Permuted and Augmented Stick-Breaking Bayesian Multinomial Regression

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Abstract

To model categorical response variables given their covariates, we propose a permuted and augmented stick-breaking (paSB) construction that one-to-one maps the observed categories to randomly permuted latent sticks. This new construction transforms multinomial regression into regression analysis of stick-specific binary random variables that are mutually independent given their covariate-dependent stick success probabilities, which are parameterized by the regression coefficients of their corresponding categories. The paSB construction allows transforming an arbitrary cross-entropy-loss binary classifier into a Bayesian multinomial one. Specifically, we parameterize the negative logarithms of the stick failure probabilities with a family of covariate-dependent softplus functions to construct nonparametric Bayesian multinomial softplus regression, and transform Bayesian support vector machine (SVM) into Bayesian multinomial SVM. These Bayesian multinomial regression models are not only capable of providing probability estimates, quantifying uncertainty, and producing nonlinear classification decision boundaries, but also amenable to posterior simulation. Example results demonstrate their attractive properties and appealing performance.

Keywords: Discrete choice models, logistic regression, nonlinear classification, softplus regression, support vector machines

1 Introduction

Inferring the functional relationship between a categorical response variable and its covariates is a fundamental problem in physical and social sciences. Random utility models, including both the logit and probit models as special examples, are widely used to address this problem. For discrete choice analysis in econometrics [Greene, 2003, Train, 2009], these models assume that among a set of S alternatives, an individual makes the choice that maximizes his/her utility $U_{is} = V_{is} + \varepsilon_{is}$, where $i \in \{1, \ldots, N\}$ indexes the individual, $s \in \{1, \ldots, S\}$ indexes the choice, and V_{is} and ε_{is} represent the observable and unobservable parts of U_{is}, respectively. Let the prime symbol denote the transpose operation. If V_{is} is set as the inner product of the individual-specific covariate vector $\boldsymbol{x}_i = (1, x_{i1}, \ldots, x_{iP})'$ and choice-specific regression-coefficient vector $\boldsymbol{\beta}_s \in \mathbb{R}^{P+1}$, which means $V_{is} = \boldsymbol{x}_i' \boldsymbol{\beta}_s$, then marginalizing out $\boldsymbol{\varepsilon}_i = (\varepsilon_{i1}, \ldots, \varepsilon_{iS})'$ leads to multinomial logistic regression (MLR) if all ε_{is} follow the extreme value distribution [McFadden, 1973, Greene, 2003, Train, 2009], and multinomial probit regression if $\boldsymbol{\varepsilon}_i$ follows a multivariate normal distribution [Albert and Chib, 1993, McCulloch and Rossi, 1994, McCulloch et al., 2000, Imai and van Dyk, 2005].

Distinct from random utility models, we consider a novel discrete choice modeling framework built on a new stick-breaking construction of the multinomial distribution. Given a one-to-one mapping between the category and stick indices, rather than assuming an individual compares its random utilities across all categories at once to make the decision, we assume an individual makes a sequence of binary random decisions in $\{0, 1\}$, the sth of which chooses "1" with a probability determined by a function of the covariate vector of the individual and the regression coefficients of the s categories mapped to the first s sticks. The choice of the individual is the category mapped to the stick that is the first to choose "1," or the category mapped to stick S if all the first $S - 1$ sticks choose "0." This framework transforms the problem of regression analysis of categorical variables into the problem of inferring the one-to-one mapping between the category and stick indices, and performing regression analysis of binary stick-specific random variables.

Both MLR and the proposed stick-breaking discrete choice models use the multinomial distribution to link a categorical response variable with its covariate-dependent multinomial probability parameters. Though sharing that similarity, they are distinct in that MLR is invariant to the permutation of the category labels, whereas given a fixed category-stick mapping, the proposed stick-breaking models purposely destruct that invariance. We are motivated to introduce this new framework for discrete choice modeling mainly to facilitate efficient Bayesian inference via data augmentation, introduce nonlinear decision boundaries, and relax a well-recogonized restrictive model assumption of MLR, as described below.

An important motivation is to extend efficient Bayesian inference available to binary regression to multinomial one. For the proposed stick-breaking models, the binary stick-specific random variables of an individual are constructed to be conditionally independent given their stick-specific probabilities, which are parameterized by the covariates of the individual and the regression coefficients of the corresponding categories. Under this setting, one can solve multinomial regression by solving conditionally independent binary ones. The only requirement is that the underlying binary regression model uses the cross entropy loss. In other words, we require each stick-specific binary random variable to be linked via the Bernoulli distribution to its corresponding stick-specific covariate-dependent probability parameter.

Another important motivation is to improve the model capacity of MLR, which is a linear multinomial regression model in the sense that it uses the intersection of $S-1$ linear hyperplanes to separate one class from the others. By choosing nonlinear binary regression models with cross entropy loss, we are able to introduce nonlinearity into the proposed stick-breaking models for nonlinear multinomial regression. We are also motivated to relax the *independence of irrelevant alternative* (IIA) assumption, an inherence property of MLR that requires the probability ratio of any two choices to be independent of the presence or characteristics of any other alternatives [McFadden, 1973, Greene, 2003, Train, 2009]. In contrast to MLR with the IIA assumption, the proposed stick-breaking models make the probability ratio of two choices depend on the characteristics of other alternatives, as long

as the two sticks that both choices are mapped to are not next to each other.

In light of these considerations, we will first extend softplus regressions recently proposed in Zhou [2016], a family of cross-entropy-loss binary classifiers that can introduce nonlinear classification decision boundaries and include logistic regression as a special case, to construct Bayesian multinomial softplus regressions (MSRs). Under the proposed framework, while it is natural to extend a cross-entropy-loss binary classifier into a Bayesian multinomial one, it is less straightforward to extend the widely used support vector machine (SVM) [Boser et al., 1992, Cortes and Vapnik, 1995, Cristianini and Shawe-Taylor, 2000], a max-margin classifier that uses the hinge loss rather than cross entropy loss. Though there has been significant effort in extending binary SVMs into multinomial ones [Crammer and Singer, 2002, Lee et al., 2004, Liu and Yuan, 2011], the resulted extensions typically only provide the predictions of deterministic class labels. By contrast, we extend the Bayesian binary SVMs in Sollich [2002] and Mallick et al. [2005] under the proposed framework to construct Bayesian multinomial SVMs (MSVMs), which naturally provide predictive class probabilities.

We will show that the proposed Bayesian MSRs and MSVMs, which all generalize the stick-breaking construction to perform Bayesian multinomial regression, are not only capable of placing nonlinear decision boundaries between different categories, but also amenable to posterior simulation via data augmentation. Another attractive feature shared by all these proposed Bayesian algorithms is that they can be used to not only predict class probabilities but also quantify model uncertainty.

The remainder is organized as follows. In Section 2 we briefly review MLR and discuss the restrictions of its stick-breaking construction. In Section 3 we introduce the permuted and augmented stick-breaking (paSB) representation of the multinomial likelihood, show how to extend under it a binary classifier using the cross entropy loss into a multinomial one, discuss the inference of the stick-dependent variables and category-sticking mapping, and show how the IIA assumption is relaxed. Under the paSB framework, we show how to transform softplus regressions and support vector machines into Bayesian multinomial

regression models in Sections 4 and 5, respectively. We provide experimental results in Section 6 and conclude the paper in Section 7. All proofs are deferred to the Appendix.

2 Multinomial logistic regression and stick breaking

In this section we first briefly review multinomial logistic regression (MLR). We then use the stick-breaking construction to show how to generate a categorical random variable as a sequence of dependent binary variables, and further discuss a naive approach to transform binary logistic regression under stick breaking into multinomial regression.

2.1 Multinomial logistic regression

MLR that parameterizes the probability of each category given the covariates as

$$P(y_i = s \,|\, \boldsymbol{x}_i, \{\boldsymbol{\beta}_s\}_{1,S}) = p_{is},\ p_{is} = e^{\boldsymbol{x}_i'\boldsymbol{\beta}_s} \big/ \big(\textstyle\sum_{j=1}^{S} e^{\boldsymbol{x}_i'\boldsymbol{\beta}_j} \big) \tag{1}$$

is widely used, where $\boldsymbol{x}_i \in \mathbb{R}^{P+1}$ consists of $x_{i1} = 1$ and P covariates, and $\boldsymbol{\beta}_s \in \mathbb{R}^{P+1}$ consists of the regression coefficients for the sth category [McCullagh and Nelder, 1989, Albert and Chib, 1993, Holmes and Held, 2006]. Without loss of generality, one may choose category S as the reference category by setting all the elements of $\boldsymbol{\beta}_S$ as 0, making $e^{\boldsymbol{x}_i'\boldsymbol{\beta}_S} = 1$ almost surely (a.s.). For MLR, if data i is assigned to the category with the largest p_{is}, then one may consider that category s resides within a convex polytope [Grünbaum, 2013], defined by the set of solutions to $S-1$ inequalities as $\boldsymbol{x}'(\boldsymbol{\beta}_j - \boldsymbol{\beta}_s) \le 0$, where $j \in \{1, \ldots, s-1, s+1, \ldots, S\}$.

Despite its popularity, MLR is a linear classifier in the sense that it uses the intersection of $S-1$ linear hyperplanes to separate one class from the others. As a classical discrete choice model in econometrics, it makes the independence of irrelevant alternatives (IIA) assumption, implying that the unobserved factors for choice making are both uncorrelated and having the same variance across all alternatives [McFadden, 1973, Train, 2009]. Moreover, while its log likelihood is convex and there are efficient iterative algorithms to find the maximum likelihood or maximum a posteriori solutions of $\boldsymbol{\beta}_s$, the absence of conjugate priors on $\boldsymbol{\beta}_s$

makes it difficult to derive efficient Bayesian inference. For Bayesian inference, Polson et al. [2013] has introduced the Polya-Gamma data augmentation for logit models, and combined it with the data augmentation technique of Holmes and Held [2006] for the multinomial likelihood to develop a Gibbs sampling algorithm for MLR. This algorithm, however, has to update $\boldsymbol{\beta}_s$ one at a time while conditioning on all $\boldsymbol{\beta}_j$ for $j \neq s$. Thus it may not only lead to slow convergence and mixing, especially when the number of categories S is large, but also prevent us from parallelizing the sampling of $\{\boldsymbol{\beta}_s\}_{1,S}$ within each MCMC iteration.

2.2 Stick breaking

Suppose y_i is a random variable drawn from a categorical distribution with a finite vector of probability parameters $(p_{i1}, \ldots, p_{iS})$, where $S < \infty$, $p_{is} \geq 0$, and $\sum_{s=1}^{S} p_{is} = 1$. Instead of directly using $y_i \sim \sum_{s=1}^{S} p_{is}\delta_s$, one may consider generating y_i using the multinomial stick-breaking construction that sequentially draws binary random variables

$$b_{is} \,\big|\, \{b_{ij}\}_{j<s} \sim \text{Bernoulli}\left[\left(1 - \textstyle\sum_{j<s} b_{ij}\right)\pi_{is}\right], \quad \pi_{is} = \dfrac{p_{is}}{1 - \sum_{j<s} p_{ij}} \tag{2}$$

for $s = 1, 2, \ldots, S$. Note that $\pi_{iS} = 1$ and $b_{iS} = 1 - \sum_{j=1}^{S-1} b_{ij}$ by construction. Defining $y_i = s$ if and only if $b_{is} = 1$ and $b_{ij} = 0$ for all $j \neq s$, then one has a strick-breaking representation for the multinomial probability parameter as

$$P(y_i = s \,|\, \{\pi_{is}\}_{1,S}) = P(b_{is} = 1)\textstyle\prod_{j\neq s} P(b_{ij} = 0) = \pi_{is}\prod_{j<s}(1 - \pi_{ij}), \tag{3}$$

which, as expected, recovers p_{is} by substituting the definitions of π_{is} shown in (2).

The finite stick-breaking construction in (3) can be further generalized to an infinite setting, as widely used in Bayesian nonparametrics [Hjort et al., 2010]. For example, the stick-break construction of Sethuraman [1994] represents the length of the kth stick using the product of k stick-specific probabilities that are independent, and identically distributed (i.i.d.) beta random variables. It represents a size-biased random permutation of a Dirich-

let process [Ferguson, 1973] random draw, which includes countably infinite atoms whose weights sum to one. The stick-breaking construction of Sethuraman [1994] has also been generalized to represent a draw from a random probability measure that is more general than the Dirichlet process [Pitman, 1996, Ishwaran and James, 2001, Wang et al., 2011a]. Related to this paper, one may further consider making the stick-specfic probabilities depend on the covariates [Dunson and Park, 2008, Chung and Dunson, 2009, Ren et al., 2011]. For example, the logistic stick-breaking process of Ren et al. [2011] uses the product of k covariate-dependent logistic functions to parameterize the probability of the kth stick. To implement a stick-breaking process mixture model, truncated stick-breaking representations that truncate the number of sticks are commonly used, with inference developed via both Gibbs sampling [Ishwaran and James, 2001, Dunson and Park, 2008, Rodriguez, 2011] and variational approximation [Blei and Jordan, 2006, Kurihara et al., 2007, Ren et al., 2011].

2.3 Logistic stick breaking

The stick-breaking construction parameterizes each p_{is} with the product of s probability parameters and links each y_i with a unit-norm binary vector $(b_{i1}, \ldots, b_{iS})$, where $b_{iy_i} = 1$ and $b_{ij} = 0$ a.s. if $j \neq y_i$. Following the logistic stick-breaking construction of Ren et al. [2011], one may represent p_{is} with (3) and parameterize the logit of each π_{is} with a latent Gaussian variable w_{is} as $\pi_{is} = e^{w_{is}} / \sum_{j=1}^{S} e^{w_{ij}}$. To model observed or latent multinomial variables, a stick-breaking procedure, closely related to that of Ren et al. [2011], is used in Khan et al. [2012] to transform the modeling of multinomial probability parameters into the modeling of the logits of binomial probability parameters using Gaussian latent variables. As shown in Linderman et al. [2015], this procedure allows using the Polya-Gamma data augmentation, without requiring the assistance of the technique of Holmes and Held [2006], to construct Gibbs sampling that simultaneously updates all categories in each MCMC iteration, leading to improved performance over the one proposed in Polson et al. [2013].

The simplification brought by the stick-breaking representation, which stochastically arranges its categories in decreasing order, comes with a clear change in that it removes the

invariance of the multinomial distribution to label permutation. For stick-breaking process mixture models, whose cluster labels are often arbitrary and non-identifiable, the imposed size-biased random permutation [Perman et al., 1992] may not be an issue for an MCMC algorithm that allows the latent cluster labels to switch during MCMC iterations [Jasra et al., 2005], but may still clearly degrade the performance of a variational Bayes algorithm without an appropriate relabelling procedure [Kurihara et al., 2007].

While the loss of invariance to label permutation may not pose a major issue for mixture modeling, it appears to be a major obstacle when applying stick breaking for multinomial regression. If naively following the logistic stick-breaking construction of Ren et al. [2011], as also used in Khan et al. [2012] and Linderman et al. [2015], to parameterize the logit of each stick probability using the inner product of the covariate and corresponding regression coefficient vectors, and then multiply the first k covariate-dependent stick probabilities to parameterize the probability of the kth category for multinomial regression, the performance is often found to be sensitive to how the labels of the S categories are ordered. Though the seemingly undesirable sensitivity to label permutation could turn into a favorable model property if label asymmetry is desired, it may result in more restrictive geometric constraints on the classification decision boundaries than those of MLR if label symmetry is desired, especially if the S categories are not labeled in an optimal order.

More specifically, if one constructs a multinomial regression model by letting $\text{logit}(\pi_{is}) = w_{is} = \boldsymbol{x}_i'\boldsymbol{\beta}_s$, which means $\pi_{is} = (1 + e^{-\boldsymbol{x}_i'\boldsymbol{\beta}_s})^{-1}$, then one has

$$p_{is} = \left(1 + e^{-\boldsymbol{x}_i'\boldsymbol{\beta}_s}\right)^{-1} \prod_{j<s} \left(1 + e^{\boldsymbol{x}_i'\boldsymbol{\beta}_j}\right)^{-1},$$

which clearly tends to impose fewer geometric constraints on the classification decision boundaries of a category with a smaller s. For example, $p_{i1} = \left(1 + e^{-\boldsymbol{x}_i'\boldsymbol{\beta}_1}\right)^{-1}$ is larger than 50% if $\boldsymbol{x}_i'\boldsymbol{\beta}_1 > 0$ while $p_{i2} = \left(1 + e^{\boldsymbol{x}_i'\boldsymbol{\beta}_1}\right)^{-1}\left(1 + e^{-\boldsymbol{x}_i'\boldsymbol{\beta}_2}\right)^{-1}$ is possible to be larger than 50% only if both $\boldsymbol{x}_i'\boldsymbol{\beta}_1 < 0$ and $\boldsymbol{x}_i'\boldsymbol{\beta}_2 > 0$. We will use an example to illustrate this type

of geometric constraints in Section 6.1. Under the logistic stick-breaking construction, not only could the performance be sensitive to how the S different categories are ordered, but the imposed geometric constraints could also be overly restrictive even if the categories are appropriately ordered. Below we first address the first issue by introducing a permuted and augmented stick-breaking representation for a multinomial model, and then address the second issue by introducing the ability to model nonlinearity.

3 Permuted and augmented stick breaking

To turn the seemingly undesirable sensitivity of the stick-breaking construction to label permutation into a favorable model property, when label asymmetry is desired, and mitigate performance degradation, when label symmetry is desired, we introduce a permuted and augmented stick-breaking (paSB) construction for a multinomial distribution, making it straightforward to extend an arbitrary binary classifier with cross entropy loss into a Bayesian multinomial one. The paSB construction infers a one-to-one mapping between the labels of the S categories and the indices of the S latent sticks, transforming the problem of modeling a multinomial random variable into that of modeling S conditionally independent binary ones. Note that there are $S!$ one-to-one label-stick mappings, which quickly becomes too large to exhaustively search for the best mapping as S increases. Our experiments will show that the proposed MCMC algorithm can quickly escape from a purposely poorly initialized mapping and subsequently switch between many different mappings that all lead to similar performance, suggesting an effective search space that is considerably smaller than $S!$.

3.1 Category-stick mapping and data augmentation

The proposed paSB construction randomly maps a category to one and only one of the S latent sticks and makes the augmented Bernoulli random variables $\{b_{is}\}_{1,S}$ conditionally independent to each other given $\{\pi_{is}\}_{1,S}$. Denote $\boldsymbol{z} = (z_1, \ldots, z_S)$ as a permutation of $(1, \ldots, S)$, where $z_s \in \{1, \ldots, S\}$ is the index of the stick that category s is mapped to. Given the label-sticking mapping $\boldsymbol{z}$, let us denote $p_{is}(\boldsymbol{z})$ as the multinomial probability of

category s, and $\pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)$ as the covariate-dependent stick probability that is associated with the covariates of observation i and the stick that category s is mapped to. For notational convenience, we will write $\pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)$ as π_{iz_s} and $\pi_{ij}(\boldsymbol{x}_i, \boldsymbol{\beta}_{s:z_s=j})$ as π_{ij}. We emphasize that here the sth regression-coefficient vector $\boldsymbol{\beta}_s$ is always associated with both category s and the corresponding stick probabily π_{iz_s}, a construction that will facilitate the inference of the label-sticking mapping $\boldsymbol{z}$. The following Theorem shows how to generate a categorical random variable of S categories with a set of S conditionally independent Bernoulli random variables, which is key to transforming the problem of solving multinomial regression into the problem of solving S binary regressions independently.

Theorem 1. *Suppose* $y_i \sim \sum_{s=1}^{S} p_{is}(\boldsymbol{z})\delta_s$, *where* $[p_{i1}(\boldsymbol{z}), \ldots, p_{iS}(\boldsymbol{z})]$ *is a multinomial probability vector whose elements are constructed as*

$$p_{is}(\boldsymbol{z}) = (\pi_{iz_s})^{\mathbf{1}(z_s \neq S)} \prod_{j<z_s} (1 - \pi_{ij}), \tag{4}$$

then y_i *can be equivalently generated under the permuted and augmented stick-breaking (paSB) construction as*

$$y_i \sim \sum_{s=1}^{S} \left\{ [\mathbf{1}(b_{iz_s} = 1)]^{\mathbf{1}(z_s \neq S)} \textstyle\prod_{j<z_s} \mathbf{1}(b_{ij} = 0) \right\} \delta_s \,, \tag{5}$$

$$b_{ij} \sim \text{Bernoulli}(\pi_{ij}), \quad j \in \{1, \ldots, S\}. \tag{6}$$

Distinct from the conventional stick breaking in (2) that maps category s to stick s and makes b_{is} depend on $b_{ij}, j = 1, \ldots, s-1$, under the new construction in (6), the S categories are now randomly permuted and then one-to-one mapped to S sticks. The augmented binary random variables $\{b_{ij}\}_j$ become mutually independent given $\{\pi_{ij}\}_j$. Given y_i, we still have $b_{ij} = 0$ for $j < z_{y_i}$ and $b_{iz_{y_i}} = 1$ a.s., but impose no restriction on any b_{ij} for $j > z_{y_i}$, whose conditional posteriors given y_i and π_{ij} remain the same as their priors: $b_{ij} \sim \text{Bernoulli}(\pi_{ij})$. These changes are key to appropriately ordering the latent sticks, more

flexibly parameterizing π_{iz_s} and hence $p_{is}(\boldsymbol{z})$, and maintaining tractable inference.

We refer to this new construction as permuted and augmented stick breaking (paSB), where the one-to-one mapping between the category labels and stick indices can be selected from one of $S!$ permutations and $\{b_{iz_s}\}_{1,S}$ are introduced as Bernoulli auxiliary variables. Note that while there is a one-to-one mapping between y_i and $\{b_{is}\}_{1,S}$ under the conventional stick-breaking construction, given the category-stick mapping $\boldsymbol{z}$, there is a one-to-many mapping between y_i and $\{b_{iz_s}\}_{1,S}$ under the paSB representation if $z_{y_i} \neq S$.

With paSB, the problem of inferring the functional relationship between the categorical response y_i and the corresponding covariates $\boldsymbol{x}_i$ is now transformed into the problem of modeling S conditionally independent binary regressions as

$$b_{iz_s} \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}_s \sim \text{Bernoulli}[\pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)],\ i = 1, \ldots, N,\ s = 1, \ldots, S.$$

Note that the only requirement for the binary regression model under paSB is that it uses the Bernoulli likelihood. In other words, it uses the cross entropy loss [Murphy, 2012] as

$$-\sum_{i=1}^{N} \ln P(b_{iz_s} \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}_s) = \sum_{i=1}^{N} \{-b_{iz_s} \ln \pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s) - (1 - b_{iz_s}) \ln[1 - \pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)]\}\,.$$

A basic choice is paSB logistic regression that lets

$$\pi_{iz_s}(\boldsymbol{x}_i, \boldsymbol{\beta}_s) = 1/(1 + e^{-\boldsymbol{x}_i \boldsymbol{\beta}_s}),$$

which becomes the same as the logistic-stick breaking construction described in Section 2.3 if $z_s = s$ for all $s \in \{1, \ldots, S\}$. Moving beyond logistic stick breaking, below we will discuss how to generalize softplus regressions and support vector machines (SVMs), which are more powerful binary classifiers that can produce nonlinear classification decision boundaries.

In addition to paSB, we define permuted and augmented reverse stick breaking (parSB) in the following Corollary.

Corollary 2. *Suppose* $y_i \sim \sum_{s=1}^{S} p_{is}\delta_s$ *and*

$$p_{is}(\boldsymbol{z}) = (1-\pi_{iz_s})^{\mathbf{1}(z_s\neq S)} \prod_{j<z_s} \pi_{ij}\,, \tag{7}$$

then y_i *can also be generated under the permuted and augmented reverse stick-breaking (parSB) representation as*

$$y_i \sim \sum_{s=1}^{S} \Big\{ [\mathbf{1}(b_{iz_s}=0)]^{\mathbf{1}(z_s\neq S)} \prod_{j<z_s} \mathbf{1}(b_{ij}=1) \Big\} \delta_s\,, \tag{8}$$

$$b_{ij} \sim \text{Bernoulli}(\pi_{ij}), \quad j \in \{1,\ldots,S\}. \tag{9}$$

Generally speaking, if $\pi_{iz_s}(\boldsymbol{x}_i, -\boldsymbol{\beta}_s) = 1-\pi_{iz_s}(\boldsymbol{x}_i,\boldsymbol{\beta}_s)$, which is the case for logistic stick breaking with $\pi_{iz_s} = (1+e^{-\boldsymbol{x}_i'\boldsymbol{\beta}_s})^{-1}$ and Bayesian SVMs to be discussed in Section 5, then there is no need to introduce parSB as an addition to paSB. However, if $\pi_{iz_s}(\boldsymbol{x}_i, -\boldsymbol{\beta}_s) \neq 1-\pi_{iz_s}(\boldsymbol{x}_i,\boldsymbol{\beta}_s)$, which is the case for softplus regressions to be introduced in Section 4, then there are potential benefits to combine parSB with paSB.

3.2 Inference of stick variables and category-stick mapping

Below we first describe Gibbs sampling for the augmented stick variables $\{b_{ij}\}_{1,S}$, and then introduce a Metropolis-Hastings (MH) step to infer the category-stick mapping $\boldsymbol{z}$. Given the category label y_i, stick probability π_{ij}, and $\boldsymbol{z}$, we sample b_{ij} as

$$(b_{ij} \,|\, y_i, \pi_{ij}, \boldsymbol{z}) \sim \mathbf{1}(j = z_{y_i}) + \mathbf{1}(j > z_{y_i})\text{Bernoulli}(\pi_{ij}), \tag{10}$$

for $j = 1,\ldots,S-1$, and let

$$b_{iS} = \mathbf{1}(z_{y_i} = S). \tag{11}$$

This means we let $b_{ij}=0$ if $j < z_{y_i}$, $b_{ij}=1$ if $j = z_{y_i}$, draw b_{ij} from Bernoulli(π_{ij}) if $z_{y_i} < j < S$, and let $b_{iS}=1$ if and only if $z_{y_i} = S$. Note that to compute $p_{is}(\boldsymbol{z})$ defined in (4) for $s \in \{1,\ldots,S\}$, where stick S is used as the reference stick, it is necessary to

have π_{ij} for $j \in \{1, \ldots, S-1\}$ but not necessary to have π_{iS}. Despite having no impact on computing $\{p_{is}\}_{1,S}$, we infer π_{iS} (*i.e.*, sample the regression-coefficient vector $\boldsymbol{\beta}_{s':z_{s'}=S}$) under the likelihood $\prod_{i=1}^{N} \text{Bernoulli}(b_{iS}; \pi_{iS})$ and use it in the Metropolis-Hastings step, as described in (12) shown below, to decide whether to switch the mappings of two different categories, one of which is mapped to the reference stick S. Once we have an MCMC sample of $\{b_{ij}\}_{1,S}$, we then essentially solve independently S binary classification problems, the jth of which can be expressed as $b_{ij} \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}_{s:z_s=j} \sim \text{Bernoulli}[\pi_{ij}(\boldsymbol{x}_i, \boldsymbol{\beta}_{s:z_s=j})]$.

Analogously, for parSB, $\{b_{ij}\}_{1,S}$ can be sampled as $(b_{ij} \,|\, y_i, \pi_{ij}, \boldsymbol{z}) \sim \mathbf{1}(j < z_{y_i}) + \mathbf{1}(j > z_{y_i})\text{Bernoulli}(\pi_{ij})$ for $j = 1, \ldots, S-1$, and $b_{iS} = 1 - \mathbf{1}(z_{y_i} = S)$, which means for parSB, we let $b_{ij} = 1$ if $j < z_{y_i}$, let $b_{ij} = 0$ if $j = z_{y_i}$, draw b_{ij} from $\text{Bernoulli}(\pi_{ij})$ if $z_{y_i} < j < S$, and let $b_{iS} = 0$ if and only if $z_{y_i} = S$.

Since stick-breaking multinomial classification is not invariant to the permutation of its class labels, it may perform substantially worse than it could be if the inherent geometric constraints implied by the current ordering of the labels make it difficult to adapt the decision boundaries to the data. Our solution to this problem is to infer the one-to-one mapping between category labels and stick indices from the data. We construct a Metropolis-Hastings (MH) step within each Gibbs sampling iteration, with a proposal of switching two sticks that categories c and c', $1 \le c < c' \le S$, are mapped to, by changing the current category-stick one-to-one mapping from $\boldsymbol{z} = (z_1, \ldots, z_c, \ldots, z_{c'}, \ldots, z_S)$ to $\boldsymbol{z}' = (z'_1, \ldots, z'_S) := (z_1, \ldots, z_{c'}, \ldots, z_c, \ldots, z_S)$. Assuming a uniform prior on $\boldsymbol{z}$ and proposing (c, c') uniformly at random from one of the $\binom{S}{2} = S!/[2!(S-2)!]$ possibilities, we would accept the proposal with probability

$$\min\left\{\prod_i \frac{\prod_{s=1}^{S}[p_{is}(\boldsymbol{z}')]^{\mathbf{1}(y_i=s)}}{\prod_{s=1}^{S}[p_{is}(\boldsymbol{z})]^{\mathbf{1}(y_i=s)}},\ 1\right\} = \min\left\{\prod_i \frac{\prod_{s=1}^{S}\left[(\pi_{iz'_s})^{\mathbf{1}(z'_s\neq S)}\prod_{j<z'_s}(1-\pi_{ij})\right]^{\mathbf{1}(y_i=s)}}{\prod_{s=1}^{S}\left[(\pi_{iz_s})^{\mathbf{1}(z_s\neq S)}\prod_{j<z_s}(1-\pi_{ij})\right]^{\mathbf{1}(y_i=s)}},\ 1\right\}. \tag{12}$$

3.3 Sequential decision making

In econometrics, a discrete choice model typically assumes that an individual makes a choice that maximizes his/her latent utility [Hanemann, 1984]. Instead of examining the utilities of all choices before making the decision, the paSB construction is characterized by a sequential decision making process, described as follows. In step one, an individual decides whether to select the choice mapped to stick 1, or to select a choice among the remaining alternatives, *i.e.*, choices $\{s : z_s \in \{2, \ldots, S\}\}$ that are not mapped to stick 1. If the individual selects the choice mapped to stick 1, then the sequential process is terminated, otherwise the choice mapped to stick 1 is eliminated and the individual proceeds to step two, in which he/she would follow the same procedure to either select the choice mapped to stick 2 or proceed to the next step to select a choice among the remaining alternatives, *i.e.*, choices $\{s : z_s \in \{3, \ldots, S\}\}$ that are not mapped to the first two sticks. The individual, reconsidering none of the eliminated choices, will keep making a *one-vs-remaining* decision at each step until the termination of the sequential decision making process.

This unique sequential decision making procedure relaxes the independence of irrelevant alternatives (IIA) assumption, as described in the following Lemma.

Lemma 3. *Under the paSB construction, the probability ratio of two choices are influenced by the success probabilities of the sticks that lie between these two choices' corresponding sticks. In other words, the probability ratio of two choices will be influenced by some other choices if they are not mapped to adjacent sticks.*

From Lemma 3 it is clear that the paSB construction could adjust how two choices' probability ratio depends on the other alternatives by controlling the distance between the two sticks that they are mapped to, providing a unique way to relax the IIA assumption. While the widely used MLR can be considered as a random utility maximization model with the IIA assumption, the paSB multinomial logistic model performs sequential random utility maximization that relaxes the IIA assumption, as described in Lemma 5 in the Appendix.

4 Bayesian multinomial softplus regression

Logistic regression is a cross-entropy-loss binary classifier that can be straightforwardly extended into paSB multinomial logistic regression (paSB-MLR). However, logistic regression is a linear classifier that uses a single hyperplane to separate one class from the other. To introduce nonlinear classification decision boundaries, we consider extending softplus regression of Zhou [2016], a multi-hyperplane binary classifier that uses the cross entropy loss, into multinomial softplus regression (MSR) under paSB. Softplus regression uses the interaction of multiple hyperplanes to construct a union of convex-polytope-like confined spaces to enclose the data labeled as "1," which are hence separated from the data labeled as "0". It is constructed by thresholding at one a latent Poisson count, the distribution of whose Poisson rate is the convolution of the probability density functions of K experts, each of which corresponds to the stack of T gamma distributions with covariate-dependent scale parameters. The number of experts K and the number of layers T can be considered as the two model parameters that determine the nonlinear capacity of the model. Note that a gamma process can be used to support a potentially countably infinite number of experts. For this reason, one can set K as large as permitted by computation and relies on the gamma process's inherent shrinkage mechanism to turn off unneeded model capacity (not all K experts will be used if K is sufficiently large).

4.1 paSB and parSB extensions of softplus regressions

We first follow Zhou [2016] to define

$$\varsigma(x_1, \ldots, x_t) = \ln\left(1 + e^{x_t} \ln\left\{1 + e^{x_{t-1}} \ln\left[1 + \ldots \ln\left(1 + e^{x_1}\right)\right]\right\}\right) \tag{13}$$

as the stack-softplus function. Note that if $t = 1$, the stack-softplus function reduces to softplus function $\varsigma(x) = \ln(1 + e^x)$, which is often considered as a smoothed version of the rectifier function as rectifier$(x) = \max(0, x)$ that has become the dominant nonlinear activation function for deep neural networks [Nair and Hinton, 2010, Glorot et al., 2011,

Krizhevsky et al., 2012, LeCun et al., 2015]. We then parameterize $\lambda_{iz_s} = -\ln(1-\pi_{iz_s})$, the negative logarithms of the failure probabilities of the stick that category s is mapped to, as

$$\lambda_{iz_s} = \sum_{k=1}^{\infty} r_{sk}\, \varsigma\big(\boldsymbol{x}'\boldsymbol{\beta}_{sk}^{(2)}, \ldots, \boldsymbol{x}'\boldsymbol{\beta}_{sk}^{(T+1)}\big), \tag{14}$$

where the countably infinite atoms $(\boldsymbol{\beta}_{sk}^{(2)}, \ldots, \boldsymbol{\beta}_{sk}^{(T+1)})$ and their weights $\{r_{sk}\}_k$ constitute a draw from a gamma process $G_s \sim \mathrm{GaP}(G_0, 1/c_s)$ [Ferguson, 1973], with G_0 as a finite and continuous base distribution over a complete separable metric space Ω and $1/c_s$ as a scale parameter. In other words, we let $b_{iz_s} \sim \mathrm{Bernoulli}(\pi_{iz_s})$ or

$$b_{iz_s} \sim \mathrm{Bernoulli}\left[1 - \prod_{k=1}^{\infty}\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T+1)}}\ln\Big\{1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T)}}\ln\Big[1+\ldots\ln\Big(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(2)}}\Big)\Big]\Big\}\right)^{-r_{sk}}\right]. \tag{15}$$

As shown in Theorem 10 of Zhou [2016], b_{iz_s} can be equivalently generated from a hierarchical model that convolves countably infinite stacked gamma distributions, with covariate-dependent scales, as

$$\begin{aligned}
\theta_{isk}^{(T)} &\sim \mathrm{Gamma}\left(r_{sk}, e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T+1)}}\right),\\
&\cdots\\
\theta_{isk}^{(t)} &\sim \mathrm{Gamma}\left(\theta_{isk}^{(t+1)}, e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(t+1)}}\right),\\
&\cdots\\
\theta_{isk}^{(1)} &\sim \mathrm{Gamma}\left(\theta_{isk}^{(2)}, e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(2)}}\right),\\
b_{iz_s} = \mathbf{1}(m_{is}\geq 1),\ m_{is} &= \sum_{k=1}^{\infty} m_{isk}^{(1)},\ m_{isk}^{(1)} \sim \mathrm{Pois}(\theta_{isk}^{(1)}),
\end{aligned} \tag{16}$$

the marginalization of whose latent variables lead to (15). We consider the combination of (16) and either paSB in (5) or parSB in (8) as the nonparametric Bayesian hierarchical model for multinomial softplus regression (MSR) that is defined below.

Definition 1 (Multinomial Softplus Regression)**.** *With a draw from a gamma process for*

each category that consists of countably infinite atoms $\boldsymbol{\beta}_{sk}^{(2:T+1)}$ *with weights* $r_{sk} > 0$*, where* $\boldsymbol{\beta}_{sk}^{(t)} \in \mathbb{R}^{P+1}$*, given the covariate vector* $\boldsymbol{x}_i$ *and category-stick mapping* $\boldsymbol{z}$*, MSR parameterizes* p_{is}*, the multinomial probability of category* s*, under the paSB construction as*

$$p_{is}(\boldsymbol{z}) = \left[1 - \prod_{k=1}^{\infty} \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T+1)}} \ln\left\{1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T)}} \ln\left[1+\ldots \ln\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(2)}}\right)\right]\right\}\right)^{-r_{sk}}\right]^{\mathbf{1}(z_s \neq S)}$$
$$\times \prod_{j:z_j<z_s} \left[\prod_{k=1}^{\infty} \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(T+1)}} \ln\left\{1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(T)}} \ln\left[1+\ldots \ln\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(2)}}\right)\right]\right\}\right)^{-r_{jk}}\right], \quad (17)$$

and parameterizes p_{is} *under the parSB construction as*

$$p_{is}(\boldsymbol{z}) = \left[\prod_{k=1}^{\infty} \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T+1)}} \ln\left\{1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(T)}} \ln\left[1+\ldots \ln\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{sk}^{(2)}}\right)\right]\right\}\right)^{-r_{sk}}\right]^{\mathbf{1}(z_s \neq S)}$$
$$\times \prod_{j:z_j<z_s} \left[1 - \prod_{k=1}^{\infty} \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(T+1)}} \ln\left\{1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(T)}} \ln\left[1+\ldots \ln\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_{jk}^{(2)}}\right)\right]\right\}\right)^{-r_{jk}}\right]. \quad (18)$$

For the convenience of implementation, we truncate the number of atoms of the gamma process at K by choosing a discrete base measure for each category as $G_{s0} = \sum_{k=1}^{K} \frac{\gamma_{s0}}{K} \delta_{\boldsymbol{\beta}_{sk}^{(2:T+1)}}$, under which we have $r_{sk} \sim \text{Gamma}(\gamma_{s0}/K, 1/c_{s0})$ as the prior distribution for the weight of expert k in category s. For each category, we expect only some of its K experts to have non-negligible weights if K is set large enough, and we may use $\sum_k \mathbf{1}\big(\sum_i m_{isk}^{(1)} > 0\big)$, where $m_{isk}^{(1)}$ is defined in (16), to measure the number of active experts inferred from the data.

4.2 Geometric constraints for MSR

Since by definition we have $p_{is}(\boldsymbol{z}) = \pi_{iz_s}\big(1 - \sum_{j<s} p_{is}(\boldsymbol{z})\big) = \pi_{iz_s} \prod_{j<z_s}(1-\pi_{ij})$ in MSR, it is clear that if π_{ij} for all $j < z_s$ are small and π_{iz_s} is the first one to have a large probability value close to one, y_i will be likely assigned to category s regardless of how large the values of $\{\pi_{ij}\}_{j>z_s}$ are. To motivate the use of the seemingly over-parameterized sum-stack-softplus function in (14), we first consider the simplest case of $K = T = 1$. Without loss of generality, let us assume that the category-stick mapping is fixed at $\boldsymbol{z} = (1, \ldots, S)$.

Lemma 4. *For paSB-MSR with* $K = T = 1$ *and* $\boldsymbol{z} = (1, \ldots, S)$*, the set of solutions to* $p_{is}(\boldsymbol{z}) > p_0$ *in the covariate space are bounded by a convex polytope defined by the intersection*

of s linear hyperplanes.

Note that the binary softplus regression with $K = T = 1$ is closely related to logistic regression, and reduces to logistic regression if $r = 1$ [Zhou, 2016]. With Lemma 4, it is clear that even if an optimal category-stick mapping $\boldsymbol{z}$ is provided, paSB-MSR with $K = T = 1$ may still clearly underperform MLR. This is because category s uses a single hyperplane to separate itself from the remaining $S - s$ categories, and hence uses the interaction of at most s hyperplanes to separate itself from the other $S - 1$ categories. By contrast, MLR uses a convex polytope bounded by at most $S - 1$ hyperplanes for each of the S categories.

When $K > 1$ and/or $T > 1$, an exact theoretical analysis is beyond the scope of this paper. Instead we provide some qualitative analysis by borrowing related geometric-constraint analysis for softplus regressions in Zhou [2016]. To enclose category s to separate it from the remaining $S - s$ categories in the covariate space, paSB-MSR with $K > 1$ and $T = 1$ uses the complement of a convex-polytope-bounded space, paSB-MSR with $K = 1$ and $T > 1$ uses a convex-polytope-like confined space, and paSB-MSR with both $K > 1$ and $T > 1$ uses a union of convex-polytope-like confined spaces. For parSB-MSR, the interpretation is the same if $K = T = 1$. If $K + T > 1$, the interpretation is the same except a convex polytope in paSB will be replaced with the complement of a convex polytope, and vise versa.

5 Bayesian multinomial support vector machine

Support vector machines (SVMs) are max-margin binary classifiers that typically minimize a regularized hinge loss objective function as

$$l(\boldsymbol{\beta}, \nu) = \sum_{i=1}^{N} \max(1 - b_i \boldsymbol{x}_i' \boldsymbol{\beta}, 0) + \nu R(\boldsymbol{\beta}),$$

where $b_i \in \{-1, 1\}$ represents the binary label for the ith observation, $R(\boldsymbol{\beta})$ is a regularization function that is often set as the L_1 or L_2 norm of $\boldsymbol{\beta}$, ν is a tuning parameter, and $\boldsymbol{x}_i'$ is the ith row of the design matrix $\mathbf{X} = (\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n)'$. For linear SVMs, $\boldsymbol{x}_i$ is the covariate vector

of the ith observation, whereas for nonlinear SVMs, one typically set the (i, j)th element of $\mathbf{X}$ as the kernel distance between the covariate vector of the ith observation and the jth support vector. The decision boundary of a binary SVM is $\{\boldsymbol{x} : \boldsymbol{x}'\boldsymbol{\beta} = 0\}$ and an observation is assigned the label $y_i = \text{sign}(\boldsymbol{x}'\boldsymbol{\beta})$, which means $b_i = 1$ if $\boldsymbol{x}'\boldsymbol{\beta} \geq 0$ and $b_i = -1$ if $\boldsymbol{x}'\boldsymbol{\beta} < 0$.

5.1 Bayesian binary SVMs

It is shown in Polson et al. [2011] that the exponential of the negative of the hinge loss can be expressed as a location-scale mixture of normals as

$$\begin{aligned} L(b_i \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}) &= \exp\left[-2\max(1 - b_i \boldsymbol{x}_i'\boldsymbol{\beta}, 0)\right] \\ &= \int_0^\infty \frac{1}{\sqrt{2\pi\omega_i}} \exp\left[-\frac{1}{2}\frac{(1 + \omega_i - b_i \boldsymbol{x}_i'\boldsymbol{\beta})^2}{\omega_i}\right] d\omega_i. \end{aligned} \tag{19}$$

Consequently, $L(\boldsymbol{b} \,|\, \mathbf{X}, \boldsymbol{\beta}) = \prod_i L(b_i \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}) = \exp\{-2\sum_i \max(1 - b_i \boldsymbol{x}_i'\boldsymbol{\beta}, 0)\}$ can be regarded as a pseudo likelihood in the sense that it is unnormalized with respect to $\boldsymbol{b} = (b_1, \ldots, b_N)' \in \{-1, 1\}^N$. This location-scale normal mixture representation of the hinge loss allows developing close-form Gibbs sampling update equations for the regression coefficients $\boldsymbol{\beta}$ via data augmentation, as discussed in detail in Polson et al. [2011] and further generalized in Henao et al. [2014] to construct nonlinear SVMs amenable to Bayesian inference. While data augmentation has made it feasible to develop Bayesian inference for SVMs, it has not addressed a common issue that SVMs provide the predictions of deterministic class labels but not class probabilities. For this reason, below we discuss how to allow SVMs predict class probabilities while maintaining tractable Bayesian inference via data augmentation.

Following Sollich [2002] and Mallick et al. [2005], by defining the joint distribution of $\boldsymbol{\beta}$ and $\{\boldsymbol{x}_i\}_i$ to be proportional to $\prod_i [L(1 \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}) + L(-1 \,|\, \boldsymbol{x}_i, \boldsymbol{\beta})]$, one may define the conditional distribution of the binary label $b_i \in \{-1, 1\}$ as

$$P(b_i \,|\, \boldsymbol{x}_i, \boldsymbol{\beta}) = \begin{cases} \dfrac{1}{1 + e^{-2b_i \boldsymbol{x}_i\boldsymbol{\beta}}}, & \text{for } |\boldsymbol{x}_i'\boldsymbol{\beta}| \leq 1; \\ \dfrac{1}{1 + e^{-b_i[\boldsymbol{x}_i\boldsymbol{\beta} + \text{sign}(\boldsymbol{x}_i'\boldsymbol{\beta})]}}, & \text{for } |\boldsymbol{x}_i'\boldsymbol{\beta}| > 1; \end{cases} \tag{20}$$

which defines a probabilistic inference model that has the same maximum a posteriori (MAP) solution as that of a binary SVM for a given dataset. Note for MAP inference, the penalty term $\nu R(\boldsymbol{\beta})$ of the regularized hinge loss can be related to a corresponding prior distribution imposed on $\boldsymbol{\beta}$, such as the Gaussian, Laplace, or spike-and-slab priors [Polson et al., 2011].

5.2 paSB multinomial support vector machine

Generalizing previous work in constructing Bayesian binary SVMs [Sollich, 2002, Mallick et al., 2005, Polson et al., 2011], below we develop multinomial SVMs that not only have tractable Bayesian inference via data augmentation, but also predict class probabilities and quantify model uncertainties. These properties differ our extension of binary SVMs to multinomial ones from those proposed in Crammer and Singer [2002], Lee et al. [2004], Liu and Yuan [2011]. A Bayesian multinomial SVM that predicts class probabilities has also been proposed before in Zhang and Jordan [2006], which, however, does not have a data augmentation procedure to sample the regression coefficients in closed form, and consequently, relies on a random-walk Metropolis-Hastings procedure that may be difficult to tune.

Redefining the label sample space from $b_i \in \{-1, 1\}$ to $b_i \in \{0, 1\}$, we may rewrite (20) as $b_i \,|\, \boldsymbol{x}_i, \boldsymbol{\beta} \sim \text{Bernoulli}[\pi_{i,\text{svm}}(\boldsymbol{x}_i, \boldsymbol{\beta})]$, where

$$\pi_{i,\text{svm}}(\boldsymbol{x}_i, \boldsymbol{\beta}) = \begin{cases} \dfrac{1}{1 + e^{-2\boldsymbol{x}_i\boldsymbol{\beta}}}, & \text{for } |\boldsymbol{x}_i'\boldsymbol{\beta}| \leq 1; \\ \dfrac{1}{1 + e^{-\boldsymbol{x}_i\boldsymbol{\beta} - \text{sign}(\boldsymbol{x}_i'\boldsymbol{\beta})}}, & \text{for } |\boldsymbol{x}_i'\boldsymbol{\beta}| > 1. \end{cases} \tag{21}$$

The Bernoulli likelihood based cross-entropy-loss binary classifier, whose covariate-dependent probabilities are parameterized as in (21), is exactly what we need to extend the binary SVM into a multinomial classifier under paSB introduced in Theorem 1. More specifically, given the category-stick mapping $\boldsymbol{z}$, with the success probabilities of the stick that category s is mapped to parameterized as $\pi_{iz_s,\text{rvm}}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)$ and binary stick variables drawn as $b_{iz_s} \sim \text{Bernoulli}[\pi_{iz_s,\text{rvm}}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)]$, we have the following definition.

Definition 2 (paSB multinomial SVM)**.** *Under the paSB construction, given the covari-*

ate vector $\boldsymbol{x}_i$ and category-stick mapping $\boldsymbol{z}$, multinomial support vector machine (MSVM) parameterizes p_{is}, the multinomial probability of category s, as

$$p_{is}(\boldsymbol{z}) = [\pi_{iz_s,\text{svm}}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)]^{\mathbf{1}(z_s \neq S)} \prod\nolimits_{j:z_j<z_s} \pi_{iz_j,\text{svm}}(\boldsymbol{x}_i, \boldsymbol{\beta}_j). \tag{22}$$

Note that there is no need to introduce parSB-MSVM in addition to paSB-MSVM, since by definition, we have $\pi_{iz_s,\text{rvm}}(\boldsymbol{x}_i, -\boldsymbol{\beta}_s) = 1 - \pi_{iz_s,\text{rvm}}(\boldsymbol{x}_i, \boldsymbol{\beta}_s)$ for all s.

6 Example results

Constructed under the paSB framework, a multinomial regression model of S categories is characterized by not only how the S stick-specific binary classifiers with cross entropy loss parameterize their covariate-dependent probability parameters, but also how its S categories are one-to-one mapped to S latent sticks. To investigate the unique properties of a paSB multinomial regression model, we will study the benefits of both inferring an appropriate one-to-one mapping between the category labels and stick indices and increasing the modeling capacity of the underlying binary regression model.

For illustration purpose, we will focus on multinomial softplus regression (MSR) that extends a binary softplus regression model under paSB. A binary softplus regression model can adjust its two parameters—the number of experts K and the number of layers per expert T—to control its capability in modeling nonlinear binary classification decision boundaries. More specifically, as described in detail in Zhou [2016], when $K = T = 1$, softplus regression is related to logistic regression in using a single hyperplane in the covariate space to separate one class from the other; when $K > 1$ and $T = 1$, it generalizes logistic regression in using the interaction of up to K hyperplanes to enclose negatively labeled observations; when $K = 1$ and $T > 1$, it uses the interaction of up to T hyperplanes to enclose positively labeled observations; and when $K > 1$ and $T > 1$, it uses the union of convex-polytope-like confined spaces to enclose positively labeled observations.

6.1 Influence of binary regression model capacity

We first consider the Iris data set with $S = 3$ categories. We choose the sepal and petal lengths as the two dimensional covariates to illustrate the performance of MSR under four different settings, where we fix $\boldsymbol{z} = (1, 2, 3)$, which means category s is mapped to stick s for all s, but choose different model capacities by varying K and T.

Examining the relative 2D spatial locations of the observations, where the blue, black, and gray points are labeled as category 1, 2, and 3, respectively, one can imagine that setting $\boldsymbol{z} = (2, 1, 3)$, which means mappings categories 2, 1, and 3 to the 1st, 2nd, and 3rd sticks, respectively, will already lead to excellent class separations for MSR with $K = T = 1$, according to the analysis in Section 4.2 and also confirmed by our experimental results (not shown for brevity). More specifically, with the 2nd, 1st, and 3rd categories mapped to the 1st, 2nd, and 3rd sticks, respectively, one can first use a single hyperplane to separate category 2 (black points) from both categories 1 (blue points) and 3 (gray points), and then use another hyperplane to separate category 1 (blue points) from category 3 (gray points).

However, when the mapping is fixed at $\boldsymbol{z} = (1, 2, 3)$, as shown in the first row of Figure 1, MSR with $K = T = 1$ performs poorly and fails to separate out category 1 (blue points) right in the beginning. This is not surprising since MSR with $K = T = 1$ is only equipped with a single hyperplane to separate the category that the first stick is mapped to (category $z_1 = 1$ in this case) from the others, whereas for this dataset it is apparent at least two hyperplanes are required to separate the blue points from the black and gray ones. MSR with $K = 5$ and $T = 1$ also fails to work with $\boldsymbol{z} = (1, 2, 3)$, as shown in the third row of Figure 1, which is also not surprising since it can only use the complementary of a convex-polytope-bound confined space to enclose category $z_1 = 1$, but it is apparent that the blue points can not be enclosed in this manner. Despite purposely enforcing an unfavorable category-stick mapping, once we increase T, the performance quickly improves, which is expected since $T > 1$ allows using a single (if $K = 1$) or a union (if $K > 1$) of convex-polytope-like confined spaces to separate one category from the others (by enclosing the positively labeled observations in

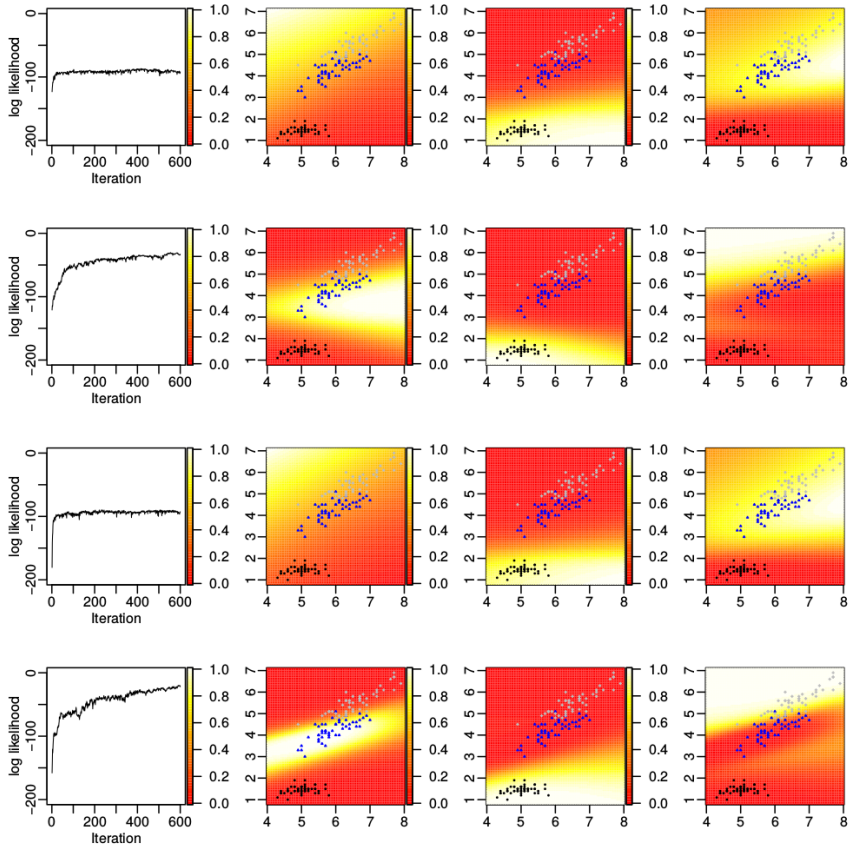


Figure 1: Log likelihood and predictive probability heat map for 2-D iris data with a fixed $\boldsymbol{z} = (1, 2, 3)$. Blue points are labeled as category 1, black 2 and gray 3. For row 1, $K = 1$, $T = 1$, row 2 $K = 1$, $T = 3$, row 3 $K = 5$, $T = 1$, and row 4 $K = 5$, $T = 3$. Column 1 shows the trace plots of log likelihood with the corresponding K and T. Column 2 to 4 show the predictive probability heat maps of category 1 (blue), 2 (black) and 3 (gray), respectively.

each stick-specific binary classification task).

The results in Figure 1 show that even an unoptimized category-stick mapping, which is unfavorable to MSR with small K and/or T, is enforced, empowering each stick-specific binary regression model with a higher capacity (using larger K and/or T) can still allow MSR to achieve excellent separations between different categories. It is also simple to show that for the data set in Figure 1, even if one chooses low-capacity stick-specific binary regression models by setting $T = 1$, one can still achieve good performance with MSR if the category-stick mapping is set as $\boldsymbol{z} = (2, 1, 3)$, $\boldsymbol{z} = (3, 1, 2)$, $\boldsymbol{z} = (2, 3, 1)$, or $\boldsymbol{z} = (3, 2, 1)$. That is to say, as long as it is not category 1 (blue points) that is mapped to stick 1, MSR with $T = 1$ is able to provide satisfactory performance. But when it is, one can increase T to increase the

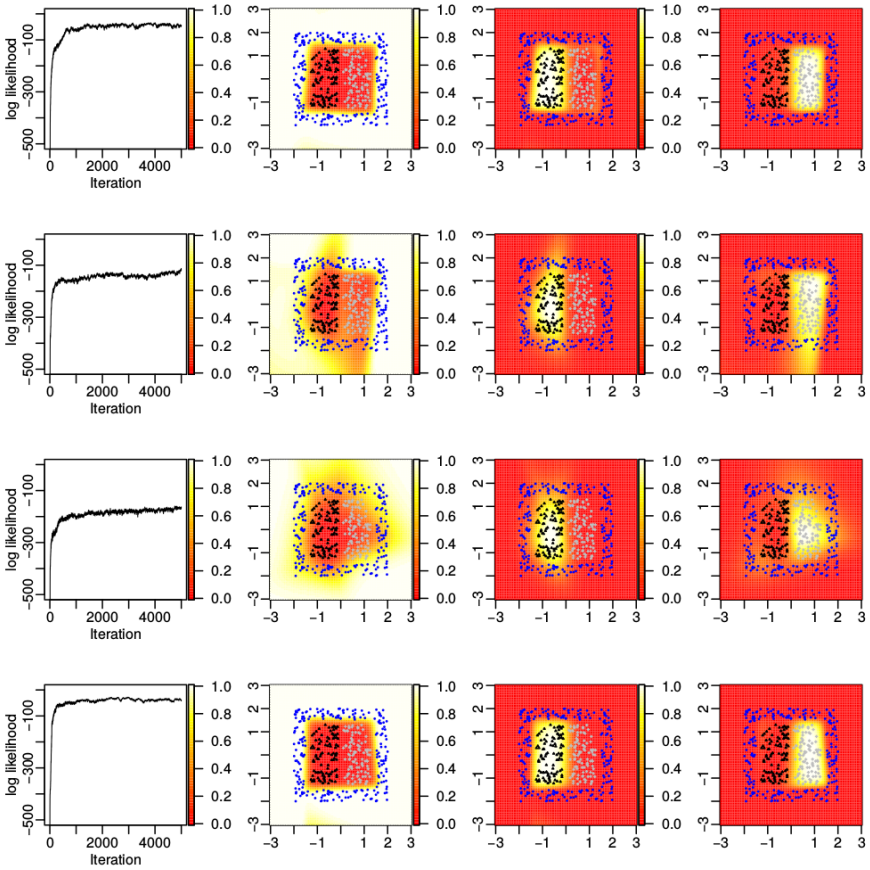


Figure 2: Log likelihoods and predictive probability heat maps for the square data with $K = T = 10$. Blue points are labeled as category 1, black 2 and gray 3. Fix $\boldsymbol{z} = (1, 2, 3)$ for row 1, $(2, 1, 3)$ for row 2, and $(3, 1, 2)$ for row 3. For row 4, we sample $\boldsymbol{z}$ within MCMC iterations. Column 1 shows the log-likelihood trace plots with the corresponding $\boldsymbol{z}$'s. Column 2 to 4 show the predictive probability heat maps of class 1 (blue), 2 (black) and 3 (gray), respectively.

capacity of each stick-specific binary regression model and hence that of MSR to mitigate the restrictions imposed by mapping category 1 to stick 1.

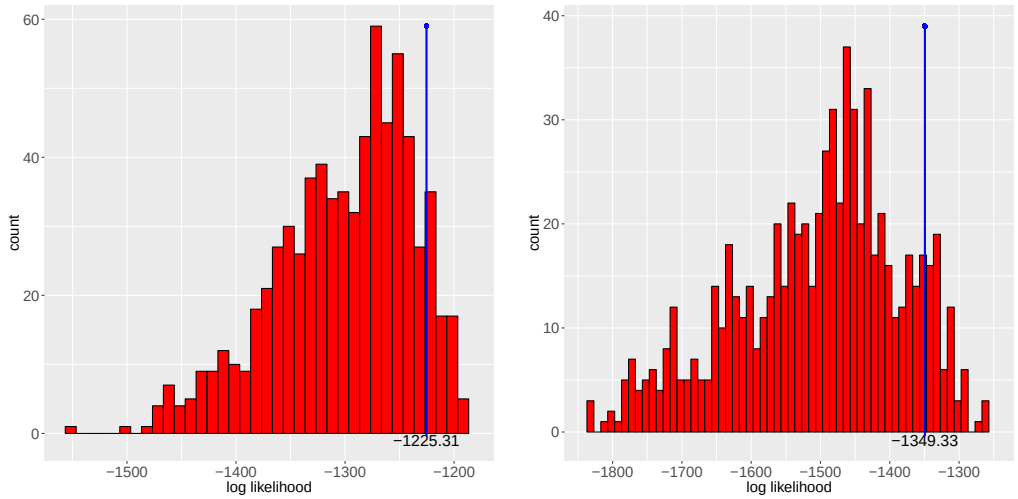
6.2 Influence of category-stick mapping and its inference

The Iris data set in Figure 1 provides an instructive example to show not only the importance of increasing the model capacity if a poor category-stick mapping is imposed, but also the importance of optimizing the category-stick mapping if the capacities of these stick-specific binary regression models are limited. To further illustrate the benefits of inferring an appropriate category-stick mapping $\boldsymbol{z}$, we consider the "square" data set shown in Figure 2. We show that for MSR, even both K and T are sufficiently large to allow each stick-specific

binary regression model to have a high enough capacity, whether an optimal category-stick mapping is selected may still clearly matter for the performance. As shown in the first three rows of Figure 2, three different $\boldsymbol{z}$'s are considered and $\boldsymbol{z} = (1, 2, 3)$ (shown in the first row) is found to perform the best. As shown in the fourth row, we sample $\boldsymbol{z}$ using (12) within each MCMC iteration and achieve a result that seems as good as fixing $\boldsymbol{z} = (1, 2, 3)$. In fact, we find that our inferred mappings switch between $\boldsymbol{z} = (1, 2, 3)$ and $\boldsymbol{z} = (1, 3, 2)$ during MCMC iterations, indicating that the Markov chain is mixing well. These results suggest the importance of both learning the mapping $\boldsymbol{z}$ from the data and allowing the stick-specific binary classifiers to have enough capacities to model nonlinear classification decision boundaries.

When sampling $\boldsymbol{z} = (z_1, \ldots, z_S)$ that the S categories are mapped to, although $S!$ permutations of $(1, \ldots, S)$ can become enormous as S increases, the effective search space could be much smaller if many different mappings imply similar likelihoods and if a few extremely poor mappings can be easily avoided. Rather than searching for the best mapping, the proposed MH step, proposing two indices z_j and $z_{j'}$ to switch in each iteration, is a simple but effective strategy to escape from the mappings that lead to poor fittings. Note that the probability of a z_j not being proposed to switch after t MCMC iterations is $[(S-2)/S]^t$. Even if S is as large as 100, that probability is less than 10^{-8} at $t = 1000$. Also note that $S/2$ is the expected number of iterations after which a z_j is proposed to switch at least once.

Figure 3 empirically demonstrates the effectiveness of permuting $\boldsymbol{z}$ on the satimage dataset, using MSRs with $K = 5$, $T = 3$, and $\boldsymbol{z}$ fixed at each of the $6! = 720$ possible one-to-one category-stick mappings. Each log likelihood is averaged over those of the corresponding model's collected MCMC samples. Panels (a) and (b) show the log-likelihood histograms for MSRs constructed under augmented SB (aSB) and augmented reversed SB (arSB), respectively. Both histograms are clearly left skewed, indicating under both aSB and arSB, only a small proportion of the 720 different category-stick mappings lead to very poor fittings. The blue vertical lines at -1203.82 in (a) and -1350.21 in (b) are the log likelihoods for paSB and parSB, respectively, in both of which the category-stick mapping



(a) aSB (b) arSB

Figure 3: Log-likelihood histograms for MSRs using all 720 possible category-stick mappings, constructed under (a) augmented stick breaking (aSB) and (b) augmented and reversed stick breaking (arSB). The blue lines in (a) and (b) correspond to the log likelihoods of paSB-MSR and parSB-MSR, respectively.

$\boldsymbol{z}$ is updated by a MH step in each MCMC iteration. Only 20 (97) out of 720 aSB-MSRs (arSB-MSRs) have a higher likelihood than paSB-MSR (parSB-MSR).

Since in the stick-breaking construction, the binary classifier that separates a category mapped to a smaller-indexed stick from the others utilizes fewer constraints, the classification can be poor if the complexity of the decision boundary goes beyond the nonlinear modeling capacity of the binary classifier. However, even with a low-capacity binary classifier, the performance could be significantly improved if that difficult-to-separate category is mapped to a larger-indexed stick, for which there are fewer categories left to be separated in its "one-vs-remaining" binary classification problem. Examining the $\boldsymbol{z}$'s associated with the 100 lowest log likelihoods in Figure 3, we find there are 51 mappings belonging to the set $\{\boldsymbol{z} : z_5 = 1 \text{ or } z_6 = 1\}$ in aSB, and 77 belonging to $\{\boldsymbol{z} : z_3 = 1 \text{ or } z_6 = 1\}$ in arSB, which suggests that separating Categories 5 or 6 (Categories 3 or 6) from all the other categories might be beyond the capacity of a binary softplus regression with $K = 5$, $T = 3$ under the aSB (arSB) construction. But if breaking the sticks associated with these categories at late stages, we only need to separate them from fewer remaining categories, which could be much

easier. We have further examined the other 620 arrangements, and found no evident patterns. These observations suggest that the effective search space of the mapping $\boldsymbol{z}$ is considerably smaller than $S!$, and the proposed MH step is effective in escaping poor mappings.

In paSB-MSVM, we use a Gaussian radial basis function kernel, whose kernel width is cross validated from a set of predefined candidates. We find its performance to be sensitive to the setting of the kernel width, which is a common issue for conventional SVMs [Cherkassky and Ma, 2004, Soares et al., 2004, Chang et al., 2005]. If an appropriate kernel width could be identified through cross validation, we find that learning the mapping $\boldsymbol{z}$ becomes less important for paSB-MSVM to perform well. However, if the kernel width is not well selected, which can happen if all candidate kernel widths are far from the optimal value, the binary classifier for each category may not have enough capacity for nonlinear classification and the learning of the category-stick mapping $\boldsymbol{z}$ is found to be important.

6.3 Turning off unneeded model capacities

While one can adjust both K and T to control the capacity of binary softplus regression, for MSR, the total number of experts K is a truncation level that can be set as large as permitted by the computation budget. This is because the truncated gamma process used by each stick-specific binary softplus regression shrinks the weights of unnecessary experts towards zeros. Figure 4 shows in decreasing order the inferred weights of the experts belonging to each of the 3 categories of the square dataset. These weights are inferred by MSR with $K = T = 10$ and the learning of $\boldsymbol{z}$, as in the fourth row of Figure 2. It is clear from Figure 4 that only a small number of experts are inferred with non-negligible weights in the posterior, and the number of active experts and their weights clearly indicate the complexity of the corresponding classification decision boundaries shown in the fourth row of Figure 2. We note that while T is a parameter to be set by the user, we find increasing it increases model capacity, without observing clear signs of overfitting for all the data considered here.

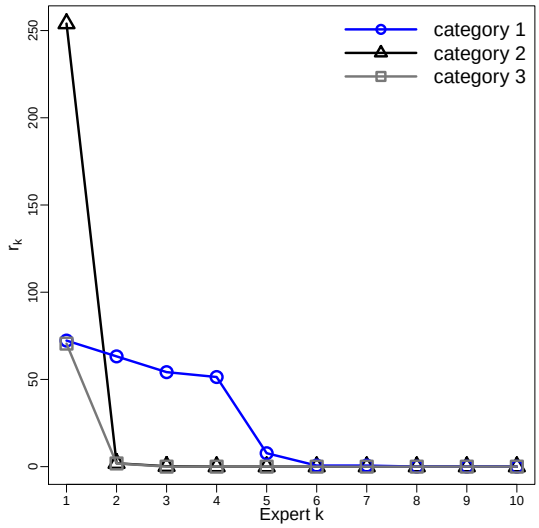


Figure 4: Inferred expert weights r_k in descending order for each category of the square data with $K = T = 10$.

6.4 Results on benchmark data sets

To further evaluate the performance of the proposed paSB multinomial regression models, we consider paSB multinomial logistic regression (paSB-MLR), MSRs, and paSB multinomial support vector machine (paSB-MSVM). We compare their performance with those of L_2 regularized multinomial logistic regression (L_2-MLR), support vector machine (SVM), and adaptive multi-hyperplane machine (AMM), and consider the following benchmark multi-class classification datasets: iris, wine, glass, vehicle, waveform, segment, vowel, dna and satimage. We also include the synthetic square data shown in Figure 2 for comparison. We consider MSRs with (K, T) as $(1, 1)$, $(1, 3)$, $(5, 1)$ and $(5, 3)$, respectively. We provide detailed descriptions on the data and experimental settings in the Appendix.

We summarize in Table 1 the classification error rates of various models, where those of MSRs are calculated by averaging over both paSB and parSB. Setting SVM as a benchmark, we normalize to 1 the SVM's average error rate. The bottom row of Table 1 presents the average normalized error rates (ANER) of all the models with SVM as a normalization baseline. It is clear from Table 1 that an MSR whose K or T is sufficiently large generally outperforms paSB-MLR, L_2-MLR, and AMM, and increasing K and T can in general further

Table 1: Comparison of the classification error rates (%) of paSB-MLR, paSB-MSVM, MSRs with various K and T (results column 3 to 6), L_2-MLR, SVM, and AMM.

	paSB-MLR	paSB-MSVM	$K=1$ $T=1$	$K=1$ $T=3$	$K=5$ $T=1$	$K=5$ $T=3$	L_2-MLR	SVM	AMM
square	59.52	0	57.14	15.08	0	0	53.17	4.76	16.67
iris	4.00	3.33	4.67	4.00	4.00	4.00	3.33	4.00	4.67
wine	4.44	2.78	2.78	2.22	2.78	2.22	3.89	2.78	3.89
glass	35.35	29.30	33.49	26.05	31.16	32.09	35.81	28.84	37.67
vehicle	23.23	17.32	22.44	17.32	17.72	15.75	22.44	14.17	21.89
waveform	17.87	15.76	19.84	16.62	15.67	15.04	15.80	15.02	18.54
segment	7.36	7.98	6.20	6.49	6.45	5.63	9.04	5.77	12.47
vowel	59.31	36.36	50.22	48.70	45.24	46.32	58.87	37.23	52.47
dna	5.06	5.31	4.13	4.47	4.55	4.22	5.23	4.55	5.43
satimage	20.65	8.90	16.65	14.45	12.85	12.00	17.95	8.50	15.31
ANER	2.56	0.97	2.35	1.33	1.02	0.96	2.37	1	1.67

reduce its error rate. This is especially evident when there are classes in a dataset that are not linearly separable, as indicated by a clearly higher error rate of L_2-MLR in comparison to that of SVM. One may notice that paSB-MLR and MSR with $K = T = 1$ have similar performance, which is expected as MSR with $K = T = 1$ is constructed under the same paSB framework, by extending a linear binary classifier that is slightly more general than logistic regression into a multinomial one. Also noticed is that both classifiers' performance are similar to L_2-MLR, suggesting the effectiveness of the proposed strategy to infer a one-to-one label-stick mapping, which helps mitigate the potential adverse effects of having asymmetric class labels. Comparable error rates to SVM on these benchmark datasets, delivered by both paSB-MSVM and MSRs with large enough capacities, further indicate the success of the paSB framework in transforming a binary classifier with cross entropy loss into a Bayesian multinomial one.

To further check whether a paSB model is attractive when fast out-of-sample prediction is desired, we consider using only the MCMC sample that has the highest likelihood among the collected ones for all paSB models, and summarize in Table 3 of the Appendix the classification error rates of various models, with the number of inferred support vectors or active hyperplanes included in parenthesis. Following the definition of active experts in Zhou [2016], we define for MSRs the number of active hyperplanes as $T\sum_s^S \widetilde{K}_s$ where $\widetilde{K}_s$ is

the number of active experts for class s. The number of active hyperplanes determines the computational complexity for out-of-sample prediction with a single MCMC sample, which is $O(T\sum_s^S \widetilde{K}_s)$. Since the error rates of MSRs in Table 3 are calculated by averaging over both paSB and parSB, the number of active hyperplanes is $T\sum_s^S(\widetilde{K}_s^{(paSB)} + \widetilde{K}_s^{(parSB)})$.

Shown in Figure 5 in the Appendix are boxplots of the number of each category's active experts for MSR with $K = 5$ and $T = 3$. It is clear that except for several categories of satimage that require all $K = 5$ experts for parSB-MSR, $K = 5$ is large enough to provided the needed model capacity under all the other scenarios. The bottom two rows of Tabel 3 present the average normalized error rate (ANER) and average normalized number of hyperplanes (ANH) of all the models (active hyperplanes for MSRs and support vectors for SVM and paSB-MSVM), with SVM as a normalization baseline. As shown in Table 3, MSRs with sufficiently large K and/or T are comparable to both SVM and paSB-SVM in terms of the error rates, while clearly outperforming them in terms of the number of (active) hyperplanes and hence computational complexity for out-of-sample predictions. While MSR with $K = T = 1$ and paSB-MLR generally perform worse than SVM in terms of the error rates, they use much fewer hyperplanes and hence have significantly lower computation for out-of-sample predictions. In summary, MSR whose upbound for the number of active expects K and number of layers for each expert T can both be adjusted to control its capacity of modeling nonlinearity, can achieve a good compromise between the accuracy and computational complexity for out-of-sample prediction of multinomial class probabilities.

7 Conclusions

To transform a cross-entropy-loss binary classifier into a Bayesian multinomial regression model and derive efficient Bayesian inference, we develop a novel permuted and augmented stick-breaking (paSB) construction. Inferring a one-to-one mapping between the category labels and stick indices, paSB links a category random variable y_i to latent stick-specific Bernoulli random variables $\{b_{is}\}_{1,S}$, which are conditionally independent given their covariate-

dependent probability parameters $\{\pi_{is}\}_{1,S}$, where π_{is} is linked to the regression coefficients of the category that is mapped to stick s. We consider transforming a binary softplus regression model to a multinomial one by parameterizing each covariate-dependent π_{is} with a potentially countably infinite number of regression coefficient vectors, only a small finite subset of which are often inferred to have non-negligible weights in the posterior. We also consider transforming a Bayesian binary SVM to a multinomial one under the paSB framework, relying on the kernel trick to model nonlinearity. We develop a Gibbs sampling algorithm with closed-form update equations, using novel data augmentation and marginalization techniques, as well as an efficient Metropolis-Hastings step, which allows two labels to switch their corresponding sticks in each MCMC iteration, to sample the one-to-one category-stick mapping. We illustrate instructive model properties with synthetic data and demonstrate promising performance on standard benchmark datasets for multi-class classification.

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Permuted and Augmented Stick-Breaking Bayesian Multinomial Softplus Regression: Appendix

A Additional Lemma and Proofs

Proof of Theorem 1. The conditional probability of y_i given $\{z_s, \pi_{is}\}_{1,S}$ can be expressed as

$$\begin{aligned} P(y_i = s \,|\, \{z_s, \pi_{is}\}_{1,S}) &= \textstyle\sum_{b_{ij}:j>z_s} \left[P(b_{iz_s}=1)\right]^{\mathbf{1}(z_s \neq S)} \left[\prod_{j<z_s} P(b_{ij}=0)\right] \left[\prod_{j>z_s} P(b_{ij})\right] \\ &= \left[P(b_{iz_s}=1)\right]^{\mathbf{1}(z_s \neq S)} \left[\prod_{j<z_s} P(b_{ij}=0)\right] \textstyle\sum_{b_{ij}:j>z_s} \left[\prod_{j>z_s} P(b_{ij})\right], \end{aligned}$$

which becomes the same as (4) by applying (6) and $\sum_{b_{ij}:j>z_s}\left[\prod_{j>z_s} P(b_{ij})\right]=1$. □

Proof of Lemma 3. Under the paSB construction, the probability ratio of categories (choices) s and $s+d$ is a function of the stick success probabilities $\pi_{z_s}, \pi_{z_{(s+1)}}, \cdots, \pi_{z_{(s+d)}}$. More specifically,

$$\frac{p_{i(s+d)}(\boldsymbol{z})}{p_{is}(\boldsymbol{z})} = \frac{\pi_{iz_{(s+d)}}^{\mathbf{1}(z_{(s+d)} \neq S)} \left[\prod_{z_s \leq j < z_{(s+d)}} (1-\pi_{ij})\right]^{\delta(z_s \leq z_{(s+d)})}}{\pi_{iz_s}^{\mathbf{1}(z_s \neq S)} \left[\prod_{z_{(s+d)} \leq j < z_s} (1-\pi_{ij})\right]^{\delta(z_s > z_{(s+d)})}}. \tag{23}$$

□

Proof of Lemma 4. Since $p_{is}(\boldsymbol{z}) = \left[1 - \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_s}\right)^{-r_s}\right]^{\mathbf{1}(s \neq S)} \prod_{j<s} \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_j}\right)^{-r_j}$ when $K = T = 1$ and $\boldsymbol{z} = (1, \ldots, S)$, the set of solutions to $p_{is} > p_0$ are bounded by the set of solutions to $\left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_j}\right)^{-r_s} > p_0,\ j \in \{1, \ldots, s-1\}$, and $1 - \left(1+e^{\boldsymbol{x}_i'\boldsymbol{\beta}_s}\right)^{-r_s} > p_0$, and hence bounded by the convex polytope defined by the set of solutions to the s inequalities as

$$\boldsymbol{x}_i'[(-1)^{\mathbf{1}(j=s)}\boldsymbol{\beta}_j] < (-1)^{\mathbf{1}(j=s)} \ln\left\{\left[p_0^{\mathbf{1}(j\neq s)}(1-p_0)^{\mathbf{1}(j=s)}\right]^{-\frac{1}{r_j}} - 1\right\}, \quad j \in \{1, \ldots, s\}. \tag{24}$$

□

Lemma 5. *Without loss of generality, let us assume that the category-stick mapping is fixed at* $\boldsymbol{z} = (1, 2, \cdots, S)$. *The paSB multinomial logistic model that assigns choice* $s \in \{1, \ldots, S\}$

for individual i with probability $p_{is} = (\pi_{is})^{\mathbf{1}(s \neq S)} \prod_{j<s}(1-\pi_{ij})$, where $\pi_{is} = 1/(1+e^{-W_{is}})$, can be considered as a sequential random utility maximization model. This model selects choice s once $U_{is} > \sum_{j \geq s} U_{ij}$ is observed for $s = 1, \ldots, S$, where U_{is} are defined as

$$
\begin{aligned}
U_{i1} &= U_{i2} + \cdots + U_{iS} + W_{i1} + \varepsilon_{i1}, \\
&\cdots \\
U_{is} &= \sum_{j>s} U_{ij} + W_{is} + \varepsilon_{is}, \\
&\cdots \\
U_{i(S-1)} &= W_{i(S-1)} + \varepsilon_{i(S-1)}, \\
U_{iS} &= 0,
\end{aligned}
$$

and $\varepsilon_{is} \overset{i.i.d.}{\sim} \text{Logistic}(0,1)$ are independent, and identically distributed (i.i.d.) random variables following the standard logistic distribution.

Proof of Lemma 5. Note that $P(\varepsilon < x) = 1/(1+e^{-x})$ if $\varepsilon \sim \text{Logistic}(0,1)$. First consider the choice of individual i be $y_i = 1$, which would happen with probability

$$
P(y_i = 1) = P\left(U_{i1} > \sum\nolimits_{j \geq 1} U_{ij}\right) = P(\varepsilon_{i1} > -W_{i1}) = 1/(1+e^{-W_{i1}}) = \pi_{i1} = p_{i1}.
$$

Then for $s = 2, \cdots, S-1$,

$$
\begin{aligned}
P(y_i = s) &= P(y_i = s \,|\, y_i > s-1) P(y_i > s-1) \\
&= P\left(U_{is} > \sum\nolimits_{j>s} U_{ij}\right) \prod\nolimits_{j \leq s-1} P\left(U_{ij} < \sum\nolimits_{j'>j} U_{ij'}\right) \\
&= P(\varepsilon_{is} > -W_{is}) \prod\nolimits_{j \leq s-1} P(\varepsilon_{ij} < -W_{ij}) \\
&= \pi_{is} \prod\nolimits_{j \leq s-1} (1-\pi_{ij}) \\
&= p_{is}.
\end{aligned}
$$

Finally, $P(y_i = S) = 1 - \sum_{j<S} P(y_i = j) = \prod_{j<S}(1 - \pi_{ij}) = p_{iS}$. □

B Experimental settings and additional results

The table below summarizes the size of training and testing sets, and the number of covariates and classes. The training and testing sets are predefined for vehicle, vowel, dna and satimage. Note that the training set and the validation set were combined as training. We divide the other datasets into training and testing as follows. For iris, wine, and glass, five random partitions are taken such that for each partition the training set accounted for 80% of the whole dataset while the testing set 20%. The classification error rate is calculated by averaging the error rates of all five random partitions. For square, waveform, and segment, only one random partition is taken, where 70% of the square dataset are used as training and the remaining 30% as testing, and 10% of both the waveform and segment datas are used as training and the remaining 90% as testing.

Table 2: Multiclass datasets used in experiments for model comparison.

	square	iris	wine	glass	vehicle	waveform	segment	vowel	dna	satimage
Train size	294	120	142	171	592	500	231	528	2000	4435
Test size	126	30	36	43	254	4500	2079	462	1186	2000
Covariate	2	4	13	9	18	21	19	10	180	36
Class	3	3	3	6	4	3	7	11	3	6

We compare paSB-MLR, paSB-MSVM, and MSR with three other models, including L_2 regularized multinomial logistic regression (L_2-MLR), support vector machine (SVM), and adaptive multi-hyperplane machine (AMM). For paSB-MSVM, we use the spike-and-slab prior to select the kernel bases and set 0.5 the probability of spike at 0, which is referred to as a uniform prior by Polson et al. [2011]. A Gaussian radial basis function (RBF) kernel is used and the kernel width is selected by 3-fold cross validation from $(2^{-10}, 2^{-9}, \ldots, 2^{10})$. We run 1000 MCMC iterations and discard the first 500 as burn-in samples. For MSR, we try both paSB and parSB with (K, T) set as $(1, 1)$, $(1, 3)$, $(5, 1)$, or $(5, 3)$. We run 10000 MCMC iterations and discard the first 5000 as burn-in samples. The predictive probability

is calculated by averaging the Monte Carlo average predictive probabilities from paSB and parSB MSRs. An observation in the testing set is classified to the category associated with the largest predictive probability.

We use the L_2-MLR provided by the LIBLINEAR package of Fan et al. [2008] to train a linear classifier, where a bias term is included and the regularization parameter C is five-fold cross-validated on the training set from $(2^{-10}, 2^{-9}, \ldots, 2^{15})$. We also classify an observation to the category associated with the largest predictive probability. For SVM and paSB-MSVM, a Gaussian RBF kernel is used and three-fold cross validation is adopted to tune both the regularization parameter C and kernel width γ on training sets. We use the LIBSVM package [Chang and Lin, 2011] to three-fold cross-validate C and γ from $(2^{-10}, 2^{-9}, \ldots, 2^{10})$, and choose the default settings for all the other parameters.

We consider adaptive multi-hyperplane machine (AMM) of Wang et al. [2011b], as implemented in the BudgetSVM[1] (Version 1.1) software package Djuric et al. [2013]. We use the batch version of the algorithm. Important parameters of the AMM include both the regularization parameter ν and training epochs E. As also mentioned by Kantchelian et al. [2014], we do not observe the testing errors of AMM to strictly decrease as E increased. Thus, in addition to cross validating the regularization parameter ν on the training set from $\{10^{-7}, 10^{-6}, \ldots, 10^{-2}\}$, as done in Wang et al. [2011b], for each ν, we tried $E \in \{5, 10, 20, 50, 100\}$ sequentially until the cross-validation error begins to decrease, *i.e.*, under the same ν, we choose $E = 20$ if the cross-validation error of $E = 50$ is greater than that of $E = 20$. We use the default settings for all the other parameters, and calculate average classification error rates.

[1] `http://www.dabi.temple.edu/budgetedsvm/`

Table 3: Comparison of classification error rates (%) of paSB-MLR, paSB-MSVM, MSRs with various K and T (results column 3 to 6), L_2-MLR, SVM, and AMM, using the collected MCMC sample with the highest log likelihood. The number of active hyperplanes/support vectors used for out-of-sample predictions are shown in parenthesis.

	paSB-MLR	paSB-MSVM	$K=1$ $T=1$	$K=1$ $T=3$	$K=5$ $T=1$	$K=5$ $T=3$	L_2-MLR	SVM	AMM
square	53.17(2)	0(256)	57.14(4)	13.49(12)	1.59(10)	0.79(33)	53.17(2)	4.76(22)	16.67(7)
iris	2(2)	3.33(97.6)	4.67(4)	4.67(12)	4(5.4)	3.33(12)	3.33(2)	4(35)	4.67(8.6)
wine	8.33(2)	2.14(125.8)	4.45(4)	4.45(12)	6.67(4)	3.34(12)	3.89(2)	2.78(77.2)	3.89(7.8)
glass	39.07(5)	30.23(137.6)	35.35(10)	30.7(30)	33.02(10.4)	35.81(33.2)	35.81(5)	28.84(118)	37.67(23.8)
vehicle	25.98(3)	17.71(592)	23.62(6)	21.65(18)	18.9(12)	16.93(33)	22.44(3)	14.17(259)	21.89(17)
waveform	18.78(2)	16.56(500)	19.73(4)	17.11(12)	17.07(6)	17.11(18)	15.8(2)	15.02(210)	18.54(11.6)
segment	7.07(6)	9.86(231)	8.61(12)	8.37(36)	7.31(13)	7.79(36)	9.04(6)	5.77(87)	12.47(11.4)
vowel	61.69(10)	44.37(528)	51.73(20)	50(60)	48.05(36)	51.73(114)	58.87(10)	37.23(349)	52.47(26.6)
dna	6.58(2)	7.25(1701)	5.56(4)	5.73(12)	6.07(7)	5.82(12)	5.23(2)	4.55(1274)	5.43(18.6)
satimage	21.35(5)	9.5(4315)	15.8(10)	14.7(30)	13.25(34)	11.95(102)	17.95(5)	8.5(1652)	15.31(16.8)
ANER	2.59	1.06	2.49	1.51	1.28	1.12	2.37	1	1.67
ANH	0.03	3.00	0.07	0.20	0.11	0.33	0.03	1	0.12

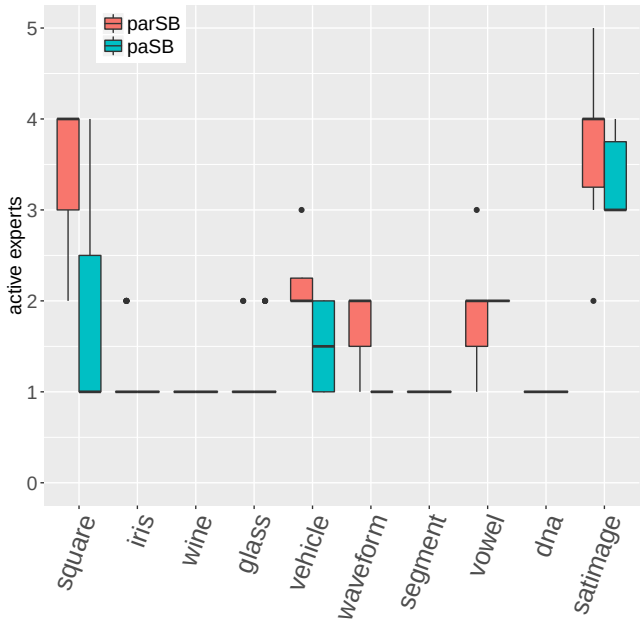

Figure 5: Boxplots of the number of active experts used by paSB/parSB MSRs.