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# FAIR BAYESIAN MODEL-BASED CLUSTERING

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## ABSTRACT

Fair clustering has become a socially significant task with the advancement of machine learning and the growing demand for trustworthy AI. Group fairness ensures that the proportions of each sensitive group are similar in all clusters. Most existing fair clustering methods are based on the  $K$ -means clustering and thus require the distance between instances and the number of clusters to be given in advance. To resolve this limitation, we propose a fair Bayesian model-based clustering called Fair Bayesian Clustering (FBC). We develop a specially designed prior which puts its mass only on fair clusters, and implement an efficient MCMC algorithm. The main advantage of FBC is its flexibility in the sense that it can infer the number of clusters, can process data where the choice of a reasonable distance is difficult (e.g., categorical data), and can reflect a constraint on the sizes of each cluster. We illustrate these advantages by analyzing real-world datasets.

## 1 INTRODUCTION

With the rapid development of machine learning-based technologies, algorithmic fairness has been considered as an important social consideration when making machine learning-based decisions. Among diverse tasks combined with algorithmic fairness, fair clustering (Chierichetti et al., 2017) has received much interest, which ensures that clusters maintain demographic fairness across sensitive attributes such as gender or race. However, most of existing fair clustering methods can be seen as modifications of  $K$ -means clustering algorithms, and thus they require (i) the number of clusters to be fixed and (ii) the distance between two instances given a priori, limiting their adaptability to various kinds of real-world datasets, where the optimal number of clusters is unknown and/or it is hard to define a reasonable distance (e.g., categorical data).

Among standard (fairness-agnostic) clustering approaches, various Bayesian models that can infer the number of clusters have been proposed including mixture models with unknown components (Richardson & Green, 1997; Nobile & Fearnside, 2007; McCullagh & Yang, 2008; Miller & Harrison, 2018) and mixture of Dirichlet process models (Ferguson, 1973; Antoniak, 1974; Escobar & West, 1995; Neal, 2000). For fair Bayesian mixture models, we first modify the standard Bayesian mixture model so that a prior concentrates on fair mixture models (called the fair prior) and so does the posterior distribution. In general, however, computation of the posterior on a constraint parameter space would be computationally demanding and frequently infeasible if the constraint is not designed carefully (Brubaker et al., 2012; Sen et al., 2018; Duan et al., 2020).

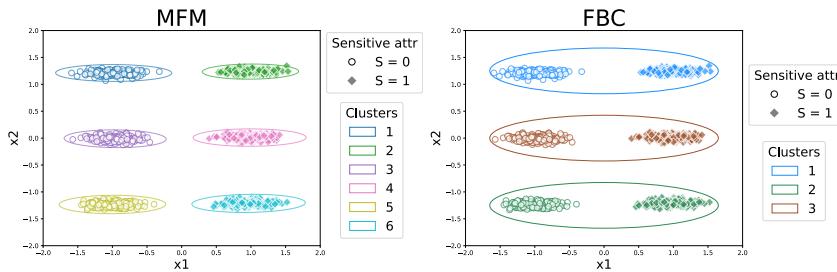
To address such limitations of existing fair clustering methods and to leverage the flexibility of Bayesian model-based approaches, we aim to develop a fair clustering algorithm based on a Bayesian framework. In Bayesian frameworks, the goal is to explore high-posterior regions of the parameter space. In the context of fair clustering, however, the posterior should be explored only within the fair region. In turn, this requires that the prior mass to be concentrated on the fair space, rather than on the entire unconstrained space. Motivated by this, we develop a fair prior based on the idea of matching instances from different sensitive groups, which has already been successfully implemented for fair supervised learning (Kim et al., 2025a) and non-Bayesian fair clustering (Chierichetti et al., 2017; Kim et al., 2025b), but this is the first attempt for Bayesian fair clustering. An important advantage is that our proposed fair prior does not involve any explicit constraint on the parameters and thus posterior approximation by an MCMC algorithm can be done without much difficulty. Our matching-based formulation in Section 2 is, to our knowledge, the first to explicitly construct such a prior restricted to the fair space.

054 A further benefit of our proposed algorithm is that it can be applied to both cases when the number  
 055 of clusters is known (fixed) and unknown. To infer the unknown number of clusters, we treat the  
 056 number of clusters as a parameter to be inferred. Specifically, we propose a fair Bayesian mixture  
 057 model and develop an MCMC algorithm to approximate the posterior distribution of the number  
 058 of clusters as well as the cluster centers and cluster assignments. Figure 1 presents an example  
 059 where the choice of the number of clusters under the fairness constraint a priori would be difficult  
 060 in practice.

061 Beyond the inference of the number of clusters, our proposed algorithm has further benefits: (i) it  
 062 can be applied to various data types, since it is a model-based clustering method, and (ii) it can  
 063 perform clustering under the constraint that the cluster sizes must be upper-bounded, since it is a  
 064 Bayesian clustering.

065 Our main contributions are summarized as follows:

- 067 ◊ We propose a definition of the fair mixture model and develop a novel MCMC algorithm  
 068 to approximate the posterior distribution of fair mixture models, called Fair Bayesian Clus-  
 069 tering (FBC).
- 070 ◊ Experimentally, we show that FBC (i) is competitive to existing non-Bayesian fair cluster-  
 071 ing methods when the number of clusters is given, (ii) can infer a proper number of clusters  
 072 well when the number of clusters is unknown, (iii) can use both continuous and categorical  
 073 data, and (iv) can infer fair clusters under certain constraints on the sizes of each cluster.



083 Figure 1: Toy example comparing two Bayesian clustering methods with and without consider-  
 084 ing fairness. MFM (Mixture of Finite Mixtures (Miller & Harrison, 2018)) is a standard Bayesian  
 085 method that infers  $K$ . Data are synthetically generated from the 6-component Gaussian mixture  
 086 dataset (see Section E.1 for details), and MFM infers  $K = 6$ , whereas the optimal number of clusters  
 087 obtained by FBC is  $K = 3$ . This example indicates that the choice of  $K$  by use of fairness-agnostic  
 088 clustering algorithms would be misleading for fair clustering.

## 090 1.1 RELATED WORKS

092 **Fair clustering** Given a pre-specified sensitive attribute (e.g., gender or race), the concept of fair  
 093 clustering is first introduced by Chierichetti et al. (2017), with the aim of ensuring that the proportion  
 094 of each sensitive group within each cluster matches the overall proportion in the entire dataset. This  
 095 fairness criterion is commonly referred to as group fairness, and is also known as proportional fairness.  
 096 Recently, several algorithms have been developed to maximize clustering utility under fairness  
 097 constraints: Chierichetti et al. (2017); Backurs et al. (2019) transform training data to fair representa-  
 098 tions to achieve fairness guarantee prior to clustering, Kleindessner et al. (2019); Ziko et al. (2021);  
 099 Li et al. (2020); Zeng et al. (2023) incorporate fairness penalties directly during the clustering pro-  
 100 cess, and Bera et al. (2019); Harb & Lam (2020) refine cluster assignments with fixed pre-determined  
 101 cluster centers. These methods, however, require the number of clusters to be given in advance. This  
 102 limitation, i.e., the lack of fair clustering algorithms that are adaptive to the unknown number of  
 103 clusters, serves as the motivation for this study. In addition, model-based clustering can be applied  
 104 to data for which a meaningful distance is difficult to define (e.g., categorical data).

105 **Bayesian model-based clustering** The mixture model is a model-based clustering approach,  
 106 where each instance (or observation) is assumed to follow a mixture of parametric distributions  
 107 independently (Ouyang et al., 2004; Reynolds et al., 2009). Popular examples of parametric distri-  
 108 butions are the Gaussian (Maugis et al., 2009; Yang et al., 2012; Zhang et al., 2021), the student-t

(Peel & McLachlan, 2000), the skew-normal (Lin et al., 2007), and the categorical (Pan & Huang, 2014; McLachlan & Peel, 2000).

Bayesian approaches have been popularly used for inference of model-based clustering since they can infer the number of clusters as well as cluster centers. There are several well-defined Bayesian model-based clustering with unknown number of clusters including Mixture of Finite Mixtures (MFM) (Richardson & Green, 1997; Nobile & Fearnside, 2007; McCullagh & Yang, 2008; Miller & Harrison, 2018) and Dirichlet Process Mixture (DPM) (Ferguson, 1973; Antoniak, 1974; Escobar & West, 1995; Neal, 2000). There also exist various MCMC algorithms for MFM and DPM, such as Reversible Jump Markov Chain Monte Carlo (RJMCMC) (Richardson & Green, 1997) and Jain-Neal split-merge algorithm (Jain & Neal, 2004).

## 2 FAIR MIXTURE MODEL FOR CLUSTERING

We consider group fairness, as it is one of the most widely studied notions of fairness (Chierichetti et al., 2017; Backurs et al., 2019; Ziko et al., 2021; Li et al., 2020; Zeng et al., 2023; Bera et al., 2019; Harb & Lam, 2020; Kim et al., 2025b). For simplicity, we only consider a binary sensitive attribute, but provide a method of treating a multinomial sensitive attributes in Section C. Let  $s \in \{0, 1\}$  be a binary sensitive attribute known a priori. We define two sets of instances (observed data) from the two sensitive groups as  $\mathcal{D}^{(s)} = \{X_i^{(s)} : X_i^{(s)} \in \mathcal{X} \subseteq \mathbb{R}^d\}_{i=1}^{n_s}$  for  $s \in \{0, 1\}$ , where  $\mathcal{X}$  is the support of  $X$ ,  $n_s$  is the number of instances in the sensitive group  $s$ , and  $d$  is the number of features. Let  $\mathcal{D} := \mathcal{D}^{(0)} \cup \mathcal{D}^{(1)}$  be the set of the entire instances.

**Standard mixture model** The standard finite mixture model (Ouyang et al., 2004; Reynolds et al., 2009; Maugis et al., 2009; Yang et al., 2012; Zhang et al., 2021) without fairness is given as

$$X_1, \dots, X_n \stackrel{\text{i.i.d.}}{\sim} \sum_{k=1}^K \pi_k f(\cdot | \theta_k) \quad (1)$$

where  $n := n_0 + n_1$  and  $X_i := X_i^{(0)}$  for  $i \in \{1, \dots, n_0\}$  and  $X_i^{(1)}$  for  $i \in \{n_0 + 1, \dots, n_0 + n_1\}$ . In view of clustering,  $K$  is considered to be the number of clusters,  $\pi := (\pi_k)_{k=1}^K \in \mathcal{S}_K$  (the  $K$ -dimensional simplex) are the proportions of instances belonging to the  $k^{\text{th}}$  cluster, and  $f(\cdot | \theta_k)$  is the density of instances in the  $k^{\text{th}}$  cluster.

An equivalent representation of the above model can be made by introducing latent variables  $Z_i \in [K]$ ,  $i \in [n]$  as the following. Note that the latent variable  $Z_i$  takes the role of the cluster assignment of  $X_i$  for all  $i \in [n]$ . That is, when  $Z_i = k$ , we say that  $X_i$  belongs to the  $k^{\text{th}}$  cluster.

$$Z_1, \dots, Z_n \stackrel{\text{i.i.d.}}{\sim} \text{Categorical}(\pi) \quad (2)$$

$$X_i | Z_i \sim f(\cdot | \theta_{Z_i}) \quad (3)$$

**Fair mixture model** To define a fair mixture model, we first generalize the formulation of the standard finite mixture model in Equations (2) and (3) by considering the dependent latent variables, which we call the *generalized finite mixture model* in this paper. Let  $\mathbf{Z} := (Z_1, \dots, Z_n)$ . Then, the generalized finite mixture model is defined as:

$$\mathbf{Z} \sim G(\cdot) \quad (4)$$

$$X_i | Z_i \sim f(\cdot | \theta_{Z_i}) \quad (5)$$

where  $G$ , i.e., the joint distribution of  $\mathbf{Z}$ , has its support on  $[K]^n$ . When  $G$  is equal to  $\text{Categorical}(\pi)^n$  (i.e.,  $Z_i, \forall i \in [n]$  independently follows  $\text{Categorical}(\pi)$ ), the generalized mixture model becomes the standard finite mixture model in Equations (2) and (3).

We also define the (group) fairness level of  $\mathbf{Z}$ :

$$\Delta(\mathbf{Z}) := \frac{1}{2} \sum_{k=1}^K \left| \sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k) / n_0 - \sum_{j=1}^{n_1} \mathbb{I}(Z_j^{(1)} = k) / n_1 \right| \in [0, 1] \quad (6)$$

162 where  $Z_i^{(0)} = Z_i$  for  $i \in \{1, \dots, n_0\}$  and  $Z_j^{(1)} = Z_{j+n_0}$  for  $j \in \{1, \dots, n_1\}$ . We say that  $\mathbf{Z}$  is *fair with fairness level  $\epsilon$*  if  $\mathbf{Z} \in \mathcal{Z}_\epsilon^{\text{Fair}}$ , where  $\mathcal{Z}_\epsilon^{\text{Fair}} := \{\mathbf{Z} : \Delta(\mathbf{Z}) \leq \epsilon\}$ . In turn, for a given generalized mixture model, if the support  $G$  is confined on  $\mathcal{Z}_\epsilon^{\text{Fair}}$ , we say it is fair with level  $\epsilon$ . Note that the notion of  $\Delta$  has been already implemented in previous works (Kim et al., 2025b). See Section A.4 for more details.

## 168 2.1 CHOICE OF $G$ FOR PERFECT FAIRNESS: $\Delta(\mathbf{Z}) = 0$

170 The art of Bayesian analysis of the fair mixture model is to parameterize  $G$  such that posterior  
171 inference becomes computationally feasible. For example, we could consider  $\text{Categorical}(\boldsymbol{\pi})^n$  (the  
172 distribution of independent  $Z_i$ ) restricted to  $\mathcal{Z}_0^{\text{Fair}}$  as a candidate for  $G$ . While developing an MCMC  
173 algorithm for this distribution would not be impossible, but it would be quite challenging.

174 In this section, we propose a novel distribution for  $G$  in the perfectly fair (i.e.,  $\Delta(\mathbf{Z}) = 0$ ) mixture  
175 model with which a practical MCMC algorithm for posterior inference can be implemented. To  
176 explain the main idea of our proposed  $G$ , we first consider the simplest case of balanced data where  
177  $n_0 = n_1$  in Section 2.1.1. We then discuss how to handle the case of  $n_0 \neq n_1$  in Section 2.1.2.

### 179 2.1.1 CASE OF $n_0 = n_1$

181 Let  $\bar{n} := n_0 = n_1$ . A key observation is that any fair  $\mathbf{Z}$  corresponds to a matching map between  
182  $[\bar{n}]$  and  $[\bar{n}]$  (a permutation on  $[\bar{n}]$ ), which is stated in Proposition 2.1 with its proof in Section A.  
183 Figure 2 illustrates the relationship between a fair  $\mathbf{Z}$  and a matching map  $\mathbf{T} : [\bar{n}] \rightarrow [\bar{n}]$ .

184 **Proposition 2.1.**  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}} \iff \text{There exists a matching map } \mathbf{T} \text{ such that } Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}, \forall j \in [\bar{n}]$ .

186 We utilize the above proposition to define a fair distribution  $G$ . The main idea is that  $G$  *assigns two*  
187 *matched data to a same cluster once a matching map is given*. To be more specific, the proposed  
188 distribution is parametrized by  $\boldsymbol{\pi}$  and  $\mathbf{T}$ , which is defined by  $Z_1^{(0)}, \dots, Z_{\bar{n}}^{(0)} \stackrel{\text{i.i.d.}}{\sim} \text{Categorical}(\boldsymbol{\pi})$  and  
189  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ . It is easy to see that  $G$  is perfectly fair. We write  $G(\cdot | \boldsymbol{\pi}, \mathbf{T})$  for such a distribution.

191 Denote  $\mathcal{Z}^{\text{Fair}}(\mathbf{T})$  as the support of  $G(\cdot | \boldsymbol{\pi}, \mathbf{T})$ . Note  
192 that  $\mathcal{Z}^{\text{Fair}}(\mathbf{T}) \subset \mathcal{Z}_0^{\text{Fair}}$ , so one might worry that  
193 the support of  $G(\cdot | \boldsymbol{\pi}, \mathbf{T})$  is too small. Proposition  
194 2.1, however, implies that  $\cup_{\mathbf{T} \in \mathcal{T}} \mathcal{Z}^{\text{Fair}}(\mathbf{T}) = \mathcal{Z}_0^{\text{Fair}}$ ,  
195 where  $\mathcal{T}$  is the set of all matching maps, and thus we  
196 can put a prior mass on  $\mathcal{Z}_0^{\text{Fair}}$  by putting a prior on  $\mathbf{T}$   
197 (as well as  $\boldsymbol{\pi}$ ) accordingly.

198 A crucial benefit of the proposed  $G$  is that  $\boldsymbol{\pi}$  and  $\mathbf{T}$   
199 are not intertwined, hence they can be selected in-  
200 dependently. As a result, we can find a fair mixture  
201 model without any additional parameter constraints.  
202 It is noteworthy that, conditional on  $\mathbf{T}$ , the fair mix-  
203 ture model can be written similarly to the standard mixture model in Equations (4) and (5) as :

$$(Z_1^{(0)}, \dots, Z_{\bar{n}}^{(0)}) \sim \text{Categorical}(\boldsymbol{\pi})^{\bar{n}} \quad (7)$$

$$X_{\mathbf{T}(j)}^{(0)}, X_j^{(1)} | Z_{\mathbf{T}(j)}^{(0)} \stackrel{\text{ind}}{\sim} f(\cdot | \theta_{Z_{\mathbf{T}(j)}^{(0)}}) \quad (8)$$

### 208 2.1.2 CASE OF $n_0 \neq n_1$

210 Without loss of generality, we assume that  $n_0 < n_1$  such that  $n_1 = \beta n_0 + r$  for nonnegative integers  
211  $\beta$  and  $r < n_0$ . We first consider the case of  $r = 0$  because we can modify  $G$  for the balanced  
212 case easily. When  $r \neq 0$ , the situation is complicated since there is no one-to-one correspondence  
213 between fairness and matching map, and thus we propose a heuristic modification.

214 **Case of  $r = 0$  :** A function  $\mathbf{T}$  from  $[n_1]$  to  $[n_0]$  is called a *matching map* if (i) it is onto and (ii)  
215  $|\mathbf{T}^{-1}(i)| = \beta$  for all  $i \in [n_0]$ . Let  $\mathcal{T}$  be the set of all matching maps. Then, we have Proposition 2.2,

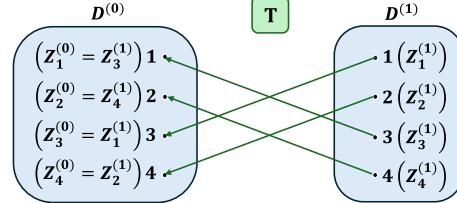


Figure 2: An example of fair  $\mathbf{Z}$  when  $\bar{n} = 4$ , where  $\mathbf{T}$  is given as  $(\mathbf{T}(1), \mathbf{T}(2), \mathbf{T}(3), \mathbf{T}(4)) = (3, 4, 1, 2)$ .

216 which is similar to Proposition 2.1 for the balanced case. See Section A for its proof. Note that for  
 217 this case,  $\mathbf{T}$  can be seen as a map to build fairlets.  
 218

219 **Proposition 2.2.**  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}} \iff \text{There exists a matching map } \mathbf{T} \text{ s.t. } Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}, \forall j \in [n_1].$   
 220

221 For given  $\boldsymbol{\pi} \in \mathcal{S}_K$  and  $\mathbf{T} \in \mathcal{T}$ , we define a fair distribution  $G(\cdot|\boldsymbol{\pi}, \mathbf{T})$  as  $Z_1^{(0)}, \dots, Z_{n_0}^{(0)} \stackrel{\text{i.i.d.}}{\sim}$   
 222 Categorical( $\boldsymbol{\pi}$ ) and  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ . Similar to the balanced case, we have  $\cup_{\mathbf{T} \in \mathcal{T}} \mathcal{Z}^{\text{Fair}}(\mathbf{T}) = \mathcal{Z}_0^{\text{Fair}}$ .  
 223

224 **Case of  $r > 0$ :** It can be shown (see Proposition A.1 in Section A for the proof) that for a given  
 225 fair  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$ , there exists a function  $\mathbf{T}$  from  $[n_1]$  to  $[n_0]$  such that it is onto,  $|\mathbf{T}^{-1}(i)|$  is either  $\beta$   
 226 or  $\beta + 1$  and  $|R_{\mathbf{T}}| = r$ , where  $R_{\mathbf{T}} = \{i : |\mathbf{T}^{-1}(i)| = \beta + 1\}$ . Let  $\mathcal{T}$  be the set of all such matching  
 227 maps (functions satisfying these conditions).  
 228

229 A difficulty arises since the converse is not always true. To resolve this difficulty, we propose a  
 230 heuristic modification of the definition of ‘fairness of  $\mathbf{Z}$ ’. Let  $R$  be a subset of  $[n_0]$  with  $|R| = r$ ,  
 231 and let  $\mathcal{T}_R$  be a subset of  $\mathcal{T}$  such that  $R_{\mathbf{T}} = R$ . Then, we say that  $\mathbf{Z}$  is fair if there exists  $\mathbf{T} \in \mathcal{T}_R$   
 232 such that  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ . Note that a fair  $\mathbf{Z}$  may not belong to  $\mathcal{Z}_0^{\text{Fair}}$  but the violation of fairness  
 233 would be small when  $|C_k^{(0)}|/n_0 \approx |C_k^{(0)} \cap R|/r$ . A theoretical upper bound on the fairness violation  
 234 ( $\Delta(\mathbf{Z})$ ) is given in Proposition A.3, and it becomes zero when  $|C_k^{(0)}|/n_0 = |C_k^{(0)} \cap R|/r$  as shown  
 235 in Proposition A.2.  
 236

237 In this paper, we consider two feasible candidates for  $R$ : (i) a random subset of  $[n_0]$  and (ii) the  
 238 index of samples closest to the cluster centers obtained by a certain clustering algorithm to  $\mathcal{D}^{(0)}$   
 239 with  $K = r$ . Finally, we can define  $G(\cdot|\boldsymbol{\pi}, \mathbf{T})$  for  $\boldsymbol{\pi} \in \mathcal{S}_K$  and  $\mathbf{T} \in \mathcal{T}_R$  similarly to that for the  
 240 balanced case. See Section A.1 for the detailed discussion and the motivation of the two candidates.  
 241 Our numerical studies in Section 5.4 confirm that the two proposed choices of  $R$  work quite well.  
 242

## 243 2.2 CHOICE OF $G$ FOR NON-PERFECT FAIRNESS: $\Delta(\mathbf{Z}) > 0$

244 Once  $\boldsymbol{\pi} \in \mathcal{S}_K$  and  $\mathbf{T} \in \mathcal{T}_R$  are given, we can modify  $G(\cdot|\boldsymbol{\pi}, \mathbf{T})$  to have a distribution whose  
 245 support is included in  $\mathcal{Z}_{\varepsilon}^{\text{Fair}}$ . The main idea of the proposed modification is to select  $m$  many samples  
 246 from  $\mathcal{D}^{(1)}$  and to assign independent clustering labels to them instead of matching them to the  
 247 corresponding samples in  $\mathcal{D}^{(0)}$ . Let  $E$  be a subset of  $[n_1]$  with  $|E| = m$ . We consider a latent  
 248 variable  $\mathbf{T}_0 : [n_1] \rightarrow [n_0]$  that is an arbitrary function from  $[n_1]$  to  $[n_0]$ . Then, we let  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$   
 249 for  $j \in [n_1] \setminus E$  and  $Z_j^{(1)} = Z_{\mathbf{T}_0(j)}^{(0)}$  for  $j \in E$ . In other words,  $\mathcal{D}^{(1)}$  is masked by  $E$ : (i) the masked  
 250 data in  $E$  are assigned by  $\mathbf{T}_0$ , (ii) while the unmasked data in  $[n_1] \setminus E$  are still assigned by  $\mathbf{T}$ . It  
 251 can be shown that the support of the distribution  $G(\cdot|\boldsymbol{\pi}, \mathbf{T}, \mathbf{T}_0, E)$  belongs to  $\mathcal{Z}_{\varepsilon}^{\text{Fair}}$  with  $\varepsilon = m/n_1$ ,  
 252 provided that  $r = 0$ . See Proposition A.4 in Section A for the theoretical proof.  
 253

## 254 3 FAIR BAYESIAN MODELING

255 We first propose a fair mixture model based on Equations (7) and (8) as:  
 256

$$\boldsymbol{\pi}|K \sim \text{Dirichlet}_K(\gamma, \dots, \gamma), \gamma > 0 \quad (9)$$

$$Z_i^{(0)}|\boldsymbol{\pi} \stackrel{\text{i.i.d.}}{\sim} \text{Categorical}(\cdot|\boldsymbol{\pi}), \quad \forall i \in [n_0] \quad (10)$$

$$Z_j^{(1)} = \begin{cases} Z_{\mathbf{T}(j)}^{(0)}, & \forall j \in [n_1] \setminus E \\ Z_{\mathbf{T}_0(j)}^{(0)}, & \forall j \in E \end{cases} \quad (11)$$

$$X_i^{(0)}|Z_i^{(0)} \sim f(\cdot|\theta_{Z_i^{(0)}}), X_j^{(1)}|Z_j^{(1)} \sim f(\cdot|\theta_{Z_j^{(1)}}) \quad (12)$$

257 In this model,  $\boldsymbol{\theta} = (\theta_1, \theta_2, \dots)$ ,  $E$ ,  $\mathbf{T}$  and  $\mathbf{T}_0$  as well as the number of clusters  $K$  are the parameters  
 258 to be inferred. Aprior, we assume that each parameter is independent:  $K \sim p_K(\cdot)$ ,  $E \sim p_E(\cdot)$ ,  $\mathbf{T} \sim$   
 259  $p_{\mathbf{T}}(\cdot)$ ,  $\mathbf{T}_0 \sim p_{\mathbf{T}_0}(\cdot)$ , and  $\theta_1, \theta_2, \dots, \stackrel{\text{ind}}{\sim} H$ .  
 260

270 **Prior for  $K$**  For  $K$ , we consider  $K \sim p_K(\cdot)$ , where  $p_K$  is a probability mass function on  
 271  $\{1, 2, \dots\}$ . In this study, we use  $\text{Geometric}(\kappa)$ ,  $\kappa \in (0, 1)$  for  $p_K$  following (Miller & Harrison,  
 272 2018), where  $\kappa$  is a hyperparameter. Further, we could consider a hierarchical prior for  $\kappa$  as well to  
 273 reduce the dependency of posterior to the selection of  $\kappa$  (see Section D for details).  
 274

275 **Prior for  $\theta$**  Usually, we choose a conjugate distribution of  $f(\cdot|\theta)$  for  $H$ . For example, when  $f(\cdot|\theta)$   
 276 is the density of the Gaussian distribution, and  $\theta$  consists of the mean vector and diagonal covariance  
 277 matrix as  $\theta = (\boldsymbol{\mu}, \boldsymbol{\lambda}^{-1}) \in \mathbb{R}^d \times \mathbb{R}^d$ , where  $\boldsymbol{\mu} = (\mu_j)_{j=1}^d$  and  $\boldsymbol{\lambda} = (\lambda_j)_{j=1}^d$ . We set  $\lambda_j = \lambda$  for  
 278 all  $j \in [d]$  where  $(\mu_j, \lambda), j \in [d]$  is independent and follow  $\lambda \sim \text{Gamma}(a, b)$  for some  $a, b$  and  
 279  $\mu_j | \lambda \sim \mathcal{N}(0, \lambda^{-1}), j \in [d]$  for  $H$ .  
 280

281 **Prior for  $\mathbf{T}, \mathbf{T}_0$ , and  $E$**  Motivated by (Volkovs & Zemel, 2012), we construct a prior of  $\mathbf{T}$  with its  
 282 support  $\mathcal{T}_R$  based on the energy defined in Definition 3.1 below. The energy of a random matching  
 283 map  $\mathbf{T}$  is defined as below, which measures the similarity between two matched data. See Sec-  
 284 tion E.2 for the choice of  $D$  in Definition 3.1. For the prior, we let  $p_{\mathbf{T}}(\mathbf{T}) \propto e(\mathbf{T}) \mathbb{I}(\mathbf{T} \in \mathcal{T}_R)$ . For  
 285  $\mathbf{T}_0$ , we use the uniform distribution on  $\Pi_n$ . For  $E$ , we use the uniform distribution on  $[n_1 : m]$ ,  
 286 where  $[n_1 : m]$  is the collection of all subsets of  $[n_1]$  with size  $m$ .  
 287

288 **Definition 3.1** (Energy of a matching map). Let  $D : \mathcal{X} \times \mathcal{X} \rightarrow \mathbb{R}_+$  be a given distance and  
 289  $\Pi_n := \{\mathbf{T} : [n_1] \rightarrow [n_0]\}$ . Given  $\mathbf{T} \in \Pi_n$ , the energy of  $\mathbf{T}$  is defined by  $e(\mathbf{T}) = e(\mathbf{T}; \tau) :=$   
 290  $\exp\left(-\sum_{j=1}^{n_1} D\left(X_{\mathbf{T}(j)}^{(0)}, X_j^{(1)}\right) / n_1 \tau\right)$ , where  $\tau > 0$  is a pre-specified temperature constant.  
 291

### 3.1 EQUIVALENT REPRESENTATIONS

293 We here present the equivalent representations of Equations (9) to (12), which enable practical im-  
 294 plementation of an MCMC inference algorithm. The proof could be done by modifying the proof  
 295 of Miller & Harrison (2018), but we present the detailed proofs in Propositions B.1 to B.3 of Sec-  
 296 tion B.3 for the readers' sake.  
 297

298 **Model** For a given partition  $\mathcal{C}$  of  $[n_0]$ , an equivalent generative model to the proposed fair mixture  
 299 model in Equations (9) to (12) is:

$$\phi_c \stackrel{\text{i.i.d.}}{\sim} H, c \in \mathcal{C} \quad (13)$$

$$X_i^{(0)} \stackrel{\text{ind}}{\sim} f(\cdot|\phi_c) \quad i \in c \quad (14)$$

$$X_j^{(1)} \stackrel{\text{ind}}{\sim} \begin{cases} f(\cdot|\phi_c) & \forall j \in [n_1] \setminus E \text{ s.t. } \mathbf{T}(j) \in c \\ f(\cdot|\phi_c) & \forall j \in E \text{ s.t. } \mathbf{T}_0(j) \in c. \end{cases} \quad (15)$$

306 **Priors** The prior for  $\mathcal{C}$  in this equivalent representation is  $p_{\mathcal{C}}(\mathcal{C}|\mathbf{T}, \mathbf{T}_0, E) = p_{\mathcal{C}}(\mathcal{C}) =$   
 307  $V_{n_0}(t) \prod_{c \in \mathcal{C}} \gamma^{(|c|)}$ , where  $t = |\mathcal{C}|$ ,  $V_{n_0}(t) = \sum_{k=1}^{\infty} \frac{k_{(t)}}{(\gamma k)^{(n_0)}} p_K(k)$ ,  $(\gamma k)^{(n_0)} = (\gamma k + n_0 - 1)! / (\gamma k -$   
 308  $1)!$  and  $k_{(t)} = k! / (k - t)!$ . See Miller & Harrison (2018) for the derivation. The prior of  $(\mathbf{T}, \mathbf{T}_0, E)$   
 309 remains the same as the prior in Section 3.  
 310

311 When  $K$  is unknown and treated as a random variable, we use the following equivalent repre-  
 312 sentation of the proposed fair Bayesian mixture model, as done in Miller & Harrison (2018).  
 313 When  $K$  is known as  $k_*$ , we only need to modify  $p_K$  in the prior for  $\mathcal{C}$ . In specific, we modify  
 314  $p_K(k) = \mathbb{I}(k = k_*)$  in  $V_{n_0}(t)$ , and the others remain the same.  
 315

## 316 4 INFERENCE ALGORITHM: FBC

318 We develop an MCMC algorithm for the equivalent representations of the proposed fair Bayesian  
 319 mixture model in Section 3.1. Here, we denote  $\Phi$  as the mixture parameters to be sampled (i.e.,  
 320  $\Phi = \mathcal{C}$  when  $H$  is conjugate, or  $\Phi = (\mathcal{C}, \phi)$  when  $H$  is non-conjugate, where  $\phi := (\phi_c : c \in \mathcal{C})$ ).  
 321

322 The posterior sampling of  $(\mathbf{T}, \mathbf{T}_0, E, \Phi) \sim p(\mathbf{T}, \mathbf{T}_0, E, \Phi | \mathcal{D})$  is done by a Gibbs sampler: (i) sam-  
 323 pling  $(\mathbf{T}, \mathbf{T}_0, E) \sim p(\mathbf{T}, \mathbf{T}_0, E | \Phi, \mathcal{D})$ , and (ii) sampling  $\Phi \sim p(\Phi | \mathbf{T}, \mathbf{T}_0, E, \mathcal{D})$ . We name the  
 324 proposed MCMC inference algorithm as **Fair Bayesian Clustering (FBC)**. In the subsequent two

324 subsections, we explain how to sample  $(\mathbf{T}, \mathbf{T}_0, E)$  and  $\Phi$  from their conditional posteriors, respec-  
 325 tively, by using a Metropolis-Hastings (MH) algorithm. We also discuss the extension of FBC for  
 326 handling a multinomial sensitive attribute in Section C, with experiments on a real dataset.  
 327

328 **STEP 1 ▷ Sampling**  $(\mathbf{T}, \mathbf{T}_0, E) \sim p(\mathbf{T}, \mathbf{T}_0, E | \Phi, \mathcal{D})$   
 329

330 • **(Proposal)** For the proposal distribution of  $(\mathbf{T}', \mathbf{T}'_0, E')$  from  $(\mathbf{T}, \mathbf{T}_0, E)$ , we first assume that  
 331  $\mathbf{T} \rightarrow \mathbf{T}'$ ,  $\mathbf{T}_0 \rightarrow \mathbf{T}'_0$  and  $E \rightarrow E'$  are independent. For the proposal of  $\mathbf{T} \rightarrow \mathbf{T}'$ , we randomly  
 332 select two indices  $i_1$  and  $i_2$  from  $[n_1]$ , and define:  
 333

$$334 \quad \mathbf{T}'(j) := \begin{cases} \mathbf{T}(j) & \text{for } j \notin [n_1] \setminus \{i_1, i_2\} \\ 335 \quad \mathbf{T}(i_2) & \text{for } j = i_1 \\ 336 \quad \mathbf{T}(i_1) & \text{for } j = i_2. \end{cases} \quad (16)$$

337 We swap only two indices to guarantee  $\mathbf{T}' \in \mathcal{T}_R$ . For  $\mathbf{T}_0 \rightarrow \mathbf{T}'_0$ , we randomly select an index  
 338  $j' \in [n_1]$ , then set  $\mathbf{T}'_0(j') = i$  where  $i \sim \text{Unif}([n_0])$  and  $\mathbf{T}'_0(j) = \mathbf{T}_0(j)$  for  $j \neq j'$ . For  
 339  $E \rightarrow E'$ , we randomly swap two indices, one from  $E$  and the other from  $[n_1] \setminus E$ . See Figure 7  
 340 in Section B.2 for an illustration of the proposal.  
 341

342 • **(Acceptance / Rejection)** As the randomness in the proposal of  $\mathbf{T}', \mathbf{T}'_0$  and  $E'$  does not depend  
 343 on  $\mathbf{T}, \mathbf{T}_0$  and  $E$ , the proposal density ratio  $q((\mathbf{T}', \mathbf{T}'_0, E') \rightarrow (\mathbf{T}, \mathbf{T}_0, E)) / q((\mathbf{T}, \mathbf{T}_0, E) \rightarrow$   
 344  $(\mathbf{T}', \mathbf{T}'_0, E'))$  is equal to 1. Hence, the acceptance probability of a proposal  $(\mathbf{T}', \mathbf{T}'_0, E')$  is  
 345

$$346 \quad \alpha(\mathbf{T}', \mathbf{T}'_0, E') = \min \{1, e(\mathbf{T}') \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}', \mathbf{T}'_0, E') / e(\mathbf{T}) \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}, \mathbf{T}_0, E)\}. \quad (17)$$

347 See Section B.2 for the calculation details of the acceptance probability. We repeat the MH sam-  
 348 pling of  $(\mathbf{T}', \mathbf{T}'_0, E')$  multiple times before sampling  $\Phi$ , which helps accelerate convergence.  
 349 In our experiments, we perform this repetition 10 times. This additional computation is mini-  
 350 mal, even for large datasets, since the acceptance probability requires calculating the likelihood  
 351 only for instances whose assigned clusters change. The maximum number of such instances with  
 352 changed clusters is 4 (2 for  $\mathbf{T}'$ , 1 for  $\mathbf{T}'_0$  and 1 for  $E'$ ).  
 353

354 **STEP 2 ▷ Sampling**  $\Phi \sim p(\Phi | \mathbf{T}, \mathbf{T}_0, E, \mathcal{D})$  Sampling from  $p(\Phi | \mathbf{T}, \mathbf{T}_0, E, \mathcal{D})$  can be done simi-  
 355 lar to the sampling algorithm for the standard mixture model when  $(\mathbf{T}, \mathbf{T}_0, E)$  is given. Specifically,  
 356 we mimic the procedure of Miller & Harrison (2018), which utilizes DPM inference algorithms from  
 357 Neal (2000); MacEachern & Müller (1998). See Section B.3 for details of this sampling step.  
 358

359 [Algorithm 1](#) below provides the pseudo-code of our proposed FBC algorithm, and we empirically  
 360 confirm the convergence of this two-step MCMC algorithm in Section E.4. See Figure 6 in Sec-  
 361 tion B.1 for a visualization of the algorithm.  
 362

---

**Algorithm 1** FBC (Fair Bayesian model-based Clustering) algorithm

---

363  
 364 1: **Inputs:** Data  $(\mathcal{D} = \mathcal{D}^{(0)} \cup \mathcal{D}^{(1)})$ , Maximum number of iterations for inference ( $\text{max}_{\text{iter}}$ ).  
 365 2: Initialize  $\Phi^{(0)}, \mathbf{T}^{(0)}, \mathbf{T}_0^{(0)}, E^{(0)}$   
 366 3: **for**  $t = 1$  to  $\text{max}_{\text{iter}}$  **do**  
 367 4:   (STEP 1) Propose  $(\mathbf{T}', \mathbf{T}'_0, E')$  and compute the acceptance probability  $\alpha(\mathbf{T}', \mathbf{T}'_0, E')$   
 368 5:   Sample  $u \sim \text{Uniform}(0, 1)$   
 369 6:   **if**  $u < \alpha(\mathbf{T}', \mathbf{T}'_0, E')$  **then**  
 370 7:     Accept  $\mathbf{T}^{(t)} = \mathbf{T}', \mathbf{T}_0^{(t)} = \mathbf{T}'_0, E^{(t)} = E'$   
 371 8:   **else**  
 372 9:     Reject  $\mathbf{T}^{(t)} = \mathbf{T}^{(t-1)}, \mathbf{T}_0^{(t)} = \mathbf{T}_0^{(t-1)}, E^{(t)} = E^{(t-1)}$   
 373 10:   **end if**  
 374 11:   (STEP 2) Sample  $\Phi^{(t)}$  from posterior  $p(\Phi | \mathbf{T}^{(t)}, \mathbf{T}_0^{(t)}, E^{(t)}, \mathcal{D})$   
 375 12: **end for**  
 376 13: **Return:** Posterior samples  $\left\{ \left( \Phi^{(t)}, \mathbf{T}^{(t)}, \mathbf{T}_0^{(t)}, E^{(t)} \right) \right\}_{t=1}^{\text{max}_{\text{iter}}}.$   


---

378     **Intuitive understanding of FBC** From an optimization perspective, our Bayesian formulation can  
 379     be viewed as an analogue of a cost-fairness decomposition: (i) the likelihood plays the role of the  
 380     clustering cost, and (ii) the fair prior space plays a role of the fairness constraint. In other words, we  
 381     design the fair-constrained space via the prior, while our MCMC algorithm stochastically searches  
 382     for both the parameters and the matchings within this fair-constrained space.  
 383

## 384     5 EXPERIMENTS

 385

386     In this section, we empirically show that FBC (i) performs competitive to existing baselines in  
 387     terms of the trade-off between clustering utility and fairness level; (ii) infers the number of clusters  
 388      $K$  reasonably well; (iii) is easily applicable when data contain both continuous and categorical  
 389     variables; (iv) can perform well under certain constraints on the cluster sizes.  
 390

391     **Datasets and performance measures** We analyze three real benchmark datasets: ADULT (Becker  
 392     & Kohavi, 1996), BANK (Moro et al., 2014), and DIABETES (Smith et al., 1988). All features in the  
 393     datasets are continuous and so we use the Gaussian mixture model. We standardize all features of  
 394     data to have zero mean and unit variance. Note that the three datasets include binary class labels.  
 395

396     For clustering utility, we consider the `Cost` (i.e., the average distance to the center of the assigned  
 397     cluster from each data point), which is defined as:  $\text{Cost} := \sum_{k=1}^K \sum_{X_i \in C_k} \|X_i - \hat{\mu}_k\|^2 / n$ , where  
 398      $C_k := C_k^{(0)} \cup C_k^{(1)}$  is the set of data assigned to the  $k^{\text{th}}$  cluster. Here,  $\hat{\mu}_k := \sum_{X_i \in C_k} X_i / |C_k|$  de-  
 399     notes the center of the  $k^{\text{th}}$  cluster. We additionally consider a density-based measure `NLD` (Negative  
 400     Log Density). For baseline methods, we fit Gaussian for each cluster, then compute the weighted  
 401     sum of negative log-likelihood. For FBC, we report the negative log posterior density for `NLD`. As  
 402     the datasets include binary class labels, we also evaluate `Acc` (classification accuracy). To calculate  
 403     `Acc`, we assign labels as follows: for each cluster, we set the label of every element to the cluster's  
 404     majority label. Lower `Cost` / Lower `NLD` / Higher `Acc` imply a better clustering utility.  
 405

406     For fairness level, we consider two measures: (i)  $\Delta(\mathcal{Z})$  defined in Equation (6) and (ii) the bal-  
 407     ance (`Bal`) defined as  $\text{Bal} := \min_{k \in [K]} \text{Bal}_k$ , where  $\text{Bal}_k := \min\{|C_k^{(0)}|/|C_k^{(1)}|, |C_k^{(1)}|/|C_k^{(0)}|\}$   
 408     which is popularly considered in recent fair clustering literature (Backurs et al., 2019; Ziko et al.,  
 409     2021; Esmaili et al., 2021; Kim et al., 2025b). We abbreviate  $\Delta(\mathcal{Z})$  by  $\Delta$  in this section. See  
 410     Section E.1 for details about the datasets and measures.

411     **Baselines and implementation details** For a fairness-agnostic method, we consider the Mixtures  
 412     of Finite Mixtures (MFM) algorithm proposed by (Miller & Harrison, 2018). For baseline fair clus-  
 413     tering methods, we consider several existing non-Bayesian approaches: SFC (Backurs et al., 2019),  
 414     VFC (Ziko et al., 2021), and FCA (Kim et al., 2025b). SFC is a **scalable fairlet-based fair clustering**  
 415     **method**, VFC is an in-processing approach by adding a fairness regularizer, and FCA is a recent work  
 416     using the matching map for fair  $K$ -means clustering. Whenever  $r > 0$ , we set  $R$  (in Section 2.1.2)  
 417     as a random subset of  $[n_0]$  of size  $r$ . Omitted experimental details are given in Section E.2.  
 418

### 419     5.1 FAIR CLUSTERING PERFORMANCE (KNOWN $K$ )

 420

421     **Comparison of FBC to existing fair clustering algorithms** We investigate whether FBC yields  
 422     reasonable clustering results compared to baselines when  $K$  is fixed at  $k_*$ , by assessing the trade-  
 423     off between utility (`Cost`, `NLD`, and `Acc`) and fairness ( $\Delta$  and `Bal`). That is, we set  $p_K(k) =$   
 424      $\mathbb{I}(K = k_*)$  in FBC. We run each algorithm to achieve the maximum fairness (e.g.,  $\Delta \approx 0$ ) for a fair  
 425     comparison. Table 1 shows the results, suggesting that FBC is competitive to the baselines when  $K$   
 426     is fixed at  $k_* = 10$ . Detailed comparisons are given as follows.  
 427

428     First, compared to SFC and VFC: FBC yields superior utility than SFC (i.e., lower `Cost` and `NLD`  
 429     and higher `Acc`) in almost all cases, while both methods achieve near-perfect fairness; FBC attains  
 430     a higher level of fairness than VFC in every case (lower  $\Delta$  and higher `Bal`), with only slight losses  
 431     in utility; indeed, on ADULT dataset, FBC even achieves higher accuracy.

432     Second, compared to FCA: FBC performs highly competitive utility and fairness, whereas FCA and  
 433     FBC are conceptually similar in the sense that both are based on matching map. Although FCA

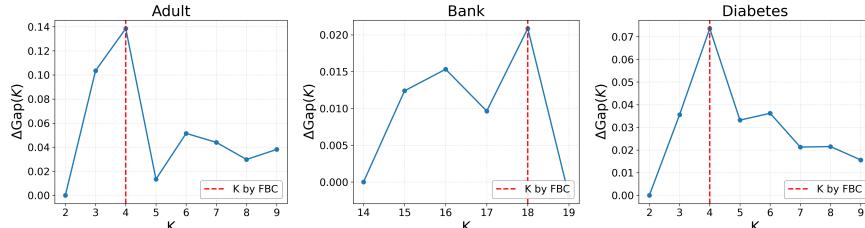
432 directly minimizes cost whereas FBC focuses on the posterior density, it is surprising that FBC  
 433 attains competitive Costs. This result suggests that the matching map  $\mathbf{T}$  in our MCMC inference  
 434 may be also optimal in frequentist-view of the Cost minimizing approach. Furthermore, Table 2 in  
 435 Section E.3.1 shows that FBC requires less computation time (near 50% of FCA). This is because  
 436 FCA optimizes  $\mathbf{T}$  by solving linear program at each iteration, while FBC searches  $\mathbf{T}$  stochastically.  
 437

438 Table 1: Comparison of utility (Cost, NLD, Acc) and fairness ( $\Delta$ , Bal) for  $k_* = 10$ . See Table 3  
 439 in Section E.3.1 for the similar results for  $k_* = 2$ . **Bold-faced values and underlined values** (Cost  
 440 and  $\Delta$ ) indicate the best and second-best values, respectively, among the methods that achieve near-  
 441 perfect fairness levels.

443	Dataset	Measure	SFC	VFC	FCA	FBC ✓
444	ADULT	Cost ( $\downarrow$ )	3.129	1.702	<b>1.869</b>	<u>1.954</u>
445		NLD ( $\downarrow$ )	6.498	6.134	6.174	6.242
446		Acc ( $\uparrow$ )	0.763	0.765	0.785	0.781
447		$\Delta$ ( $\downarrow$ )	0.006	0.039	<b>0.001</b>	<b>0.001</b>
448		Bal ( $\uparrow$ )	0.491	0.277	0.493	0.491
449	BANK	Cost ( $\downarrow$ )	2.868	1.552	<b>1.785</b>	<u>1.787</u>
450		NLD ( $\downarrow$ )	6.828	6.270	6.357	6.302
451		Acc ( $\uparrow$ )	0.893	0.893	0.891	0.890
452		$\Delta$ ( $\downarrow$ )	0.003	0.040	<b>0.001</b>	0.004
453		Bal ( $\uparrow$ )	0.647	0.513	0.648	0.615
454	DIABETES	Cost ( $\downarrow$ )	5.115	3.077	<b>3.441</b>	<u>3.757</u>
455		NLD ( $\downarrow$ )	9.381	8.946	9.033	9.088
456		Acc ( $\uparrow$ )	0.656	0.724	0.690	0.693
457		$\Delta$ ( $\downarrow$ )	0.057	0.217	<b>0.004</b>	<u>0.013</u>
458		Bal ( $\uparrow$ )	0.824	0.083	0.929	0.882

459 **Fairness level control of FBC** We also numerically confirm that the fairness level can be con-  
 460 trolled by  $m$  (the size of  $E$ ). Figure 8 in Section E presents the trade-off between  $m$  and the fairness  
 461 levels  $\Delta$  and Bal, showing that a smaller  $m$  usually results in a fairer clustering.

## 463 5.2 REASONABLE INFERENCE OF $K$ (UNKNOWN $K$ )

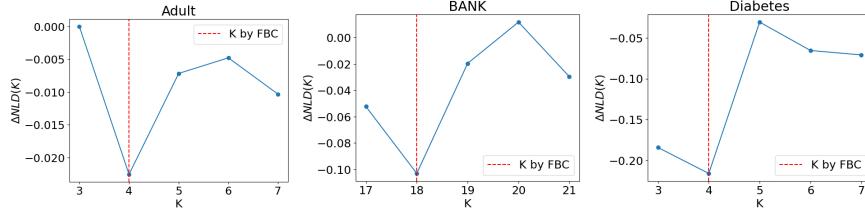


473 Figure 3:  $K$  vs.  $\Delta\text{Gap}(K)$  of FCA on (left) ADULT, (center) BANK, and (right) DIABETES datasets.  
 474 Red vertical dashed lines indicate the  $K$  inferred by FBC.  
 475

477 **Cluster quality** When  $K$  is unknown, FBC treats it as a random variable and infer as  $K = 4, 18$ ,  
 478 and 4 for ADULT, BANK, and DIABETES datasets, respectively, and these are at the posterior modes  
 479 (Figure 9 in Section E.3.2). To assess the optimality of the inferred  $K$  in view of cluster quality, we  
 480 consider the Gap statistic (Tibshirani et al., 2002), a well-known measure developed to determine  
 481 the optimal  $K$  based on within-cluster dispersions. We run FCA for various  $K$ s, calculate the Gap  
 482 statistic for each  $K$ , and then plot  $\Delta\text{Gap}(K) = \text{Gap}(K) - \text{Gap}(K-1)$  for  $K \geq 2$  with  $\text{Gap}(2) = 0$ .  
 483 The elbow, i.e., the largest increase, occurs at the  $K$  inferred by FBC (see Figure 3).

484 We further evaluate the trade-off performance compared to the baseline methods. That is, we run  
 485 baseline algorithms with  $K$ s inferred by FBC, then compare the trade-off performance. Table 5 in  
 Section E.3.2 presents the results, suggesting that FBC is still competitive to the baselines.

486 **Density estimation** As FBC is a model-based approach, it can be used for not only clustering but  
 487 also density estimation. Similar to the Gap statistic, Figure 4 shows the difference  $\Delta \text{NLD}(K) =$   
 488  $\text{NLD}(K) - \text{NLD}(K-1)$  in posterior densities (on test data) for various  $K$ 's in FBC, which suggests  
 489 that the inferred ones are optimal in view of density estimation (i.e., achieves the elbow in NLD on  
 490 the test data). More details are given in E.3.2.



491  
 492 Figure 4:  $K$  vs.  $\Delta \text{NLD}(K)$  of FBC with fixed  $K$  on (left) ADULT, (center) BANK, and (right)  
 493  
 494 DIABETES datasets. Red vertical dashed lines indicate the  $K$  inferred by FBC.  
 495  
 496

### 501 5.3 FLEXIBILITIES OF FBC

502 **Applicability to various data types** FBC accommodates both continuous and categorical data as  
 503 long as the likelihood of the mixture model is defined. We empirically compare FBC with FairDen  
 504 (Krieger et al., 2025), which likewise supports categorical data as well. Section E.3.3 details the  
 505 analysis, where Table 6 shows that (i) using both continuous and categorical data improves the  
 506 utility (Acc), highlighting the limitation of distance-based clustering methods that operate only on  
 507 continuous data; and (ii) FBC outperforms FairDen in terms of the fairness–utility trade-off.  
 508

509 **Clustering under size constraints** FBC can also flexibly work under cluster size constraints  
 510 (i.e., the upper bound of cluster size) with a slight modification to the inference algorithm. Sec-  
 511 tion E.3.4 details how we incorporate the size constraint in FBC; results in Table 7 shows that under  
 512 the size constraint, FBC achieves lower Cost while attaining perfect fairness, outperforming the  
 513 post-processing method of Bera et al. (2019).  
 514

### 515 5.4 ABLATION STUDIES

516 We conduct ablation studies on three topics: (i) Impact of the temperature constant  $\tau$  in the prior  
 517 of  $\mathbf{T}$  defined in Definition 3.1; (ii) Validity of the two proposed heuristic approaches of selecting  $R$   
 518 in Section 2.1.2; (iii) Influence of the covariance structure in the Gaussian mixture model. Details  
 519 and results are given in Section E.3.5, showing the robustness on  $\tau$  and  $R$ , and that using a more  
 520 complex covariance improves density estimation (lower NLD) while maintaining high fairness level.  
 521

## 522 6 CONCLUDING REMARKS

523 In this paper, we proposed a fair Bayesian mixture model for fair clustering with unknown number  
 524 of clusters and developed an efficient MCMC algorithm called FBC. A key advantage of FBC is its  
 525 ability to infer the number of clusters.

526 A problem not pursued in this work is the assignment of new data to the learned clusters. FBC  
 527 requires matched instances to be assigned to the same cluster, but the inferred matching map is only  
 528 available for the training data. To address this, one may approximate the learned matching map using  
 529 a parametric model and apply it to new test data. We leave this approach as future work.

540     **Ethics Statement** The fairness notion we consider in this study, i.e., group (or proportional) fairness,  
 541     is widely examined in recent literature. All the datasets we consider are publicly available. We  
 542     believe this research can contribute to avoid discriminatory results in clustering, rather than creating  
 543     new ethical concerns.

544     **Reproducibility Statement** For theoretical results, we document full proofs and mathematical  
 545     definitions for the stated theorems, in Appendix. For experimental results, we state implementation  
 546     details across the main body and Appendix, and further include the source files in the supplementary  
 547     materials.

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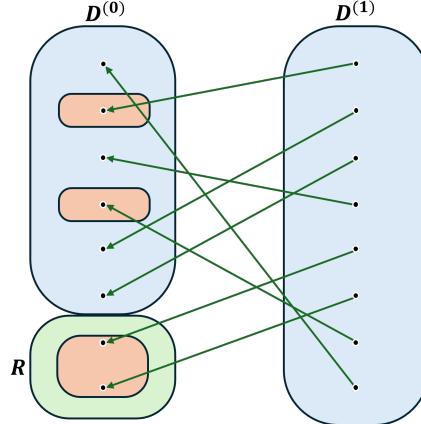
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APPENDIX

705 A DETAILS AND THEORIES FOR SECTION 2

706 A.1 HANDLING THE CASE OF  $r > 0$

709 As explained in Section 2.1.2, we need to resolve the issue that the matching map  $\mathbf{T}$  does not  
710 always corresponds to a fair  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$ , for the case of  $r > 0$ . That is, there exists  $\mathbf{Z}$  that satisfies  
711  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$  for some  $\mathbf{T} \in \mathcal{T}$  but is not fair. In turn, a sufficient condition of  $\mathbf{Z}$  with  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$   
712 for some  $\mathbf{T} \in \mathcal{T}$  to be fair is that  $|C_k^{(0)}|/n_0 = |C_k^{(0)} \cap R_{\mathbf{T}}|/r$ , where  $C_k^{(0)} = \{i : Z_i^{(0)} = k\}$  for  
713  $k \in [K]$  (see Proposition A.2 for the proof). That is, fairness of  $\mathbf{Z}$  depends on both  $\mathbf{T}$  and  $\mathbf{Z}^{(0)}$ ,  
714 which would make the computation of the posterior inference expensive.

715 Let  $\mathbb{P}_{n_0}$  and  $\mathbb{P}_R$  be the empirical distributions of  $\{X_i^{(0)}, i \in [n_0]\}$  and  $\{X_i^{(0)}, i \in R\}$ , respectively.  
716 If  $\mathbb{P}_{n_0}(\cdot) = \mathbb{P}_R(\cdot)$ , we have  $|C_k^{(0)}|/n_0 = |C_k^{(0)} \cap R|/r$ , and thus any fair  $\mathbf{Z}$  belongs to  $\mathcal{Z}_0^{\text{Fair}}$ .  
717 This observation suggests us to choose  $R$  such that  $\{X_i^{(0)}, i \in R\}$  represents the original data  
718  $\{X_i^{(0)}, i \in [n_0]\}$  well. Hence, as previously stated, we suggest two candidates of  $R$ , (i) a random  
719 subset and (ii) cluster centers. For (ii), the cluster centers can be found by  $K$ -medoids algorithm.  
720



736 Figure 5: An illustration on the modification for the case of  $r > 0$ . Orange-indicated points are  
737 upsampled indices from  $[n_0]$  to construct  $R$ .  
738

740 A.2 PROOFS

741 **Proposition 2.1** Assume that  $n_0 = n_1 = \bar{n}$ . Then, we have:  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}} \iff$  There exists a  
742 matching map  $\mathbf{T}$  such that  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}, \forall j \in [\bar{n}]$ .  
743

745 *Proof of Proposition 2.1.* See the proof of Proposition 2.2, as this proposition is a special case of  
746 Proposition 2.2, with  $\beta = 1$ .  $\square$   
747

748 **Proposition 2.2** Assume that  $n_1 = \beta n_0$  for some positive integer  $\beta$ . Then, we have:  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$   
749  $\iff$  There exists a matching map  $\mathbf{T}$  such that  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}, \forall j \in [n_1]$ .  
750

751 *Proof of Proposition 2.2.* ( $\implies$ ) Recall that  $C_k^{(0)} = \{i : Z_i^{(0)} = k\}$  and  $C_k^{(1)} = \{j : Z_j^{(1)} = k\}$ .  
752 Note that  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$  implies  $\beta|C_k^{(0)}| = |C_k^{(1)}|$  for all  $k \in [K]$ . Hence, for all  $k \in [K]$ , there exists  
753 an onto map  $\mathbf{T}_k$  from  $C_k^{(1)}$  to  $C_k^{(0)}$  such that  $|\mathbf{T}_k^{-1}(i)| = \beta$  for all  $i \in C_k^{(0)}$ . Letting  $\mathbf{T}(j) :=$   
754  $\sum_{k=1}^K \mathbf{T}_k(j) \mathbb{I}(j \in C_k^{(1)}), j \in [n_1]$  concludes the proof.  
755

( $\Leftarrow$ ) Suppose that there exists a matching map  $\mathbf{T}$  such that  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$  for all  $j \in [n_1]$ . Then, we have  $\beta|C_k^{(0)}| = |C_k^{(1)}|$  for all  $k \in [K]$ . Hence,  $\sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k)/n_0 = |C_k^{(0)}|/n_0 = \beta|C_k^{(0)}|/n_1 = |C_k^{(1)}|/n_1 = \sum_{j=1}^{n_1} \mathbb{I}(Z_j^{(1)} = k)/n_1$ , which implies  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$ .  $\square$

Propositions A.1 and A.2 below support the claims in Section 2.1.2. For enhanced readability, we first recall some notations/assumptions:

- $n_1 = \beta n_0 + r$ .
- $\mathbf{T} : [n_1] \rightarrow [n_0]$  is a function such that it is onto,  $|\mathbf{T}^{-1}(i)|$  is either  $\beta$  or  $\beta+1$  and  $|R_{\mathbf{T}}| = r$ , where  $R_{\mathbf{T}} = \{i : |\mathbf{T}^{-1}(i)| = \beta+1\}$ . Let  $\mathcal{T}$  be the set of all such matching maps (functions satisfying these conditions).
- Let  $R_{\mathbf{T}} = \{i : |\mathbf{T}^{-1}(i)| = \beta+1\}$  for a given  $\mathbf{T} : [n_1] \rightarrow [n_0]$ .
- For given  $Z_i^{(0)}, i \in [n_0]$  and  $Z_j^{(1)}, j \in [n_1]$ , we define  $C_k^{(0)} = \{i : Z_i^{(0)} = k\}$  and  $C_k^{(1)} = \{j : Z_j^{(1)} = k\}$  for  $k \in [K]$ .

**Proposition A.1.** Assume that  $r > 0$ . For a given fair  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$ , there exists a function  $\mathbf{T} \in \mathcal{T}$ .

*Proof of Proposition A.1.* Since  $\mathbf{Z} \in \mathcal{Z}^{\text{Fair}}$ , for all  $k \in [K]$  we have  $|C_k^{(1)}| = \frac{n_1}{n_0} |C_k^{(0)}|$ , which is an integer. Let  $k^* = \arg \min_k |C_k^{(0)}|$  and  $\alpha = \frac{r|C_{k^*}^{(0)}|}{n_0} \in \mathbb{N}$ . Then, we can construct  $\mathbf{T}_{k^*} : C_{k^*}^{(1)} \rightarrow C_{k^*}^{(0)}$  so that exactly  $\alpha$  elements of  $C_{k^*}^{(1)}$  have preimage size  $\beta+1$ , and the remaining  $|C_{k^*}^{(1)}| - \alpha$  have size  $\beta$ .

Next, for each  $l \neq k^*$ , set  $a_l = \frac{|C_l^{(0)}|}{|C_{k^*}^{(0)}|} \in \mathbb{N}$ , so that  $|C_l^{(0)}| = a_l |C_{k^*}^{(0)}|$  and  $|C_l^{(1)}| = a_l |C_{k^*}^{(1)}|$ . Define  $\alpha_l = a_l \alpha$ , and similarly construct  $\mathbf{T}_l : C_l^{(1)} \rightarrow C_l^{(0)}$  so that exactly  $\alpha_l$  points in  $C_l^{(1)}$  have preimage size  $\beta+1$ , and the remaining  $|C_l^{(1)}| - \alpha_l$  have size  $\beta$ .

Finally, let  $\mathbf{T}(j) := \sum_{k=1}^K \mathbf{T}_k(j) \mathbb{I}(j \in C_k^{(1)})$ ,  $j \in [n_1]$ . Then,  $\mathbf{T}$  is onto, each  $\mathbf{T}_k$  has size  $\beta$  or  $\beta+1$ , and  $|R_{\mathbf{T}}| = \sum_{k=1}^K \alpha_k = \alpha \sum_{k=1}^K a_k = \alpha \cdot \frac{n_0}{|C_{k^*}^{(0)}|} = \frac{r|C_{k^*}^{(0)}|}{n_0} \cdot \frac{n_0}{|C_{k^*}^{(0)}|} = r$ , which completes the proof.  $\square$

**Proposition A.2.** Assume that  $r > 0$ . For a given  $\mathbf{T}$ , let  $\mathbf{Z}$  with  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ ,  $j \in [n_1]$ . If  $\mathbf{T} \in \mathcal{T}$  satisfied  $|C_k^{(0)}|/n_0 = |C_k^{(0)} \cap R_{\mathbf{T}}|/r$  for all  $k \in [K]$ , we have that  $\mathbf{Z} \in \mathcal{Z}_0^{\text{Fair}}$ .

*Proof of Proposition A.2.* Fix a  $k \in [K]$ . By definition of  $\mathbf{Z}$  that  $C_k^{(1)} = \{j : Z_j^{(1)} = k\} = \{j : Z_{\mathbf{T}(j)}^{(0)} = k\}$ , we have that

$$|C_k^{(1)}| = \sum_{i \in C_k^{(0)}} |\mathbf{T}^{-1}(i)| = \sum_{i \in C_k^{(0)}} (\beta + \mathbb{I}(i \in R_{\mathbf{T}})) = \beta |C_k^{(0)}| + |C_k^{(0)} \cap R_{\mathbf{T}}|.$$

By the sufficient condition  $|C_k^{(0)} \cap R_{\mathbf{T}}| = (r/n_0) |C_k^{(0)}|$  and since  $n_1 = \beta n_0 + r$ , it follows that

$$|C_k^{(1)}| = \beta |C_k^{(0)}| + \frac{r}{n_0} |C_k^{(0)}| = \frac{\beta n_0 + r}{n_0} |C_k^{(0)}| = \frac{n_1}{n_0} |C_k^{(0)}|,$$

which concludes the proof.  $\square$

**Proposition A.3.** Assume that  $r > 0$ . Let  $\mathbf{T} \in \mathcal{T}$  and define  $\mathbf{Z}$  by  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ ,  $j \in [n_1]$ . Then, the fairness level  $\Delta(\mathbf{Z})$  is uniformly bounded as

$$\Delta(\mathbf{Z}) \leq \frac{r(n_0 - r)}{n_0 n_1} = \max_{\mathbf{Z}} \Delta(\mathbf{Z}),$$

where the maximum (i.e., the worst-case) is attained when all instances in  $R_{\mathbf{T}}$  are assigned to the same cluster.

810  
811 *Proof.* For  $k \in [K]$ , let  $C_k^{(1)} = \{j : Z_j^{(1)} = k\}$  and define  $p_k^{(0)} := \frac{|C_k^{(0)}|}{n_0}$  and  $p_k^{(1)} := \frac{|C_k^{(1)}|}{n_1}$ . By the  
812 definition of  $\mathbf{Z}$ , we have  $C_k^{(1)} = \{j : Z_j^{(1)} = k\} = \{j : Z_{\mathbf{T}(j)}^{(0)} = k\}$ , so

$$813 \quad |C_k^{(1)}| = \sum_{i \in C_k^{(0)}} |\mathbf{T}^{-1}(i)| = \sum_{i \in C_k^{(0)}} (\beta + \mathbb{I}(i \in R_{\mathbf{T}})) = \beta |C_k^{(0)}| + |C_k^{(0)} \cap R_{\mathbf{T}}|. \\ 814 \quad 815$$

816 Hence

$$817 \quad p_k^{(0)} - p_k^{(1)} = \frac{|C_k^{(0)}|}{n_0} - \frac{\beta |C_k^{(0)}| + |C_k^{(0)} \cap R_{\mathbf{T}}|}{n_1} = \frac{r}{n_1} p_k^{(0)} - \frac{|C_k^{(0)} \cap R_{\mathbf{T}}|}{n_1}. \quad (18) \\ 818 \quad 819$$

820 Define  $q_k := \frac{|C_k^{(0)} \cap R_{\mathbf{T}}|}{r}$ ,  $k \in [K]$ . Then  $q_k \geq 0$  and  $\sum_{k=1}^K q_k = 1$ , so  $\mathbf{q} = (q_1, \dots, q_K)$  is a  
821 probability vector. Then, from Equation (18) we can write

$$822 \quad p_k^{(0)} - p_k^{(1)} = \frac{r}{n_1} (p_k^{(0)} - q_k), k \in [K], \quad (19) \\ 823 \quad 824$$

825 and therefore we have

$$826 \quad \Delta(\mathbf{Z}) = \frac{1}{2} \sum_{k=1}^K |p_k^{(0)} - p_k^{(1)}| = \frac{r}{2n_1} \sum_{k=1}^K |p_k^{(0)} - q_k| = \frac{r}{2n_1} \|\mathbf{p}^{(0)} - \mathbf{q}\|_1, \quad (20) \\ 827 \quad 828 \quad 829$$

830 where  $\mathbf{p}^{(0)} = (p_1^{(0)}, \dots, p_K^{(0)})^\top$ . Since  $\mathbf{p}^{(0)}$  and  $\mathbf{q}$  are probability vectors, we have  $\|\mathbf{p}^{(0)} - \mathbf{q}\|_1 \leq 2$ .  
831 and thus  $\Delta(\mathbf{Z}) \leq \frac{r}{n_1}$ .

832 Moreover, the  $\ell_1$  distance  $\|\mathbf{p}^{(0)} - \mathbf{q}\|_1$  is maximized over all probability vectors  $\mathbf{q}$  at an extreme  
833 point of the simplex, that is, at some  $\mathbf{q} = e_{k^*}$  with  $(e_{k^*})_{k^*} = 1$  and  $(e_{k^*})_k = 0$  for  $k \neq k^*$ . Such  
834 a vector corresponds exactly to the case where all indices in  $R_{\mathbf{T}}$  belong to a single cluster  $C_{k^*}^{(0)}$ ,  
835 that is,  $R_{\mathbf{T}} \subset C_{k^*}^{(0)}$ . Hence this configuration yields the worst-case (maximal) value of  $\Delta(\mathbf{Z})$ , so it  
836 suffices to focus on this case.

837 Under  $R_{\mathbf{T}} \subset C_{k^*}^{(0)}$ , we have  $|C_{k^*}^{(0)} \cap R_{\mathbf{T}}| = r$ ,  $|C_k^{(0)} \cap R_{\mathbf{T}}| = 0$  for  $k \neq k^*$ . Plugging this into  
838 Equation (18) yields  $p_{k^*}^{(0)} - p_{k^*}^{(1)} = \frac{r}{n_1} p_{k^*}^{(0)} - \frac{r}{n_1} = \frac{r}{n_1} (p_{k^*}^{(0)} - 1)$ , and for  $k \neq k^*$ , we have  
839  $p_k^{(0)} - p_k^{(1)} = \frac{r}{n_1} p_k^{(0)}$ . Therefore, we get  $|p_{k^*}^{(0)} - p_{k^*}^{(1)}| = \frac{r}{n_1} |p_{k^*}^{(0)} - 1| = \frac{r}{n_1} (1 - p_{k^*}^{(0)})$ , and for  
840  $k \neq k^*$ , we have  $|p_k^{(0)} - p_k^{(1)}| = \frac{r}{n_1} p_k^{(0)}$ . Using the definition of  $\Delta(\mathbf{Z})$ ,

$$841 \quad \Delta(\mathbf{Z}) = \frac{1}{2} \sum_{k=1}^K |p_k^{(0)} - p_k^{(1)}| = \frac{1}{2} \left( \frac{r}{n_1} (1 - p_{k^*}^{(0)}) + \sum_{k \neq k^*} \frac{r}{n_1} p_k^{(0)} \right). \\ 842 \quad 843$$

844 Since  $\sum_{k \neq k^*} p_k^{(0)} = 1 - p_{k^*}^{(0)}$ , we obtain

$$845 \quad \Delta(\mathbf{Z}) = \frac{1}{2} \cdot \frac{r}{n_1} \left( 1 - p_{k^*}^{(0)} + 1 - p_{k^*}^{(0)} \right) = \frac{r}{n_1} (1 - p_{k^*}^{(0)}). \\ 846 \quad 847$$

848 Finally, because  $R_{\mathbf{T}} \subset C_{k^*}^{(0)}$  and  $|R_{\mathbf{T}}| = r$ , we have  $|C_{k^*}^{(0)}| \geq r$ , so that  $p_{k^*}^{(0)} = \frac{|C_{k^*}^{(0)}|}{n_0} \geq \frac{r}{n_0}$ . Hence

$$849 \quad \Delta(\mathbf{Z}) = \frac{r}{n_1} (1 - p_{k^*}^{(0)}) \leq \frac{r}{n_1} \left( 1 - \frac{r}{n_0} \right), \\ 850 \quad 851$$

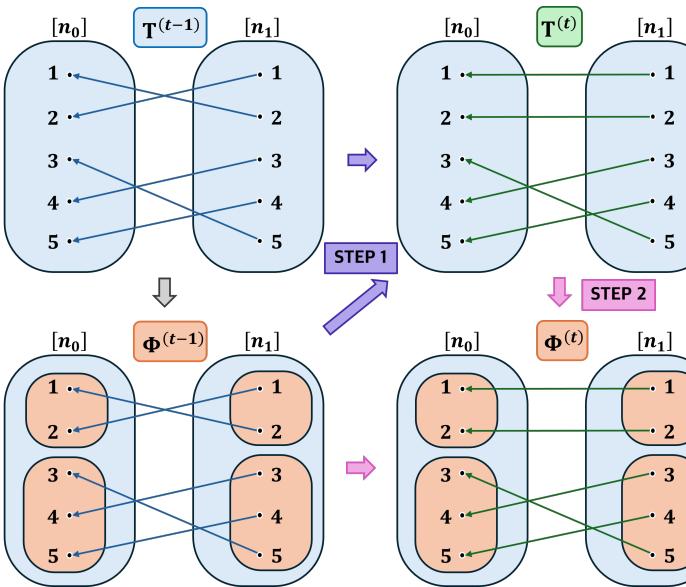
852 which completes the proof. □

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864 A.3 FOR NON-PERFECT FAIRNESS  
865866 **Proposition A.4.** Assume that  $r = 0$ . Let  $\mathbf{T}$  and  $\mathbf{T}_0$  be the maps defined in Section 2.2 for a given  
867  $m \leq n_1$ . Then, for any  $\mathbf{Z}$  satisfying  $Z_j^{(1)} = Z_{\mathbf{T}(j)}^{(0)}$ ,  $j \in [n_1] \setminus E$  and  $Z_j^{(1)} = Z_{\mathbf{T}_0(j)}^{(0)}$ ,  $j \in E$ , we  
868 have that  $\mathbf{Z} \in \mathcal{Z}_{m/n_1}^{\text{Fair}}$ .  
869870 *Proof of Proposition A.4.* We first note the following two facts: (i)  $\sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i \in [n_0]} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j \in [n_1]} \mathbb{I}(Z_{\mathbf{T}(j)}^{(0)} = k) \right| = 0$  for any given  $\mathbf{T}$  due to the assumption  $r = 0$ . (ii) For any  $\mathbf{T}$   
871 and  $\mathbf{T}_0$ , there exist nonnegative integers  $m_1, \dots, m_K$  with  $\sum_k m_k = 2m$  such that for each  $k$ ,  
872  $\left| \sum_{j \in E} \mathbb{I}(Z_{\mathbf{T}(j)}^{(0)} = k) - \sum_{j \in E} \mathbb{I}(Z_{\mathbf{T}_0(j)}^{(0)} = k) \right| = m_k$ . Therefore,  
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874 
$$\begin{aligned} \Delta(\mathbf{Z}) &= \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i \in [n_0]} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j \in [n_1]} \mathbb{I}(Z_j^{(1)} = k) \right| \\ &= \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i \in [n_0]} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j \in [n_1] \setminus E} \mathbb{I}(Z_j^{(1)} = k) - \frac{1}{n_1} \sum_{j \in E} \mathbb{I}(Z_j^{(1)} = k) \right| \\ &= \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i \in [n_0]} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j \in [n_1] \setminus E} \mathbb{I}(Z_{\mathbf{T}(j)}^{(0)} = k) - \frac{1}{n_1} \sum_{j \in E} \mathbb{I}(Z_{\mathbf{T}_0(j)}^{(0)} = k) \right| \\ &\leq \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i \in [n_0]} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j \in [n_1]} \mathbb{I}(Z_{\mathbf{T}(j)}^{(0)} = k) \right| \\ &\quad + \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_1} \sum_{j \in E} \mathbb{I}(Z_{\mathbf{T}(j)}^{(0)} = k) - \frac{1}{n_1} \sum_{j \in E} \mathbb{I}(Z_{\mathbf{T}_0(j)}^{(0)} = k) \right| \\ &= 0 + \frac{1}{2} \frac{1}{n_1} \sum_{k=1}^K m_k = \frac{m}{n_1}. \end{aligned}$$

895 Thus  $\Delta(\mathbf{Z}) \leq m/n_1$ , so  $\mathbf{Z} \in \mathcal{Z}_{m/n_1}^{\text{Fair}}$ . □  
896897 A.4 RELATIONSHIP BETWEEN  $\Delta$  AND  $\text{BAL}$   
898899 Two fairness measures -  $\Delta$  and  $\text{Bal}$  - that we consider in this work are closely related, as proven in  
900 Kim et al. (2025b). For readers' sake, we provide a rigorous statement below.901 **Proposition A.5** (Proposition 4.2. of Kim et al. (2025b)). Suppose  $n_0 \leq n_1$ . For given cluster  
902 assignments  $Z_i^{(0)}$ ,  $i \in [n_0]$  and  $Z_j^{(1)}$ ,  $j \in [n_1]$ , we have  $\max_{k \in [K]} \left| \frac{\sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k)/n_0}{\sum_{j=1}^{n_1} \mathbb{I}(Z_j^{(1)} = k)/n_1} - \frac{n_0}{n_1} \right| \leq c\Delta$ ,  
903 where  $c = \frac{n_0}{n_1} \max_{k \in [K]} \frac{n_1}{\sum_{j=1}^{n_1} \mathbb{I}(Z_j^{(1)} = k)}$ . This implies that the difference between balance and the  
904 balance of perfect fairness ( $= n_0/n_1$ ) is bounded by  $\Delta$ .  
905906 Furthermore, experimental results in Section 5 also numerically support the use of  $\Delta$  in the sense  
907 that controlling  $\Delta$  effectively controls  $\text{Bal}$ .  
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918 B DETAILS OF FBC  
919920 B.1 HIGH-LEVEL UNDERSTANDING  
921922 **Flow diagram** We provide a flow diagram of FBC in Figure 6, which is a visualization of Algo-  
923 rithm 1. Note that it focuses on the perfect fairness case with  $n_0 = n_1$  for simplicity. FBC iteratively  
924 obtains MCMC samples by a Gibbs sampler: STEP 1 provides a matching function at the time step  
925 ( $t$ ), and STEP 2 yields a mixture parameter at the time step ( $t$ ).946 Figure 6: A flow diagram of FBC.  
947948 **Understanding FBC in view of fairlets** For simplicity, let ignore  $\mathbf{T}_0$  and  $E$ , and consider only  
949 the perfect-fairness case with  $\mathbf{T}$ . In this setting,  $\mathbf{T}$  can be seen as a map to build fairlets, and we treat  
950  $\mathbf{T}$  as a random variable to perform posterior inference. Inspired by MFM (Miller & Harrison, 2018)  
951 which obtains MCMC samples of model parameters, we integrate the MH algorithm into the original  
952 MCMC procedure to yield posterior samples of  $\mathbf{T}$ . We also theoretically validate this proposed  
953 algorithm in Section B.3. Moreover, for reasonable initialization and prior for  $\mathbf{T}$ , we incorporate  
954 ideas from optimal transport inspired of the the fairlet-based approaches. A crucial difference is  
955 that, we update  $\mathbf{T}$  for higher clustering utility (e.g., higher log-likelihood or lower clustering cost)  
956 rather than using a fixed  $\mathbf{T}$ , as fairlet-based approaches do.957 B.2 DETAILS OF STEP 1 (SAMPLING  $\mathbf{T}, \mathbf{T}_0, E$ ) IN SECTION 4  
958959 In this section, we first provide a detailed explanation about the calculation of  $\alpha'(\mathbf{T}', \mathbf{T}'_0, E)$  in  
960 Equation (17). First, we have that

$$\begin{aligned}
 \alpha'(\mathbf{T}', \mathbf{T}'_0, E') &= \frac{p(\mathbf{T}', \mathbf{T}'_0, E' | \Phi, \mathcal{D}) q((\mathbf{T}', \mathbf{T}'_0, E') \rightarrow (\mathbf{T}, \mathbf{T}_0, E))}{p(\mathbf{T}, \mathbf{T}_0, E | \Phi, \mathcal{D}) q((\mathbf{T}, \mathbf{T}_0, E) \rightarrow (\mathbf{T}', \mathbf{T}'_0, E'))} \\
 &= \frac{p(\mathbf{T}', \mathbf{T}'_0, E') \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}', \mathbf{T}'_0, E') q((\mathbf{T}', \mathbf{T}'_0, E') \rightarrow (\mathbf{T}, \mathbf{T}_0, E))}{p(\mathbf{T}, \mathbf{T}_0, E) \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}, \mathbf{T}_0, E) q((\mathbf{T}, \mathbf{T}_0, E) \rightarrow (\mathbf{T}', \mathbf{T}'_0, E'))} \\
 &= \frac{e(\mathbf{T}') \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}', \mathbf{T}'_0, E')}{e(\mathbf{T}) \mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}, \mathbf{T}_0, E)},
 \end{aligned}$$

961 where the last equality holds since  
962

963 
$$q((\mathbf{T}', \mathbf{T}'_0, E') \rightarrow (\mathbf{T}, \mathbf{T}_0, E)) = q((\mathbf{T}, \mathbf{T}_0, E) \rightarrow (\mathbf{T}', \mathbf{T}'_0, E'))$$

964 and  $p(\mathbf{T}', \mathbf{T}'_0, E')/p(\mathbf{T}, \mathbf{T}_0, E) = e(\mathbf{T}')/e(\mathbf{T})$ , because the priors of  $\mathbf{T}_0$  and  $E$  are uniform.

972 For the likelihood ratio, if we use a conjugate prior which enables the calculation of marginal likelihood, we have  
 973

$$\frac{\mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}', \mathbf{T}'_0, E')}{\mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}, \mathbf{T}_0, E)} = \frac{\prod_{c \in \mathcal{C}} m(X^c | \mathbf{T}', \mathbf{T}'_0, E')}{\prod_{c \in \mathcal{C}} m(X^c | \mathbf{T}, \mathbf{T}_0, E)},$$

977 where

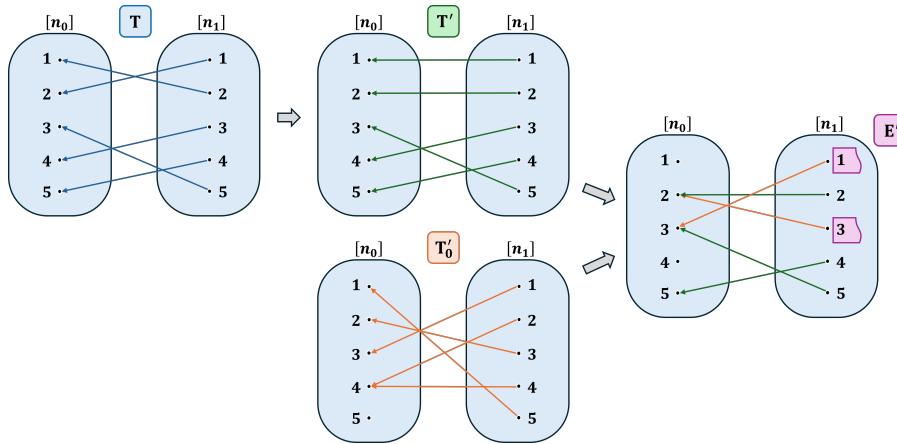
$$m(X^c | \mathbf{T}, \mathbf{T}_0, E) = \int_{\Theta} \left[ \prod_{i \in c} f(X_i^{(0)} | \phi_c) \prod_{j \in J(c; \mathbf{T}, \mathbf{T}_0, E)} f(X_j^{(1)} | \phi_c) \right] H(d\theta), \quad (21)$$

981  $J(c; \mathbf{T}, \mathbf{T}_0, E) := \{j \in E : \mathbf{T}_0(j) \in c\} \cup \{j \in [n_1] \setminus E : \mathbf{T}(j) \in c\}$  for  $c \in \mathcal{C}$  and  $X^c = \{X_i^{(0)} : i \in c\} \cup \{X_j^{(1)} : j \in J(c; \mathbf{T}, \mathbf{T}_0, E)\}$  for  $c \in \mathcal{C}$ . For a non-conjugate  $H$ , we have  
 982  
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$$\frac{\mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}', \mathbf{T}'_0, E')}{\mathcal{L}(\mathcal{D}; \Phi, \mathbf{T}, \mathbf{T}_0, E)} = \frac{\prod_{c \in \mathcal{C}} \left[ \prod_{i \in c} f(X_i^{(0)} | \phi_c) \prod_{j \in J(c; \mathbf{T}', \mathbf{T}'_0, E')} f(X_j^{(1)} | \phi_c) \right]}{\prod_{c \in \mathcal{C}} \left[ \prod_{i \in c} f(X_i^{(0)} | \phi_c) \prod_{j \in J(c; \mathbf{T}, \mathbf{T}_0, E)} f(X_j^{(1)} | \phi_c) \right]}.$$

984 Note that these calculations are derived from the equivalent representation in Section 3.1.  
 985

986 Next, we provide an illustration of the proposal from STEP 1 in Figure 7.  $\mathbf{T}'$  of the green line is  
 987 randomly swapped from  $\mathbf{T}$  of the blue line.  $\mathbf{T}'_0$  of the orange line is a random proposal.  $\mathbf{E}'$  of the  
 988 pink region is a random proposal of the given size. The final matching is visualized as the lines of  
 989 the final diagram.  
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1009 Figure 7: An illustration of the proposal from STEP 1.  
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### 1112 B.3 DETAILS OF STEP 2 (SAMPLING $\Phi$ ) IN SECTION 4

1113 Here, we consider the following two cases. When  $m(X^c | \mathbf{T}, \mathbf{T}_0, E)$  can be easily computed (e.g.,  
 1114  $H$  is a conjugate prior), we sample  $\mathcal{C} \sim p(\mathcal{C} | \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E)$ . Otherwise, when  $m(X^c | \mathbf{T}, \mathbf{T}_0, E)$  is  
 1115 intractable, we sample  $(\mathcal{C}, \phi) \sim p(\mathcal{C}, \phi | \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E)$ . If the marginal likelihood is computable, a  
 1116 direct adaptation of Algorithm 3 from Neal (2000); MacEachern & Müller (1998) is applicable.  
 1117 Otherwise, when the marginal likelihood is not computable, Algorithm 8 from Neal (2000) can be  
 1118 applied. Wherever the meaning is clear, we abbreviate  $J(c; \mathbf{T}, \mathbf{T}_0, E)$  by  $J(c)$  in this section.  
 1119

1120 **Conjugate prior** The modification of Algorithm 3 for FBC is described as below.  
 1121

1. Initialize  $\mathcal{C} = \{[n_0]\}$  (i.e., a single cluster)
2. Repeat the following steps  $N$  times, to obtain  $N$  samples. For  $i = 1, \dots, n_0$ : Remove  
 element  $i \in [n_0]$  and its matched elements in  $J(\{i\}; \mathbf{T}, \mathbf{T}_0, E) := \{j \in E : \mathbf{T}_0(j) = i\} \cup \{j \in [n_1] \setminus E : \mathbf{T}(j) = i\}$  from  $\mathcal{C}$ . Then, place them

1026           • to  $c' \in \mathcal{C} \setminus i$  with probability  
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 1028            $\propto (|c'| + \gamma) \frac{m(X^{c'} \cup X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)}{m(X^{c'} | \mathbf{T}, \mathbf{T}_0, E)}$   
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 1030           where  $X^{\{i\}} := \{X_i^{(0)}\} \cup \{X_j^{(1)} : j \in J(\{i\})\}$ .  
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 1032           • to a new cluster with probability  
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 1034            $\propto \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)$   
 1035  
 1036           where  $t$  is a number of clusters when  $X^{\{i\}}$  are removed.

1037           **Proposition B.1.** *The above modification of Algorithm 3 of Neal (2000) is a valid Gibbs sampler.*

1040           *Proof of Proposition B.1.* The posterior density can be formulated as follows:

$$\begin{aligned} p(\mathcal{C} | \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto p(\mathcal{C}) \cdot p\left(X_{1:n_0}^{(0)}, X_{1:n_1}^{(1)} | \mathcal{C}, \mathbf{T}, \mathbf{T}_0, E\right) \\ &= V_{n_0}(t) \prod_{c \in \mathcal{C}} \gamma^{|c|} \cdot \prod_{c \in \mathcal{C}} m(X^c | \mathbf{T}, \mathbf{T}_0, E) \end{aligned}$$

1047           To justify the proposed modification of Algorithm 3, we only need to calculate the probabilities  
 1048           of placing  $X_i^{(0)}$  and its matched elements  $\{X_j^{(1)} : j \in J(c(i))\}$ : (i) to an existing partition  $c'$ , or  
 1049  
 1050           (ii) to a new cluster. Let  $\mathcal{C}_{-i}$  be the collection of clusters where  $X_i^{(0)}$  and its matched elements  
 1051            $\{X_j^{(1)} : j \in J(\{i\})\}$  are removed from  $\mathcal{C}$ . The calculation can be done as follows:

1053           (i) to existing  $c'$ :

1055           The term  $\gamma^{|c'|}$  in the prior term  $p(\mathcal{C}) \propto V_{n_0}(t) \prod_{c \in \mathcal{C}} \gamma^{|c|}$  changes to  $\gamma^{|c'|+1}$  for this  
 1056           particular  $c'$ . The marginal likelihood  $m(X^{c'})$  changes to  $m(X^{c'} \cup X^{\{i\}})$  for this particular  
 1057            $c'$ . Hence, we have the following conditional probability:

$$\begin{aligned} p(i \rightarrow c' | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto \frac{\gamma^{|c'|+1}}{\gamma^{|c'|}} \frac{m(X^{c'} \cup X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)}{m(X^{c'} | \mathbf{T}, \mathbf{T}_0, E)} \\ &= (|c'| + \gamma) \frac{m(X^{c'} \cup X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)}{m(X^{c'} | \mathbf{T}, \mathbf{T}_0, E)} \end{aligned}$$

1064           (ii) to a new cluster:

1066           The prior term  $V_{n_0}(t) \prod_{c \in \mathcal{C}} \gamma^{|c|}$  changes into  $V_{n_0}(t+1) [\prod_{c \in \mathcal{C}} \gamma^{|c|}] \gamma$ . Hence, we have  
 1067           the following conditional probability:

$$\begin{aligned} p(i \rightarrow \text{new} | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E) \end{aligned}$$

1073           □

1074           **Non-conjugate prior** When using a non-conjugate prior, we can use Algorithm 8 instead of Algo-  
 1075           rithm 3. The outline of implementation of Algorithm 8 for FBC can be formulated similar to those  
 1076           of Algorithm 3, as below.

1077           1. Initialize  $\mathcal{C} = \{[n_0]\}$  (i.e., a single cluster) with  $\phi_{[n_0]} \sim H$ .

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2. Repeat the following steps  $N$  times, to obtain  $N$  samples. For  $i = 1, \dots, n_0$ : Remove element  $i \in [n_0]$  and its matched elements in  $J(\{i\})$  from  $\mathcal{C}$ . Then, generate  $m$  independent auxiliary variables  $\phi^{(1)}, \dots, \phi^{(m)} \sim H$ . Compute the assignment weights as:

$$w_{c'} = (|c'| + \gamma) \prod_{x \in X^{\{i\}}} f(x|\phi_{c'}), \quad c' \in \mathcal{C} \setminus i,$$

$$w_{\text{aux},h'} = \frac{\gamma}{m} \frac{V_{n_0}(t+1)}{V_{n_0}(t)} \prod_{x \in X^{\{i\}}} f(x|\phi^{(h')}), \quad h' = 1, \dots, m,$$

where  $X^{\{i\}} := \{X_i^{(0)}\} \cup \{X_j^{(1)} : j \in J(\{i\})\}$  and  $t$  is a number of clusters when  $X^{\{i\}}$  are removed. Then, place them

- to  $c' \in \mathcal{C} \setminus i$  with probability  $\propto w_{c'}$ , or
- to a new randomly chosen cluster  $h$  among  $m$  auxiliary components, with probability  $\propto w_{\text{aux},h}$ .

Then, discard all auxiliary variables which are not chosen.

**Proposition B.2.** *The above modification of Algorithm 8 of Neal (2000) is a valid Gibbs sampler.*

*Proof of Proposition B.2.* To justify the proposed modification of Algorithm 8, we only need to calculate the probabilities of replacing  $X^{\{i\}}$ : (i) to an existing partition  $c'$ , or (ii) to a new cluster.

The calculation can be done as follows:

(i) to existing  $c'$ :

The term  $\gamma^{|c'|}$  in the prior term  $p(\mathcal{C}) \propto V_{n_0}(t) \prod_{c \in \mathcal{C}} \gamma^{|c|}$  changes to  $\gamma^{|c'|+1}$  for this particular  $c'$ . The likelihood is multiplied by  $\prod_{x \in X^{\{i\}}} f(x|\phi_{c'})$  for this particular  $c'$ . Hence, we have the following conditional probability:

$$\begin{aligned} p(i \rightarrow c' | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto \frac{\gamma^{|c'|+1}}{\gamma^{|c'|}} \prod_{x \in X^{\{i\}}} f(x|\phi_{c'}) \\ &= (|c'| + \gamma) \prod_{x \in X^{\{i\}}} f(x|\phi_{c'}). \end{aligned}$$

(ii) to a new cluster: A new cluster  $h$  is chosen uniformly among the auxiliary  $m$  components. Then, we have the following conditional probability by Monte-Carlo approximation:

$$\begin{aligned} p(i \rightarrow \text{new} | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E) \\ &= \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} \int_{\Theta} \left[ \prod_{x \in X^{\{i\}}} f(x|\phi) \right] H(d\phi) \\ &\approx \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} \frac{1}{m} \sum_{h'=1}^m \prod_{x \in X^{\{i\}}} f(x|\phi^{(h')}) \\ &= \sum_{h'=1}^m w_{\text{aux},h'}. \end{aligned}$$

From the fact that  $h$  is uniformly chosen among  $m$ -auxiliary components, we have the conditional probability to a new cluster  $h$  as follows:

$$\begin{aligned} p(i \rightarrow h | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) &\propto p(i \rightarrow h | i \rightarrow \text{new}, \cdot) p(i \rightarrow \text{new} | \mathcal{C}_{-i}, \mathcal{D}, \mathbf{T}, \mathbf{T}_0, E) \\ &\propto \frac{w_{\text{aux},h}}{\sum_{h'=1}^m w_{\text{aux},h'}} \cdot \sum_{h'=1}^m w_{\text{aux},h'} \\ &= w_{\text{aux},h}. \end{aligned}$$

□

1134     **The case when  $K$  is known** When to perform FBC with fixed  $K$ , we only need to consider a point  
 1135     mass prior for  $K$ . Let  $p_K(K) = \mathbb{I}(K = k_*)$  for some fixed  $k_*$ . Then, we have:  
 1136

$$1137 \quad V_{n_0}(t) = \sum_{k=1}^{\infty} \frac{k_{(t)}}{(\gamma k)^{(n_0)}} p_K(k) = \frac{(k_*)_{(t)}}{(\gamma k_*)^{(n_0)}} \mathbb{I}(t \leq k_*).$$

1140     For conjugate prior case:  
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- 1142       • probability to an existing cluster remains the same.
- 1143       • probability to a new cluster

$$1145 \quad \propto \gamma \frac{V_{n_0}(t+1)}{V_{n_0}(t)} m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E) = \gamma(k_* - t)_+ m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E).$$

1147     Hence, the probability to a new cluster vanishes when  $t$  reaches  $k_*$ .

1149     For non-conjugate prior case:  
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- 1151       • probability to an existing cluster remains the same.
- 1152       • probability to a new cluster

$$1154 \quad \propto \frac{\gamma}{m} (k_* - t)_+ \prod_{x \in X^{\{i\}}} f(x | \phi^{(h')}).$$

1156     Hence, the probability to a new cluster vanishes when  $t$  reaches  $k_*$ .

1158     **Proposition B.3.** *The above modifications of Algorithm 3, 8 of Neal (2000) is a valid Gibbs sampler  
 1159     for a finite mixture model with  $K = k_*$ .*

1160     *Proof.* Let  $E_i = \{j : Z_j^{(0)} = i\}$ , and let  $\mathcal{C}(\mathbf{Z})$  be the partition induced by  $\mathbf{Z}$ . By Dirichlet-  
 1162     multinomial conjugacy, we have:

$$1163 \quad p(\mathbf{Z}) = \int p(\mathbf{Z} | \boldsymbol{\pi}) d\boldsymbol{\pi} = \frac{\Gamma(k_* \gamma)}{\Gamma(\gamma)^{k_*}} \frac{\prod_{i=1}^{n_0} \Gamma(|E_i| + \gamma)}{\Gamma(n_0 + k_* \gamma)} = \frac{1}{(k_* \gamma)^{(n_0)}} \prod_{c \in \mathcal{C}(\mathbf{Z})} \gamma^{(|c|)},$$

1166     for  $\mathbf{Z} \in [k_*]^n$ .

1168     Therefore, for any partition  $\mathcal{C}$  of  $[n]$ , we have:

$$\begin{aligned} 1169 \quad p(\mathcal{C}) &= \sum_{\mathbf{Z} \in [k_*]^{n_0} : \mathcal{C}(\mathbf{Z}) = \mathcal{C}} p(\mathbf{Z}) \\ 1170 \quad &= \# \{ \mathbf{Z} \in [k_*]^{n_0} : \mathcal{C}(\mathbf{Z}) = \mathcal{C} \} \frac{1}{(\gamma k_*)^{(n_0)}} \prod_{c \in \mathcal{C}} \gamma^{(|c|)} \\ 1172 \quad &= \frac{(k_*)_{(t)}}{(\gamma k_*)^{(n_0)}} \prod_{c \in \mathcal{C}} \gamma^{(|c|)}, \end{aligned}$$

1177     where  $t = |\mathcal{C}|$ . □  
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1188 **C EXTENSION OF FBC FOR A MULTINARY SENSITIVE ATTRIBUTE**  
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1190 This section explains that FBC can be modified for the case of a multinary sensitive attribute (i.e.,  
1191 the number of groups  $\geq 3$ ). For simplicity, we consider three sensitive groups. Extension to more  
1192 than three groups can be done similarly.  
1193

1194 Let  $\mathcal{D}^{(2)} = \{X_i^{(2)}\}_{i=1}^{n_2}$ , along with existing  $\mathcal{D}^{(0)}, \mathcal{D}^{(1)}$ . Assume that  $n_0 \leq \min\{n_1, n_2\}$ . Similar to  
1195 the binary sensitive case, we consider  $\mathbf{T}_1 : [n_1] \rightarrow [n_0]$  and  $\mathbf{T}_2 : [n_2] \rightarrow [n_0]$  as random matching  
1196 maps from  $\mathcal{D}^{(1)}$  to  $\mathcal{D}^{(0)}$  and from  $\mathcal{D}^{(2)}$  to  $\mathcal{D}^{(0)}$ , respectively. We also consider arbitrary functions  
1197  $\mathbf{T}_{01} : [n_1] \rightarrow [n_0]$  and  $\mathbf{T}_{02} : [n_2] \rightarrow [n_0]$  and arbitrary subsets  $E_1 \in [n_1], E_2 \in [n_2]$  of sizes  $m_1$   
1198 and  $m_2$ . Let  $\mathcal{C}$  be a partition of  $[n_0]$  induced by  $\mathbf{Z}$  such that  $Z_i^{(0)} | \boldsymbol{\pi} \stackrel{\text{i.i.d.}}{\sim} \text{Categorical}(\cdot | \boldsymbol{\pi}), \forall i \in [n_0]$ .  
1199 Then, similar to Section 3.1, we consider the model  
1200

$$\begin{aligned} \phi_c &\stackrel{\text{i.i.d.}}{\sim} H, c \in \mathcal{C} \\ X_i^{(0)} &\stackrel{\text{ind}}{\sim} f(\cdot | \phi_c), i \in c \\ X_j^{(1)} &\stackrel{\text{ind}}{\sim} \begin{cases} f(\cdot | \phi_c) & \forall j \in [n_1] \setminus E_1 \text{ s.t. } \mathbf{T}_1(j) \in c \\ f(\cdot | \phi_c) & \forall j \in E_1 \text{ s.t. } \mathbf{T}_{01}(j) \in c \end{cases} \\ X_j^{(2)} &\stackrel{\text{ind}}{\sim} \begin{cases} f(\cdot | \phi_c) & \forall j \in [n_2] \setminus E_2 \text{ s.t. } \mathbf{T}_2(j) \in c \\ f(\cdot | \phi_c) & \forall j \in E_2 \text{ s.t. } \mathbf{T}_{02}(j) \in c \end{cases} \end{aligned}$$

1201 The inference algorithm can be also modified accordingly. Furthermore,  $\Delta(\mathbf{Z})$  is also generalized  
1202 as follows.  $G$   
1203

1204 **Fairness measure for a multinary sensitive attribute** Let  $B$  be the number of sensitive groups.  
1205 For  $b \in \{0, 1, \dots, B-1\}$ , let  $n_b$  be the number of samples in group  $b$ , and denote  $\{Z_i^{(b)}\}_{i=1}^{n_b}$  as the  
1206 cluster assignments of group  $b$ . Then  $\Delta(\mathbf{Z})$  is generalized as:  
1207

$$\Delta(\mathbf{Z}) := \frac{1}{2(B-1)} \sum_{k=1}^K \sum_{b=1}^{B-1} \left| \frac{1}{n_0} \sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_b} \sum_{j=1}^{n_b} \mathbb{I}(Z_j^{(b)} = k) \right| \in [0, 1]$$

1208 The  $\text{Bal}$  is also generalized as:  $\text{Bal} := \min_{k \in [K]} \text{Bal}_k$  where  
1209

$$\text{Bal}_k := \min_{b_1 \neq b_2} \left\{ \frac{|C_k^{(b_1)}|}{|C_k^{(b_2)}|}, \frac{|C_k^{(b_2)}|}{|C_k^{(b_1)}|} \right\},$$

1210 where  $C_k^{(b)}$  denotes the set of samples in group  $b$  assigned to the  $k^{\text{th}}$  cluster. Note that the above  
1211 formulation of  $\Delta(\mathbf{Z})$  with  $B = 2$  coincides with the definition of  $\Delta(\mathbf{Z})$  in the binary sensitive  
1212 case, which is defined in Equation (6). Proposition C.1 below further shows that FBC can control  
1213 the fairness level  $\Delta(\mathbf{Z})$  for a multinary sensitive attribute.  
1214

1215 **Proposition C.1.** Denote  $n_0, n_1$ , and  $n_2$  as the number of samples in three sensitive groups. Let  
1216  $\mathbf{T}_1 : [n_1] \rightarrow [n_0]$  and  $\mathbf{T}_2 : [n_2] \rightarrow [n_0]$  be matching maps from groups 1 and 2 to group 0. Consider  
1217 arbitrary functions  $\mathbf{T}_{01} : [n_1] \rightarrow [n_0], \mathbf{T}_{02} : [n_2] \rightarrow [n_0]$  and arbitrary subsets  $E_1 \in [n_1], E_2 \in$   
1218  $[n_2]$  of sizes  $m_1$  and  $m_2$ . Suppose that the assignment  $\mathbf{Z}$  satisfies:  
1219

$$\begin{aligned} \bullet \quad & Z_j^{(1)} = Z_{\mathbf{T}_1(j)}^{(0)} \text{ for } j \in [n_1] \setminus E_1 \text{ and } Z_j^{(1)} = Z_{\mathbf{T}_{01}(j)}^{(0)} \text{ for } j \in E_1, \\ \bullet \quad & Z_j^{(2)} = Z_{\mathbf{T}_2(j)}^{(0)} \text{ for } j \in [n_2] \setminus E_2 \text{ and } Z_j^{(2)} = Z_{\mathbf{T}_{02}(j)}^{(0)} \text{ for } j \in E_2. \end{aligned}$$

1220 Then, we have  
1221

$$\Delta(\mathbf{Z}) \leq \frac{1}{2} \left( \frac{m_1}{n_1} + \frac{m_2}{n_2} \right).$$

1222 *Proof of Proposition C.1.* We investigate all three pairs among the three groups: (0, 1), (0, 2), and  
1223 (1, 2).  
1224

1242 (i) Between groups 0 and 1: Since  $Z_j^{(1)} = Z_{\mathbf{T}_1(j)}^{(0)}$  for  $j \in [n_1] \setminus E_1$ , we have the following inequality  
 1243 utilizing the proof of Proposition A.4,  
 1244

$$1245 \quad 1246 \quad 1247 \quad \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_1} \sum_{j=1}^{n_1} \mathbb{I}(Z_j^{(1)} = k) \right| \leq \frac{m_1}{n_1}.$$

1248 (ii) Between groups 0 and 2: Similarly, we have  
 1249

$$1250 \quad 1251 \quad 1252 \quad 1253 \quad \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_2} \sum_{j=1}^{n_2} \mathbb{I}(Z_j^{(2)} = k) \right| \leq \frac{m_2}{n_2}.$$

1254 Combining the two terms: Taking the average, we get:  
 1255

$$1256 \quad 1257 \quad 1258 \quad 1259 \quad \Delta(\mathbf{Z}) = \frac{2}{2(3-1)} \sum_{b=1}^2 \left( \frac{1}{2} \sum_{k=1}^K \left| \frac{1}{n_0} \sum_{i=1}^{n_0} \mathbb{I}(Z_i^{(0)} = k) - \frac{1}{n_b} \sum_{j=1}^{n_b} \mathbb{I}(Z_j^{(b)} = k) \right| \right) \\ 1260 \quad 1261 \quad 1262 \quad \leq \frac{1}{2} \left( \frac{m_1}{n_1} + \frac{m_2}{n_2} \right).$$

1263  $\square$

1264 Note that we use this extended approach for BANK dataset with three sensitive groups in our ex-  
 1265 periments. See Section E.3 for the results showing that FBC works well for a multinary sensitive  
 1266 attribute.  
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1296 **D HIERARCHICAL PRIOR ON  $K$  WHEN  $K$  IS UNKNOWN**  
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1298 Here, we discuss how to consider a hierarchical prior on  $K$ , to make the sampling of  $K$  robust. A  
1299 simple idea is to consider a Beta prior on  $\kappa$ , where the prior of  $K$  is  $\text{Geometric}(\kappa)$ . Then, we can  
1300 choose one from the following two options when considering posterior inference with varying  $\kappa$ .  
1301 For simplicity, we utilize the  $\kappa$ -marginalized version in our experiments.  
1302

1303 **Marginalize  $\kappa$**  One simple idea is to marginalize  $\kappa$ , and consider the corresponding distribution  
1304 of  $K$ .  
1305

$$\kappa \sim \text{Beta}(a, b)$$

$$K|\kappa \sim \text{Geometric}(\kappa)$$

1308 We can marginalize the above hierarchy as follows:  
1309

$$\begin{aligned} \bar{p}_K(k) &= \int p_K(k|\kappa)p(\kappa)d\kappa \\ &= \int_0^1 \kappa(1-\kappa)^{k-1} \frac{\kappa^{a-1}(1-\kappa)^{b-1}}{B(a, b)} d\kappa \\ &= \frac{B(a+1, b+k-1)}{B(a, b)}. \end{aligned}$$

1317 Approximately for large  $k$ ,  $\bar{p}_K(k) \sim k^{-(a+1)}$ , which makes  $\mathbb{E}[K] < \infty$  when  $a > 1$ . Considering a  
1318 uniform prior for  $\kappa$  is equivalent with  $\text{Beta}(1, 1)$ , resulting in  $\mathbb{E}[K] = \infty$ .  
1319

1320 Note that, this is a simple change of the prior of  $K$ , which does not affect the procedure of FBC at  
1321 all. That is, we just alter the term  $p_K$  as  $\bar{p}_K$ .  
1322

1323 **Sample  $\kappa$**  An alternative is to sample  $\kappa$ . To do so, we need to investigate whether the sampling of  
1324  $\kappa$  can be well integrated to the current formulation of FBC. We have:  
1325

$$p(\kappa|K) \propto \kappa^{a-1}(1-\kappa)^{b-1} \times \kappa(1-\kappa)^{K-1} = \kappa^a(1-\kappa)^{b+K-2} \sim \text{Beta}(a+1, b+K-1)$$

1326 Then, the posterior of  $K$  given partition  $\mathcal{C}$  can be yielded as:  
1327

$$p(K|\mathcal{C}, \kappa) \propto \kappa(1-\kappa)^{K-1} \frac{(K)_t}{(\gamma K)^{(n)}}$$

1330 Hence, we can define a similar term to  $V_n(t)$  as:  
1331

$$V_n^{(\kappa)}(t) := \sum_{k=1}^{\infty} \kappa(1-\kappa)^{K-1} \frac{(k)_t}{(\gamma k)^{(n)}}$$

1334 Finally, we get  
1335

$$p(\mathcal{C}|\kappa) = V_n^{(\kappa)}(t) \prod_{c \in \mathcal{C}} \gamma^{(|c|)}$$

1338 We here can simply use a Gibbs sampler for  $\kappa$  as well as other parameters. That is, we update  $\kappa$   
1339 from:  
1340

$$p(\kappa|\mathcal{C}) \propto p(\kappa)V_n^{(\kappa)}(t)$$

1341 Note that this update requires a proper sampling algorithm such as the MH algorithm.  
1342

- 1343 • Proposal:  $\kappa' \sim \text{Beta}(a', b')$   
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1350 **E EXPERIMENTS**  
13511352 **E.1 DATASETS**  
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1354 1. Toy dataset: We build a 2D toy dataset from a 6-component Gaussian mixture model with  
1355 unit covariance matrix  $\mathbb{I}_2$ . For  $\mathcal{D}^{(0)}$ , we draw 600 samples from each  $\mathcal{N}([-5, -30], \mathbb{I}_2)/3 +$   
1356  $\mathcal{N}([-5, 0], \mathbb{I}_2)/3 + \mathcal{N}([-5, 30], \mathbb{I}_2)/3$  and Similarly for  $\mathcal{D}^{(1)}$ , we draw 600 samples from  
1357  $\mathcal{N}([-5, -29.5], \mathbb{I}_2)/3 + \mathcal{N}([-5, 0.5], \mathbb{I}_2)/3 + \mathcal{N}([-5, 30.5], \mathbb{I}_2)/3$ . As a result, the total  
1358 number of samples is 1200, with  $n_0 = n_1 = 600$ .

1359 2. ADULT: The adult income dataset is a collection of data consisting of several demographic  
1360 features including employment features. It is extracted from 1994 U.S. Census database  
1361 (Becker & Kohavi, 1996). Sensitive group sizes are (10,771 / 21,790). We use 5 continuous  
1362 features (age, fnlwgt, education-num, capital-gain, hours-per-week). For the sensitive  
1363 attribute, we use the gender (male/female) attribute.

1364 3. BANK: The bank marketing dataset is a collection of data from a Portuguese bank’s direct  
1365 marketing campaigns, each corresponding to an individual client contacted (Moro et al.,  
1366 2014). We use 6 continuous features (age, call duration, 3-month Euribor rate, number  
1367 of employees, consumer price index, and number of contacts during the campaign). For  
1368 two sensitive groups, we treat marital status as the sensitive attribute: categorized into  
1369 two groups (single/married) and exclude all ‘unknown’ entries. Sensitive group sizes are  
1370 (16,180 / 24,928).  
1371 When considering three sensitive groups, following (Ziko et al., 2021), we categorize the  
1372 marital status into three groups (single/married/divorced) and exclude all ‘unknown’ en-  
1373 tries. Sensitive group sizes are (4,612 / 11,568 / 24,928).

1374 4. DIABETES: The diabetes dataset is a collection of data spanning five years, consisting of  
1375 various physical indicators (e.g., glucose concentration, blood pressure, BMI, etc., totaling  
1376 7 features) of Pima Indian women<sup>1</sup>. Sensitive group sizes are (372 / 396). It originates from  
1377 the National Institute of Diabetes and Digestive and Kidney Diseases (Smith et al., 1988).  
1378 For the sensitive attribute, we use the binarized age attribute at the median value.

1379 **E.2 IMPLEMENTATION DETAILS**  
13801381 **Algorithms**  
1382

1383 • Baseline methods: For MFM, we employ the Julia code of Miller & Harrison (2018) with-  
1384 out modification, available on the authors’ GitHub<sup>2</sup>. Similarly, for SFC, VFC, FCA and  
1385 FairDen, we use the publicly released source codes provided by the authors<sup>3 4 5 6</sup>.

1386 • FBC: We use a conjugate prior for  $H$ . For Gaussian mixture, we use the following conjugate  
1387 prior following Miller & Harrison (2018). For  $\theta$ , we set  $a = b = 1$  in  $\mathcal{N}(\mu_j, \lambda_j^{-1})$ ,  $\lambda \sim$   
1388  $\text{Gamma}(a, b)$ ,  $\mu_j | \lambda \sim \mathcal{N}(0, \lambda^{-1})$ . For  $\mathbf{T}$ , we set the temperature  $\tau = 1.0$ . For fixed  $K$   
1389 cases, we simply set  $\gamma = 1$  for the Dirichlet distribution. We repeat the step 1 for (1, 10, 5)  
1390 for  $k_* = 10$  (for ADULT, BANK and DIABETES, respectively). We use 6000 burn-in epochs  
1391 and select a sample from the posterior mode among 4000 samples after burn-in for ADULT  
1392 and BANK, and we use 2000 burn-in epochs and select a sample from 2000 samples after  
1393 burn-in for DIABETES.

1394 For unknown  $K$  cases, we consider  $\kappa \sim \text{Beta}(21, 80)$  and  $\gamma = (10.0, 10.0, 5.0)$  for the  
1395 Dirichlet distribution to prevent the cluster numbers explode (for ADULT, BANK and DIA-  
1396 BETES, respectively). We use 8000 burn-in epochs and select a sample from the posterior  
1397 mode among 2000 samples after burn-in for ADULT, 18000 burn-in epochs and select a  
1398 sample from 2000 samples after burn-in for BANK, and we use 8000 burn-in epochs and

1399 <sup>1</sup>Diabetes: <https://github.com/aasu14/Diabetes-Data-Set-UCI>

1400 <sup>2</sup>MFM: <https://github.com/jwmi/BayesianMixtures.jl>

1401 <sup>3</sup>SFC: [https://github.com/talwagner/fair\\_clustering](https://github.com/talwagner/fair_clustering)

1402 <sup>4</sup>VFC: <https://github.com/imtiazziko/Variational-Fair-Clustering>

1403 <sup>5</sup>FCA: <https://github.com/kwkimonline/FCA>

1404 <sup>6</sup>FairDen: <https://jugit.fz-juelich.de/ias-8/fairden>

1404 select a sample from 2000 samples after burn-in for DIABETES. The choice is because,  
 1405 when  $K$  is treated as a random variable, since the parameter space with unknown  $K$  is  
 1406 much larger than that with fixed  $K$ . We also utilize the Jain-Neal split-merge sampler (Jain  
 1407 & Neal, 2004) to enable faster mixing, following the setting of Miller & Harrison (2018).  
 1408 For the choice of  $D$  in the energy, we use the Euclidean distance for continuous features  
 1409 and the Gower distance (Gower, 1971) for mixed-type data (i.e., continuous + categorical)  
 1410 which is a weighted sum of scaled euclidean distance and hamming distance (Hamming,  
 1411 1950; Huang, 1998; Zhang et al., 2006).  
 1412 For faster convergence, we partially initialize  $\mathbf{T}$  utilizing optimal transport, motivated by  
 1413 prior work showing that matching nearby instances tends to yield higher clustering utility  
 1414 (Chierichetti et al., 2017; Backurs et al., 2019; Kim et al., 2025b). In detail, we randomly  
 1415 sample some proportion from each (upsampled)  $\mathcal{D}^{(s)}$  and calculate the optimal transport  
 1416 between them, while remains are randomly matched.

## 1417 Performance measures

- 1419 • NLD: For the baseline methods, NLD is computed as follows: we first estimate a mean for  
 1420 each cluster and a single variance shared across all clusters/components, then compute the  
 1421 negative log-likelihood of the data under this fitted mixture model.
- 1423 • ACC: Even when the number of clusters differs from the number of class labels, we assign to  
 1424 each cluster the ground-truth class that appears most frequently within that cluster (majority  
 1425 vote). We then compute ACC as the fraction of samples whose predicted labels (from this  
 1426 assignment) match their ground-truth class labels.

## 1427 Hardwares

- 1429 • The Julia language is used for running FBC.
- 1430 • All our experiments are done through Julia 1.11.2, Python 3.9.16 with Intel(R) Xeon(R)  
 1431 Silver 4310 CPU @ 2.10GHz and 128GB RAM.

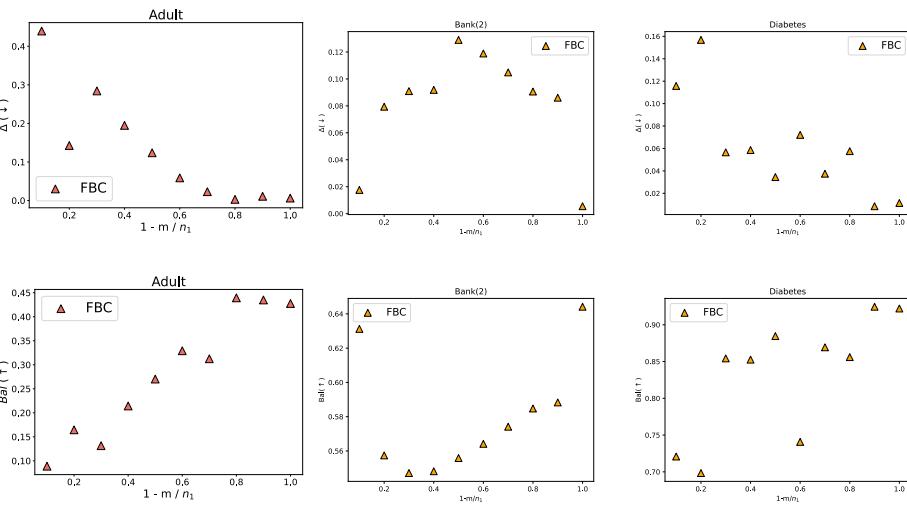
1458 E.3 EXPERIMENTAL RESULTS  
14591460 E.3.1 FAIR CLUSTERING PERFORMANCE (KNOWN  $K$ )  
14611462 **Comparison of FBC to existing fair clustering algorithms** Table 2 compares the computation  
1463 time of FBC and FCA, which suggests that FBC requires less computation time than FCA, up to  
1464 50% faster.1465 Table 2: Averaged computation time (seconds) of FBC and FCA on five random trials for  $k_* = 10$ .  
1466

Computation time	ADULT	BANK	DIABETES
FCA	1059.22	1365.32	26.71
FBC ✓	<b>599.69</b>	<b>812.08</b>	<b>12.38</b>

1471 Similar to Table 1 in the main body, we investigate whether FBC yields reasonable clustering results  
1472 compared to baselines when  $K$  is fixed at  $k_* = 2$ . We similarly run each algorithm to achieve the  
1473 maximum fairness (e.g.,  $\Delta \approx 0$ ) for a fair comparison. Table 3 shows the results, suggesting that  
1474 FBC is competitive to the baselines when  $K$  is fixed at  $k_* = 2$ .  
14751476 Table 3: Comparison of utility (Cost, NLD, Acc) and fairness levels ( $\Delta$ , Bal) for  $k_* = 2$ . **Bold**-  
1477 **faced values and underlined values (Cost and  $\Delta$ ) indicate the best and second-best values, respec-**  
1478 **tively, among the methods that achieve near-perfect fairness levels.**  
1479

Dataset	Measure	SFC	VFC	FCA	FBC ✓
ADULT	UTILITY	Cost (↓)	4.397	4.248	<b>4.237</b>
		NLD (↑)	6.684	7.129	<u>6.688</u>
	FAIRNESS	Acc (↑)	0.763	0.636	0.765
		$\Delta$ (↓)	<b>0.000</b>	0.041	<b>0.000</b>
	FAIRNESS	Bal (↑)	0.494	0.455	0.494
BANK	UTILITY	Cost (↓)	4.042	3.729	<b>3.919</b>
		NLD (↑)	7.739	7.717	7.746
	FAIRNESS	Acc (↑)	0.733	0.720	0.680
		$\Delta$ (↓)	0.003	0.084	<b>0.000</b>
	FAIRNESS	Bal (↑)	0.647	0.571	0.649
DIABETES	UTILITY	Cost (↓)	6.621	5.729	<b>5.733</b>
		NLD (↑)	9.838	9.752	<u>9.753</u>
	FAIRNESS	Acc (↑)	0.613	0.638	0.633
		$\Delta$ (↓)	0.017	0.002	0.001
	FAIRNESS	Bal (↑)	0.884	0.937	0.939

1512  
1513 **Fairness level control of FBC** Figure 8 shows the relationship between  $m$  and the fairness level,  
1514 showing that fairness level is well controlled by controlling  $m$  unless  $m$  is too large.  
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1532 Figure 8: (Top three) Trade-off between  $m$  (the size of  $E$ ) and the fairness level  $\Delta$ . Smaller  $\Delta$ , fairer  
1533 the clustering. (Bottom three) Trade-off between  $m$  (the size of  $E$ ) and the  $\text{Bal}$ . Larger  $\text{Bal}$ , fairer  
1534 the clustering.  
1535

1536 **Additional analysis: handling a multinomial sensitive attribute (BANK)** We analyze BANK with  
1537 three sensitive groups. Table 4 presents the performance comparison between VFC and FBC, show-  
1538 ing that FBC is competitive to VFC in terms of the utility-fairness trade-off. In particular, FBC  
1539 achieves better fairness levels (i.e., lower  $\Delta$  and higher  $\text{Bal}$ ), while its utility (Cost and Acc)  
1540 remains comparable.  
1541

1542 Table 4: Utility (Cost, Acc) and fairness ( $\Delta$ ,  $\text{Bal}$ ) on BANK for  $k_* = 10$ .  
1543

$K$	Measure	VFC	FBC ✓
10	UTILITY	Cost ( $\downarrow$ )	1.578
		Acc ( $\uparrow$ )	0.742
	FAIRNESS	$\Delta$ ( $\downarrow$ )	0.079
		$\text{Bal}$ ( $\uparrow$ )	0.166

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1567E.3.2 REASONABLE INFERENCE OF  $K$ 1568  
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**Cluster quality** Figure 9 draws the posterior distributions of  $K$  for the three datasets. The inferred  $K$ s for the three datasets are sampled from the posterior modes, and posterior distributions are well-concentrated around the posterior modes.

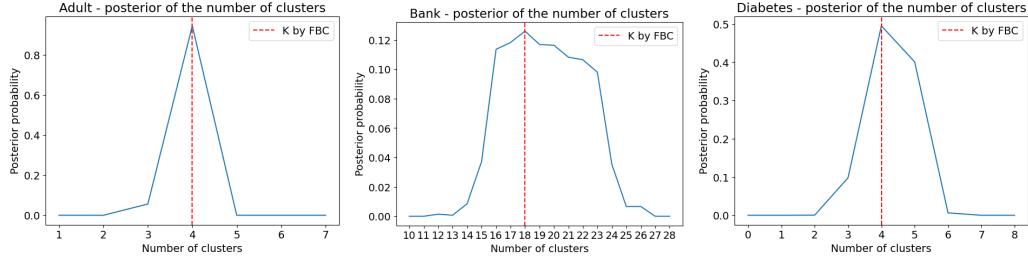
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Figure 9: Posterior distributions of  $K$  for the three datasets. Table 5 below shows that FBC still performs comparable to baseline methods when  $K$  is unknown so inferred, in terms of fairness-utility trade-off.

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Table 5: Utility (Cost, Acc) and fairness ( $\Delta$ ,  $\text{Bal}$ ) on three datasets with inferred  $K$ s. **Bold-faced** values and underlined values ( $\text{Cost}$  and  $\Delta$ ) indicate the best and second-best values, respectively, among the methods that achieve near-perfect fairness levels.

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Dataset	Measure	SFC	VFC	FCA	FBC ✓
ADULT ( $K = 4$ )	UTILITY Cost ( $\downarrow$ )	4.045	3.317	<b>3.033</b>	4.364
	UTILITY Acc ( $\uparrow$ )	0.763	0.759	0.766	0.761
	FAIRNESS $\Delta$ ( $\downarrow$ )	<u>0.001</u>	0.031	<b>0.000</b>	<b>0.000</b>
	FAIRNESS $\text{Bal}$ ( $\uparrow$ )	0.491	0.443	0.494	0.494
BANK ( $K = 18$ )	UTILITY Cost ( $\downarrow$ )	2.570	1.112	<b>1.377</b>	2.202
	UTILITY Acc ( $\uparrow$ )	0.893	0.892	0.892	0.891
	FAIRNESS $\Delta$ ( $\downarrow$ )	<u>0.003</u>	0.063	<b>0.001</b>	0.006
	FAIRNESS $\text{Bal}$ ( $\uparrow$ )	0.647	0.466	0.644	0.612
DIABETES ( $K = 4$ )	UTILITY Cost ( $\downarrow$ )	5.771	4.858	<b>4.646</b>	5.381
	UTILITY Acc ( $\uparrow$ )	0.656	0.656	0.702	0.682
	FAIRNESS $\Delta$ ( $\downarrow$ )	0.007	0.112	<b>0.001</b>	<u>0.006</u>
	FAIRNESS $\text{Bal}$ ( $\uparrow$ )	0.824	0.671	0.938	0.875

**Density estimation** We further support the optimality of  $K$  inferred by FBC, in terms of density estimation. To this end, we first split a given dataset into training/test with ratios 8:2, then run FBC on the training dataset and compute the posterior density on the test dataset. The results are given in Section 5.2 in the main body.

1620

## E.3.3 FLEXIBILITY OF FBC: APPLICABILITY TO VARIOUS DATA TYPES

1621

1622 FBC can be applied to any variable type provided that the likelihood is defined. In this analysis, we  
 1623 consider datasets which include both continuous variables and categorical variables.

1624

1625 **Dataset construction** For a baseline method, we consider FairDen, since it can also applied to both  
 1626 continuous or categorical variables. Note that we use subsampled ADULT dataset in this analysis,  
 1627 since FairDen requires high computational complexity when using the entire ADULT. In detail, it  
 1628 requires building a full  $n \times n$  similarity matrix between data points, calculating the Laplacian, and  
 1629 performing eigen-decomposition under fairness constraints. Thus the computational complexity of  
 1630 this pipeline is  $\mathcal{O}(n^2)$  in both time and memory, and involves fragile linear algebra, leading to  
 1631 numerical instability as well as computational overhead when using the entire ADULT dataset.

1632

1633 That is, we randomly select 2,000 subsamples from the entire dataset. Note that the resulting  
 1634 subsample contains 1,357 males and 643 females, so the maximum achievable value of  $\text{Bal}$  is  
 $643/1357 \approx 0.474$ .

1635

1636 In addition to continuous features used in the main analysis, we consider 2 categorical features  
 1637 (marital status and race with 7 and 5 categories, respectively).

1638

1639 **FBC for mixed-type (continuous + categorical) data** For continuous variables, we keep con-  
 1640 sidering the Gaussian mixture. For categorical variables, we consider the mixture of independent  
 1641 Multinoulli distributions, where each component  $f(\cdot|\theta_k)$  is the product of Multinoulli distribu-  
 1642 tion. In other words,  $f(\cdot|\theta_k) \sim \prod_{j=1}^{l_{\text{cate}}} \text{Cat}(\cdot; \phi_{k,j})$ , where  $\phi_{k,j} = (p_{k,j,1}, \dots, p_{k,j,l_j}) \in [0, 1]^{l_j}$ .  
 1643 Here,  $l_j$  is the number of categories of the  $j$ -th categorical feature. We use the conjugate prior as  
 $\phi_{k,j} \sim \text{Dirichlet}(\alpha, \dots, \alpha)$  with  $\alpha = 1$ .

1644

1645 **Results** The comparison results are provided in Table 6. For both FairDen and FBC, the additional  
 1646 use of categorical variables improves  $\text{Acc}$ , compared to the results with the continuous variables  
 1647 only. Note that we cannot measure  $\text{Cost}$ , which cannot be applied to categorical variables. However,  
 1648 while the use of categorical variables reduces  $\text{Bal}$  and increases  $\Delta$  in FairDen, FBC still achieves  
 1649 nearly perfect fairness in terms of  $\Delta$  and  $\text{Bal}$  for both cases, with and without categorical variables.  
 1650 In summary, FBC outperforms FairDen for both cases, with and without categorical variables.

1651

1652 Table 6: Comparison of utility ( $\text{Acc}$ ) and fairness ( $\Delta$ ,  $\text{Bal}$ ) on subsampled ADULT for  $k_* = 10$ .  
 1653 **Bold-faced** results indicate the bests. ‘c’ denotes for the results with the use of continuous variables  
 1654 only, and ‘cc’ denotes for the results with the use of both continuous and categorical variables.

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Dataset	Measure	FairDen(c)	FairDen(cc)	FBC(c) ✓	FBC(cc) ✓
ADULT(SUB)	UTILITY	0.651	0.654	0.715	<b>0.721</b>
	FAIRNESS	0.005	0.013	0.001	<b>0.001</b>
	Bal (↑)	0.466	0.451	0.472	<b>0.473</b>

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1674 E.3.4 FLEXIBILITY OF FBC: CLUSTERING UNDER SIZE CONSTRAINTS  
16751676 **FBC algorithm under the cluster size constraint** Consider a problem of searching fair clus-  
1677 ters under the constraint that the maximum size of each cluster should be bounded by  $M$ . For this  
1678 purpose, we can modify Algorithm 3 for FBC under the size constraint as:

1679 1. Initialize  $\mathcal{C} = \{[n_0]\}$  (i.e., a single cluster)  
 1680 2. Repeat the following steps  $N$  times, to obtain  $N$  samples. For  $i = 1, \dots, n_0$ : Remove  
 1681 element  $i \in [n_0]$  and its matched elements in  $J(\{i\}; \mathbf{T}, \mathbf{T}_0, E) := \{j \in E : \mathbf{T}_0(j) =$   
 1682  $i\} \cup \{j \in [n_1] \setminus E : \mathbf{T}(j) = i\}$  from  $\mathcal{C}$ . Then, place them  
 1683 • to  $c' \in \mathcal{C} \setminus i$  with probability

$$1685 \propto (|c'| + \gamma) \frac{m(X^{c'} \cup X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)}{m(X^{c'} | \mathbf{T}, \mathbf{T}_0, E)} \mathbb{I}(|c'| \leq M)$$

1688 where  $X^{\{i\}} := \{X_i^{(0)}\} \cup \{X_j^{(1)} : j \in J(\{i\})\}$ .

1689 • to a new cluster with probability  $\propto \gamma^{\frac{V_{n_0}(t+1)}{V_{n_0}(t)}} m(X^{\{i\}} | \mathbf{T}, \mathbf{T}_0, E)$ , where  $t$  is a number  
 1690 of clusters when  $X^{\{i\}}$  are removed.

1692 The modification of Algorithm 8 for FBC can be done similarly.  
16931694 **Experimental setup and Baseline method** Given  $\alpha \geq 1$ , we set the per-cluster upper bound  
 1695  $U_{\max}^{(\alpha)}(K) = \lceil \alpha \frac{n}{K} \rceil$ . That is,  $\alpha = 1$  regularizes the sizes of all clusters to the uniform size of  $n/K$ ,  
 1696 and larger  $\alpha$  allows more relaxations.  
16971698 As a baseline, we consider a post-processing fair clustering method proposed by (Bera et al., 2019),  
 1699 which aims to find fair assignments through solving a linear program with fixed pre-determined  
 1700 cluster centers. Since the size constraint is also linear with respect to the assignments, we add it with  
 1701 the parameter  $\alpha$ , when solving the linear program.  
17021703 **Results** We consider varying  $\alpha \in \{1.25, 1.50, 1.75\}$ , whose corresponding cluster size upper  
 1704 bounds are  $\{4071, 4885, 5699\}$ . Results under these size constraints are reported in Table 7. FBC  
 1705 consistently outperforms the post-processing method of Bera et al. (2019). Specifically, for Bera  
 1706 et al. (2019), the constraint does not affect the fair assignment when  $\alpha$  exceeds 1.5; in that case, the  
 1707 optimal Cost for Bera et al. (2019) is 2.748 - higher than that of FBC. These findings demonstrate  
 1708 the superiority of FBC for strictly size-constrained fair clustering.  
17091710 Various size constrained clustering algorithms have been considered (Esmaeili et al., 2020; Zhu  
 1711 et al., 2010; Höppner & Klawonn, 2008). We believe that FBC could be modified for such problems  
 1712 without much hamper similarly to what we have done for the upper bound constraint.  
17131714 Table 7: Results of utility (Cost), fairness ( $\Delta$ , Bal), and statistics on cluster sizes (min size,  
 1715 max size) on ADULT with  $k_* = 10$  under size constraints.  $\alpha$  controls the size constraint.  
1716

$\alpha$	Measure	Bera et al. (2019) under size constraint with $\alpha$	FBC ✓
1.25	UTILITY Cost ( $\downarrow$ )	2.829	2.481
	FAIRNESS $\Delta$ ( $\downarrow$ )	0.002	0.001
	FAIRNESS Bal ( $\uparrow$ )	0.492	0.493
	SIZES min / max	2,802 / 4,071	219 / 4,070
1.50	UTILITY Cost ( $\downarrow$ )	2.748	2.451
	FAIRNESS $\Delta$ ( $\downarrow$ )	0.000	0.001
	FAIRNESS Bal ( $\uparrow$ )	0.494	0.485
	SIZES min / max	2,802 / 4,128	98 / 4,885
1.75	UTILITY Cost ( $\downarrow$ )	2.748	2.439
	FAIRNESS $\Delta$ ( $\downarrow$ )	0.000	0.001
	FAIRNESS Bal ( $\uparrow$ )	0.494	0.491
	SIZES min / max	2,802 / 4,128	79 / 5,699

## E.3.5 ABLATION STUDIES

**Temperature  $\tau$**  We analyze the impact of the temperature constant  $\tau$  in the prior of  $\mathbf{T}$  defined in Definition 3.1. To do so, we set  $E = \emptyset$  and compare the utility ( $\text{Cost}$ ) and fairness levels ( $\text{Bal}$  and  $\Delta$ ) for various values of  $\tau$ . Table 8 below reports the performance of FBC for different temperature values  $\tau \in \{0.1, 1.0, 10.0\}$ . Overall, varying  $\tau$  does not affect much to the performance of FBC.

Table 8: Comparison of  $K$ ,  $\text{Cost}$ ,  $\text{Acc}$ ,  $\Delta$ , and  $\text{Bal}$  for  $\tau \in \{0.1, 1.0, 10.0\}$ .

Dataset	Measure	$\tau$		
		0.1	1.0	10.0
ADULT	$K$	4	4	4
	$\text{Cost} (\downarrow)$	4.364	4.364	4.364
	$\text{Acc} (\uparrow)$	0.761	0.761	0.761
	$\Delta (\downarrow)$	0.000	0.000	0.000
	$\text{Bal} (\uparrow)$	0.494	0.494	0.494
BANK	$K$	18	18	18
	$\text{Cost} (\downarrow)$	2.202	2.202	2.202
	$\text{Acc} (\uparrow)$	0.891	0.891	0.891
	$\Delta (\downarrow)$	0.006	0.006	0.006
	$\text{Bal} (\uparrow)$	0.612	0.612	0.612
DIABETES	$K$	4	4	4
	$\text{Cost} (\downarrow)$	5.381	5.381	5.381
	$\text{Acc} (\uparrow)$	0.682	0.682	0.682
	$\Delta (\downarrow)$	0.006	0.006	0.006
	$\text{Bal} (\uparrow)$	0.875	0.875	0.875

**Choice of  $R$  when  $r > 0$**  In this section, we compare the two choices of  $R$  in Section 2.1.2: (i) a random subset of  $[n_0]$  and (ii) the index of samples closest to the cluster centers obtained by a certain clustering algorithm to  $\mathcal{D}^{(0)}$  with  $K = r$ , which is considered in Section 2.1.2. Table 9 below provides the results, showing that the performance of the two approaches are not much different. Here, we utilized  $K$ -medoids algorithm to yield the cluster centers from  $[n_0]$ . Overall, we can conclude that FBC is not sensitive to the choice of  $R$  and the two proposed heuristic approaches work well in practice.

Table 9: Comparison of  $K$ ,  $\text{Cost}$ ,  $\text{Acc}$ ,  $\Delta$ , and  $\text{Bal}$  for the two heuristic approaches in Section 2.1.2. ‘Random’ indicates the first approach ( $R =$  a random subset of  $[n_0]$ ). and ‘Clustering’ indicates the second approach ( $R =$  centers obtained by a clustering algorithm).

Dataset	Measure	$R$	
		Random	Clustering
ADULT	$K$	4	4
	$\text{Cost} (\downarrow)$	4.364	4.364
	$\text{Acc} (\uparrow)$	0.761	0.761
	$\Delta (\downarrow)$	0.000	0.000
	$\text{Bal} (\uparrow)$	0.494	0.494
BANK	$K$	18	18
	$\text{Cost} (\downarrow)$	2.202	2.202
	$\text{Acc} (\uparrow)$	0.891	0.891
	$\Delta (\downarrow)$	0.006	0.006
	$\text{Bal} (\uparrow)$	0.612	0.612
DIABETES	$K$	4	4
	$\text{Cost} (\downarrow)$	5.381	5.381
	$\text{Acc} (\uparrow)$	0.682	0.682
	$\Delta (\downarrow)$	0.006	0.006
	$\text{Bal} (\uparrow)$	0.875	0.875

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 1783 **Variation of covariance structure** We examine how the covariance structure in the Gaussian  
 1784 mixture model affects utility and fairness of FBC. Specifically, we compare the *Unified* covariance  
 1785 used in the main analysis (a single scale parameter  $\lambda$  shared across clusters and features) with a more  
 1786 flexible one, *Isotropic* covariance (cluster-wise  $\lambda_j$ ). To do so, we split the dataset into training/test  
 1787 with 8:2 ratios, and calculate the performance on the test data. We also fix  $K = k_* = 10$  in this  
 1788 analysis.

1788 The results in Table 10 give the following implications: (i) allowing cluster-specific covariances  
 1789 improves density estimation i.e., lowers NLD, by capturing richer covariance variability; (ii) *Unified*  
 1790 offers lower Cost, since Cost assumes shared variances across clusters; (iii) fairness is achieved  
 1791 well regardless of the covariance choice: both settings maintain near-perfect fairness ( $\Delta \approx 0$  and  
 1792 high Bal).

1793  
 1794 Table 10: Comparison of utility (Cost, NLD, ACC) and fairness ( $\Delta$ , Bal).  $K$  is fixed as  $K = k_* =$   
 1795 10. *Unified* indicates the use of a single scale parameter and *Iso* indicates the use of cluster-specific  
 1796 scale parameters.

Dataset	Measure	Covariance	
		Unified	Iso
ADULT	Cost ( $\downarrow$ )	1.954	2.272
	NLD ( $\downarrow$ )	6.242	6.239
	Acc ( $\uparrow$ )	0.781	0.775
	$\Delta$ ( $\downarrow$ )	0.001	0.001
	Bal ( $\uparrow$ )	0.491	0.492
BANK	Cost ( $\downarrow$ )	1.787	1.788
	NLD ( $\downarrow$ )	6.302	6.300
	Acc ( $\uparrow$ )	0.890	0.888
	$\Delta$ ( $\downarrow$ )	0.004	0.004
	Bal ( $\uparrow$ )	0.615	0.614
DIABETES	Cost ( $\downarrow$ )	3.757	3.958
	NLD ( $\downarrow$ )	9.088	9.076
	Acc ( $\uparrow$ )	0.693	0.701
	$\Delta$ ( $\downarrow$ )	0.013	0.018
	Bal ( $\uparrow$ )	0.882	0.800

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## E.4 CONVERGENCE OF MCMC

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We assess the convergence of the MCMC algorithm by monitoring (i) the autocorrelation function of the inferred  $K$  and (ii) the negative log-likelihood (NLL) on training data (i.e., the observed instances), over sampling iterations. As is done by Miller & Harrison (2018), the results in Figures 10 and 11 of Section E.3.5 show that the MCMC algorithm converges well and finds good clusters.

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$K$ : As is done by Miller & Harrison (2018), in Figure 10, we draw the autocorrelation function  $\rho(h)$  defined as

$$\rho(h) = \text{corr}\{(K_t, K_{t+h}), t = 1, \dots\},$$

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where  $K_t$  is a posterior sample at iteration  $t$ . The autocorrelation functions amply support that the proposed MCMC algorithm converges well.

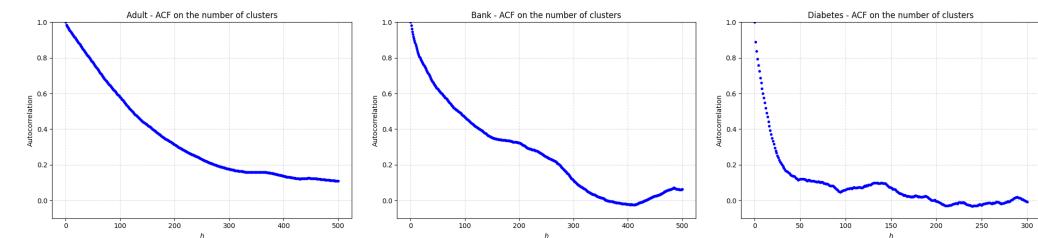
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Figure 10:  $h$  vs. Autocorrelation functions for (left) DIABETES, (center) ADULT, and (right) BANK datasets.

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NLL: Figure 11 draws the trace plots of the NLL on training data. Dramatic decreases of NLL are observed which would happen when the MCMC algorithm moves one local optimum to another local optimum. This supports the ability of FBC to explore high-posterior clusters efficiently.

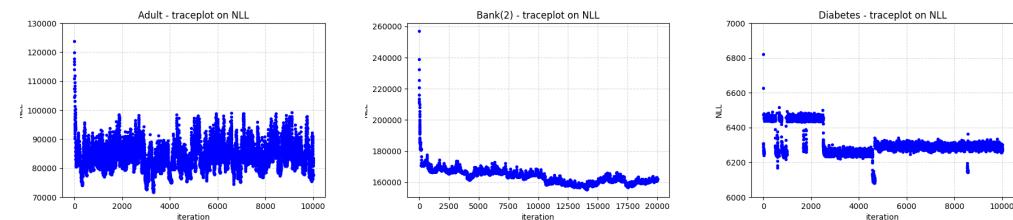
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Figure 11: Trace plots of NLL on (left) DIABETES, (center) ADULT, and (right) BANK datasets.

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1890 **F ADDITIONAL EXPERIMENTS**  
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1892 **F.1 ASSIGNMENTS FOR NEW DATA**  
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1894 Suppose the new dataset is given as  $D_0^{\text{new}} \cup D_1^{\text{new}}$ . Then, we assign instances of  $D_0^{\text{new}}$  to their nearest  
 1895 neighbors in  $D_0$ , and similarly assign instances of  $D_1^{\text{new}}$  to their nearest neighbors in  $D_1$ .

1896 We empirically validate this assignment strategy as follows: (i) we split the ADULT dataset into  
 1897 training and test sets with an 8:2 ratio; (ii) we perform FBC on the training data and then assign the  
 1898 test data according to the procedure described above.

1899 The results are reported in Table 11, where we observe that fairness on the new (test) data (in terms  
 1900 of  $\Delta$  and Balance) remains near the values of near-perfect fairness, and the NLD value is similar to  
 1901 that in Table 1, where the full dataset is used. These empirical findings suggest that the proposed  
 1902 assignment technique for new data performs well in practice.

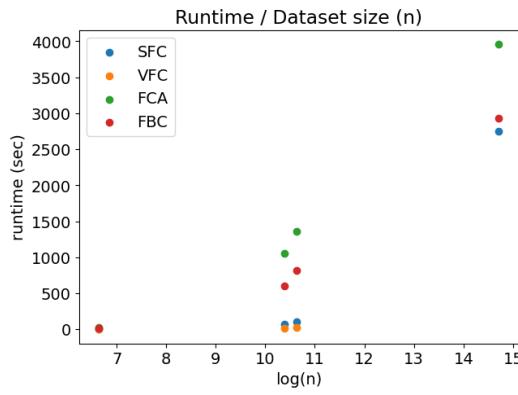
1903  
 1904 **Table 11: Performance comparison between FBC performed/evaluated on the full data and FBC**  
 1905 **performed on the training data and evaluated on the test data, on ADULT dataset.**

	NLD (↓)	$\Delta$ (↓)	Bal (↑)
Full data	6.242	0.001	0.491
New data	6.241	0.019	0.472

1911 **F.2 COMPUTATIONAL COST**  
 1912

1913 The computational complexity of the MH step (STEP 1) for  $\mathbf{T}$  does not depend on the input dimension,  
 1914 and its scale on each iteration is  $O(1)$  since it is a random swap with a fixed number of  
 1915 repetition (10 times in our experiments). The computational complexity of the mixture parameter  
 1916 sampling of each iteration (STEP 2) for  $\Phi$ , is empirically observed as  $O(n)$  in Miller & Harrison  
 1917 (2018).

1918 To further verify the scalability of FBC, we compare its runtime with baseline methods for several  
 1919 datasets. For this purpose, we plot the logarithm of dataset size ( $n$ ) vs. runtime in Figure 12 (datasets  
 1920 are DIABETES, ADULT, BANK, and CENSUS). The results show that FBC is competitive to baseline  
 1921 methods in terms of computational cost, while maintaining the nearly-best performance.



1936 **Figure 12: Scatterplot of runtime and the logarithm of dataset size.**  
 1937

1938 **F.3 PERFORMANCE ON A LARGE-SCALE DATASET**  
 1939

1940 **Known  $K$**  To validate the scalability of FBC, we conduct an additional experiment using Census  
 1941 dataset, which has a scale of millions and has been previously used in the fairness literature (Backurs  
 1942 et al., 2019; Ziko et al., 2021). It <sup>7</sup> is a sub-dataset of the 1990 US Census, consisting of 2,458,285

1943  
 7<sup>7</sup><https://archive.ics.uci.edu/dataset/116/us+census+data+1990>

1944 samples with 68 attributes. We use 25 continuous variable and consider ‘gender’ attribute as the  
 1945 sensitive attribute, similar to the approach of Backurs et al. (2019) and Ziko et al. (2021). Since it  
 1946 is noted that for CENSUS dataset, VFC fails without  $L_2$  normalization (Kim et al., 2025b), we only  
 1947 compare FBC to SFC and FCA.

1948 In Table 12, we can observe that the similar behavior to that of Table 1. While all methods achieves  
 1949 near-perfect fairness, FBC yields better Cost than SFC, and requires less computation time than  
 1950 FCA.

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1952 Table 12: Performance comparison for  $k_* = 10$  on CENSUS dataset.

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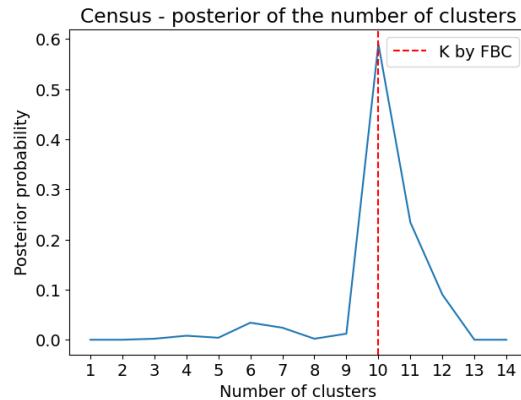
	Cost (↓)	$\Delta$ (↓)	Bal (↑)	Computation time (sec)
SFC	24.488	0.000	0.933	2753.30
FCA	11.804	0.000	0.934	3957.83
FBC ✓	12.854	0.000	0.930	2927.42

1954

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1960 **Unknown  $K$**  We further analyze the posterior density of  $K$ , to validate the inferred  $K$  is reasonable.  
 1961 Figure 13 shows the results, indicating that the inferred  $K$  is sampled from the posterior mode,  
 1962 and posterior distributions are well-concentrated around the modes, similar to Figure 9.

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1977 Figure 13: Posterior of  $K$  on CENSUS dataset.

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