Reproducible model selection using bagged posteriors

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Outline

1. Motivation
2. Methodology (Bagged posteriors)
3. Theory
4. Applications
   - Variable selection
   - Phylogenetic tree inference

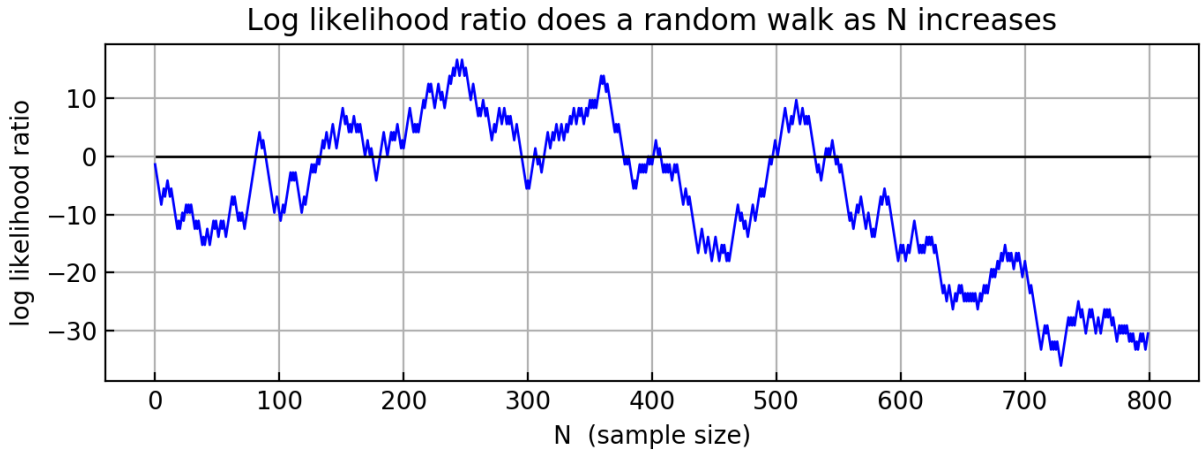
Outline

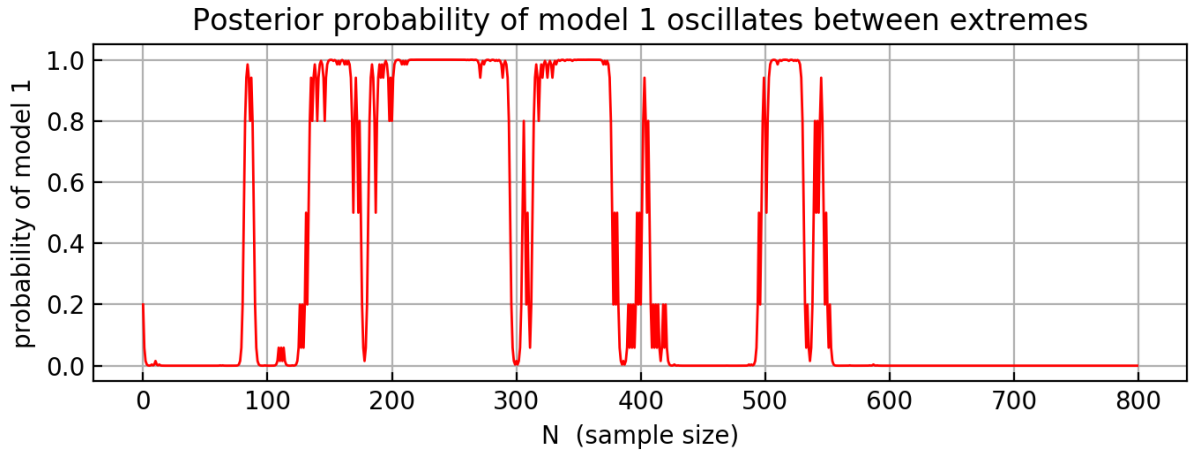
Motivation

- 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 $p = 0.501$.

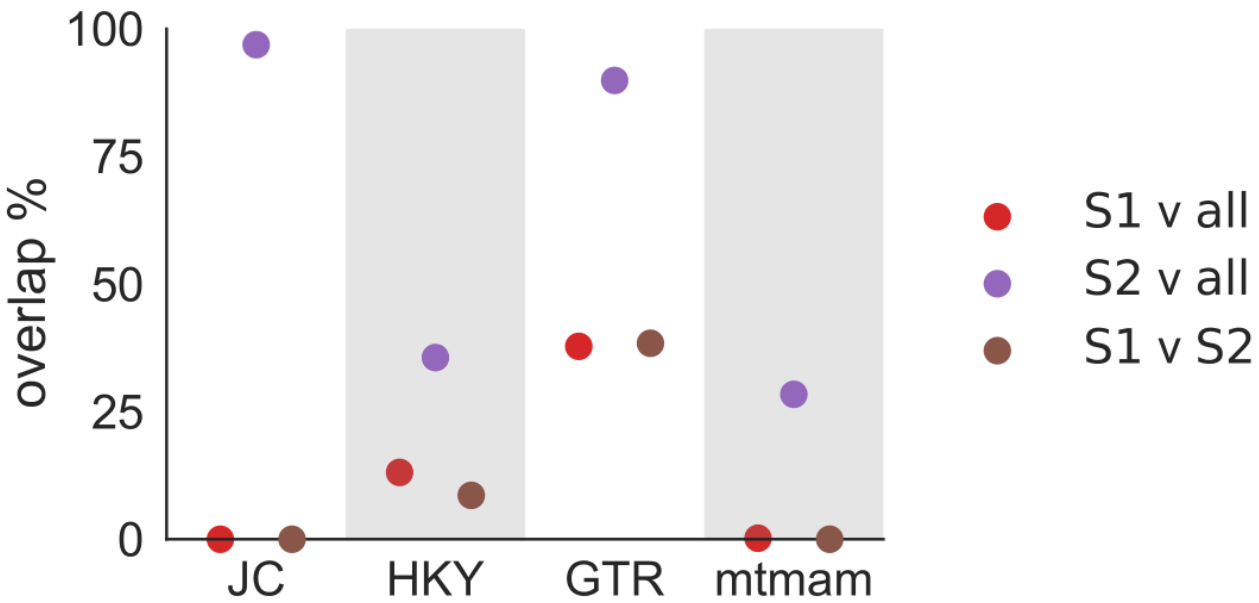




Example: Phylogenetic tree inference for whale species

- 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



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: $x^* = (x_1^*, \ldots, x_M^*)$.
  - Set of models under consideration: $\mathfrak{M} = \{\mathfrak{m}_1, \mathfrak{m}_2, \ldots\}$.
  - Posterior obtained by treating x^* as the original data set:

$$\pi(\mathfrak{m} \mid x^*) \propto \pi(\mathfrak{m}) p(x^*_{1:M} \mid \mathfrak{m}).$$

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

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

    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 $\pi^*(\mathfrak{m} \mid x)$ by generating B bootstrap datasets $x^*_{(1)}, \ldots, x^*_{(B)}$ and forming the simple Monte Carlo approximation

$$\pi^*(\mathfrak{m} \mid x) \approx \frac{1}{B} \sum_{b=1}^{B} \pi(\mathfrak{m} \mid x^*_{(b)}).$$

- Any posterior computation technique for the standard posterior can be used to compute each term $\pi(\mathfrak{m} \mid x^*_{(b)})$.
  - 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.

- Recommended choice of M:
  - Our theory suggests choosing $M = o(N)$ or $M = cN$ with $c \in (0, 1]$.
  - As a default, $M = N^{0.95}$ works well in theory and practice.
  - Even smaller M may work well under significant misspecification or when there are many models relative to the amount of data.

- 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.
- In concurrent work, we (Huggins & Miller, 2019) we have investigated bagged posteriors in the parameter inference setting.
- 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.

Outline

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
  $$\lim_{N\to\infty} \mathrm{E}_{P_0}(\Lambda_N/\sqrt{N}) = \mu_\infty \in \mathbb{R},$$
  2. $\mathrm{Var}_{P_0}(\Lambda_N/\sqrt{N}) = \sigma_\infty^2 \in (0,\infty)$ 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.:

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

- The bagged posterior probability of model 1 converges to a r.v.:

$$\pi^*(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \Phi(c^{1/2}Z)$$

where $Z \sim \mathcal{N}(\mu_\infty/\sigma_\infty, 1)$.

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

$$\pi(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \text{Bernoulli}(1/2)$$

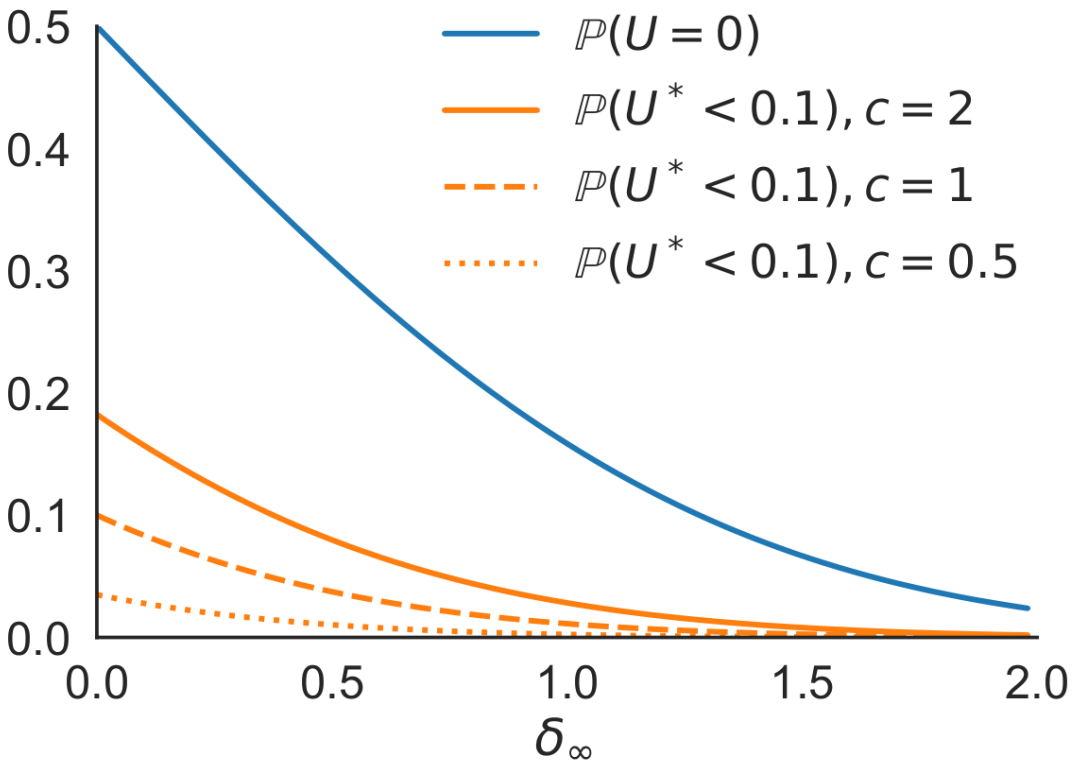
$$\pi^*(\mathfrak{m}_{1,N} \mid X_{1:N}) \xrightarrow{D} \text{Uniform}(0,1).$$

- Meanwhile, if $c = 0$ then

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

Theoretical results: Model selection

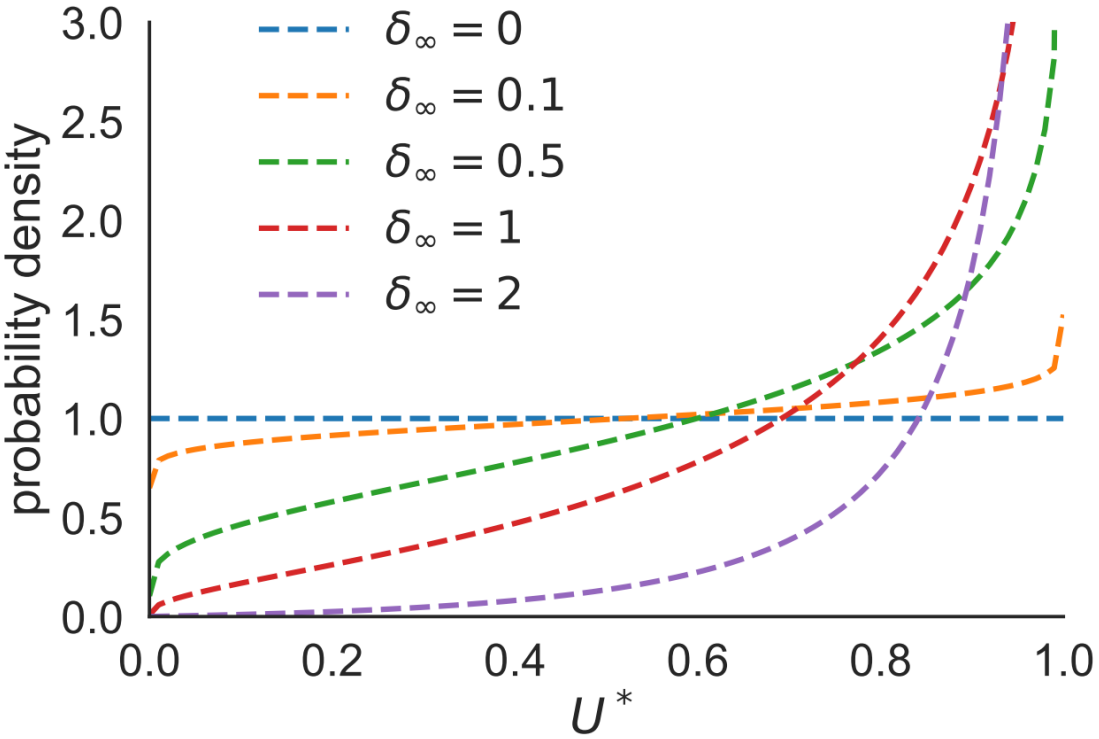
The standard posterior overwhelmingly favors the wrong model with non-negligible probability. The bagged posterior does much better.



- 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: $c = 1$.)



$$U^* = \Phi(c^{1/2} Z) \text{ where } Z \sim \mathcal{N}(\mu_\infty/\sigma_\infty, 1)$$

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

Outline

Application: Variable selection

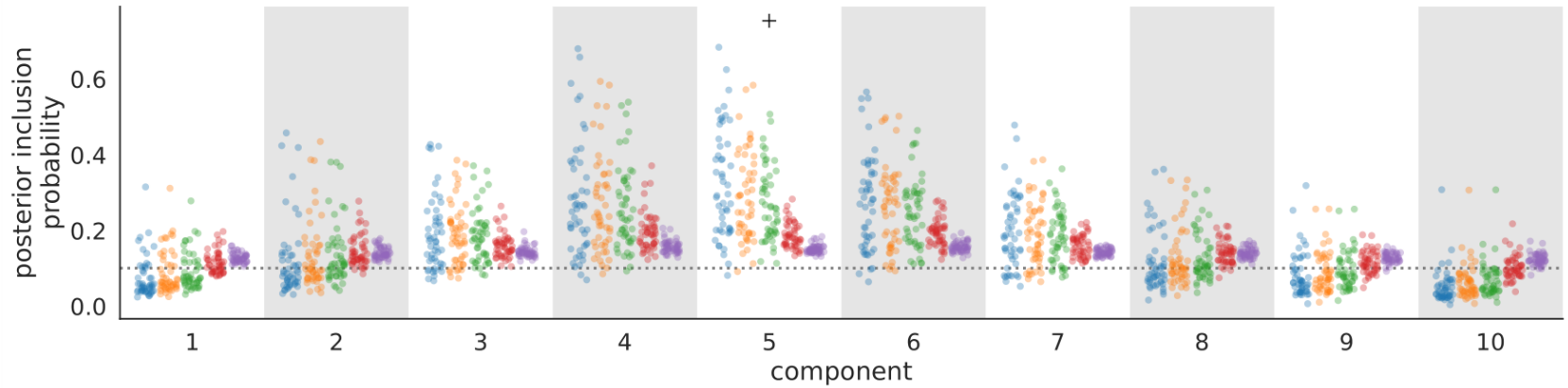
- We consider a standard Bayesian variable selection model for linear regression.
- Specifically, under the prior, each variable is included with probability q_0, independently, and we integrate out Normal and InverseGamma priors on the coefficients and variance, respectively.

- 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.

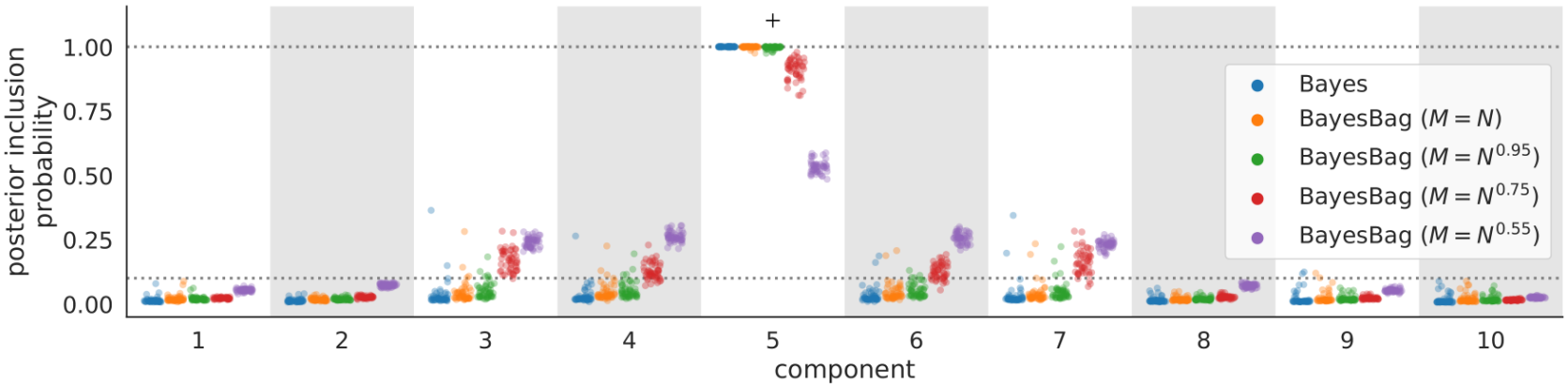
- We consider using $M = N^{\alpha}$ for $\alpha \in \{1, 0.95, 0.75, 0.55\}$ to compute the bagged posterior.

Application: Variable selection

When the model is correct, the bagged posterior with $M = N^\alpha$ is similar to the standard posterior when $\alpha = 1$ and more stable as α decreases.



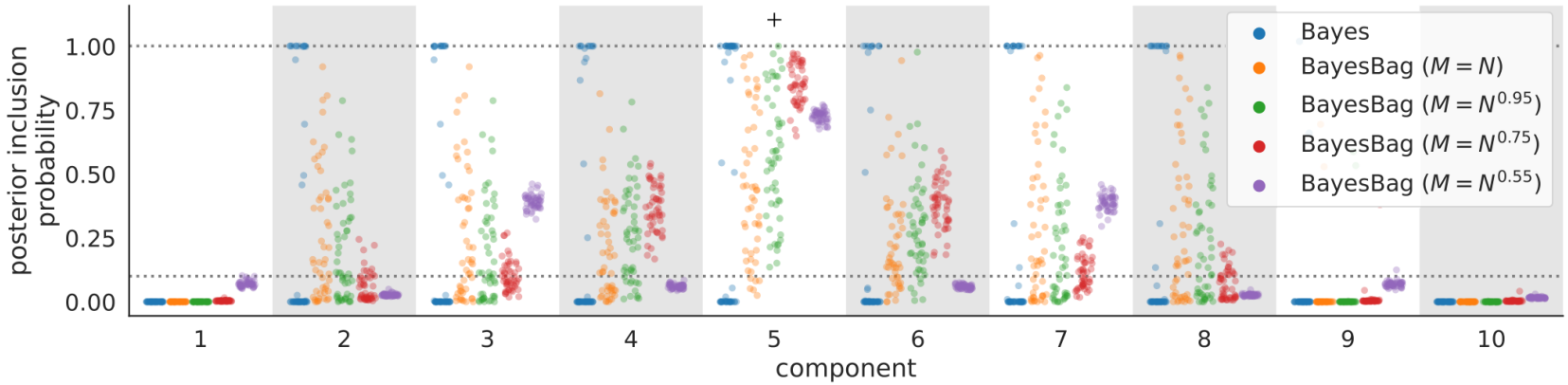
1-sparse-linear, $N = 5 \times 10^1$



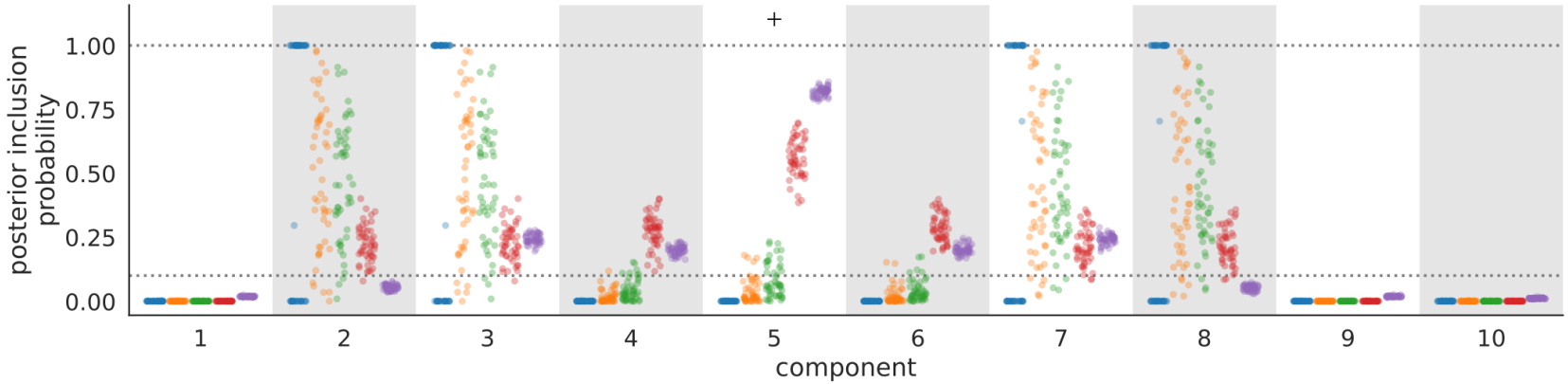
1-sparse-linear, $N = 5 \times 10^3$

Application: Variable selection

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



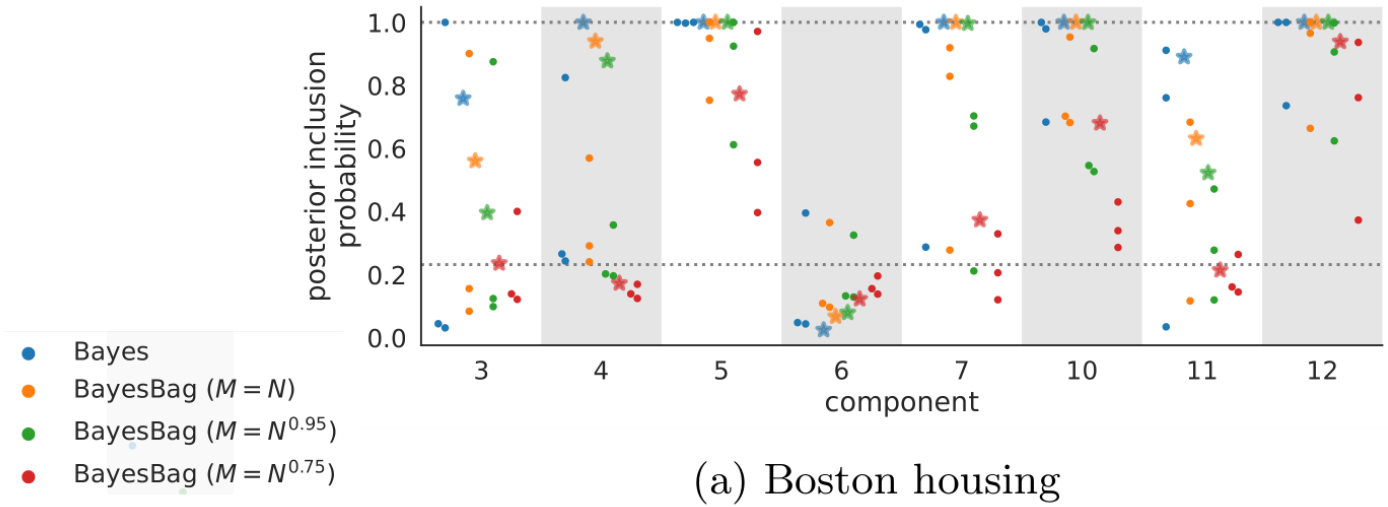
$N = 5 \times 10^3$



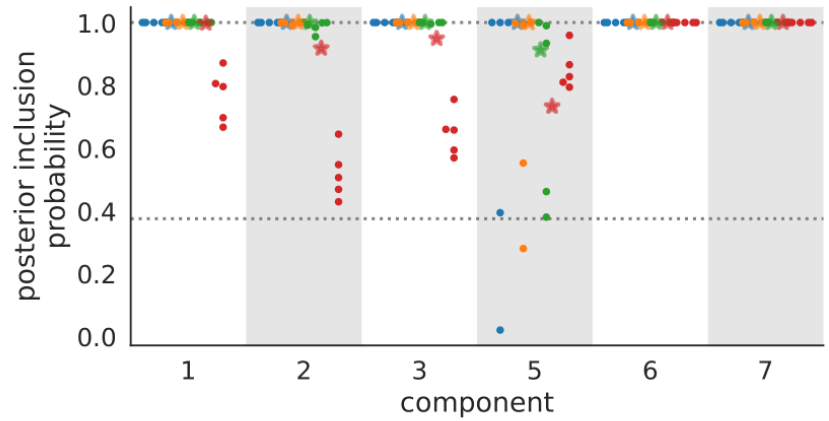
$N = 5 \times 10^4$

Application: Variable selection

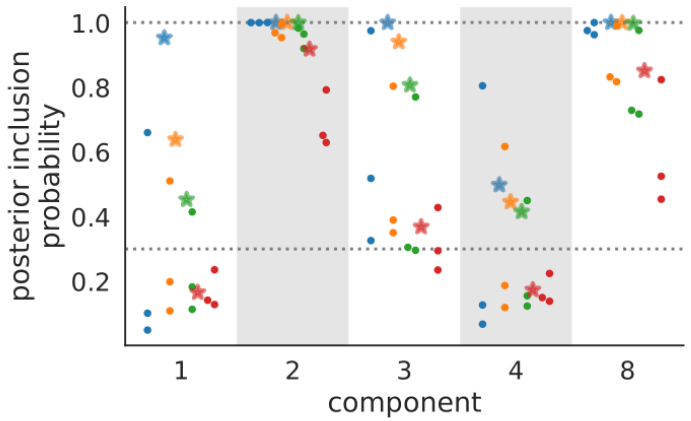
On real datasets, the bagged posterior yields greater reproducibility across subsets of the data.



(a) Boston housing



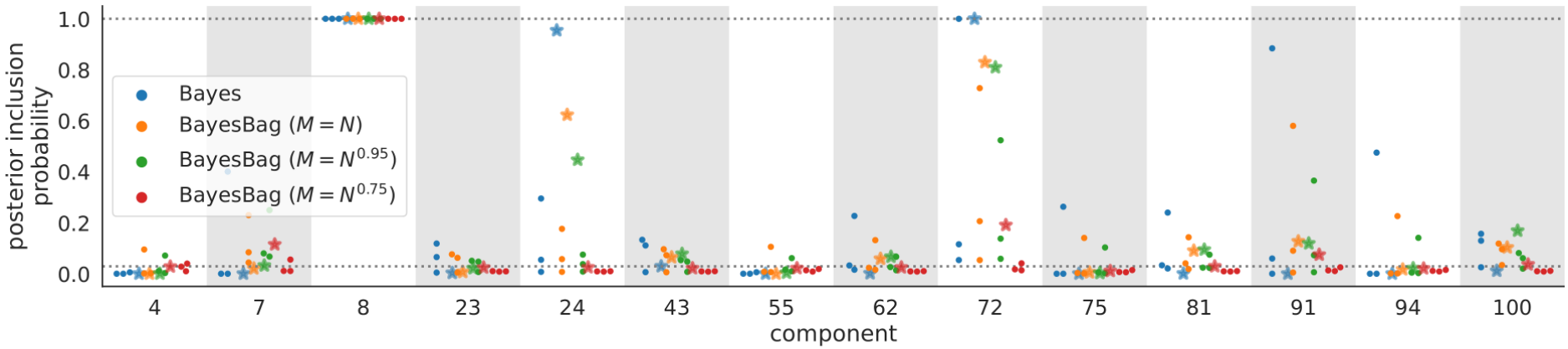
(b) California housing



(c) Diabetes

Application: Variable selection

On real datasets, the bagged posterior yields greater reproducibility across subsets of the data.

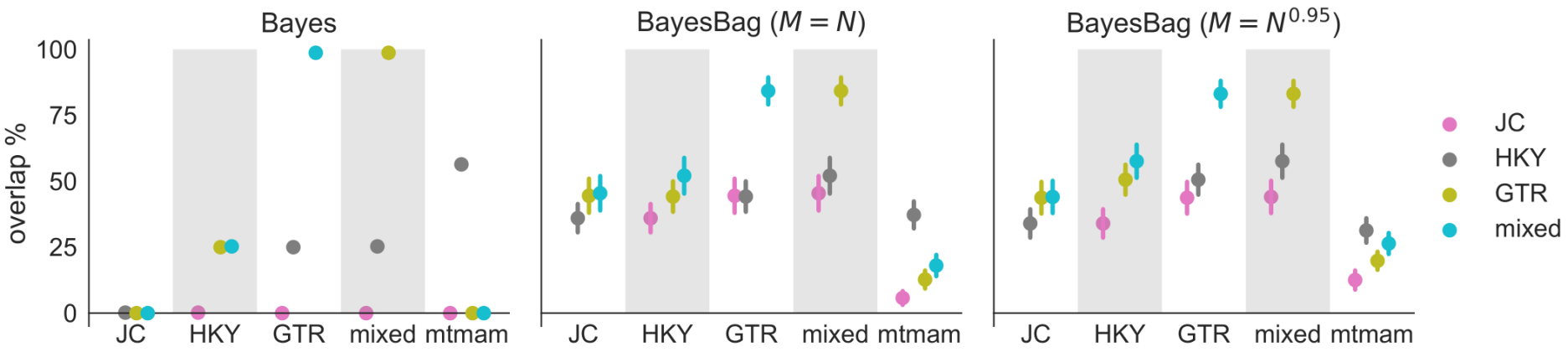


(d) Residential building

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 $M \in \{N, N^{0.95}\}$ and $B = 100$.
- To assess reproducibility, we computed the overlap of 99% highest posterior density regions for selected pairs of posteriors.

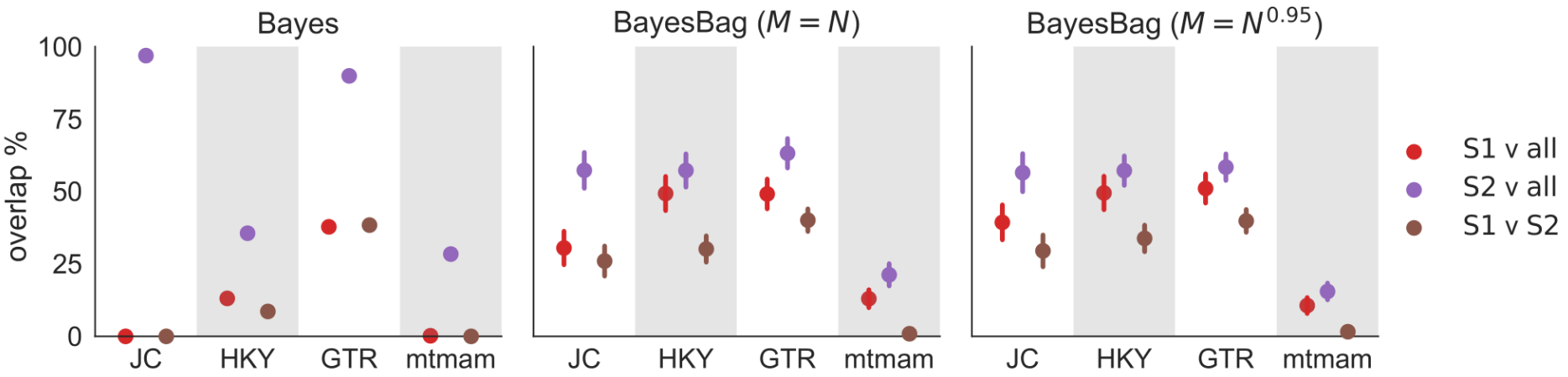
Application: Phylogenetic tree inference



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



Intra-model comparison

- 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.

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.
  - Finite-sample theory for bagged posteriors.
  - Improved model assessment/criticism techniques and theory.

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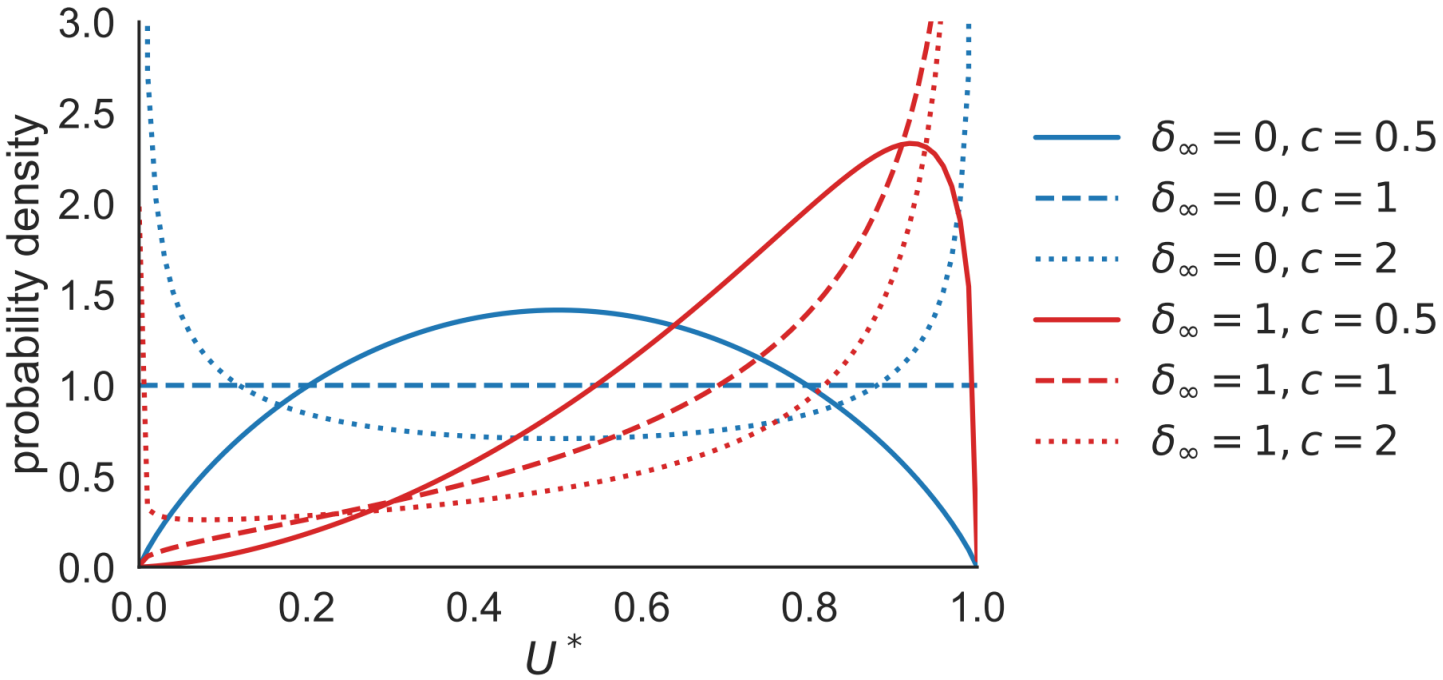
Theoretical results: Model selection

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.

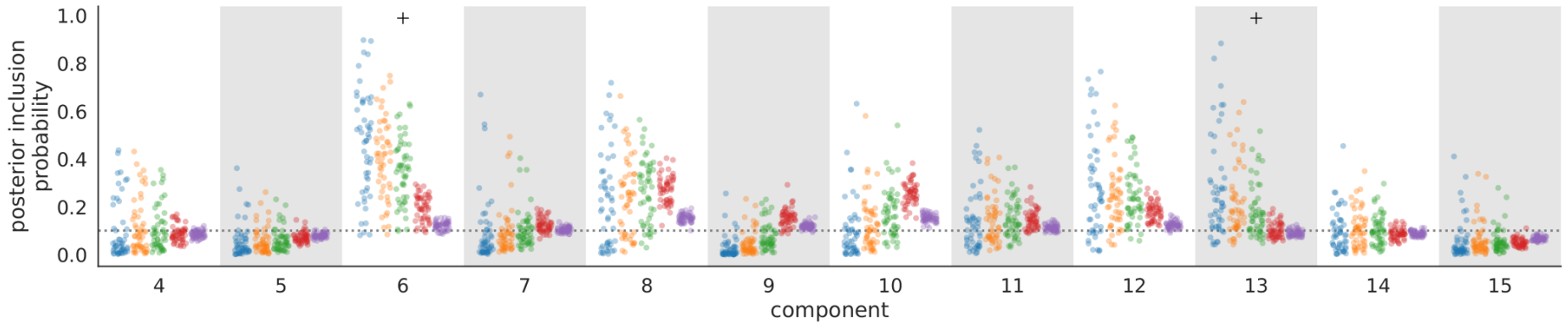
Applications: Dataset summary

Real-world datasets used in experiments. LR = linear regression, PTR = phylogenetic tree reconstruction. For PTR, N is the number of features and D is the number of species.

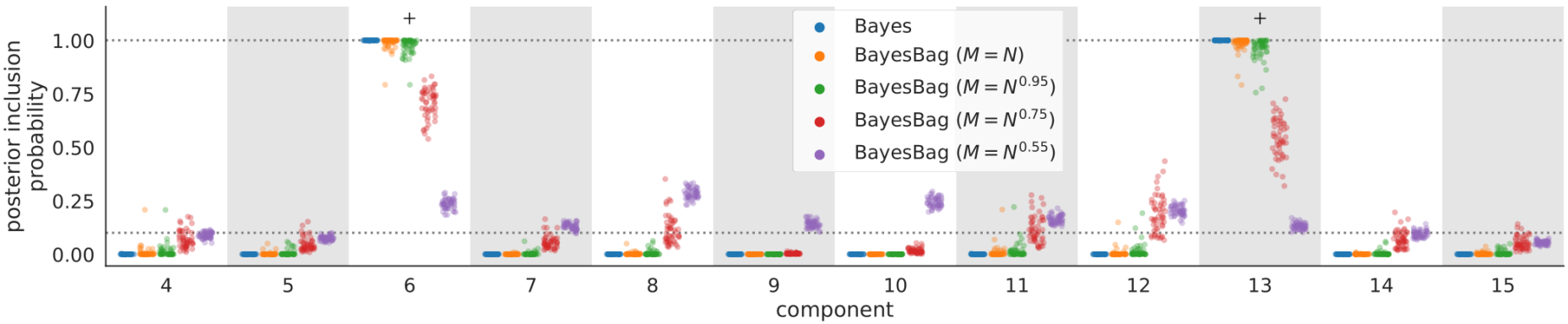
Name	Model	N	D
California housing	LR	20,650	8
Boston housing	LR	506	13
Diabetes	LR	442	10
Residential building	LR	371	105
Whale mitochondrial coding DNA	PTR	10,605	14
Whale mitochondrial amino acids	PTR	3,535	14

Application: Variable selection

When the model is correct, the bagged posterior with $M = N^\alpha$ is similar to the standard posterior when $\alpha = 1$, and more stable as α decreases.



2-sparse-linear, $N = 10^2$



2-sparse-linear, $N = 10^3$

Application: Variable selection

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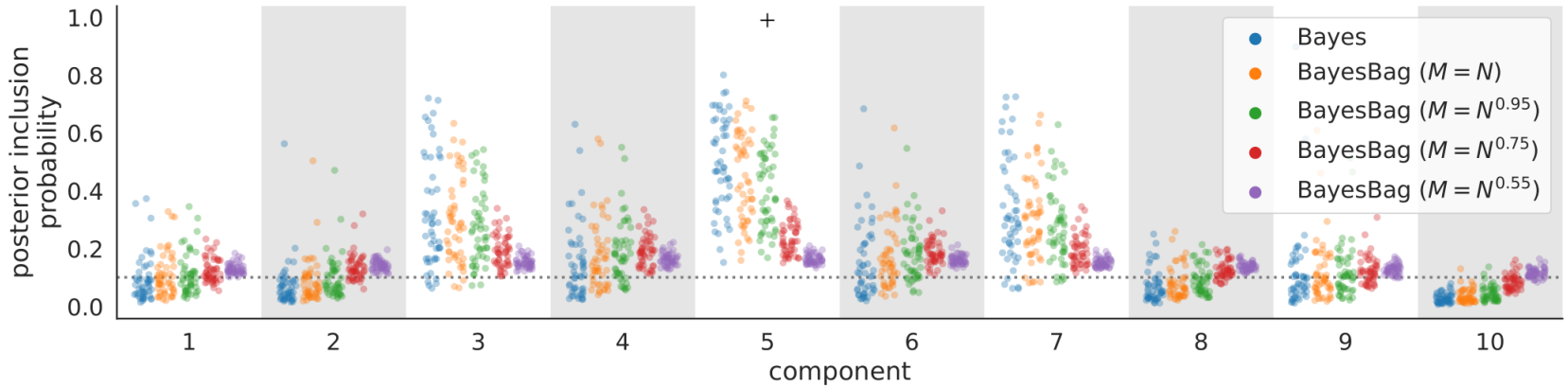
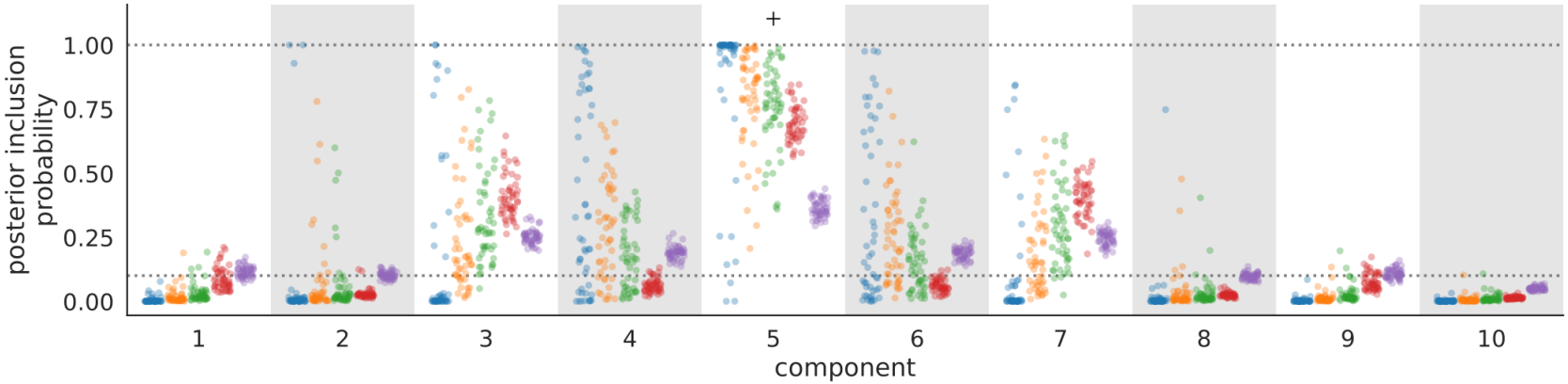


$N = 5 \times 10^1$



$N = 5 \times 10^2$