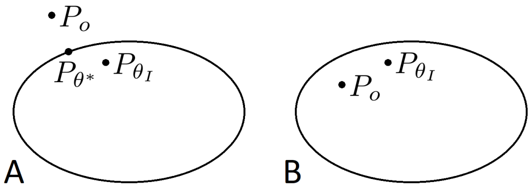
- Notation:
  - P_o = distribution of the observed data
  - θ^* = pseudo-true parameter (KL-nearest point in model to P_o)
  - θ_I = ideal parameter (the truth before perturbation)
  - We think of P_o as a perturbation of P_{θ_I}.
- Scenario A: P_o is not in the model class.
- Scenario B: P_o is in the model class, but $P_o \neq P_{\theta_I}$.



- If there is no perturbation, then $P_o = P_{\theta^*} = P_{\theta_I}$.

What is the quantity of interest?

- The choice of method depends on the quantity of interest.
- Two main perspectives:
  1. *Fitting/prediction:* Model is a tool for approximating P_o.
     - ★ Want to predict future observations.
     - ★ Pseudo-true parameter θ^* is of interest.
  2. *Inference:* Model is an idealization of a true process.
     - ★ Want to recover unknown true parameters.
     - ★ Ideal parameter θ_I is of interest.



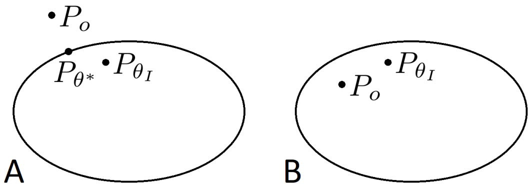
Perspective 1: Model is a tool for approximating P_o

- Pseudo-true parameter θ^* is of interest.
- Common when doing prediction using classification or regression.

- The posterior concentrates at θ^* (under regularity conditions), but ...
  - It is typically miscalibrated: credible sets do not have correct coverage.
    - ★ Kleijn & van der Vaart (2012)
    - ★ Can recalibrate using sandwich covariance (Müller, 2013, and others)
  - Slow concentration can occur, causing poor prediction performance.
    - ★ Grünwald & van Ommen (2014)
    - ★ Can fix this using a power posterior $\propto p(x|\theta)^\zeta p(\theta)$ for certain $\zeta \in (0, 1)$

Perspective 2: Model is an idealization of a true process

- Model is interpretable, but not exactly right of course.
- Ideal parameter θ_I is of interest.
- Data is from P_o, which we think of as a perturbation of P_{θ_I}.
- The objective is to understand — not to fit.
- This perspective is ubiquitous in science & medicine.



Some previous methods, categorized

- Perspective 1: Fitting/prediction, focus on pseudo-true parameter θ^*.
  - Robust adjusted likelihood (Royall & Tsou, 2003)
  - SafeBayes (Grünwald & van Ommen, 2014)
  - Modular posteriors (Jacob et al., 2017)
  - Sandwich covariance adjustment (Müller, 2013)
  - Holmes & Walker (2017)

  ... and many others.
- Perspective 2: Inference, focus on idealized parameter θ_I.
  - Coarsened posterior (M. & Dunson, 2019)
  - Nonparametric perturbation models (M., forthcoming)
- In this talk, we focus on perspective 1.

Outline

Bagged posterior (BayesBag)

- Basic idea: Use bagging on the posterior, that is, average the posterior over many bootstrapped datasets.

- More precisely:
  - Original data set: $x = (x_1, \ldots, x_N)$.
  - Bootstrapped copy of original data set: $x^* = (x_1^*, \ldots, x_M^*)$.
  - Posterior obtained by treating x^* as the original data set:

$$\pi(\theta \mid x^*) \propto \pi_0(\theta) \prod_{m=1}^{M} p_\theta(x_m^*).$$

  - The *bagged posterior* is defined by averaging these posteriors:

$$\pi^*(\theta \mid x) := \frac{1}{N^M} \sum_{x^*} \pi(\theta \mid x^*),$$

    where the sum is over all N^M possible bootstrap datasets of M samples drawn with replacement from the original dataset.

Bagged posterior (BayesBag): Practical considerations

- In practice, we approximate $\pi^*(\theta \mid x)$ by generating B bootstrap datasets $x^*_{(1)}, \ldots, x^*_{(B)}$ and forming the simple Monte Carlo approximation
$$\pi^*(\theta \mid x) \approx \frac{1}{B} \sum_{b=1}^{B} \pi(\theta \mid x^*_{(b)}).$$
- Any posterior computation technique for the standard posterior can be used to compute each term $\pi(\theta \mid x^*_{(b)})$.
  - For example, a closed-form solution, MCMC, or quadrature.
- How to choose the number of bootstrap datasets B?
  - As a default, $B \approx 50$ to 100 often suffices.
  - Formally, the Monte Carlo error can easily be estimated, since the bootstrap datasets $x^*_{(b)}$ are i.i.d. given the original dataset.

Bagged posterior (BayesBag): Practical considerations

- How to choose the bootstrap dataset size M?
  - Unlike B, bigger M is not always better.
  - The choice of M affects the concentration of the bagged posterior.
  - Thus, M is connected to calibration of uncertainty.

- Interpretation of M:
  - As a default, $M = N$ is a conservative choice that is robust to misspecification.
  - If the model is correct, then $M = 2N$ coincides with the standard posterior, asymptotically.
  - As M/N increases, the bagged posterior becomes more concentrated.

- The role of M is subtly different in the model selection setting compared to the parameter inference setting.

Previous work on bagged posteriors (BayesBag)

- Suggested by Waddell et al. (2002) and Douady et al. (2003).
  - Limited empirical study of BayesBag on phylogenetic inference.
- Independently proposed by Bühlmann (2014).
  - Limited empirical/theoretical study on a simple univariate Gaussian location model.
  - Coined the name "BayesBag", which we adopt here.
- Surprisingly, there seems to have been little empirical or theoretical investigation of bagged posteriors.
- Bagging the posterior is very different than Bayesian Bagging (Clyde & Lee, 2001) and the Bayesian Bootstrap (Rubin, 1981), which are Bayesian ways of doing bagging and bootstrap, respectively.

Principled justification via Jeffrey conditionalization

- Jeffrey conditionalization (Diaconis & Zabell, 1982; Jeffrey, 1968):
  - Assume we have a model $p(x, y)$ for some variables x and y.
  - Suppose we are informed that $p_0(x)$ is the true distribution of x.
  - Then, Jeffrey says to quantify uncertainty in y using

$$q(y) := \int p(y|x)p_0(x)dx.$$

- Now, to connect this to the bagged posterior:
  - Take $x = x_{1:N}$ and $y = \theta$.
  - If we are informed that the true distribution is $p_0^{(N)}(x_{1:N})$, then

$$q(\theta) := \int p(\theta \mid x_{1:N})p_0^{(N)}(x_{1:N})dx_{1:N}.$$

  - Plugging in the empirical distribution $\frac{1}{N}\sum_{i=1}^{N} \delta_{x_i}$ for p_0, we obtain

$$q(\theta) \approx \frac{1}{N^N} \sum_{x^*_{1:N}} p(\theta \mid x^*_{1:N}),$$

    which is precisely the bagged posterior with $M = N$.

Outline

Overview of theoretical results

- We consider the setting of i.i.d. data $X_1, \ldots, X_N \sim P_0$.
- **Model selection.** We show that if two models provide a nearly equally good fit to the data distribution P_0, then:
  - the standard posterior oscillates randomly, strongly favoring one model or the other at random.
  - the bagged posterior stabilizes the probabilities probabilities of the two models, improving reproducibility.
- **Parameter inference.** We derive the mean and covariance of the bagged posterior, and prove a Bernstein–von Mises result characterizing the asymptotic normal distribution.

Theoretical results: Model selection

- Asymptotically, we know the posterior concentrates on the model that is nearest in Kullback–Leibler (KL) divergence to the true distribution.
- To study the non-asymptotic regime via an asymptotic analysis, we consider sequences of models $\mathfrak{m}_{1,N}$ and $\mathfrak{m}_{2,N}$.
- Letting $\Lambda_N = \log \dfrac{p(X_{1:N}|\mathfrak{m}_{1,N})}{p(X_{1:N}|\mathfrak{m}_{2,N})}$ (the log-likelihood ratio), suppose:
  1. $\mathfrak{m}_{1,N}$ and $\mathfrak{m}_{2,N}$ are asymptotically comparable in the sense that
  $$\lim_{N\to\infty} \mathrm{E}(\Lambda_N/\sqrt{N}) = \mu_\infty \in \mathbb{R},$$
  2. $\mathrm{Var}(\Lambda_N/\sqrt{N}) = \sigma_\infty^2 \in (0,\infty)$ for all N, and
  3. $M/N \to c \in [0,\infty)$ as $N \to \infty$, where $M = M(N) \to \infty$.
- The effect size μ_∞/σ_∞ is the evidence in favor of model 1.

Theoretical results: Model selection

- Then as $N \to \infty$, the standard posterior probability of model 1 concentrates at 0 and 1, that is, it converges to a Bernoulli r.v.:

$$\pi(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \mathrm{Bernoulli}(\Phi(\mu_\infty/\sigma_\infty)).$$

- When $c > 0$, the bagged posterior probability of model 1 converges to a continuous r.v. with pdf

$$f(u) = \Phi'\big(c^{-1/2}\Phi^{-1}(u) - \mu_\infty/\sigma_\infty\big)c^{-1/2}/\Phi'(\Phi^{-1}(u)).$$

- When $c = 0$, the bagged posterior prob. of model 1 converges to 1/2:

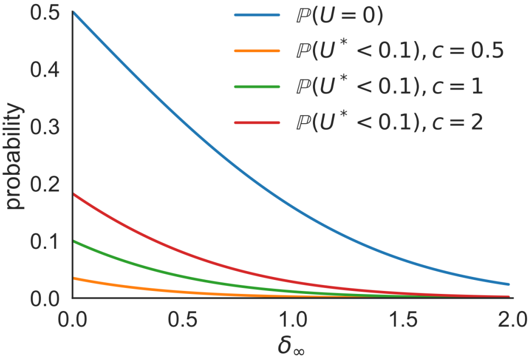
$$\pi^*(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{P} 1/2.$$

- In particular, if $\mu_\infty = 0$ and $c > 0$, then

$$\pi(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \mathrm{Bernoulli}(1/2)$$
$$\pi^*(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \mathrm{Uniform}(0,1).$$

Theoretical results: Model selection

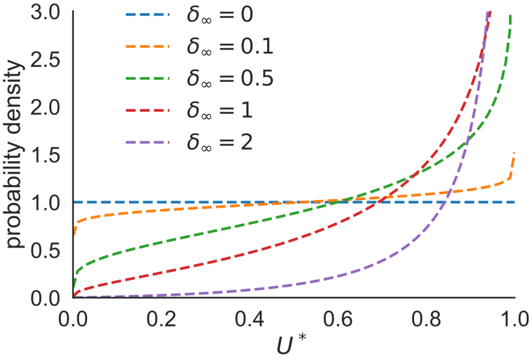
The standard posterior overwhelmingly favors the wrong model with non-negligible probability. The bagged posterior does much better.



- Standard posterior probability of model 1 converges to U.
- Bagged posterior probability of model 1 converges to U^*.
- $\delta_\infty := \mu_\infty / \sigma_\infty$ = mean effect size in favor of model 1.

Theoretical results: Model selection

The bagged posterior converges to a continuous r.v. U^* on $[0,1]$, avoiding misleading extreme probabilities close to 0 or 1. (Shown: $c = 1$.)

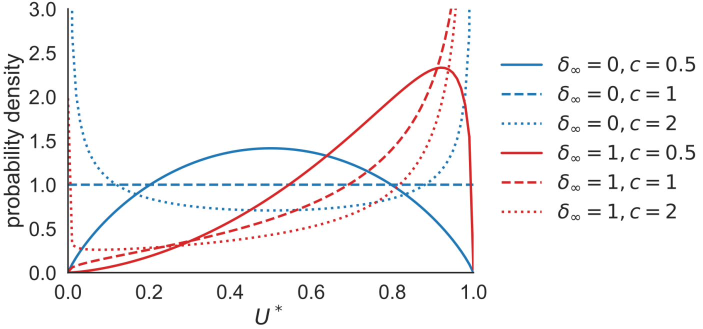


$$f_{U^*}(u) = \Phi'\big(c^{-1/2}\Phi^{-1}(u) - \mu_\infty/\sigma_\infty\big)c^{-1/2}/\Phi'(\Phi^{-1}(u))$$

- $\delta_\infty := \mu_\infty/\sigma_\infty$ = mean effect size in favor of model 1.

Theoretical results: Model selection

Choosing M smaller makes the bagged posterior tend to be more uniform over the set of plausible models.



- $c = \lim_{N\to\infty} M/N$, where $M = M(N)$.
  - For instance, $c \in \{0.5, 1, 2\}$ when $M \in \{0.5N, N, 2N\}$, respectively.
- $\delta_\infty := \mu_\infty/\sigma_\infty =$ mean effect size in favor of model 1.

Theoretical results: Parameter inference

- Now, consider the bagged posterior on a parameter $\theta \in \mathbb{R}^D$.

- Given dataset $x = x_{1:N}$, let X^* be a random bootstrap dataset.
- Let $\mu(x)$ and $\Sigma(x)$ denote the mean and covariance matrix of the standard posterior $p(\theta|x)$.

- By the law of total expectation, the mean of the bagged posterior is

$$\mathrm{E}(\mu(X^*) \mid x) = \frac{1}{N^M} \sum_{x^*} \mu(x^*).$$

- By the law of total variance, the covariance of the bagged posterior is

$$\mathrm{E}(\Sigma(X^*) \mid x) + \mathrm{Cov}(\mu(X^*) \mid x).$$

Theoretical results: Parameter inference

- Thus, the covariance of the bagged posterior decomposes as the sum of two terms:
  1. $\mathrm{E}(\Sigma(X^*) \mid x)$
     - ★ $\approx$ mean of the posterior covariance matrix under its sampling distribution.
     - ★ Bayesian model-based uncertainty averaged with respect to frequentist sampling variability.
  2. $\mathrm{Cov}(\mu(X^*) \mid x)$
     - ★ $\approx$ covariance of the posterior mean under its sampling distribution.
     - ★ Frequentist sampling-based uncertainty of the Bayesian model-based point estimate.

Theoretical results: Parameter inference

- Suppose $X_1, \ldots, X_N \sim P_0$ i.i.d., and let θ_0 minimize the KL divergence from P_0.

- For the standard posterior, by Bernstein–von Mises we know that

$$N^{1/2}(\theta - \hat{\theta}_N) | X_{1:N} \xrightarrow{D} \mathcal{N}(0, J_{\theta_0}^{-1})$$

where $\theta \sim p(\theta | X_{1:N})$, $\hat{\theta}_N$ is the MLE, and $J_{\theta_0} = -\mathrm{E}(\nabla^2 \log p_\theta(X_i))$.

- Meanwhile, we also know that the MLE is asymptotically normal:

$$N^{1/2}(\hat{\theta}_N - \theta_0) | X_{1:N} \xrightarrow{D} \mathcal{N}(0,\ J_{\theta_0}^{-1} I_{\theta_0} J_{\theta_0}^{-1}).$$

where $I_{\theta_0} = \mathrm{Cov}(\nabla \log p_\theta(X_i))$.

- Hence, asymptotically, the standard posterior is correctly calibrated if these two covariance matrices coincide.

Theoretical results: Parameter inference

- We prove a Bernstein–von Mises theorem for the bagged posterior, showing that the asymptotic covariance is
$$(J_{\theta_0}^{-1} + J_{\theta_0}^{-1} I_{\theta_0} J_{\theta_0}^{-1})/c$$
where $c = \lim_{N\to\infty} M/N$, and the asymptotic mean is the same as for the standard posterior.

- This is the asymptotic form of the total covariance decomposition.

- When the model is correct, $c = 2$ recovers the standard posterior, asymptotically, since then $J_{\theta_0}^{-1} = J_{\theta_0}^{-1} I_{\theta_0} J_{\theta_0}^{-1}$.

- In general, $c = 1$ is a safe choice, since it is guaranteed to prevent overconfident credible regions, asymptotically.

Outline

Application: Variable selection

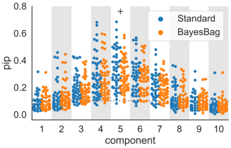
- We consider a standard Bayesian variable selection model for linear regression.
- Specifically, under the prior, each variable is included with probability q_0, independently, and we integrate out Normal and InverseGamma priors on the coefficients and variance, respectively.

- First, we simulate datasets from (1) the assumed model and (2) a model with nonlinearly transformed covariates.
- In both scenarios, the true coefficient vector is sparse.

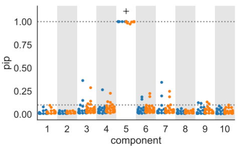
- We compute the bagged posterior using $M = N$.

Application: Variable selection

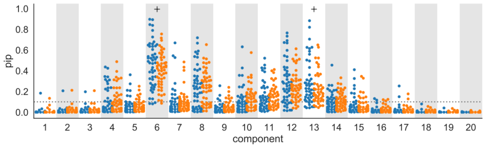
When the model is correct, the bagged and standard posteriors are similar.



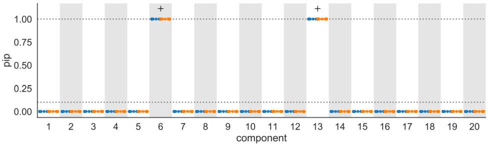
(a) 1-sparse-linear, $N = 5 \times 10^1$



(b) 1-sparse-linear, $N = 5 \times 10^3$



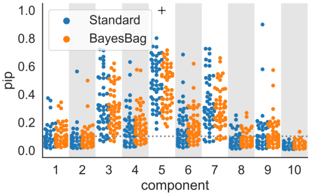
(c) 2-sparse-linear, $N = 10^2$



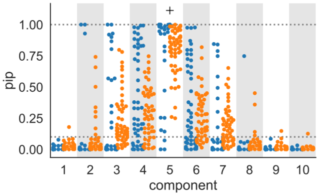
(d) 2-sparse-linear, $N = 10^4$

Application: Variable selection

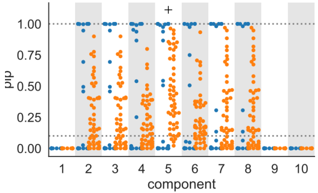
When the model is incorrect, the bagged posterior avoids the self-contradictory results produced by the standard posterior.



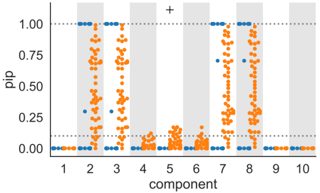
(a) $N = 5 \times 10^1$



(b) $N = 5 \times 10^2$



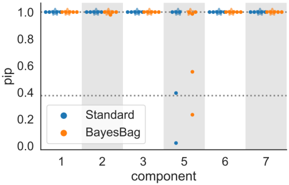
(c) $N = 5 \times 10^3$



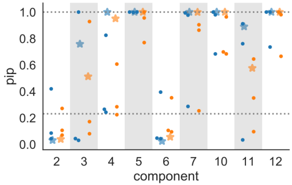
(d) $N = 5 \times 10^4$

Application: Variable selection

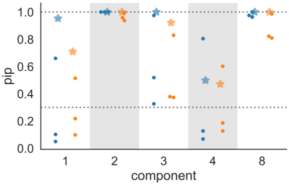
On real datasets, the difference is not dramatic, but the bagged posterior does yield greater reproducibility across subsets of the data.



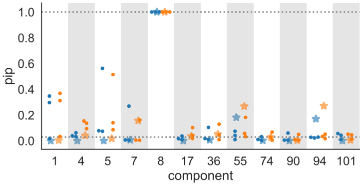
(a) California housing ($\mathcal{I} = 1.00$)



(b) Boston housing ($\mathcal{I} = 0.62$)



(c) Diabetes ($\mathcal{I} = 0.03$)

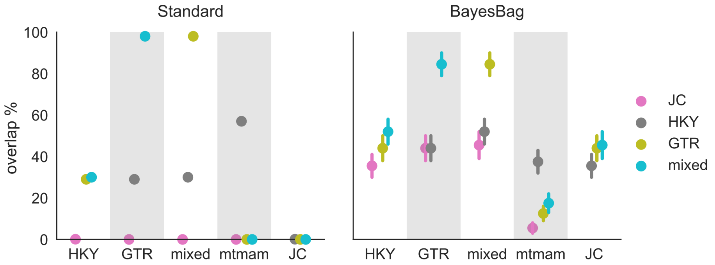


(d) Residential building ($\lambda = 16, \mathcal{I} =$ NA)

Application: Phylogenetic tree inference

- We use a standard Bayesian package for phylogenetic inference (MrBayes 3.2, Ronquist et al., 2012).
- We used the whale dataset from Yang (2008), consisting of mitochondrial DNA from 13 whale species.
- To compute the posterior on trees, MrBayes was run using five different models for the evolutionary process (JC, HKY, GTR, mixed, and mtmam).
- For the bagged posterior, we used $M = N$ and $B = 100$.
- To assess reproducibility, we computed the overlap of 99% highest posterior density regions for selected pairs of posteriors.

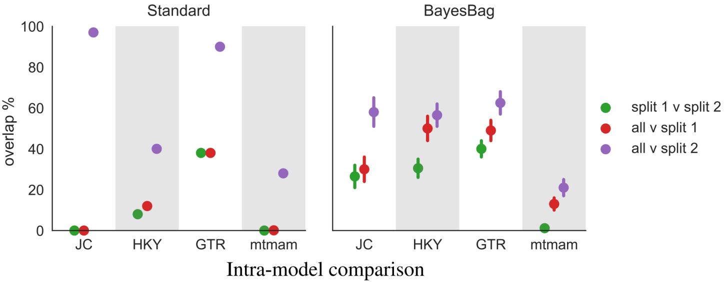
Application: Phylogenetic tree inference



Inter-model comparison

- First, we consider the posterior overlap for each pair of evolutionary models.
- The standard posteriors sometimes have extremely low overlap, suggesting poor reproducibility.
- Meanwhile, the bagged posteriors exhibit more reasonable overlaps for each pair.

Application: Phylogenetic tree inference



- Then, we split the genetic data into two parts, and compute the overlap for (1) the posteriors of the two splits, and (2) the posteriors for each split and the full data.
- Again, the standard posterior exhibits poor reproducibility, while the bagged posterior is more self-consistent.

Application: Linear regression

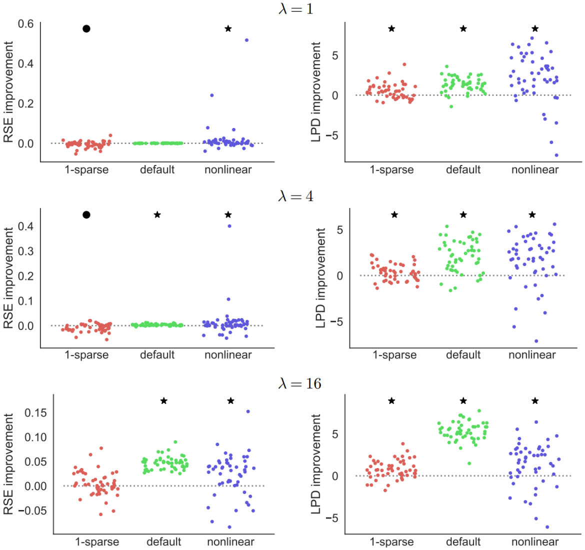
- To illustrate in the parameter inference setting, we consider a standard Bayesian linear regression model.
- As before, we use Normal and InverseGamma priors on the coefficients and variance.

- We simulate data from three scenarios:
  1. the assumed model ("default"),
  2. the coefficient vector has only one nonzero entry ("1-sparse"), and
  3. the covariates are nonlinearly transformed ("nonlinear").

- For the bagged posterior, we selected M using an approach based on our asymptotic theory (see Huggins and M., 2019 for details).

Application: Linear regression

The bagged posterior usually recovers the KL-optimal parameter better in terms of relative squared error (RSE) and log posterior density (LPD).

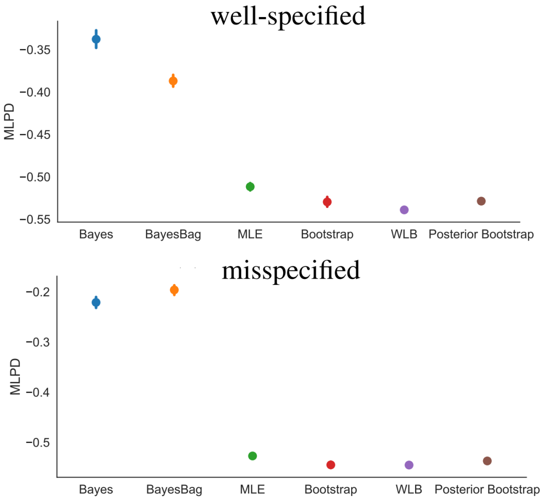


Application: Hierarchical mixed effects logistic regression

- Finally, we consider a mixed effects model from Browne and Draper (2006), applied to prenatal care data from Guatemalan communities.
- We compare the predictive performance of the standard posterior, the bagged posterior, and four methods based on maximum likelihood estimation (with the random effects integrated out):
  - the standard MLE,
  - the bootstrapped MLE,
  - the weighted likelihood bootstrap (Newton and Raftery, 1994), and
  - the posterior bootstrap (Lyddon, Walker and Holmes, 2018).

Application: Hierarchical mixed effects logistic regression

The bagged posterior performs favorably compared to the other methods in terms of mean log predictive density (MLPD).



Conclusion

- Bagging the posterior is an easy-to-use and widely applicable method that improves upon standard Bayesian inference by making it more stable, accurate, and reproducible.

- Directions for future work or improvements:
  - Extensions to non-i.i.d. settings such as time-series and spatial data.
  - Improved computation of bagged posteriors (e.g., Pierre Jacob proposed an unbiased MCMC approach).
  - Finite-sample theory for bagged posteriors.
  - Improved model assessment/criticism techniques and theory.

Robust inference and model selection using bagged posteriors

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Harvard Statistics Colloquium || Cambridge, MA || Feb 1, 2021

Slides: http://jwmi.github.io/talks/Harvard2021.pdf
Preprint 1: https://arxiv.org/abs/1912.07104
Preprint 2: https://arxiv.org/abs/2007.14845