Simulations

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In this section, we illustrate the performance of the different proposed models under different scenarios. Through these simulations, we aim at highlighting the specific properties of the models we have discussed in the previous sections, in terms of prediction of the number of unseen features in a future sample. To this end, we distinguish between two broad classes of generating mechanisms, i.e. (i.b) bounded-features scenarios, where the number of features observable in the population is bounded, that is $\exists K^* > 0$ such that $\lim_{n\to\infty} K_n = K^*$ almost surely; (ii) diverging-features scenarios, where the number of features observable in the population is unbounded, that is $\lim_{n\to\infty} K_n = \infty$ almost surely. We are going to discuss how the two classes of feature allocation models - *Mixtures of IBP* and *Mixtures of Beta-Bernoulli with N features* - are suitable for different scenarios.

Bounded-features scenarios

For these scenarios, we consider 4 ecological species detection models, as in Chiu (2022). Within these settings, the individuals are geographical sites where species of animals are collected (each species is a feature). In each scenario, the total number of species is $H = 500$ and the species occurrence probabilities $(\pi_1, \dots, \pi_H)$ are determined. We compare the Gamma mixture of IBP, the mixture of Beta-Bernoulli with Poisson prior on N and the mixture of Beta-Bernoulli with negative binomial prior on N. For each setting and each model we show the following quantities, estimated for different dimensions of the training set: (i.a) the in-sample rarefaction curve (on a single dataset), (i.b) the extrapolated rarefaction curve on the test set (on a single dataset), (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets. Specifically, we focus on the following measure of accuracy, denoted with $\nu_m^{(n)}$,

$$\nu_m^{(n)} := \frac{1}{1 + \frac{|\tilde{K}_m^{(n)} - \hat{K}_m^{(n)}|}{\tilde{K}_n}},$$

where $\tilde{K}_m^{(n)}$ is the observed number of unseen features in the test set, $\hat{K}_m^{(n)}$ is the expected value of the statistic $K_m^{(n)}$ and $\tilde{K}_n$ is the observed number of features in the training set. Note that $\nu_m^{(n)} \in (0, 1]$, with $\nu_m^{(n)} = 1$ meaning perfect estimation.

Moreover, for the mixtures of Beta-Bernoulli, we also report (iii) the posterior distribution of the total number of features (on a single dataset), (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.

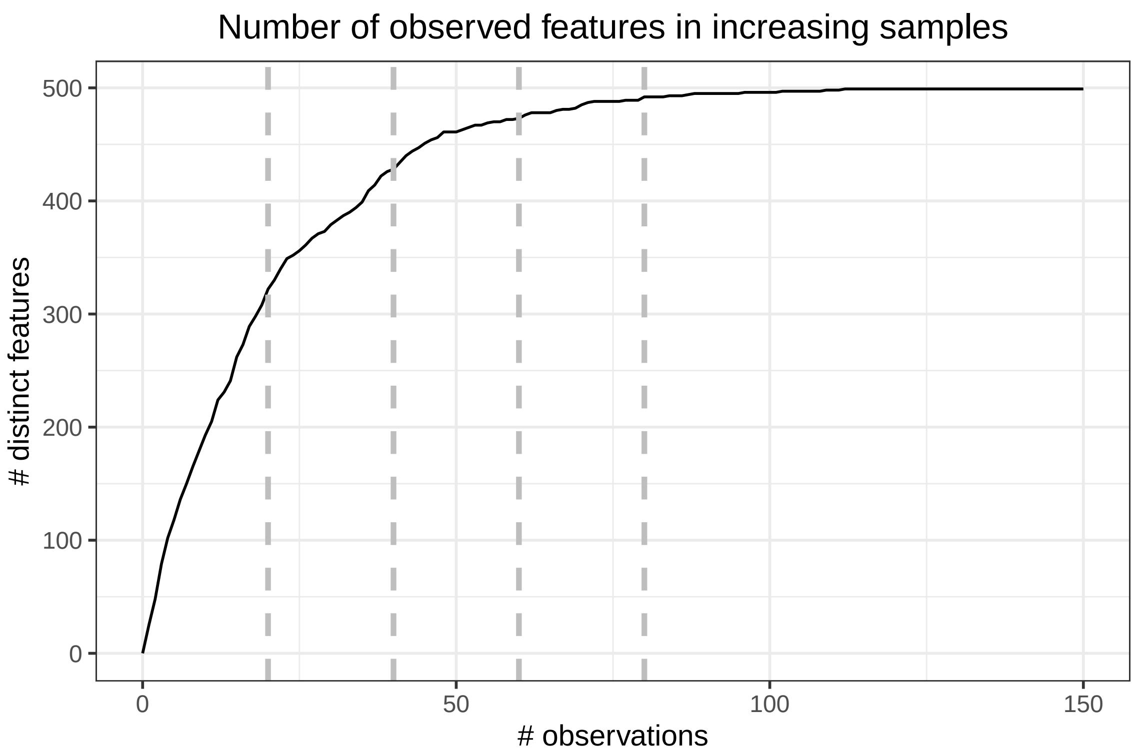
Model 1: the homogeneous model

Set $\pi_k = 0.05$, for $k = 1, \dots, H$. Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

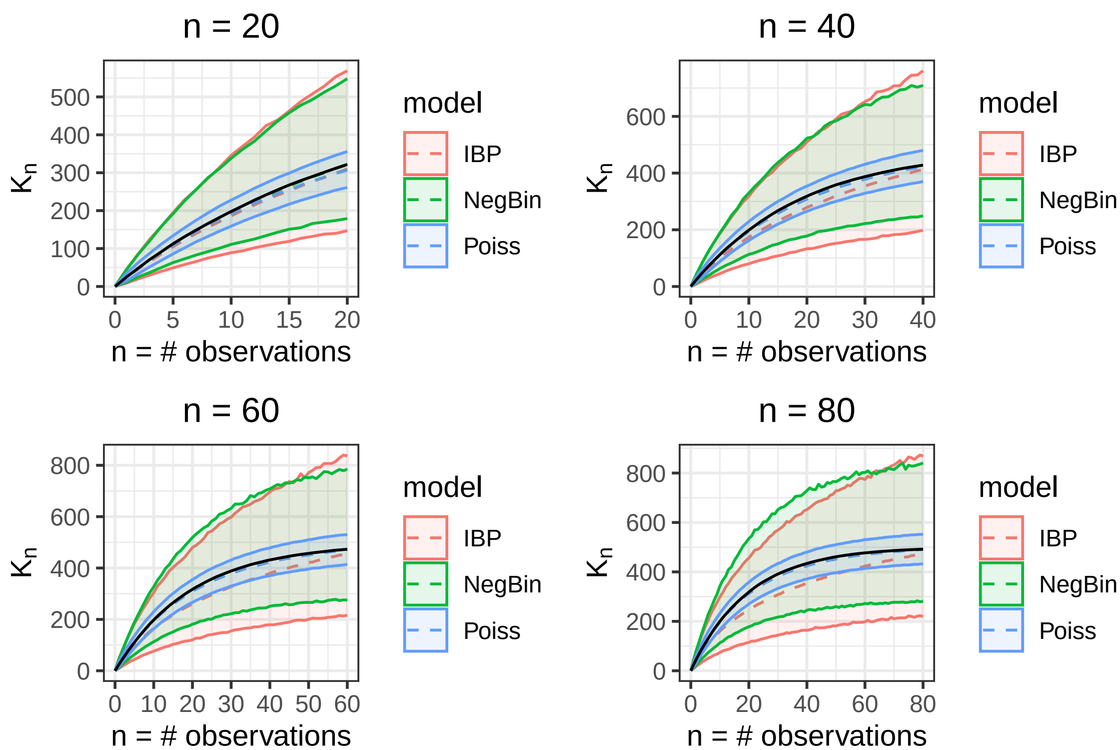
```
## L =  150
```

```
## n =  20  40  60  80
```

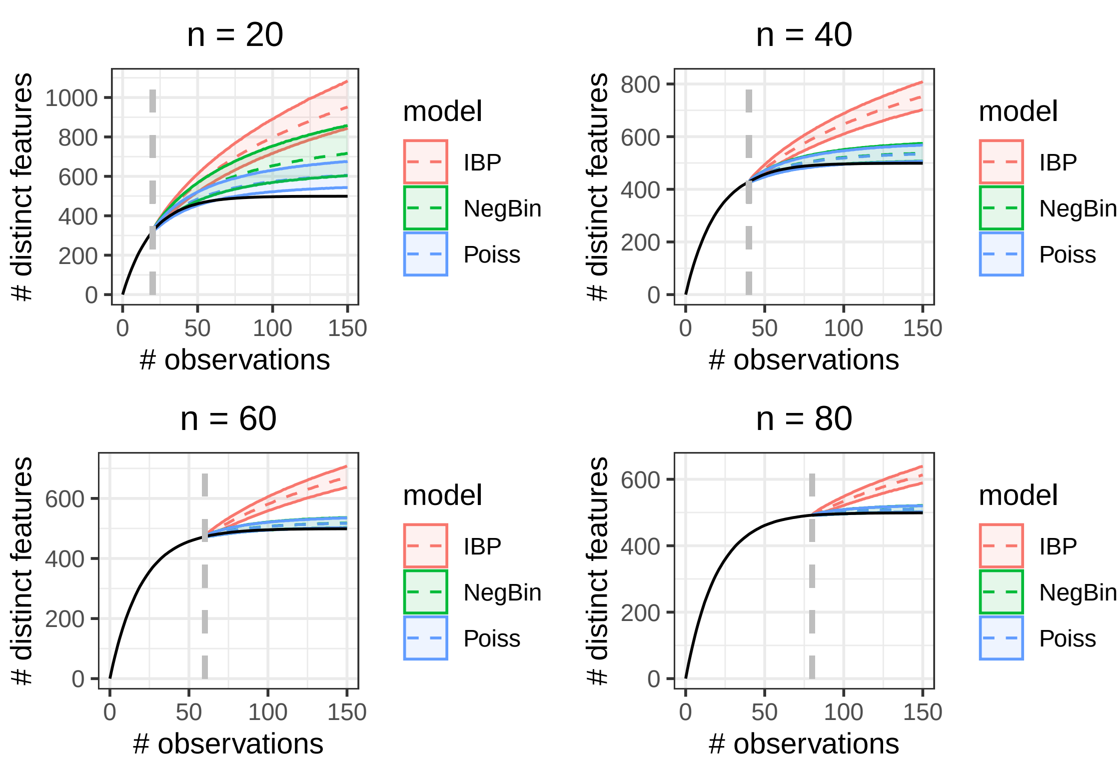
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



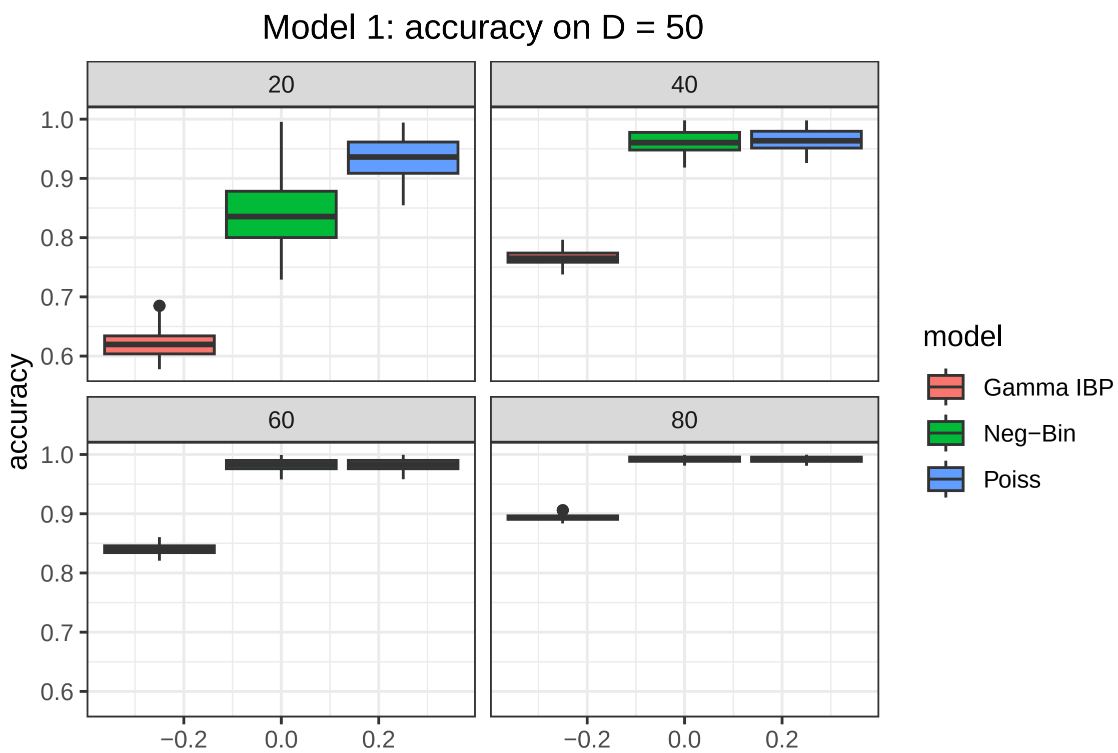
Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



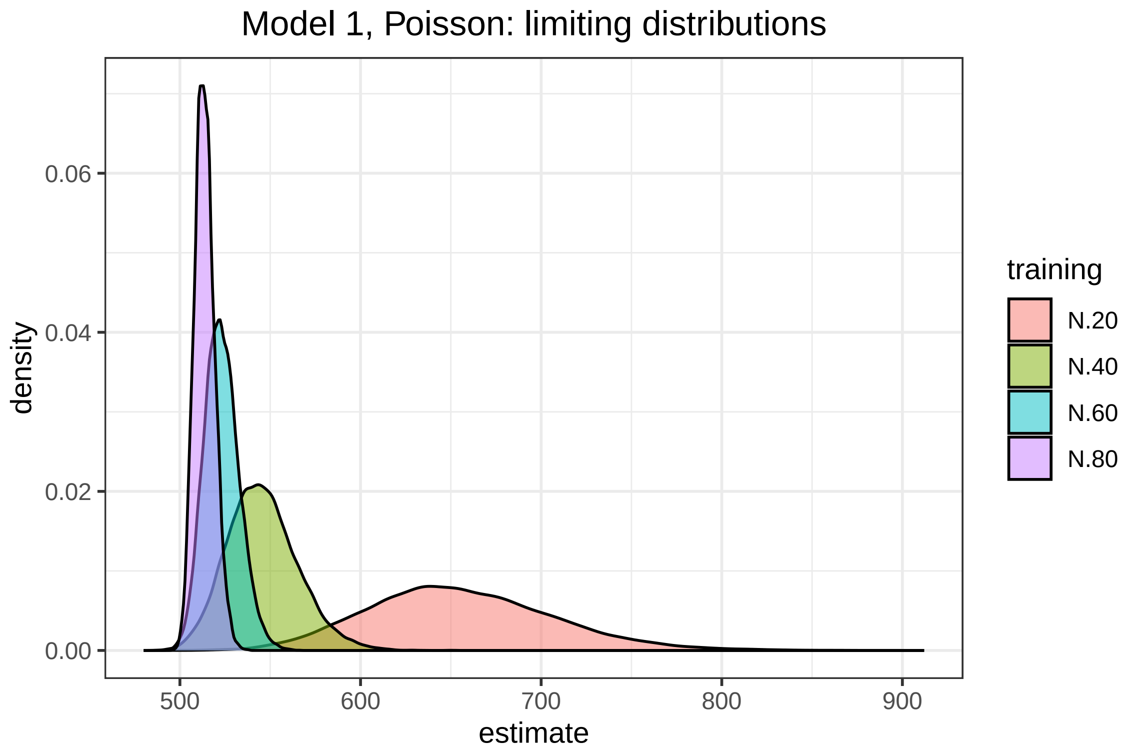
Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).

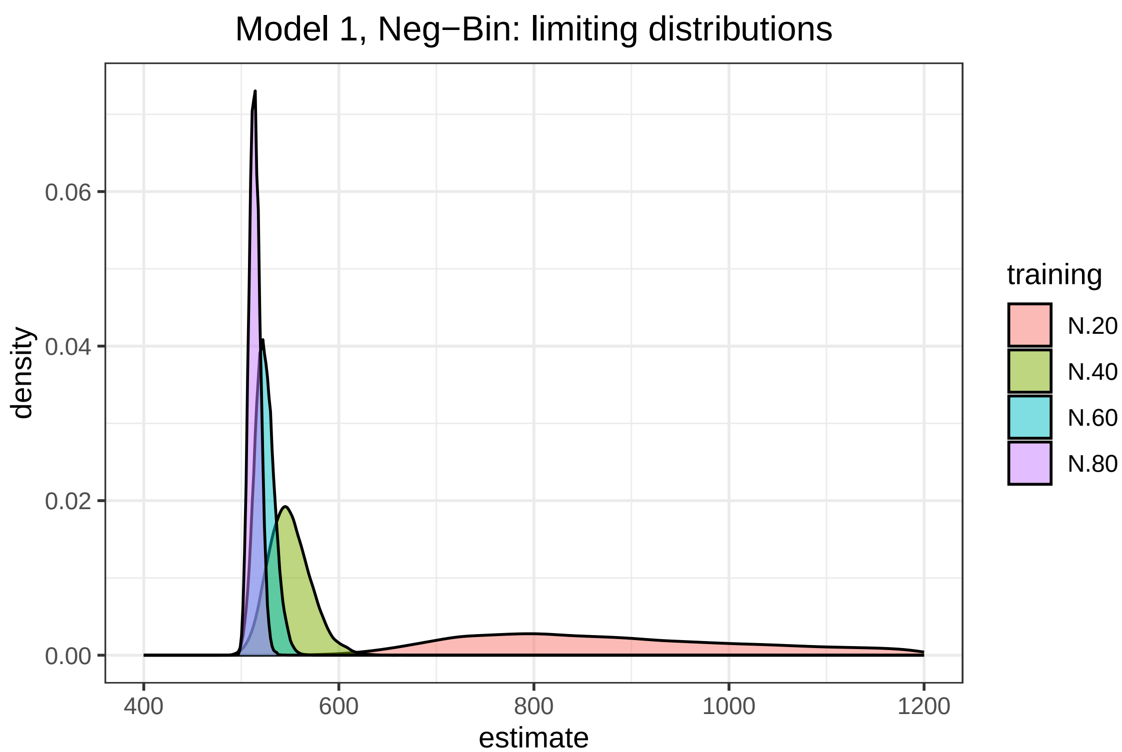


Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.

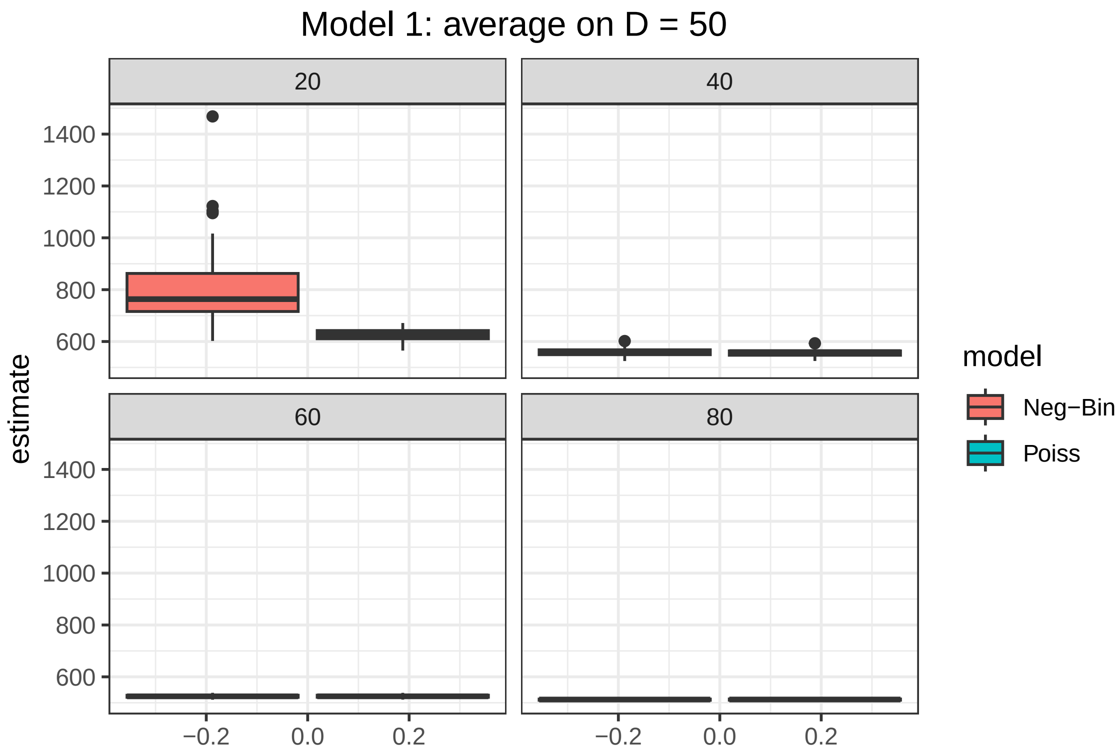


For the mixtures of Beta-Bernoulli, we report (iii) the posterior distribution of the total number of features (on a single dataset).





Finally, we report (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.



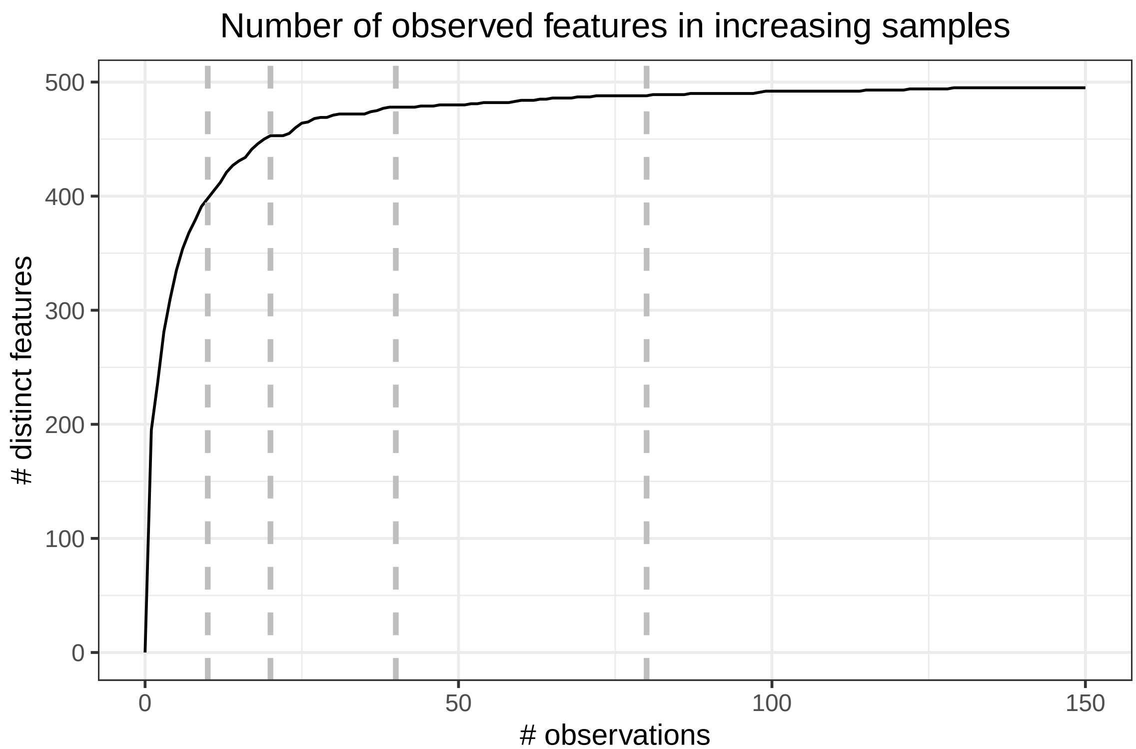
Model 2: the random uniform model

Set $\pi_k = c \cdot a_k$, for $k = 1, \ldots, H$, and $a_k \overset{iid}{\sim} \text{Uniform}(0, 1)$. Set c such that the maximum π_k is equal to 0.5. Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

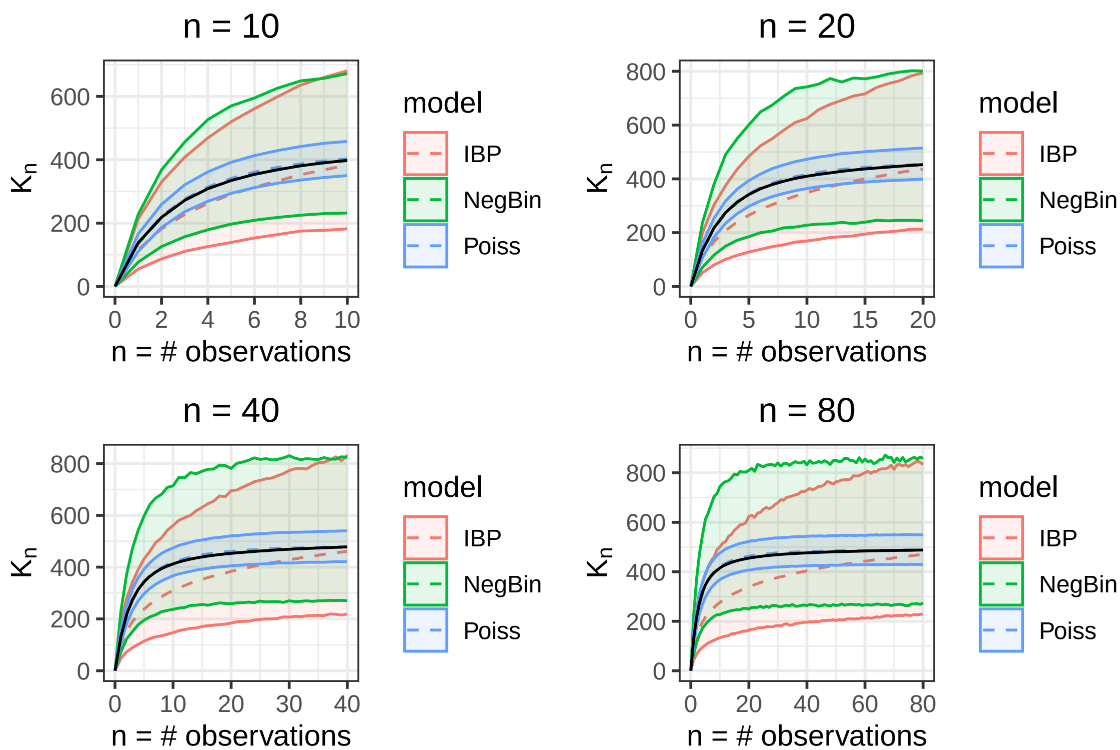
```
## L =  150
```

```
## n =  10  20  40  80
```

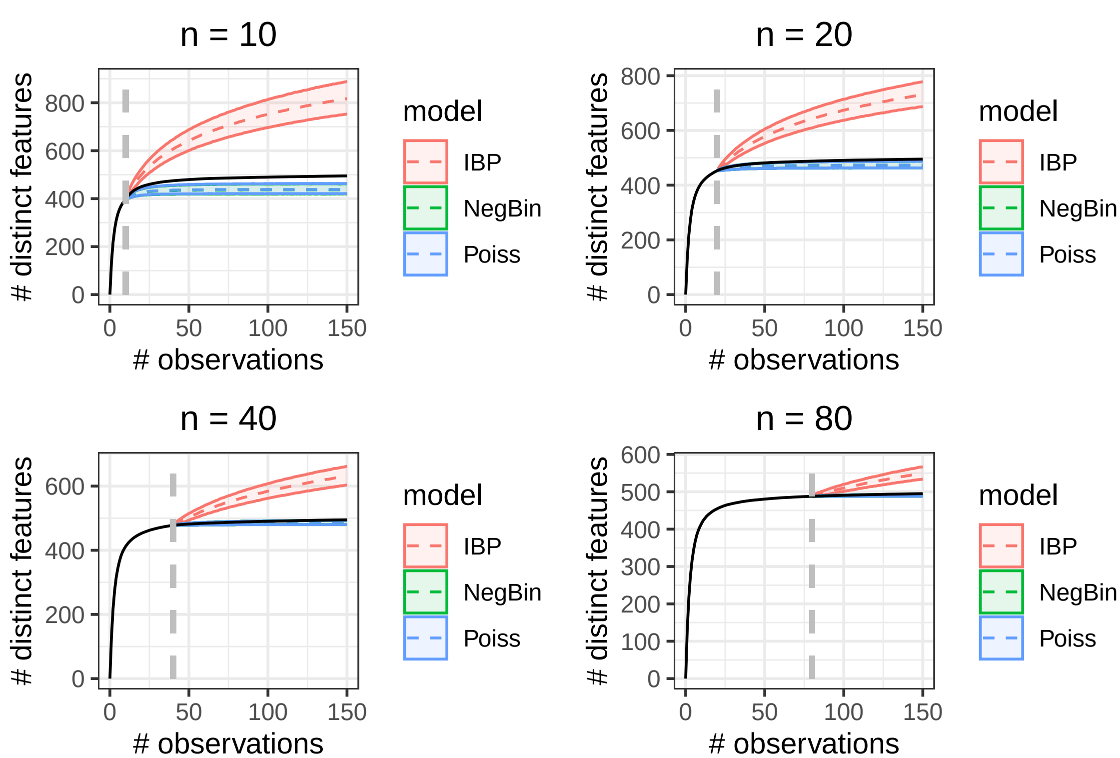
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



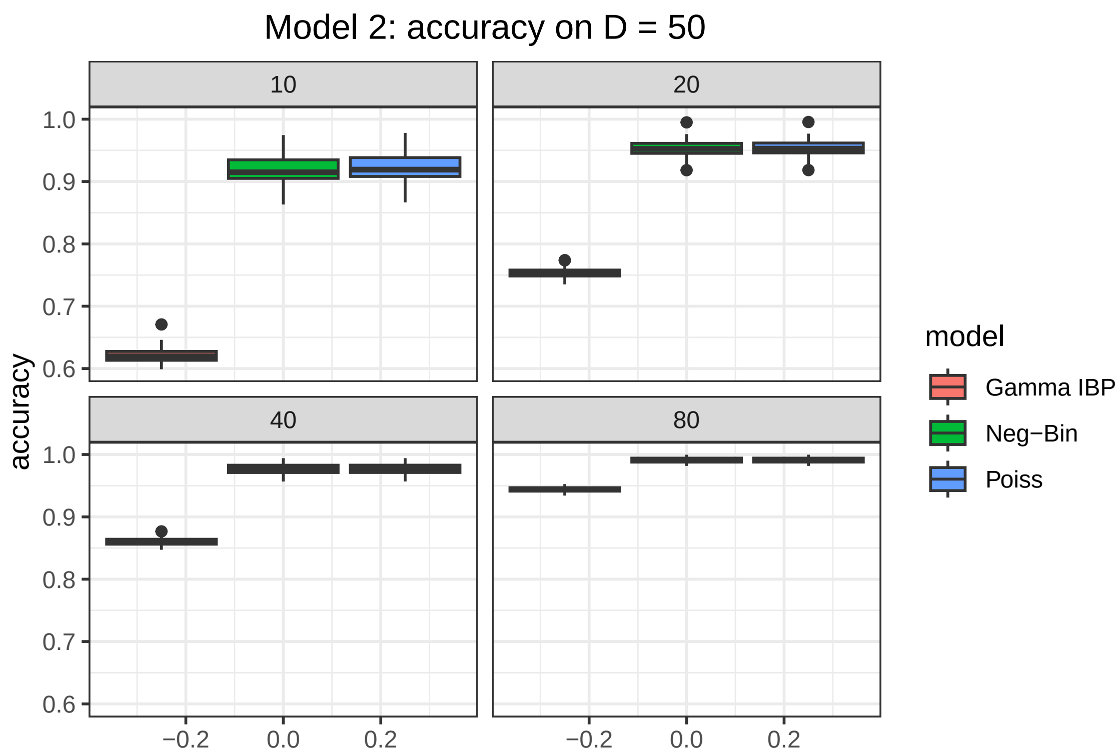
Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).

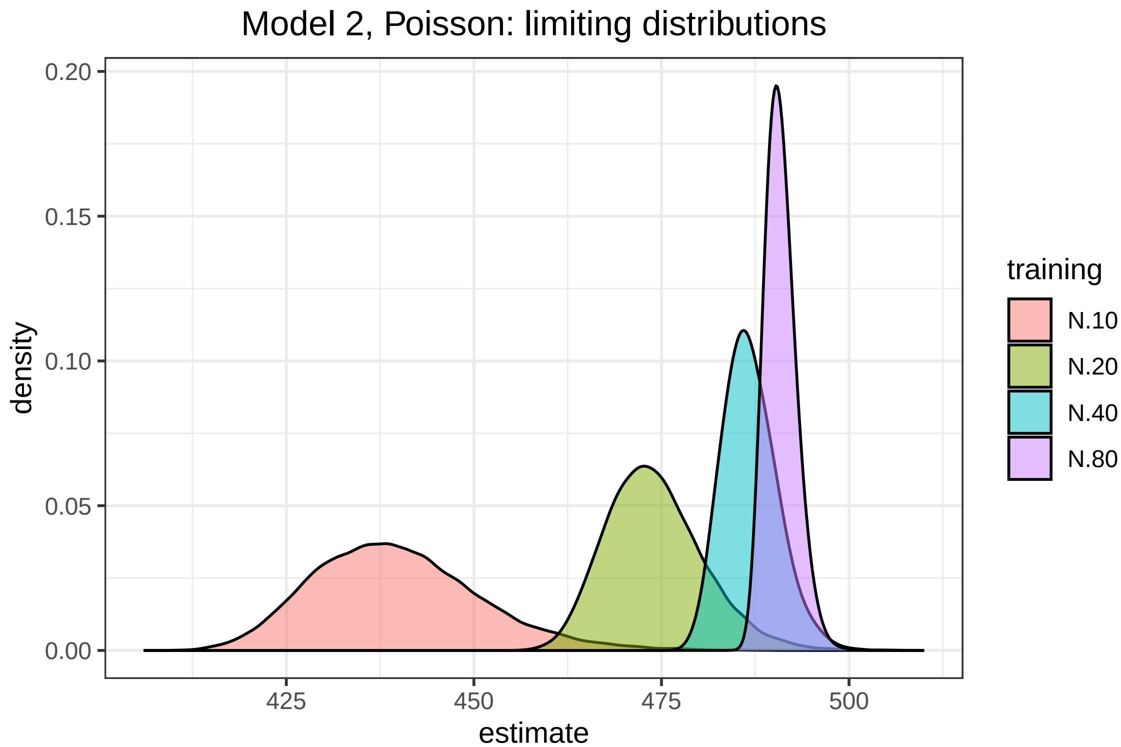


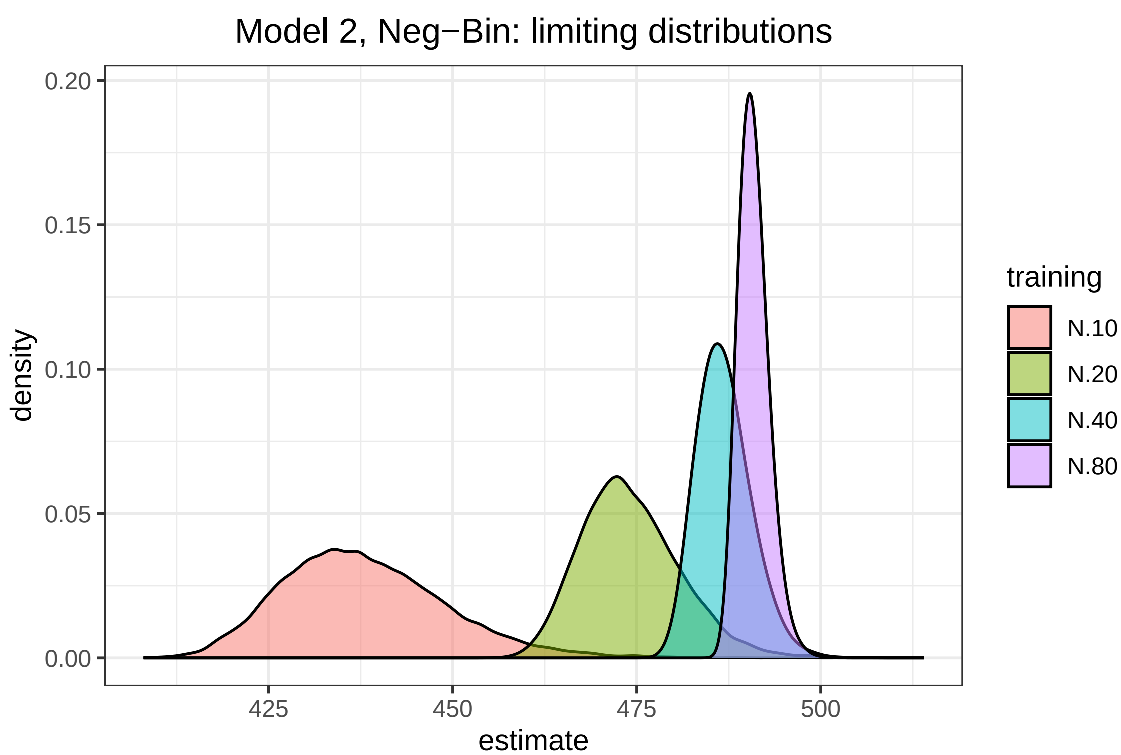
Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.



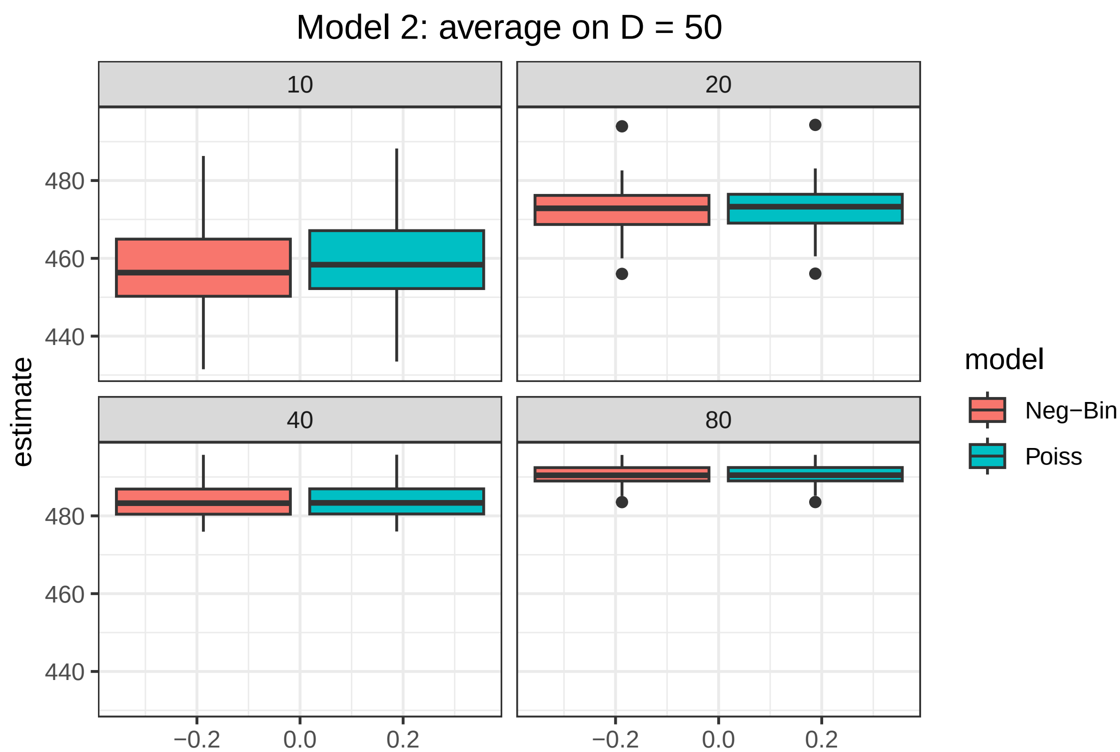
Even if the Mixture of IBP seems to reach better performance when the training set increases, this is just due to the fact the test set dimension is reducing: see the behaviour of the extrapolated rarefaction curve to get the behaviour of the model on larger test sets.

For the mixtures of Beta-Bernoulli, we report (iii) the posterior distribution of the total number of features (on a single dataset).





Finally, we report (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.



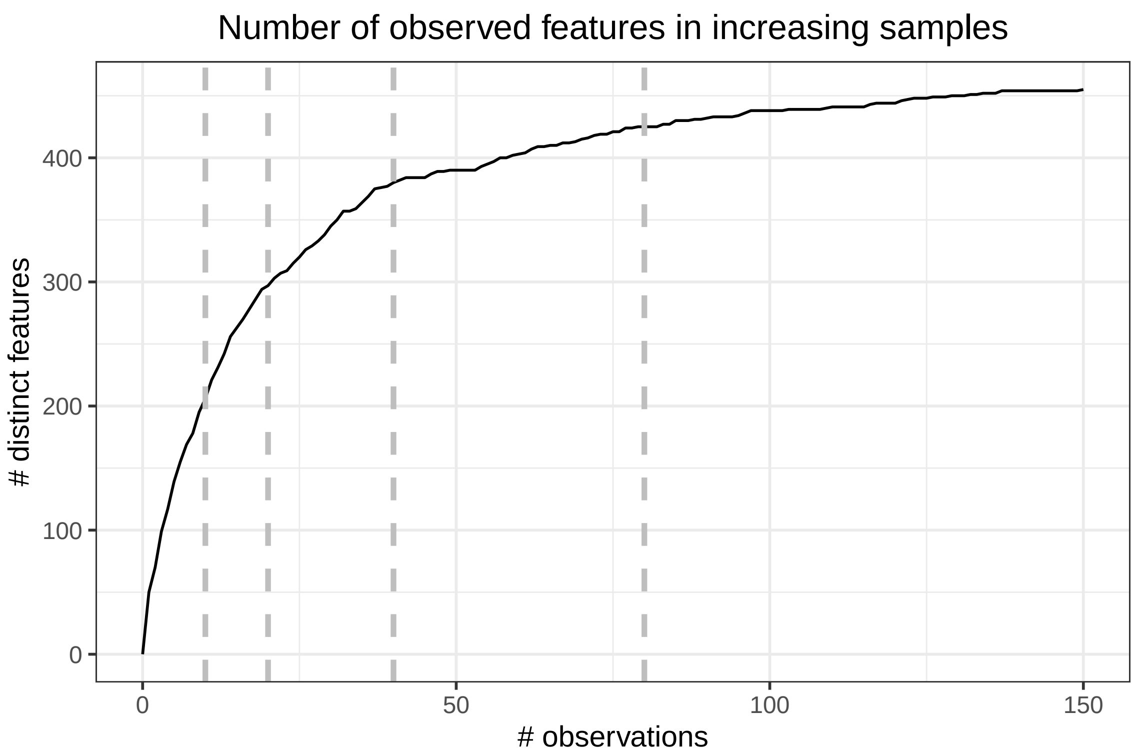
Model 3: the broken stick model

Set $\pi_k = c \cdot a_k$, for $k = 1, \ldots, H$, and $a_k \overset{iid}{\sim} \text{Exp}(1)$. Set c such that the maximum π_k is equal to 0.5. As Chiu (2022) says: "This model is commonly used in previous literature and equivalent to the Dirichlet distribution". Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

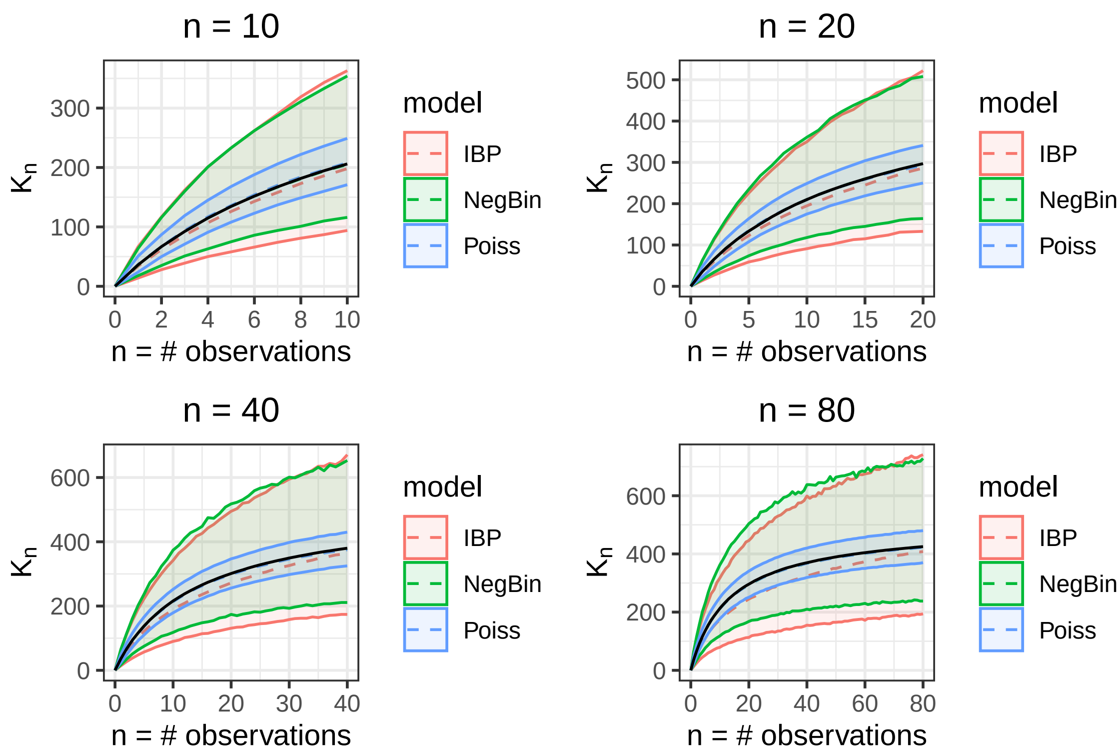
```
## L =  150
```

```
## n =  10  20  40  80
```

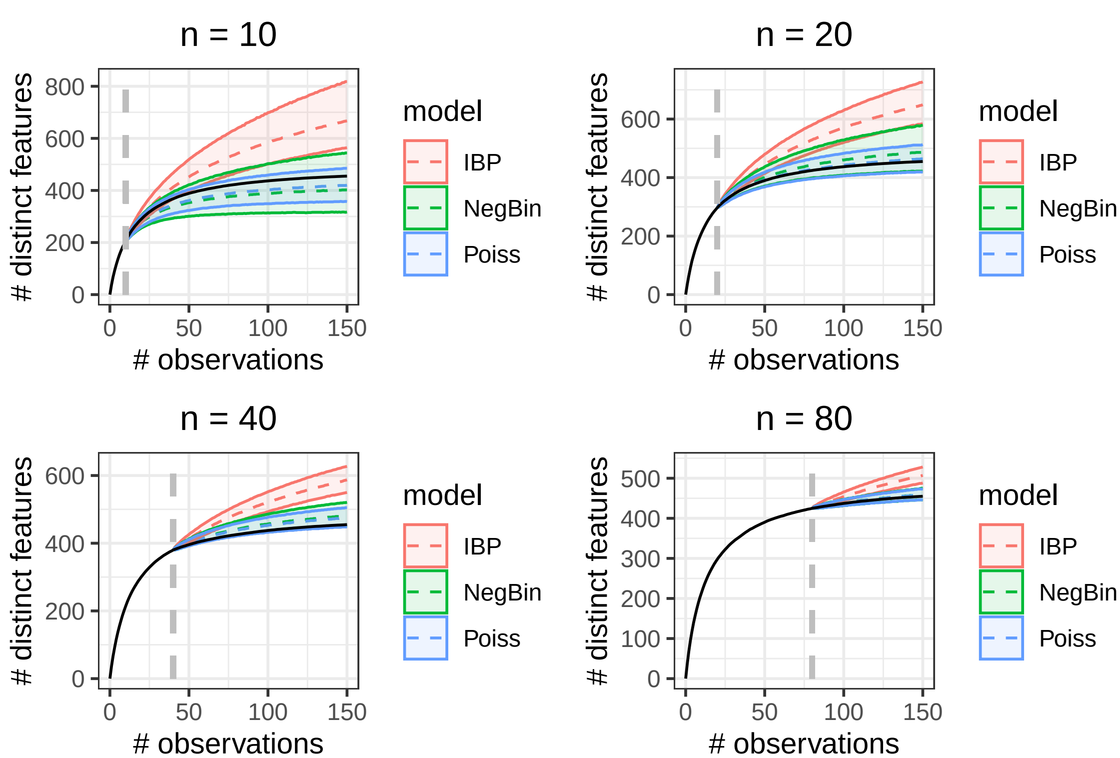
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



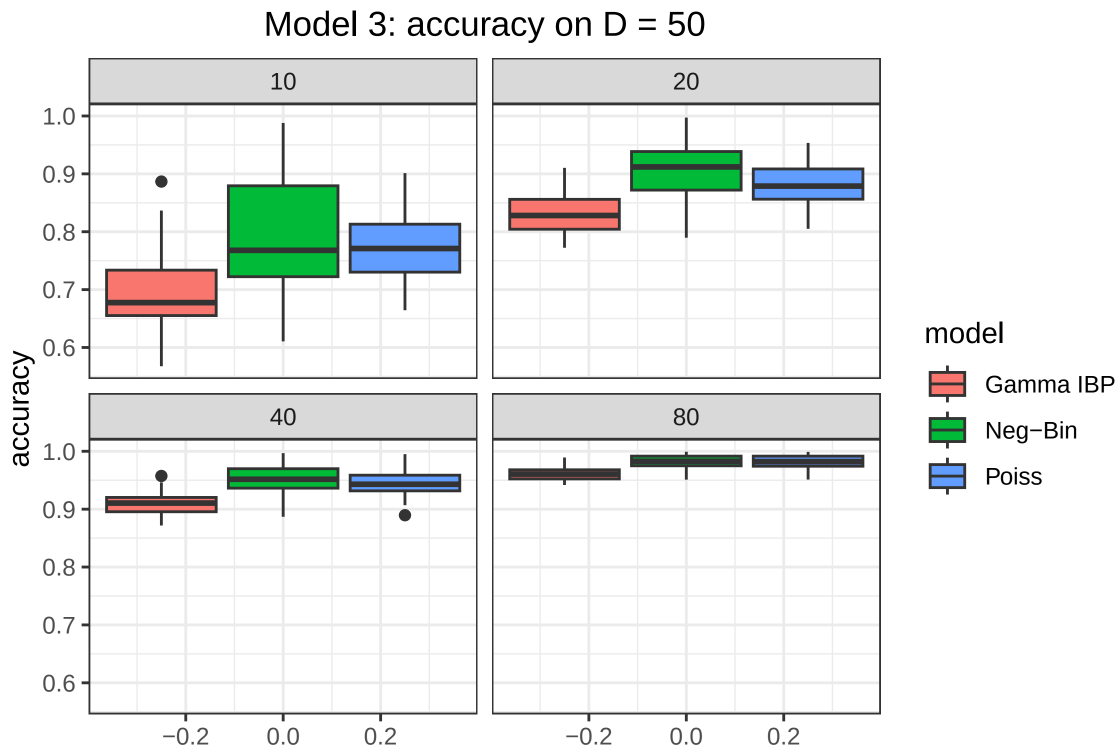
Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).

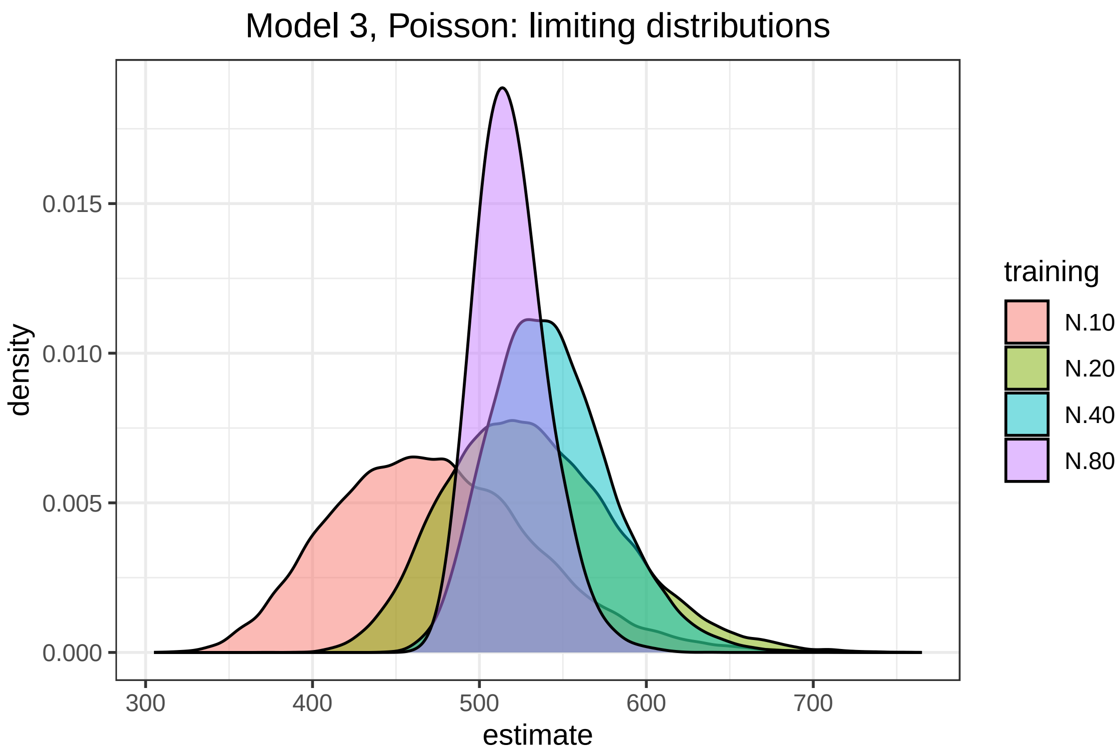


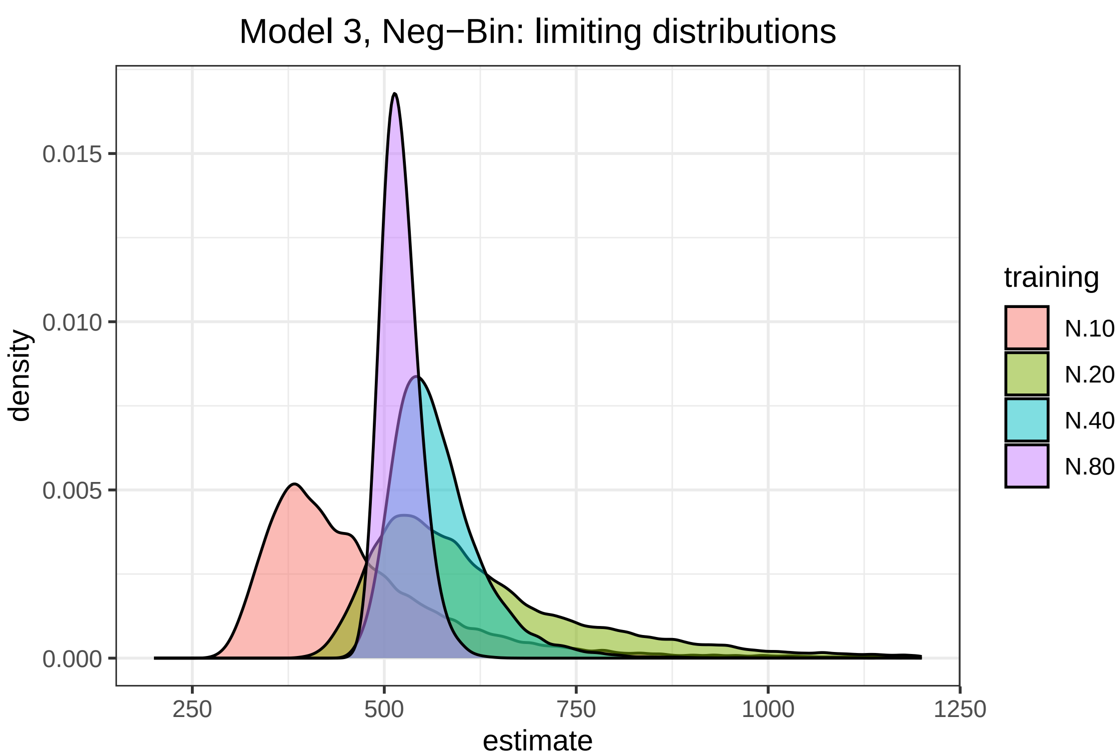
Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.



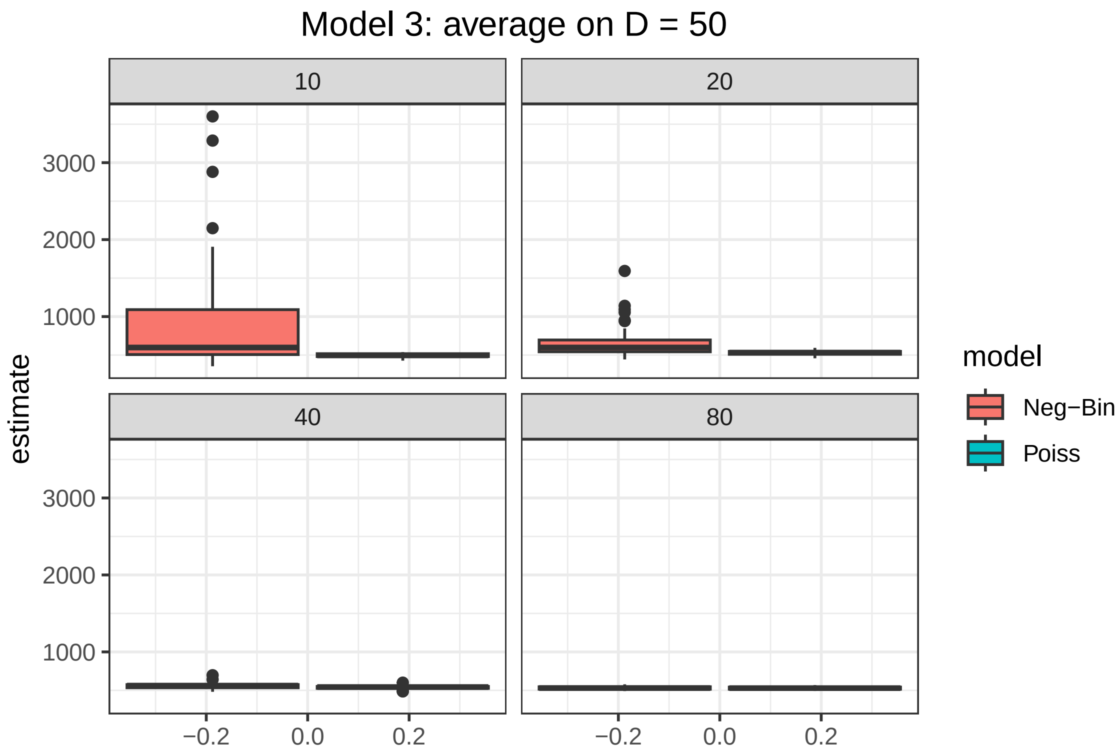
Even if the Mixture of IBP seems to reach better performance when the training set increases, this is just due to the fact the test set dimension is reducing: see the behavior of the extrapolated rarefaction curve to get the behavior of the model on larger test sets.

For the mixtures of Beta-Bernoulli, we report (iii) the posterior distribution of the total number of features (on a single dataset).





Finally, we report (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.



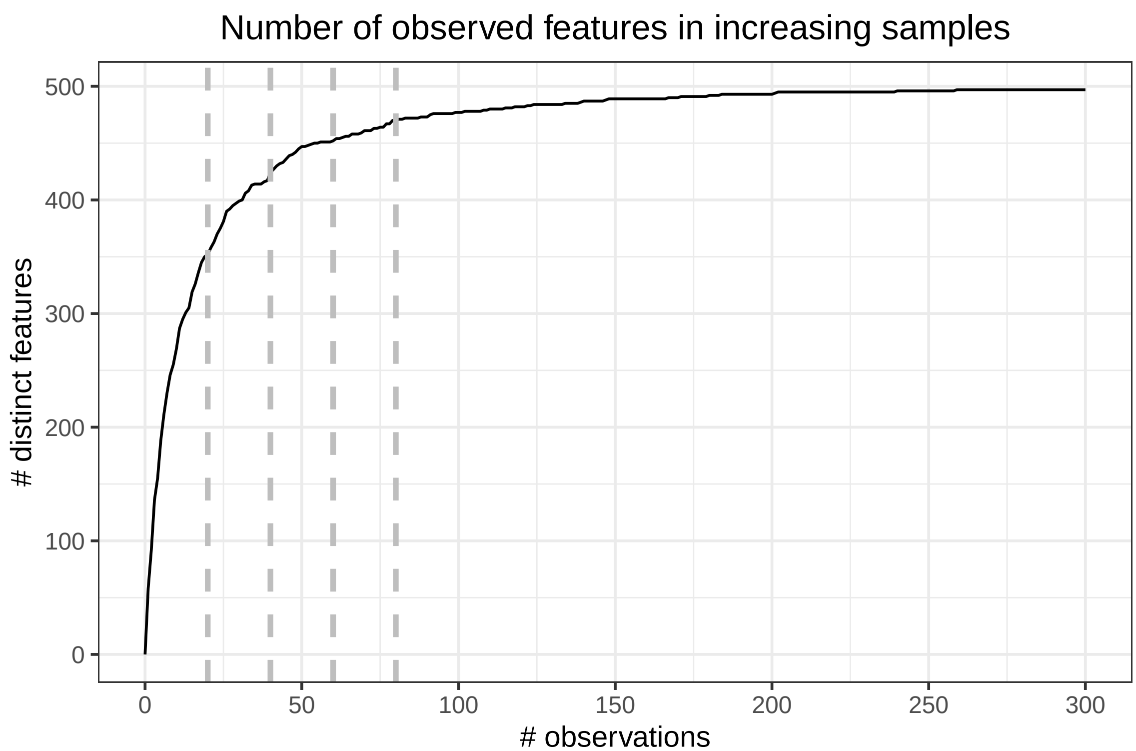
Model 4: the log-normal model

Set $\pi_k = c \cdot a_k$, for $k = 1, \dots, H$, and $a_k \overset{iid}{\sim} \log - \text{normal}(0, 1)$. Set c such that the maximum π_k is equal to 1. Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

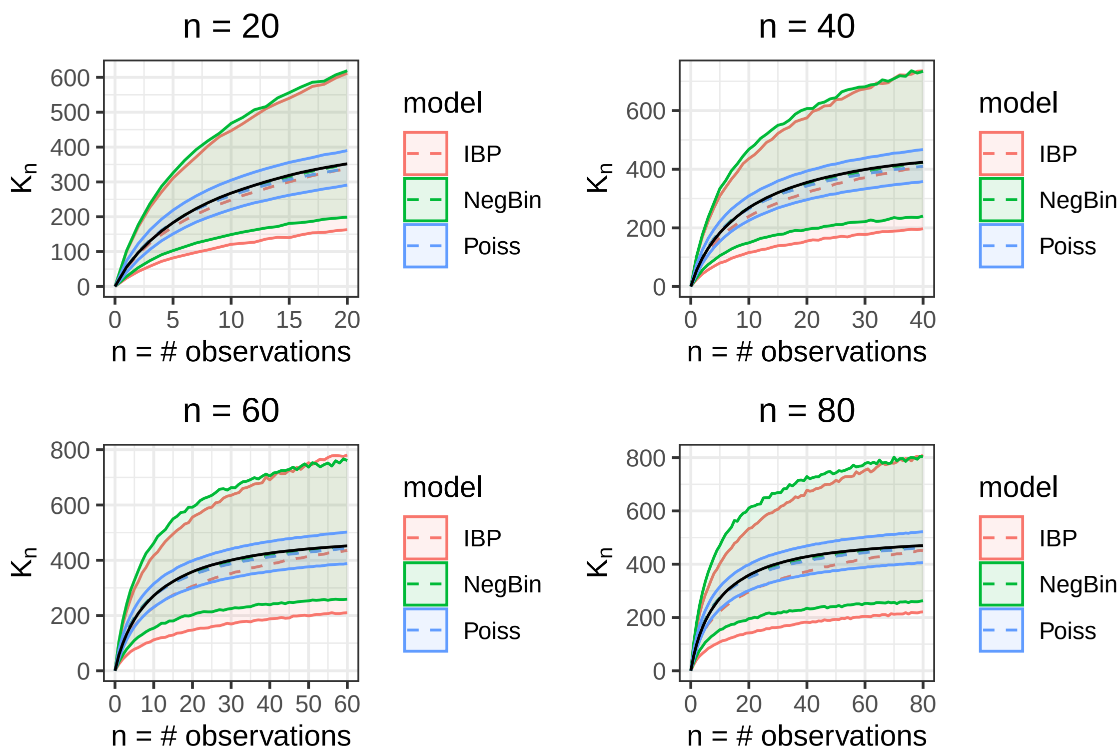
```
## L =  300
```

```
## n =  20  40  60  80
```

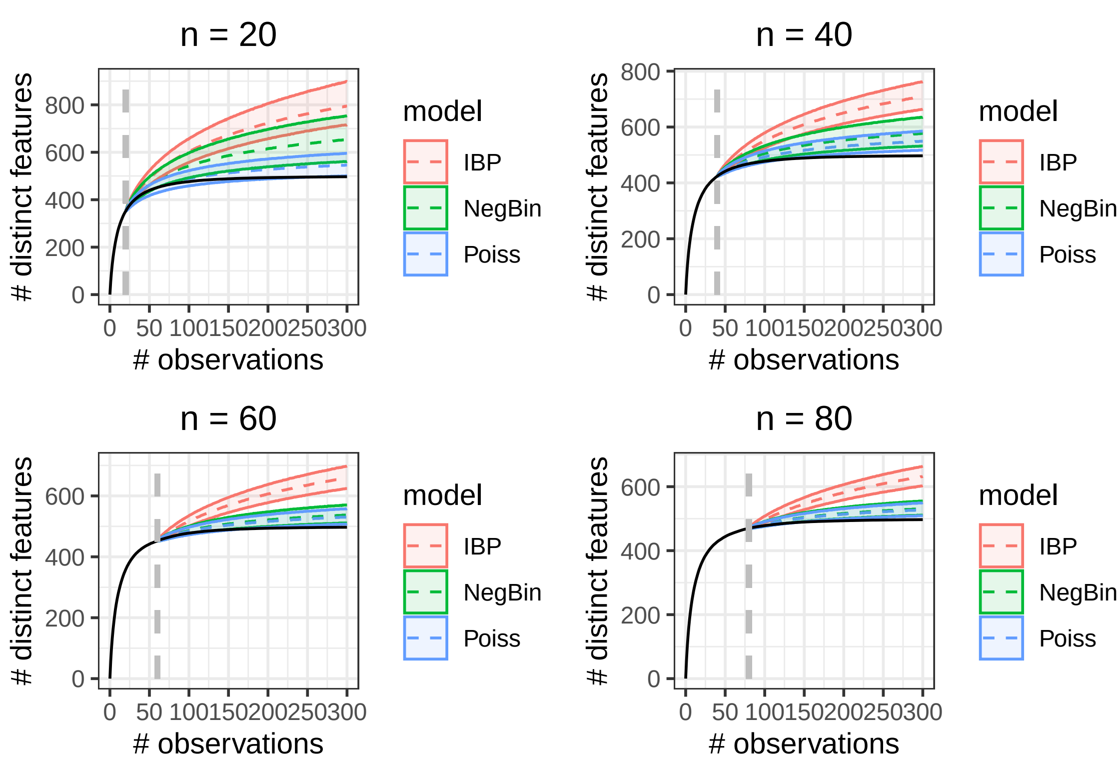
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



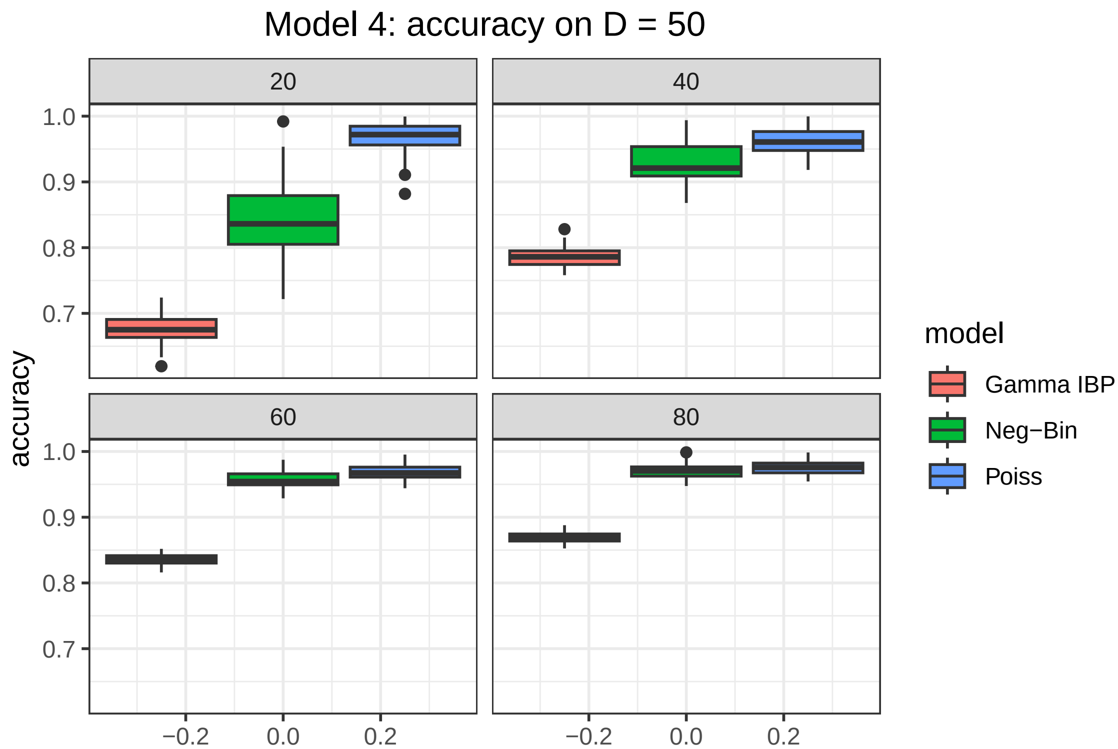
Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).

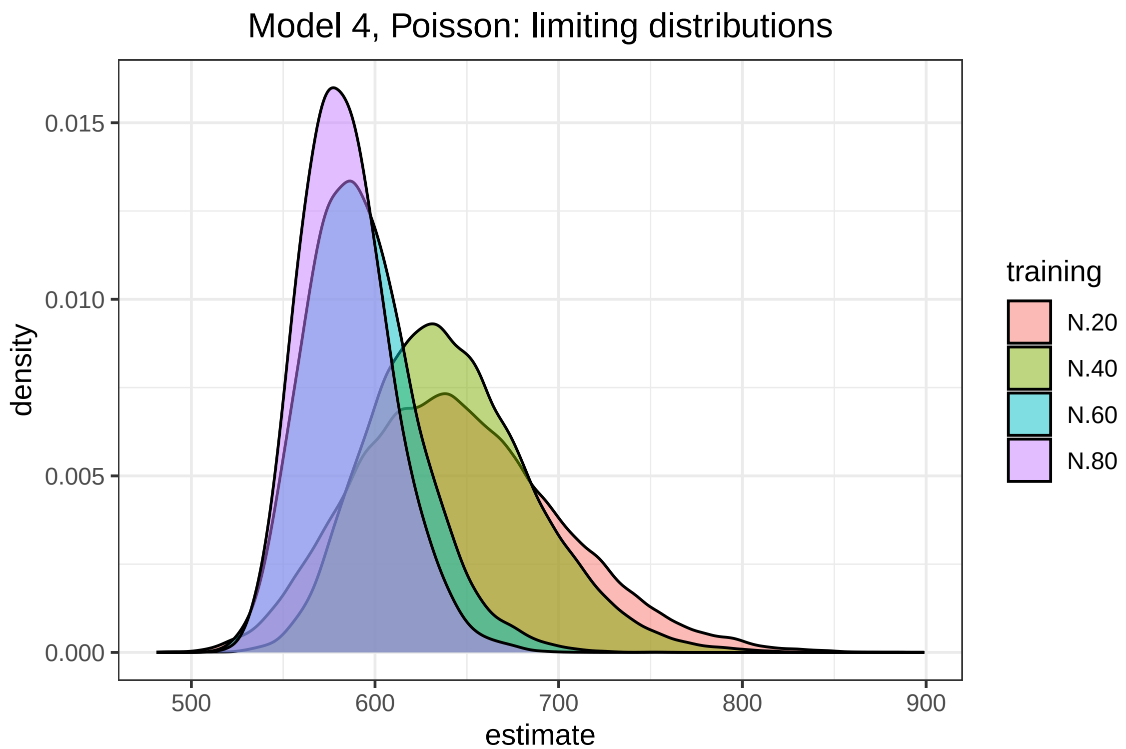


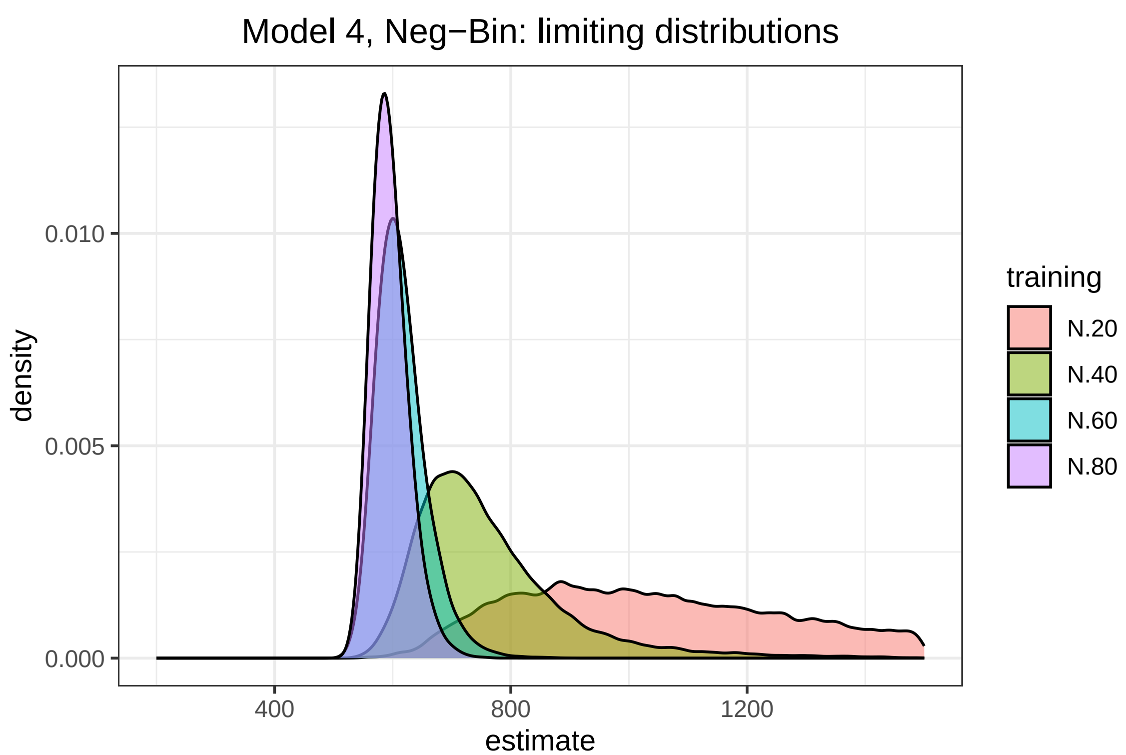
Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.



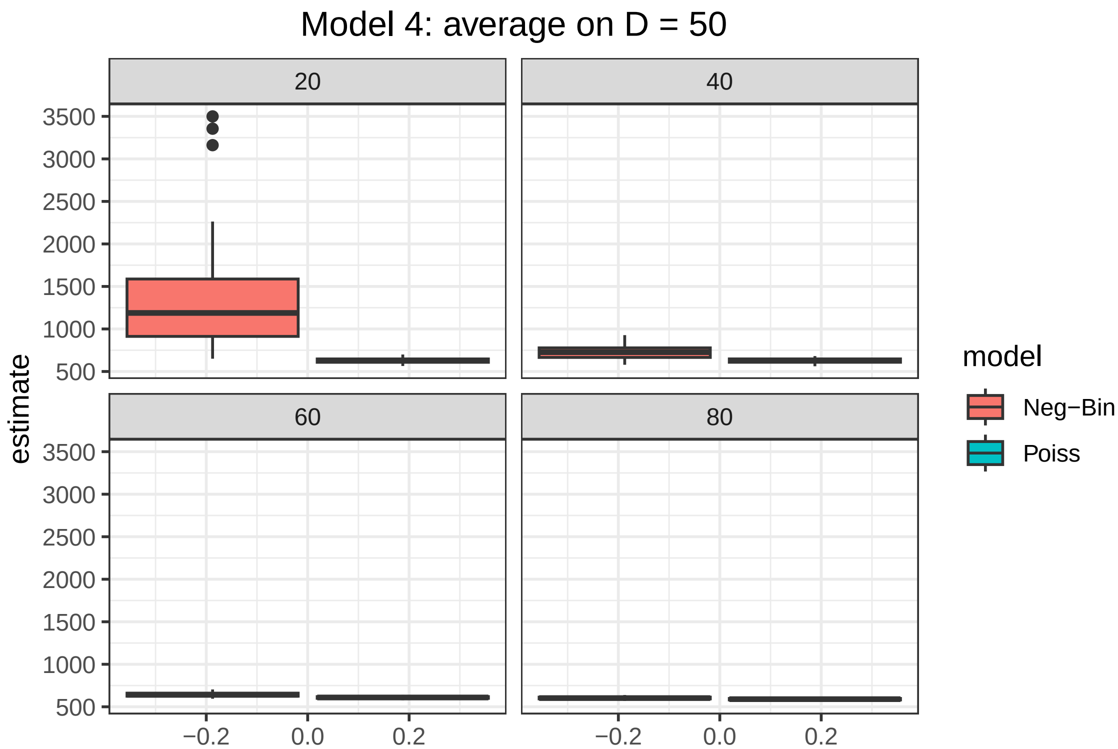
Even if the Mixture of IBP seems to reach better performance when the training set increases, this is just due to the fact the test set dimension is reducing: see the behavior of the extrapolated rarefaction curve to get the behavior of the model on larger test sets.

For the mixtures of Beta-Bernoulli, we report (iii) the posterior distribution of the total number of features (on a single dataset).





Finally, we report (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.



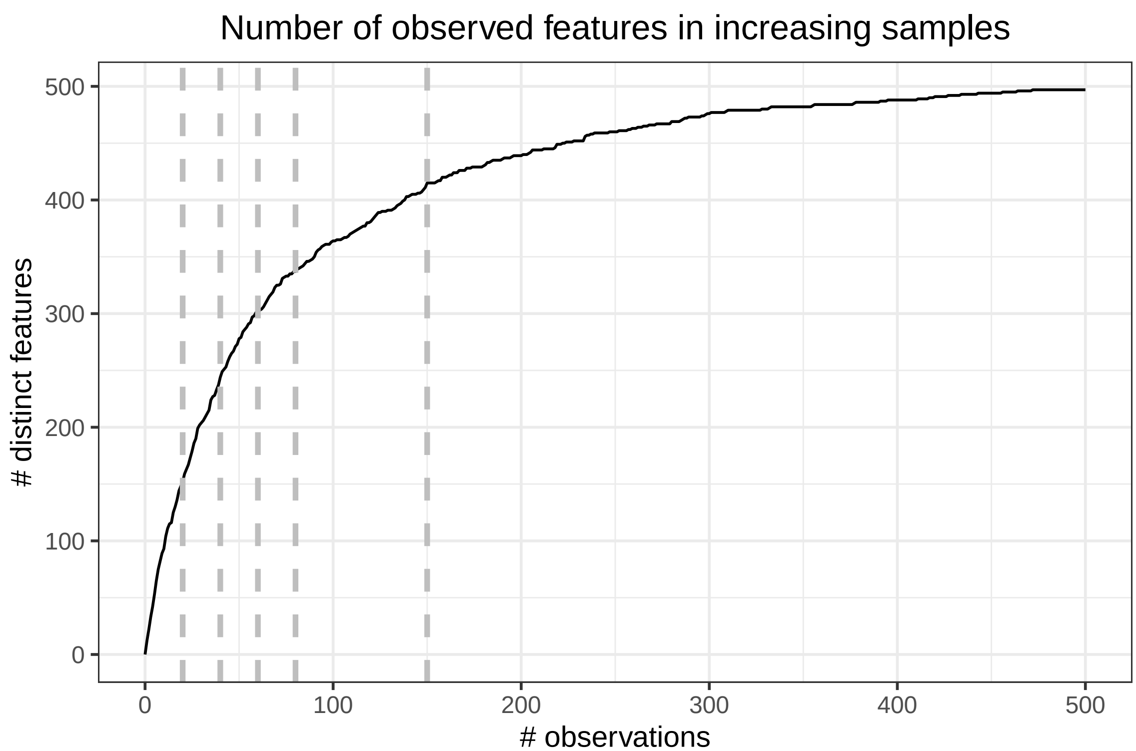
Model 5: the Zipf–Mandelbrot model

Set $\pi_k = \frac{3}{k+5}$, for $k = 1, \ldots, H$. Note that the maximum π_k is equal to 0.5. Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

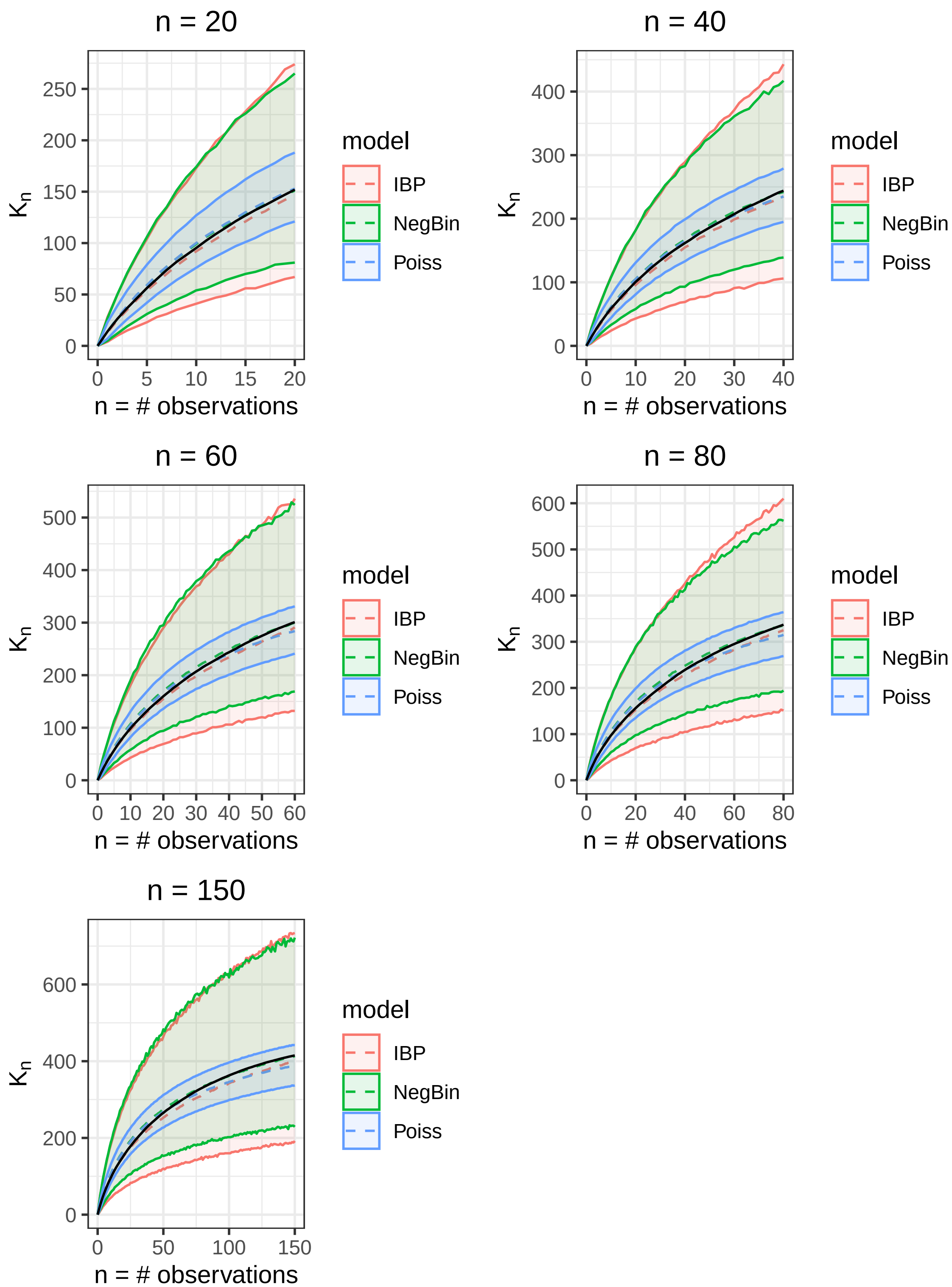
```
## L =  500
```

```
## n =  20  40  60  80  150
```

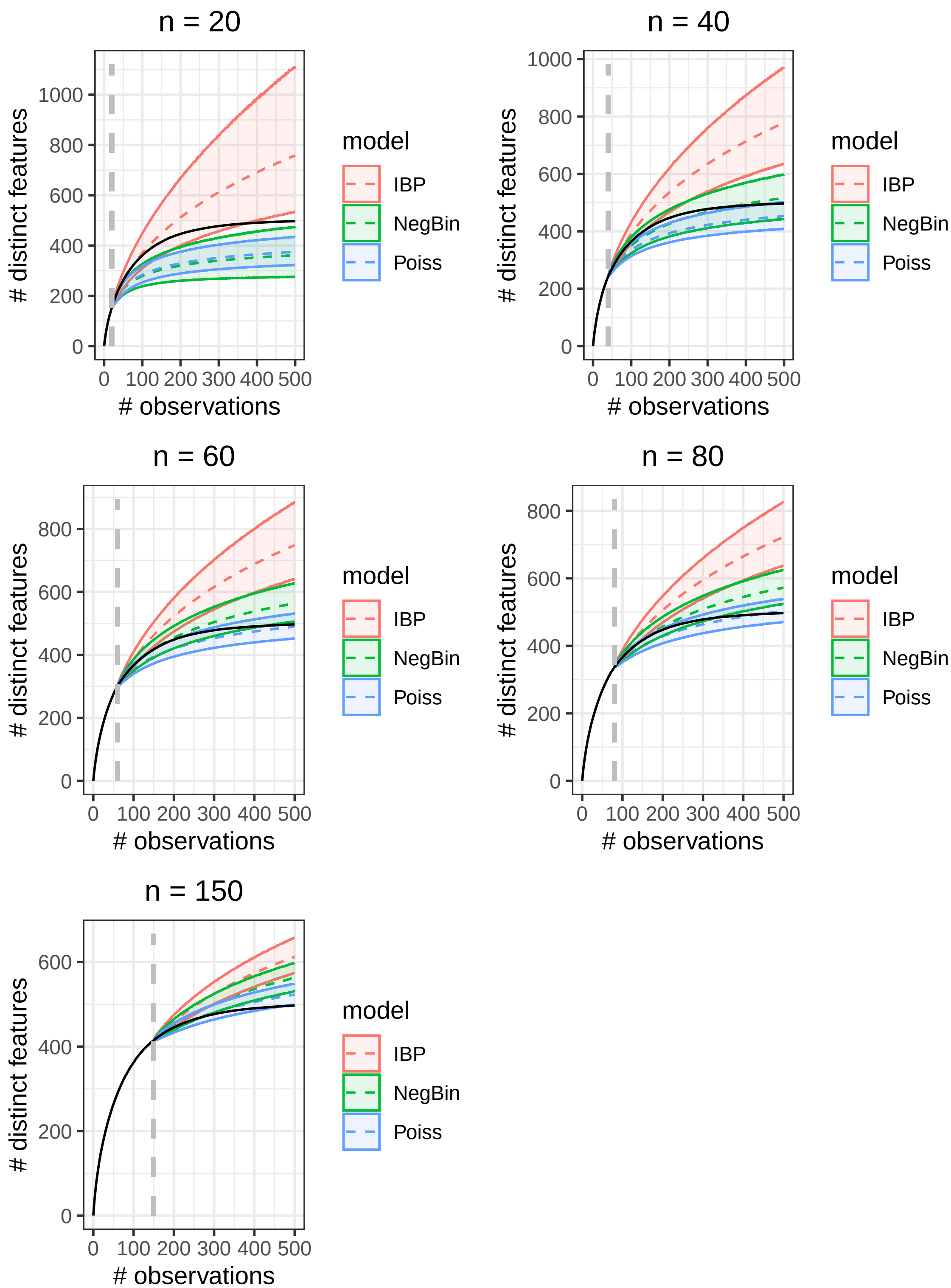
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



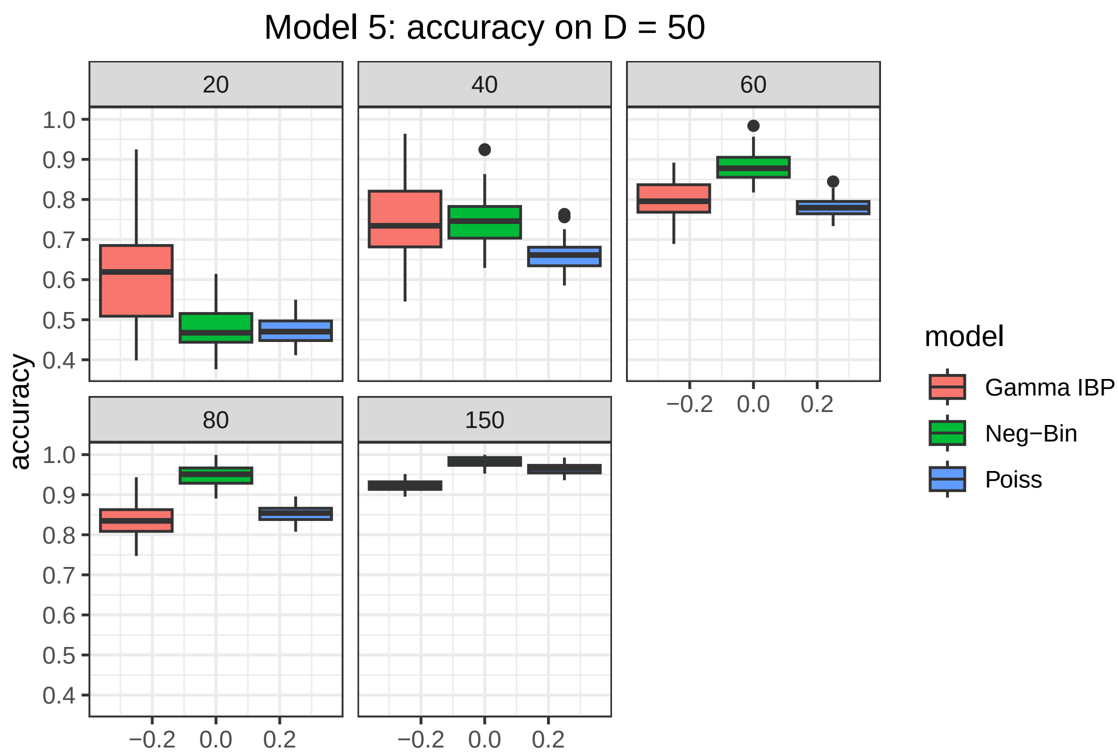
Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



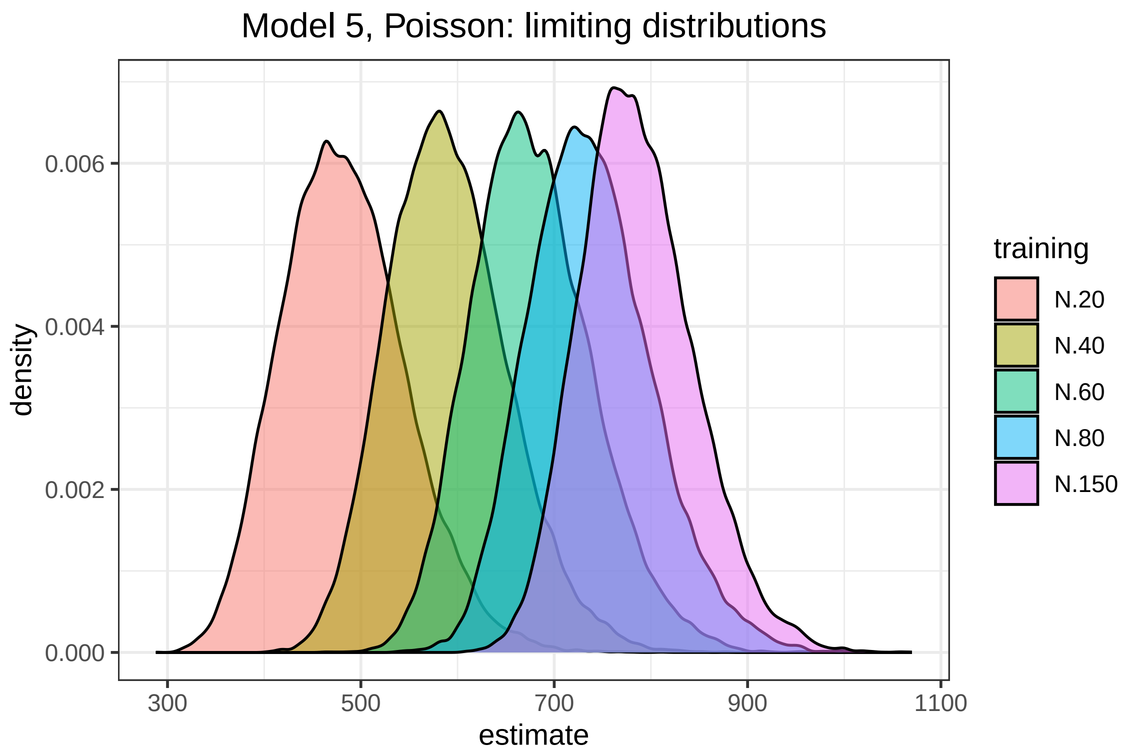
Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).

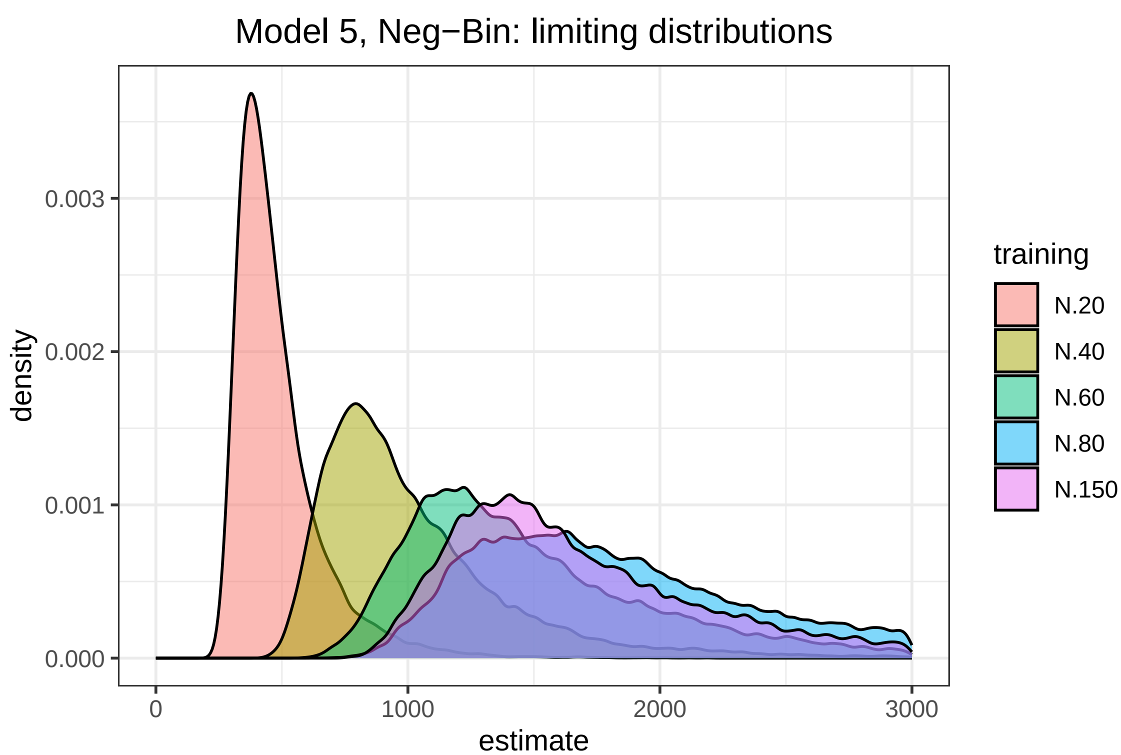


Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.

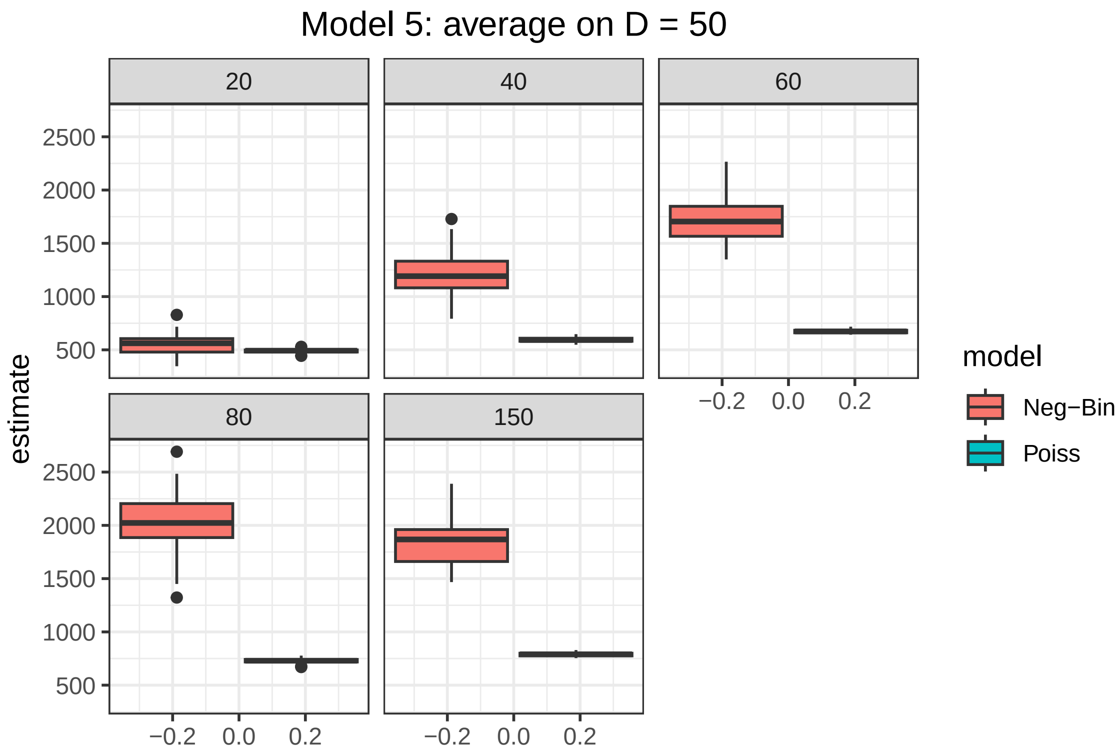


For the mixtures of Beta-Bernoulli, we report (iii) the posterior distribution of the total number of features (on a single dataset).





Finally, we report (iv) the expected value of the posterior distribution of the total number of features, over $D = 50$ replicated datasets.



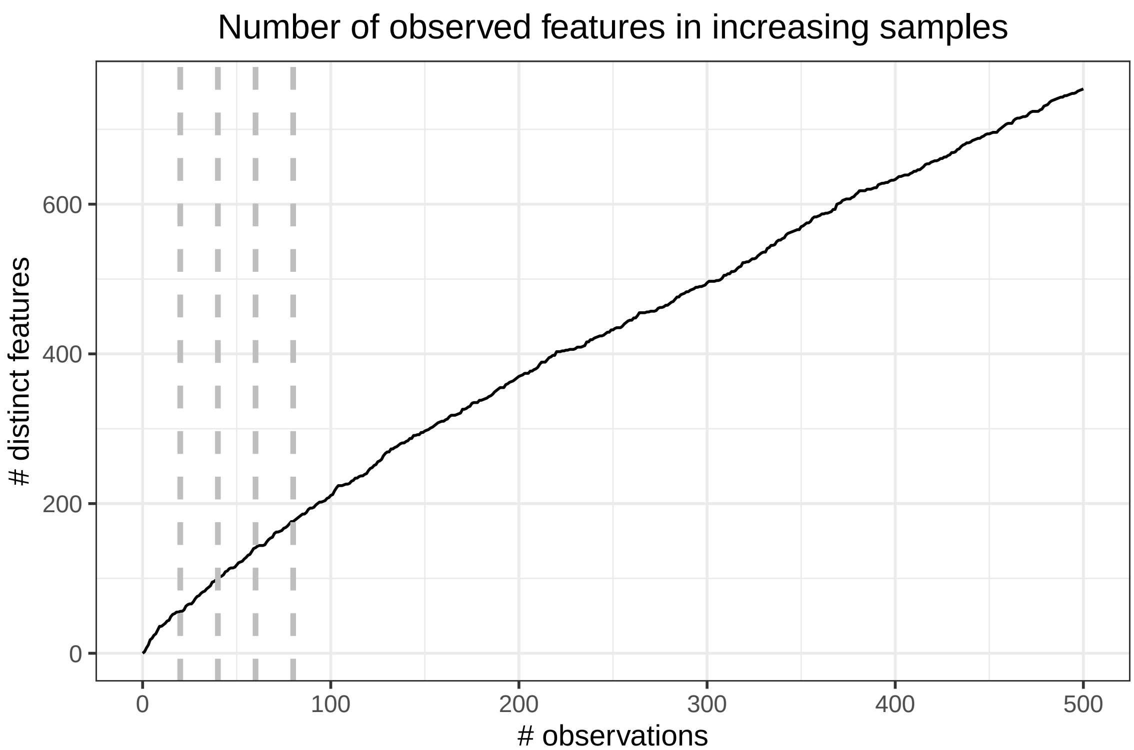
Unbounded-features scenario

Set $\pi_k = \frac{1}{(k+1)^\xi}$, for $k = 1, \ldots, H$, with $H = 10^5$ and $\xi = 1.2$. Let the total dimension of the dataset to be L, and consider different dimensions for the training set n, i.e.

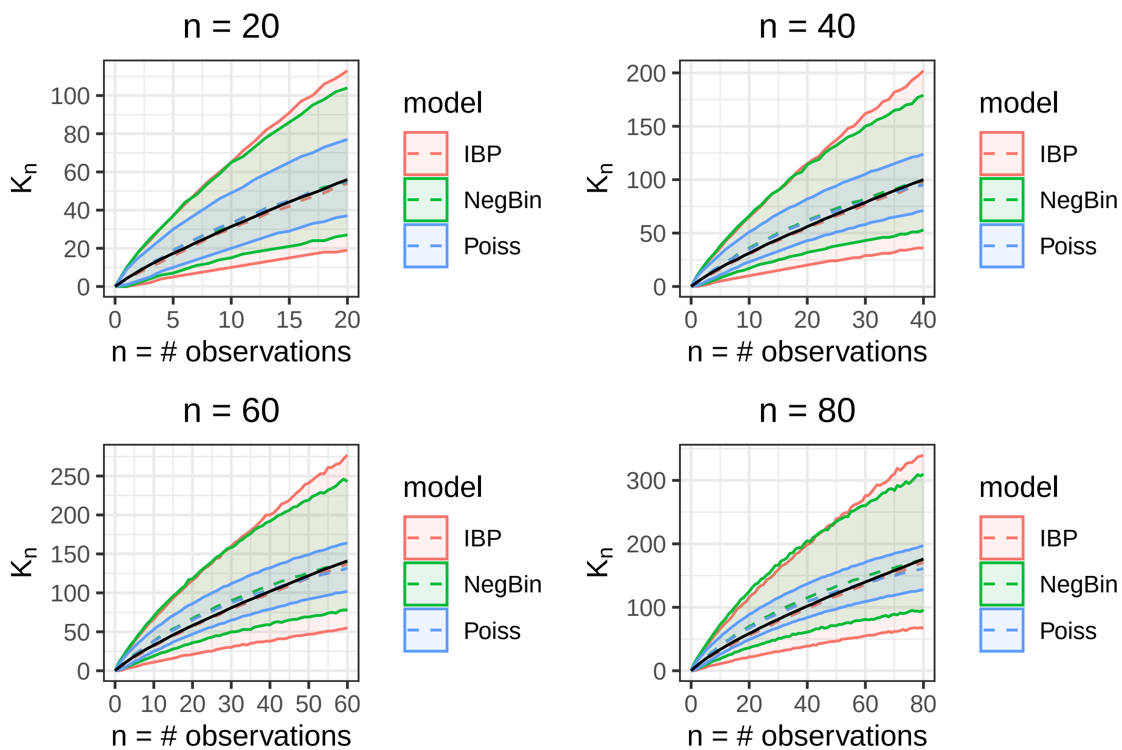
```
## L =  500
```

```
## n =  20  40  60  80
```

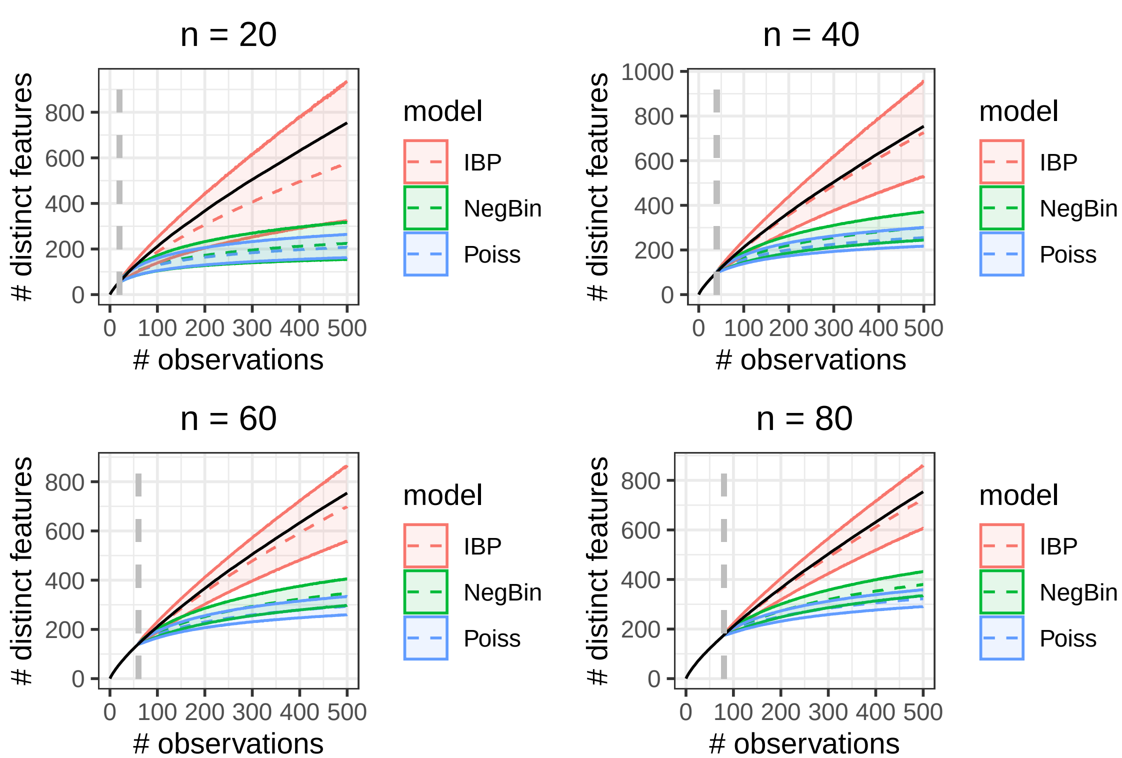
Here, the curve representing the number of observed features in increasing samples, where the grey vertical lines indicate the different training dimensions.



Here, we report (i.a) the in-sample rarefaction curve (on a single dataset).



Here, we report (i.b) the extrapolated rarefaction curve (on a single dataset).



Here, we report (ii) the accuracy of the estimated number of unseen features in the test sample, over $D = 50$ replicated datasets.