Computational Efficient Approximations of the Concordance Probability in a Big Data Setting

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Abstract

Performance measurement is an essential task once a statistical model is created. The Area Under the receiving operating characteristics Curve (AUC) is the most popular measure for evaluating the quality of a binary classifier. In this case, the AUC is equal to the concordance probability, a frequently used measure to evaluate the discriminatory power of the model. Contrary to AUC, the concordance probability can also be extended to the situation with a continuous response variable. Due to the staggering size of data sets nowadays, determining this discriminatory measure requires a tremendous amount of costly computations and is hence immensely time consuming, certainly in case of a continuous response variable. Therefore, we propose two estimation methods that calculate the concordance probability in a fast and accurate way and that can be applied to both the discrete and continuous setting. Extensive simulation studies show the excellent performance and fast computing times of both estimators. Finally, experiments on two real-life data sets confirm the conclusions of the artificial simulations.

Keywords: *AUC, C-index, clustering, efficient algorithm, performance measure*

1 Introduction

Since the beginning of this century, technological advances dramatically changed the size of data sets as well as the speed with which these data have to be processed, analyzed and evaluated. Modern data may have a huge number of observations and/or a very large number of dimensions. Recently, data is growing at an explosive rate and these massive data sets are collected at high speed from different sources, e.g. results of sensors in an industrial process or in healthcare, spatial data from mobile devices, etc. This data is often used to get insights into a certain process, which are typically obtained by predicting one response variable by using all the other explanatory variables. Many statistical models can be used for this prediction task that will turn data into knowledge and hence, it is of utmost importance to compare the performance of these various models. In this paper, it will be shown how to efficiently compute the concordance probability, a popular measure of the predictive

ability of both classification and regression problems. We will focus on the presence of a huge number of observations, to which the computing time of this measure is particularly sensitive.

For evaluating the quality of a binary classifier, the focus typically lies on the discriminatory ability of the model. For more information on the different aspects of the predictive ability, such as the difference between the discriminatory ability and the calibration, we refer to Steyerberg et al. (2010). The most widely used performance measure to check the discriminatory ability of a binary classifier is the Area Under the ROC Curve (AUC), see for example the work of Liu et al. (2008); Razavian et al. (2015); De Cnudde et al. (2019). Note that the construction of the Receiver Operating Characteristic (ROC) curve was suggested in electronic signal detection theory (Bamber, 1975). It is known that the AUC in case of a binary response variable equals exactly the concordance probability, also called the C-index (see for example Reddy and Aggarwal (2015)). The concordance probability corresponds to the probability that a randomly selected subject with outcome $Y = 1$ has a higher predicted probability $\pi(\boldsymbol{X}) = \mathrm{P}(Y = 1|\boldsymbol{X})$ than a randomly selected subject with outcome $Y = 0$, where $\boldsymbol{X}$ corresponds to the vector of variables (Pencina and D'Agostino, 2004):

$$\mathrm{C} = \mathrm{P}\Big(\pi(\boldsymbol{X}_i) > \pi(\boldsymbol{X}_j) \mid Y_i = 1, \ Y_j = 0\Big). \tag{1}$$

A pair of observations with their predictions that satisfies the above condition is called a concordant pair. Hence, the concordance probability can also be defined as the probability that a randomly selected comparable pair of observations with their predictions, is a concordant pair. The concordance probability, defined in Equation (1), normally ranges between 0.5 and 1, and the closer it is to 1, the better its discriminatory ability. If its value drops below 0.5, the predictions are consistently inconsistent. For a sample of size n, the concordance probability typically is estimated as the ratio of the number of concordant pairs n_c over the number of comparable pairs n_t:

$$\widehat{\mathrm{C}} = \frac{n_c}{n_t} = \frac{\widehat{\pi}_c}{\widehat{\pi}_c + \widehat{\pi}_d} = \frac{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} I\Big(\widehat{\pi}(\boldsymbol{x}_i) > \widehat{\pi}(\boldsymbol{x}_j), \ y_i = 1, \ y_j = 0\Big)}{\sum_{i=1}^{n-1} \sum_{j=i+1}^{n} I\Big(\widehat{\pi}(\boldsymbol{x}_i) \neq \widehat{\pi}(\boldsymbol{x}_j), \ y_i = 1, \ y_j = 0\Big)}, \tag{2}$$

where the value $\widehat{\pi}_c$ (respectively $\widehat{\pi}_d$) refers to the estimated probability that a comparable pair is concordant (respectively discordant) and $I(\cdot)$ to the indicator function. For observation i, y_i and $\widehat{\pi}(\boldsymbol{x}_i)$ correspond to the observed outcome and estimated predicted probability with $\boldsymbol{X}_i$ the vector of observed variables respectively. Note that the extra condition $\widehat{\pi}(\boldsymbol{x}_i) \neq \widehat{\pi}(\boldsymbol{x}_j)$ is added to the denominator to ensure that no ties in the predictions are taken into account (Yan and Greene, 2008). Ties namely attenuate the concordance probability to 0.5, depending on the distribution of the observations over the different risk groups, which is undesirable (Heller and Mo, 2016). According to Yan and Greene (2008), it depends on the context whether one wants to ignore ties. An estimator should therefore be able to handle both situations. Since ties only influence the actual definition of the comparable and concordant pairs, the choice of whether to include ties does not influence the expression of any definition or estimator presented here. See Yan and Greene (2008) for a more detailed treatment of the subject of ties on the concordance probability. However, the approximations that we will discuss in this paper are still applicable when one wants to include ties in the predictions, something that is often done in the classical AUC estimator.

As can be seen in Equation (2), calculating this C-index can be very time consuming for large data sets. Therefore, research was conducted to find approximations that reduce the time complexity for calculating such a discriminatory measure in a discrete setting. For example, Bouckaert (2006) provides a method for incrementally updating exact AUC curves and for calculating approximate AUC curves. A number of researchers have attempted to approximate the AUC by smooth functions (Komori, 2011; Eguchi and Copas, 2002; Ma and Huang, 2005), or more specifically polynomials

(Calders and Jaroszewicz, 2007). The most popular algorithm is introduced by Fawcett (2006), where the ROC curve is determined efficiently such that the AUC can be calculated as the area under the ROC curve. This area is obtained by approximating the integral by the trapezium rule.

In this paper, two additional approximations will be presented, which do not rely on the link between the concordance probability and the area under the ROC curve.

- k-means approximation: rather than working with the predictions of all observations of the data set, the predictions of the observations of each outcome class are reduced to the predictions of the centroids of k clusters. Afterwards, Equation (2) is applied to predictions of the latter centroids only. Due to its favorable scaling to large data sets, the k-means clustering algorithm will be used.

- Marginal approximation: For each observation of a given outcome class, its prediction is compared to all predictions of the other outcome class, meaning that there is no correlation between the pairs of both outcome classes that are considered during the estimation process. Hence, by approximating the distribution of predictions of both outcome classes separately by discrete bins and by computing the concordance probability using these bins rather than each separate observation in Equation (2), the concordance probability can be computed more efficiently.

When the response variable Y is continuous, the discriminatory ability of the model can also be of interest, especially when the ranking of the observations is of higher importance than obtaining well-calibrated predictions. Typical examples are the modelling of the claim size distribution of a non-life insurance product, or the modelling of a lifetime distribution in a churn analysis. Note that the concordance probability is particularly popular within the field of survival analysis, and many estimation methods have been proposed to compute the concordance probability in the presence of right censoring (Harrell et al., 1982; Gerds and Schumacher, 2007). As such, the basic Definition (1) is typically adapted as:

$$C = P\Big(\pi(\boldsymbol{X}_i) > \pi(\boldsymbol{X}_j) \mid Y_i > Y_j\Big), \tag{3}$$

where $\pi(\boldsymbol{X}_i)$ represents the predicted value of Y_i. However, in some situations distinguishing nearly identical observations has little practical importance. Consequently, the basic definition in (3) can be extended as follows:

$$C(\nu) = P\Big(\pi(\boldsymbol{X}_i) > \pi(\boldsymbol{X}_j) \mid Y_i - Y_j > \nu\Big), \tag{4}$$

where $\nu \geq 0$. In other words, the difference between the considered observations is at least ν. Note that in this continuous setting, there is no link with the area under the ROC curve. As a result, the aforementioned research is not suitable for this setting in case of a large data set. To our knowledge, the present paper is the first one that focuses on approximating the concordance probability in a fast and efficient manner in the continuous setting. The aforementioned k-means and marginal approximation will be adapted to the continuous setting.

Summarized, we present in this paper two computationally efficient approximations of the concordance probability for big data, both in a discrete and continuous setting, the k-means and marginal approximation. The remainder of this paper is structured as follows. Section 2 presents a detailed explanation of the two proposed approximations. The good performance of both estimators of the concordance probability is verified in an extensive simulation study in Section 3. Finally, we illustrate the practical applications of this work on two real-life examples in Section 4. The main findings and suggestions for further research are summarized in the conclusion.

2 *k*-means and marginal approximation

In this section, two approximations of the concordance probability are presented. One approximation makes use of the *k*-means clustering algorithm and will therefore be called the *k-means approximation*. The other one takes advantage of the structure of the estimation process of the concordance probability and will be denoted the *marginal approximation*. The first subsection focuses on the discrete setting, meaning that the response variable is binary. The second subsection considers the continuous setting, where the response variable is continuous.

2.1 Discrete setting

In this subsection, we consider the situation of a binary response variable Y. The *k*-means approximation can be obtained by separately applying a clustering algorithm to the predictions of each group in the definition of the concordance probability. The number of clusters k will then determine the level of approximation, hence a more precise estimate will be obtained as k increases. When the clustering algorithm is applied, only the cluster centroids will be considered for estimating the concordance probability. In other words, all cluster centroids of each group will be compared with one another. The importance of each cluster by cluster comparison is weighted by the probability that a randomly selected pair of observations belongs to the respective clusters, or:

$$\widehat{\pi}_c \approx \sum_{l=1}^{k} \sum_{m=1}^{k} I\left(\widehat{\pi}_B^l > \widehat{\pi}_A^m\right) w_B^l w_A^m,$$

$$\widehat{\pi}_d \approx \sum_{l=1}^{k} \sum_{m=1}^{k} I\left(\widehat{\pi}_B^l < \widehat{\pi}_A^m\right) w_B^l w_A^m,$$

$$\widehat{C}_{k\text{-means}} = \frac{\widehat{\pi}_c}{\widehat{\pi}_c + \widehat{\pi}_d} \approx \frac{\sum_{l=1}^{k} \sum_{m=1}^{k} I\left(\widehat{\pi}_B^l > \widehat{\pi}_A^m\right) w_B^l w_A^m}{\sum_{l=1}^{k} \sum_{m=1}^{k} I\left(\widehat{\pi}_B^l \neq \widehat{\pi}_A^m\right) w_B^l w_A^m}, \tag{5}$$

where subscript B (respectively A) refers to the group of observations of which the predictions are supposed to be higher (respectively lower) than the ones of subscript A (respectively B). The denominator of the estimator is needed to eliminate the effect of ties on the predictions. Moreover, $\widehat{\pi}_*^l$ is the centroid of the l-th cluster of group * and w_*^l the weight of the l-th cluster of group *. The latter is estimated by computing the percentage of observations of group * that belongs to cluster l, such that by definition $\sum_{l=1}^{k} w_*^l = 1$.

The marginal approximation is obtained by taking advantage of a structure that can be found in the estimation process of the concordance probability. For each observation of a given group, its prediction is compared to all predictions of the other group. As such, no correlation is present between the pairs (π_A, π_B), yielding the following expression for the bivariate distribution $F_{\pi_A, \pi_B}(\pi_A, \pi_B)$:

$$F_{\pi_A, \pi_B}(\pi_A, \pi_B) = F_{\pi_A}(\pi_A) F_{\pi_B}(\pi_B),$$

where $F_{\pi_A}(\pi_A)$ and $F_{\pi_B}(\pi_B)$ correspond to the marginal distributions of π_A and π_B respectively. Hence, when a grid with the same q boundary values $\boldsymbol{\tau} = (\tau_0 \equiv -\infty, \tau_1, \ldots, \tau_q, \tau_{q+1} \equiv +\infty)$ for the marginal distribution of both groups is placed on top of the latter bivariate distribution, the probability that a pair belongs to any of the delineated regions only depends on the marginal distributions $F_{\pi_A}(\pi_A)$ and $F_{\pi_B}(\pi_B)$. In Figure 1, an example is shown where every pair of predictions

of a given data set is plotted out. A grid is added to the scatterplot, which delineates the different regions that are used to compute the marginal approximation.
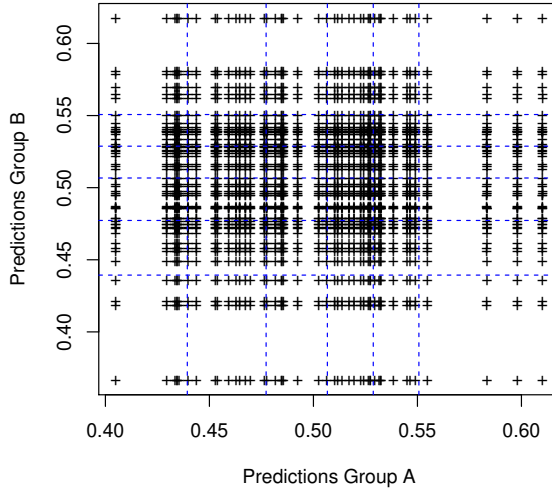

Figure 1: Scatter plot showing the different pairs that are considered in the estimation of the concordance probability. In dashed blue lines the grid lines are shown, hereby delineating the different regions of the grid.

In a next step, three different regions in the two dimensional space can be determined: regions that only contain concordant pairs, regions that contain only discordant pairs, and regions that also contain ties (induced by the grid structure). As such the latter region is considered to be a region of incomparable pairs only. For the ease of presentation, we assume that the q boundaries are the same for both groups, but this is not an absolute necessity. Remember that it is assumed that all observations of group A have a lower observed outcome value than all the observations of group B, and that the values of group A (respectively B) are plotted on the X (respectively Y)-axis. Therefore, all concordant pairs are located in the upper left part of the support of $F_{\pi_A, \pi_B}(\pi_A, \pi_B)$, whereas all discordant pairs are in the lower right part of the support of $F_{\pi_A, \pi_B}(\pi_A, \pi_B)$, and the incomparable pairs are in between both. In Figure 2, the downward dashed region (in green) corresponds to the region of the concordant pairs, the upward dashed region (in red) to the region of the discordant pairs and upward and downward dashed region (in grey) to the region of the incomparable pairs. This colouring scheme serves as an interpretation of the grid that was overlaid in Figure 1 concerning the interpretation of the different delineated regions regarding the marginal approximation.

Since only both marginal distributions $F_{\pi_A}(\pi_A)$ and $F_{\pi_B}(\pi_B)$ are needed to compute the probability that a pair belongs to a region of the support of $F_{\pi_A, \pi_B}(\pi_A, \pi_B)$, the concordance probability can be estimated as follows:

$$\widehat{\pi}_c \approx \sum_{i=1}^{q} \left(\widehat{F}_{\pi_A}(\tau_i) - \widehat{F}_{\pi_A}(\tau_{i-1}) \right) \left(1 - \widehat{F}_{\pi_B}(\tau_i) \right),$$
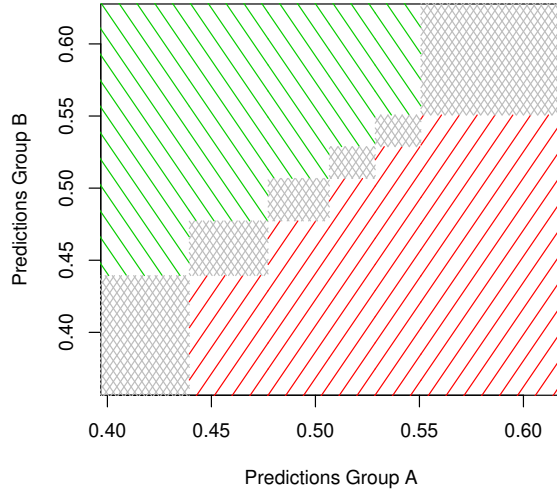
5

Figure 2: The different regions of the grid, shown in Figure 1, in which the concordant pairs (downward dashed region, in green), the discordant pairs (upward dashed region, in red) and incomparable pairs (upward and downward dashed region, in grey) are highlighted.

$$\widehat{\pi}_d \approx \sum_{i=2}^{q+1} \left(\widehat{F}_{\pi_A}(\tau_i) - \widehat{F}_{\pi_A}(\tau_{i-1}) \right) \widehat{F}_{\pi_B}(\tau_{i-1}),$$

$$\widehat{C}_{\mathrm{marg}} = \frac{\widehat{\pi}_c}{\widehat{\pi}_c + \widehat{\pi}_d}$$

$$\approx \frac{\sum_{i=1}^{q} \left(\widehat{F}_{\pi_A}(\tau_i) - \widehat{F}_{\pi_A}(\tau_{i-1}) \right) \left(1 - \widehat{F}_{\pi_B}(\tau_i) \right)}{\sum_{i=1}^{q+1} \left(\widehat{F}_{\pi_A}(\tau_i) - \widehat{F}_{\pi_A}(\tau_{i-1}) \right) \left[I(i \neq q+1) \left(1 - \widehat{F}_{\pi_B}(\tau_i) \right) + I(i \neq 1) \widehat{F}_{\pi_B}(\tau_{i-1}) \right]}.$$

Note that this methodology only yields an approximation of the estimated concordance probability of (2), and that the accuracy improves as q increases. Although $\boldsymbol{\tau}$ can be determined in many ways, we strongly recommend to base it on a set of evenly spaced percentiles of the empirical distribution of the predictions of both group A and B jointly. This is motivated by the easiness of determining the number of observation-prediction couples in each grid.

2.2 Continuous setting

Here, we consider the situation of a continuous response variable Y. Since the data structure and the design of the concordance probability is entirely different for the continuous setting as compared to the discrete setting, the approximations that were proposed in Section 2.1 will not necessarily work for this new setting. One of the key points underpinning these approximations is the existence of two independent groups. In case of a continuous response variable, two of such groups cannot be defined and therefore the previous approximations need to be adapted to the continuous setting.

6

Based on (4), the large data set can only be reduced to a smaller set of clusters, when these clusters of observations are jointly constructed based on their observed outcomes and predictions. All these clusters are uniquely characterized by their observed outcome, prediction and weight, the latter being determined by the number of observations that pertain to the cluster at hand. As a result, (4) can be computed whilst using only these representations of the clusters,

$$\widehat{\pi}_c \approx \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} I\Big(\widehat{\pi}^i > \widehat{\pi}^j, \ y^i - y^j > \nu\Big) w^i w^j,$$

$$\widehat{\pi}_d \approx \sum_{i=1}^{k-1} \sum_{j=i+1}^{k} I\Big(\widehat{\pi}^i < \widehat{\pi}^j, \ y^i - y^j > \nu\Big) w^i w^j,$$

$$\widehat{C}_{k\text{-means}}(\nu) = \frac{\widehat{\pi}_c}{\widehat{\pi}_c + \widehat{\pi}_d} \approx \frac{\sum_{i=1}^{k-1} \sum_{j=i+1}^{k} I\Big(\widehat{\pi}^i > \widehat{\pi}^j, \ y^i - y^j > \nu\Big) w^i w^j}{\sum_{i=1}^{k-1} \sum_{j=i+1}^{k} I\Big(y^i - y^j > \nu\Big) w^i w^j}, \tag{6}$$

where y^l and $\widehat{\pi}^l$ are the observed outcome and the prediction of the representation of the l-th cluster respectively; which is the centroid in case of k-means. w^l is the weight of the l-th cluster that is estimated by computing the percentage of observations belonging to cluster l, such that by definition $\sum_{l=1}^{k} w^l = 1$. Note that the number of clusters, necessary to obtain a good approximation, is likely much higher for this definition than for Definition (5) since Definition (6) needs to consider the additional condition $y^i - y^j > \nu$, which is not needed in the discrete setting. Clearly, in order to ensure that a sufficient number of clusters are comparable for larger values of ν, k should be large enough.

The marginal approximation can be adapted to the continuous setting as well. In this case, a grid will be placed on the $(Y, \pi(\boldsymbol{X}))$ space. Since the condition in Definition (4) only takes the continuous variable Y into account, the q boundary values $\boldsymbol{\tau} = (\tau_0 \equiv -\infty, \tau_1, \ldots, \tau_q, \tau_{q+1} \equiv +\infty)$ are based on the observed values of Y only. The set $\boldsymbol{\tau}$ is selected as a set of evenly spaced percentiles from the empirical distribution of the observed values for Y. The set of boundary values for dimension $\pi(\boldsymbol{X})$ does not necessarily need to be the same as the one for dimension Y. However, we will use the same boundary values nevertheless, as this will allow for better visualization of the discriminatory ability of the model over the $(Y, \pi(\boldsymbol{X}))$, as will be apparent below.

An important difference with the marginal approximation in the discrete setting is that the distance in the Y dimension between two regions needs to be larger than ν before they can be compared. Definition (4) states namely that the difference in observed values of Y should be at least ν. Therefore, regions of which the distance in the Y dimension between their lower boundary and the upper boundary of the selected region is smaller than ν, should not be considered when estimating the selected region's contribution to $\widehat{C}(\nu)$. These eliminated regions potentially contain observations of which its observed value of Y does not differ at least ν from every observation of the selected region.

Ties in the predictions need to be eliminated as well, such that regions that have exactly the same boundary values for the $\pi(\boldsymbol{X})$ dimension as the selected region, will not be considered for the estimation of $\widehat{C}(\nu)$ either. In Figure 3, these ties in predictions correspond to an upward and downward dashed horizontal rectangular region (in grey), containing the selected region. The effect of eliminating both sets of regions, is that the $(Y, \pi(\boldsymbol{X}))$ space is partitioned in two or four main regions, depending on whether the selected region is located on the border of the grid. This partitioning greatly simplifies the estimation of the contribution of the selected region, since for each of the two or four main regions, all members of the selected region either contribute to $\widehat{\pi}_c$ or $\widehat{\pi}_d$.

Interesting is that in all cases, the number of main regions that contribute to $\widehat{\pi}_c$ is always equal to the number of main regions that contribute to $\widehat{\pi}_d$. In Figure 3, the downward dashed regions (in green) correspond to the region of the concordant pairs, contributing to $\widehat{\pi}_c$, and the upward dashed regions (in red) to the region of the discordant pairs, contributing to $\widehat{\pi}_d$.

During the estimation of $\widehat{\mathrm{C}}_{\mathrm{marg}}(\nu)$, it is important to let each region-to-region comparison contribute only once. This can be obtained by only considering those main regions during the computation of the total contribution of a selected region, that are located in the same, fixed direction as compared to the selected region. For example, by only considering those main regions that are located on the right-hand side of the selected region in the $(Y, \pi(\boldsymbol{X}))$ space, i.e. those regions that have a higher observed value for Y than the one of the selected region, each region-to-region comparison will only contribute once. One might as well choose any of the other three remaining directions, i.e. on the left-hand side, below or above the selected region, as long as the same direction is used for all selected regions. Therefore, by selecting the main regions that are located on the right-hand side of the selected region only, the marginal approximation of the concordance probability can be computed as:

$$
\begin{aligned}
n_C(\nu) &\approx \sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(n_{\overrightarrow{C}, \tau_{ij}}(\nu) \right) \\
&= \sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(I\left(i \leq q, j \leq q\right) \sum_{k=i+2}^{q+1} \sum_{l=j+1}^{q+1} \left(I\left(\tau_i + \nu \leq \tau_{k-1}\right) n_{\tau_{ij}, \tau_{kl}} \right) \right), \\
n_D(\nu) &\approx \sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(n_{\overrightarrow{D}, \tau_{ij}}(\nu) \right) \\
&= \sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(I\left(i \leq q, j \geq 2\right) \sum_{k=i+1}^{q+1} \sum_{l=1}^{j-1} \left(I\left(\tau_i + \nu \leq \tau_{k-1}\right) n_{\tau_{ij}, \tau_{kl}} \right) \right), \\
\widehat{\mathrm{C}}_{\mathrm{marg}}(\nu) &= \frac{n_C(\nu)}{n_C(\nu) + n_D(\nu)} \approx \widehat{\mathrm{C}}_{\mathrm{marg}}^{\rightarrow}(\nu) = \frac{\sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(n_{\overrightarrow{C}, \tau_{ij}}(\nu) \right)}{\sum_{i=1}^{q+1} \sum_{j=1}^{q+1} \left(n_{\overrightarrow{C}, \tau_{ij}}(\nu) + n_{\overrightarrow{D}, \tau_{ij}}(\nu) \right)},
\end{aligned}
$$

where, τ_{ij} corresponds to the rectangle with values $Y \in [\tau_{i-1}, \tau_i[$ and values $\pi(\boldsymbol{X}) \in [\tau_{j-1}, \tau_j[$. Furthermore, $n_{\overrightarrow{C}, \tau_{ij}}(\nu)$ $(n_{\overrightarrow{D}, \tau_{ij}}(\nu))$ equals the number of concordant (discordant) comparisons for region τ_{ij}, and $n_{\tau_{ij}, \tau_{kl}}$ is the product of the number of elements in regions τ_{ij} and τ_{kl}.

3 Simulations

We now investigate the performance of the proposed k-means approximation and the marginal approximation for the concordance probability in an extensive simulation study. Section 3.1 investigates the approximations for the discrete setting with a binary response variable, whereas Section 3.2 focuses on the continuous setting with a continuous response variable.

3.1 Discrete setting

Data generation setup To examine the performance of the proposed estimators when the response variable is binary, a simulation study was set up on a response variable following a beta-binomial distribution with parameter n equal to 1. The beta-binomial distribution, denoted $BB(\alpha, \beta, n)$ with

$\alpha > 0$ and $\beta > 0$, is a compound probability distribution and can be seen as a binomial distribution where the parameter p (i.e. probability of success) is randomly drawn from a beta distribution, denoted $\text{Beta}(\alpha, \beta)$. Note that when $Y \sim \text{Beta}(\alpha, \beta)$, its mean μ equals $\frac{\alpha}{\alpha+\beta}$ and its concentration is defined by $\kappa = \alpha + \beta$. The concentration indicates how broad this beta distribution is: the larger the concentration, the narrower the distribution. Moreover, we focus on $\alpha > 1$ and $\beta > 1$ since the beta distribution is then unimodal. More information about the beta-binomial distribution can be found in Appendix A.

In this simulation setting, a parameter p is sampled from the beta distribution (and used for true prediction), whereas a sample of the corresponding beta-binomial distribution yields the observed value. These pairs of predicted and observed values for p are then used to calculate the proposed approximations for the concordance probability.

First, the population value of C is computed. For this, a large sample (i.e. with sample size 100,000,000) is selected from a beta distribution. Based on its mean and concentration, we considered 63 possible beta distributions (resulting in 63 population values), see Table 1 for combinations. Next, these samples are used as true rate values to sample outcomes from the binomial distribution with $n = 1$ (i.e. Bernouilli distribution). These sampled outcomes, i.e. the sampled rates, can be seen as the true predictions coming from the beta distribution. Moreover, they can be classified into two groups: the ones that have a sampled outcome equal to 0 and the ones that have a sampled outcome equal to 1. The population value is then computed by comparing the sampled rates of the 0 group with the ones of the 1 group. This population value is for each of the considered situations presented in Table 1.

A first thing to notice is that a concentration $\kappa = 15$ was not possible for extreme probabilities p, since it required α or β to be smaller than 1. As expected, we do see similarities in *complementary* probabilities; e.g. $p = 0.25$ has approximately the same population values as $p = 0.75$. In these situations, the relative size of the two groups remains the same. Moreover, the larger the concentration, the smaller the population value of the concordance probability. This can be explained by the fact that the difference between the values of the probabilities, i.e. the predictions, is small in case of a high concentration. Finally, the more extreme the probability (close to zero or close to one), the higher the concordance probability.

Table 1: The population values of C when p is sampled from different beta distributions with mean μ and concentration κ.

κ	μ						
	0.05	0.10	0.20	0.25	0.30	0.40	0.50
15		0.7234	0.6744	0.6623	0.6541	0.6448	0.6421
25	0.7347	0.6788	0.6374	0.6276	0.6208	0.6134	0.6111
50	0.6741	0.6297	0.5985	0.5912	0.5862	0.5808	0.5792
100	0.6263	0.5929	0.5701	0.5648	0.5613	0.5574	0.5562
150	0.6041	0.5762	0.5574	0.5529	0.5501	0.5469	0.5460

κ	μ					
	0.60	0.70	0.75	0.80	0.90	0.95
15	0.6448	0.6541	0.6623	0.6744	0.7234	
25	0.6134	0.6208	0.6275	0.6374	0.6788	0.7347
50	0.5808	0.5862	0.5911	0.5985	0.6297	0.6741
100	0.5574	0.5613	0.5648	0.5701	0.5929	0.6263
150	0.5469	0.5501	0.5530	0.5574	0.5762	0.6041

It is important to investigate whether the size of the population value has an effect on the algorithms. Therefore, we consider $\mu = 0.10$, for $\kappa \in \{15, 50, 150\}$ in the above setting. To determine whether the extremity of the probability affects the algorithms, the simulation study also focuses on $\mu \in \{0.10, 0.25, 0.50\}$, for $\kappa = 50$.

Evaluation setup For each of the above discussed simulation settings, 1,000 samples are generated on which the k-means approximation and the marginal approximation are applied to calculate the concordance probability. As benchmark method, we added the standard trapezium approximation of Fawcett (2006), which determines the ROC curve efficiently and then calculates the AUC as the area under the ROC curve, by approximating this integral by the trapezium rule.

This simulation study also tests the effect of using 10, 20, 100, 500 or 1,000 boundary values or clusters, while working with a data set with 500,000 or 5,000,000 observations. In case of the marginal approximation, the boundary values are evenly spaced percentiles of the empirical distribution of the predictions of both groups, as advised in Section 2.1. Focusing on the simulation setting with $\mu = 0.1$ and $\kappa = 50$, Table 2 shows the bias (based on the mean or the median) together with the mean and median run time, but also the standard deviation and the interquartile range of the computed concordance measure and run time. For the other simulation settings, the same table is constructed as can be seen in Appendix B. Note that the bias is here defined as the difference between the mean (or the median) of the estimated values and the true value, meaning that a positive bias corresponds with estimated values that are overall too large.

Table 2: This table considers the discrete simulation setting with $\mu = 0.10$ and $\kappa = 50$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This all is shown in function of the number of boundary values or clusters, for the k-means approximation, the marginal approximation and the one based on the trapezium rule. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0002	0.0041	-0.0007	0.0009	0.5616	0.5215	4.8458	4.6855
20	-0.0002	-0.0001	-0.0002	-0.0004	0.5677	0.5270	4.5939	3.9200
100	-0.0001	-0.0001	-0.0002	-0.0002	0.8358	0.7740	6.3073	6.2630
500	-0.0001	-0.0001	-0.0002	-0.0002	4.7549	4.4940	19.9356	19.7370
1,000	-0.0001	-0.0001	-0.0002	-0.0001	14.2775	13.4840	42.5733	41.8800
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0205	0.0252	0.0161	0.0216	0.1897	0.2463	1.5367	1.9117
20	0.0046	0.0059	0.0042	0.0057	0.1919	0.2690	1.4260	1.8145
100	0.0013	0.0017	0.0005	0.0007	0.1531	0.1063	0.1740	0.1490
500	0.0013	0.0017	0.0004	0.0005	0.5185	1.0410	0.5131	0.2822
1,000	0.0013	0.0017	0.0004	0.0005	1.1108	2.1002	1.2281	2.3403
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0116	0.0116	0.0115	0.0115	0.1109	0.1100	1.2258	1.2190
20	0.0060	0.0060	0.0060	0.0060	0.1112	0.1110	1.2274	1.2220
100	0.0012	0.0012	0.0011	0.0011	0.1214	0.1210	1.2867	1.2810
500	0.0002	0.0001	0.0001	0.0001	0.1683	0.1670	1.6043	1.6060
1,000	0.0000	0.0000	0.0000	0.0000	0.2244	0.2230	1.9884	1.9870
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0014	0.0018	0.0004	0.0006	0.0041	0.0020	0.0249	0.0270
20	0.0013	0.0018	0.0004	0.0006	0.0028	0.0020	0.0243	0.0280
100	0.0013	0.0017	0.0004	0.0005	0.0048	0.0040	0.0278	0.0442
500	0.0013	0.0017	0.0004	0.0005	0.0073	0.0040	0.0342	0.0540
1,000	0.0013	0.0017	0.0004	0.0005	0.0094	0.0050	0.0373	0.0560
trapezium	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
	-0.0001	-0.0001	-0.0002	-0.0001	0.3028	0.3010	3.0180	3.0180
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
	0.0013	0.0017	0.0004	0.0005	0.0081	0.0050	0.0371	0.0500

Discussion of results From Table 2, some general conclusions that are also valid in the other simulation settings, can be drawn about the bias. First of all, the bias of all approximations is low, even almost negligible. Overall, the bias of the k-means approximation and the trapezium

approximation is smaller than the bias of the marginal approximation. The latter results in a bias that is not affected by the sample size of the data, while the bias of the k-means approximation depends on the sample size. As expected, the bias decreases when the number of clusters or boundaries increases. In general, we see that the bias based on the mean and the bias based on the median are close to each other. Hence, we can conclude that there were no extreme estimates.

Table 2 also reveals some general conclusions about the run time. Primarily, the marginal approximation results in the smallest run times, opposite to the k-means approximation with the largest run times. Hence, the run time of the trapezium approximation is always smaller than the one of the k-means approximation, but larger than the run time of the marginal approximation. As expected, the run time generally increases as the number of clusters or boundary values increases. The run time also increases as the sample size increases. More specifically, we see that when the sample size increases from $n = 500,000$ to $n = 5,000,000$, the run time gets approximately ten times larger for the marginal approximation and the trapezium approximation. However, for the k-means approximation, the increment factor of the run time is shorter than ten and becomes even shorter when the number of clusters increases.

The estimates vary little as can be seen from Table 2. From the simulations, we learn that the variability of the estimated concordance probability is higher for the k-means approximation than for the marginal approximation, at least for a low number of clusters or boundary values. This can be explained by the random starting values for the clusters in the k-means clustering algorithm, combined with the low number of clusters. For more than twenty clusters or boundary values, the standard deviation and the interquartile range are the same for the two approximations. Furthermore, the standard deviation and interquartile range do not change in function of the number of boundary values for the marginal approximation, whereas we do see a reduction of variability when the number of clusters increases for the k-means approximation. Overall, the variation of the estimates decreases for each of the three algorithms when the sample size increases. For the marginal approximation we can conclude that in general the run time variability increases when the sample size increases. This conclusion cannot be made for the k-means approximation.

Until here, only general conclusions of each specific simulation setting on its own are considered. To check whether there is an effect of the size of the population value on the algorithms, Tables 2, B.2 and B.3 are compared. From these tables, we can see that the bigger the concentration (and hence the smaller the population value of the concordance probability), the smaller the bias of all approximations in most of the cases. Moreover, the true population value of the concordance probability has no effect on their run time and its variability for all algorithms. The true population value of the concordance probability has also no effect on the variability of their estimates. Another question was whether the extremity of the probability affects the algorithms. To answer this question, we compare the Tables 2, B.1 and B.4. The extremer the probability, the bigger the bias and the smaller run times of the marginal approximation. These conclusions cannot be drawn for the k-means approximation and the approximation based on the trapezium rule. For all algorithms, the extremity of the probability has no effect on the variability of the estimates and their run times.

As a conclusion, this simulation study favors the marginal approximation over the approximations based on the k-means algorithm or the trapezium rule. The marginal approximation with 500 clusters or more delivers namely estimates that are very weakly biased. Moreover, this approximation is computed faster when dealing with the really large data sets, hence better passing the sample size complexity test than the k-means approximation or the one based on the trapezium rule.
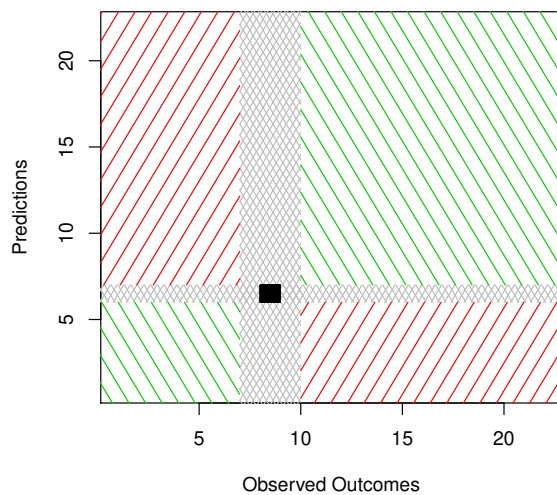
Figure 3: A grid is laid on top of the (Y, π) space in which the regions are highlighted that contain the concordant pairs (downward dashed region, in green), the discordant paired (upward dashed region in red) and incomparable pairs (upward and downward dashed region, in grey) for the region shown in an even black rectangle.

3.2 Continuous setting

In this subsection, the goal is to investigate the performance of the k-means approximation and the marginal approximation, when the response variable is continuous.

Data generation setup We suppose that the observations and predictions both follow a standard normal distribution. In this simulation, the correlation between the observations and predictions varies between the following values $\rho \in \{0, 0.25, 0.5, 0.75\}$. The parameter ν is determined such that $x\%$ of the pairwise absolute differences of the observed values is smaller than ν, with $x \in \{0, 20, 40\}$.

A first step in this simulation is to determine the correct values for ν. As these values are only based on the observations, they will be independent of the correlation ρ. Moreover, it is computationally impossible to precisely calculate these values for each sample and hence, the same values of ν will be consistently used. In order to determine these values, we first sample 10,000 observations from a standard normal distribution of which all pairwise absolute differences are calculated. The 20% and 40% percentiles of these absolute differences represent the values for ν in this specific sample, denoted by the pair $\mathbf{p}$. The above procedure is repeated 100 times, such that the means $\mathbf{q}$ of all obtained percentiles $\mathbf{p}_1, \ldots \mathbf{p}_{100}$ are a better estimate for the correct values of ν. Since the ranges of $\mathbf{p}_1, \ldots \mathbf{p}_{100}$ can still be 3%, the whole aforementioned procedure is once again repeated 100 times. The mean values of these obtained means $\mathbf{q}_1, \ldots \mathbf{q}_{100}$ are the final values for ν, i.e. $\nu \in \{0, 0.3583, 0.7416\}$ for $x \in \{0, 20, 40\}$ respectively. These estimates are more reliable since the range of these means $\mathbf{q}_1, \ldots \mathbf{q}_{100}$ is maximum 0.4%.

The next step for the simulation is to determine the population values of $C(\nu)$, for $\nu \in \{0, 0.3583, 0.7416\}$ and $\rho \in \{0, 0.25, 0.5, 0.75\}$. For each combination of ρ and ν, the concordance probability is calculated by (4) based on a sample of size 50,000. This is repeated 100 times, and the mean of these 100 concordance probabilities is denoted by m. Since the range of these concordance probabilities can still be 1.6%, the above procedure is once again repeated five times. The mean value of the aforementioned obtained means $m_1, \ldots, m_5$ is the final value for $C(\nu)$. This estimation method is more reliable since the range of these means $m_1, \ldots, m_5$ is maximum 0.8%. The final values of the concordance probability for each combination of ρ and ν are denoted in Table 3. Completely in line with our expectations, the concordance probability increases when the correlation between the predictions and observations increases. In case that ρ is strictly positive, it can be seen that the concordance probability increases in function of ν.

Table 3: The population values of the concordance probability for several combinations of ν and ρ.

	ν		
ρ	0	0.3583	0.7416
0	0.5000	0.5001	0.5001
0.25	0.5804	0.5973	0.6164
0.50	0.6666	0.7011	0.7387
0.75	0.7699	0.8233	0.8747

Evaluation setup Similar to the discrete setting, 1,000 samples are generated for each of the above described simulation settings. On these samples, the marginal approximation and the k-means approximation are applied to calculate the concordance probability. To the best of our knowledge, we have proposed the first approximations to compute the concordance probability in the continuous setting and hence no benchmark methods are available. The k-means approximation tests the effect of 10, 20, 100, 500 or 1,000 clusters, whereas the marginal approximation focuses on 10, 20 or 100 boundary values. The latter only considers small numbers of boundary values due to the lengthy run times, as will be clear from the simulation results. Moreover, the boundary values are evenly spaced percentiles of the empirical distribution of the observed values, as advised in Section 2.2. Focusing

on the simulation setting with $\rho = 0.25$ and $\nu = 0.3583$, Table 4 shows the bias (based on the mean or median) together with the mean and median run time, but also the standard deviation and the interquartile range of the computed concordance measure and run time. For the other simulation settings, the same table is constructed as can be seen in Appendix C.

Table 4: This table considers the continuous simulation setting with $\rho = 0.25$ and $\nu = 0.3583$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0181	0.0173	0.0208	0.0196	1.0409	0.9020	6.8401	5.4290
20	0.0077	0.0076	0.0097	0.0096	1.1936	0.9900	7.3614	5.9335
100	0.0014	0.0015	0.0016	0.0016	2.2619	1.6825	11.4168	10.3470
500	0.0003	0.0003	0.0003	0.0003	14.3973	14.0835	26.5740	26.1695
1,000	0.0002	0.0002	0.0002	0.0002	33.1026	34.3245	45.5225	45.2805
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0342	0.0447	0.0338	0.0436	0.5161	0.7095	2.3342	3.6027
20	0.0165	0.0235	0.0160	0.0220	0.6839	0.8413	2.4344	3.9245
100	0.0026	0.0033	0.0022	0.0029	1.4296	1.8160	2.6989	0.3110
500	0.0006	0.0009	0.0003	0.0004	9.3571	18.3248	2.5966	0.2913
1,000	0.0005	0.0007	0.0002	0.0003	16.8481	29.5448	2.8324	0.3230
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0260	0.0260	0.0259	0.0259	2.0783	2.0770	26.8437	26.8590
20	0.0119	0.0119	0.0119	0.0119	3.8648	3.8660	49.2721	49.2805
100	0.0028	0.0028	0.0028	0.0028	85.7858	85.7620	316.6178	315.9965
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0007	0.0009	0.0002	0.0003	0.0516	0.0790	1.8140	2.5202
20	0.0006	0.0008	0.0002	0.0003	0.0632	0.1060	2.9274	3.7165
100	0.0005	0.0007	0.0002	0.0002	0.7199	1.0315	8.9207	11.7882

Discussion of results From Table 4, some general conclusions that are also valid in the other continuous simulation settings, can be made about the bias. The bias is low for all approximations and there is a decrease in the bias when the number of clusters or boundaries increases. Moreover, similar to the discrete setting, the bias of the k-means approximation is smaller than the one of the marginal approximation when using the same number of clusters or boundaries. The sample size of the data has clearly no effect on the bias of the marginal approximation, as well as on the k-means approximation with 100 clusters or more.

Finally, when the number of clusters is larger than ten, we see that the bias based on the mean and the bias based on the median are almost similar. Hence, we can conclude that no extreme estimates were encountered in these cases. The same holds for all considered numbers of boundaries for the marginal approximation. A note of caution is due here, since some aforementioned conclusions are not valid in case there is no correlation between the observations and the predictions (see Appendix C). Firstly, the bias of the marginal approximation seems independent of the number of boundaries. Secondly, the bias of the k-means approximation is only smaller than the one of the marginal approximation in case of less than 100 clusters or boundary values. Once it is higher than 100, the bias of both approximations is equal.

Table 4 also reveals some general conclusions about the run time. In contrast to the discrete setting, the run time of the marginal approximation is higher than the one of the k-means approximation. More specifically, the k-means method is approximately two times faster to compute than the marginal method for ten clusters or boundary values, while for hundred clusters or boundary values, it is thirty

to fifty times faster. Next, we see that the run time generally increases as the number of clusters or boundary values increases. Note that sometimes, this is not the case when we compare the simulation results for 10 and 20 clusters. Furthermore, the run time increases as the sample size increases for both approximations. Finally, there are no extreme run times, since the mean and median run times are nearly identical.

The estimates vary little as can be seen in Table 4. From the simulations, we learn that the variability of the estimated concordance probability is higher for the k-means approximation than for the marginal approximation when the same number of clusters and boundary values is considered. The k-means approximation with more than 100 clusters has approximately the same values for the standard deviation and interquartile range of the estimates, as the marginal approximation with 10, 20 or 100 boundary values. This was expected due to the random starting values for the clusters in the k-means clustering algorithm. The latter also explains why we see a reduction of the variability when the number of clusters increases for the k-means approximation. However, for the marginal approximation the standard deviation and interquartile range of the estimates hardly change in function of the number of boundary values. Overall, the variation of the estimates decreases when the sample size increases.

Thus far, the focus was on the variability of the estimates. In Table 4, the variability of the run times is also studied. When the number of observations equals 500,000, the variability of the run time is mostly higher for the k-means approximation than for the marginal approximation. Moreover, it increases when the number of clusters or boundary values increases. For 5,000,000 observations, we still see an increase of variability when the number of clusters or boundary values increases, apart from the interquartile range for the cases with 10 or 20 clusters. Moreover, the variability of the run time is in this case typically smaller for the k-means approximation than for the marginal approximation. Going from 500,000 to 5,000,000 observations leads to an increase in the variability of the run time for the marginal approximation. For the k-means approximation, the same holds for the standard deviation (interquartile range) in case of 100 (20) clusters or less. However, a larger number of clusters results in a decrease of variability in the run time when going from 500,000 observations to 5,000,000 observations.

Finally, we also consider the effect of ρ and ν on both approximations. In general, the bias increases when the correlation increases, but it is independent of ν. Focusing on the run time, we see that it seems to be unaffected by the correlation between the observed and predicted values. As expected, the run time decreases for increasing values of ν, since larger values of ν result in smaller numbers of pairs that should be compared. Next, the variability of the run times and the estimates does not change in function of ν. However, the variability of the estimates decreases when ρ increases, whereas there is no link between the variability of the run times and ρ.

To conclude, this simulation study clearly favors the k-means approximation over the marginal one. The k-means approximation delivers namely estimates that are very weakly biased, even if the number of clusters is poorly tuned. Also, the k-means approximation is computed much faster when dealing with really large data sets, hence better passing the sample size complexity test than the marginal approximation. As a general recommendation, one should choose 100 clusters when using the k-means approximation, as the fitting time is still very small, and as this results in a low variability over the estimated concordance probability.

4 Real-life examples

In this section, two real life data sets from Kaggle[1] are used to compare the exact concordance probability with the approximations discussed in this paper. The first example focuses on the discrete setting, whereas the second one deals with a continuous response variable. Both examples are executed on a computer with specifications Intel Core i7-8650U CPU @ 1.90GHz 2.11GHz processor.

4.1 Predict Click through rate (CTR) for a website

We consider data about the click through rate (CTR) for a website related to job searches (Animesh, 2019). This data set consists of 10 variables and 1,200,890 observations, where each observation corresponds to a user's view of a job listing. One of the variables is called `apply`, which indicates whether or not the user has applied for this job listing after checking the job description. The related notebook "Let's Start" on Kaggle cleans the data first, i.e. duplicates and observations with missing values are removed. Next, the data set is split into a training and test set (respectively containing 871,290 and 81,704 observations) and finally three popular predictive models are applied: XGBoost (xgb), random forest (rf) and a Light Gradient Boosted Machine (lgbm). The main interest of this paper is on the calculation of the concordance probability of the model once the predictions are available. Normally, this measure is only determined for the test set, but since we also focus on large data sets, we consider the predictions of the entire cleaned data set as well.

In order to determine the bias of the concordance probability estimates, we first need to determine its exact value. Therefore, the data set is first split into a zero-group and a one-group, based on the value of the variable `apply`. In this case the one-group is the smallest, which is why a for loop is used for the elements in this group. In each iteration, we count the number of predictions in the zero-group that are smaller than the prediction of the considered element of the one-group. Summing up all these counts, divided by the number of considered pairs, results in the exact concordance probability. The latter can be found in Table 5 and shows that, based on the concordance probability, the third model based on a Light Gradient Boosted Machine, performs best on the test set. Moreover, it requires an excessive amount of time to calculate the concordance probability on the complete cleaned data set.

Table 5: The first three columns show the exact concordance probabilities obtained for the three different models of the CTR example, for the test set (test) or the complete cleaned data set (all). In the last three columns, the computing times are shown.

	C			run time (s)		
	lgbm	xgb	rf	lgbm	xgb	rf
test	0.5842	0.5838	0.5655	3.58	3.64	3.66
all	0.5940	0.5872	0.7052	428.20	432.33	427.16

Table 6 shows for the three predictive models the bias of the different approximations for the concordance probability discussed in this paper. First of all, the bias of all approximations is extremely low, even almost negligible. More specifically, the smallest bias is in this example obtained by approximations based not only on the trapezium rule, but also on the k-means algorithm with 1,000 clusters. However, the approximations based on the k-means algorithm do have the largest run time. The smallest run times are obtained by the marginal approximation. Moreover, comparing Tables 5 and 6 show that all approximations for the complete cleaned data set have a much smaller run time than the one of the exact calculation. Finally, general conclusions from the simulation

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[1] https://www.kaggle.com

study in the previous section are confirmed in this example, e.g. the bias decreases when the number of boundaries increases, the run time increases when the number of clusters and/or observations increases and so on.

Table 6: In the left part of this table, we can see the bias of the concordance probability estimates for the CTR example, based on the k-means approximation, the marginal approximation and the one based on the trapezium rule. The right part shows the corresponding run times of these approximations.

| | bias | | | | | | run time (s) | | | | | |
| | test | | | all | | | test | | | all | | |
k-means	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf
10	-0.0193	-0.0365	0.0359	0.0096	-0.0273	0.0069	0.12	0.17	0.10	1.61	1.89	1.08
20	-0.0074	0.0067	-0.0129	0.0036	0.0025	0.0017	0.31	0.26	0.22	1.55	2.23	2.89
100	0.0004	-0.0004	-0.0001	0.0003	0.0001	-0.0002	0.48	0.48	0.27	2.58	4.31	1.67
500	0.0001	0.0001	0.0000	0.0000	-0.0000	-0.0001	4.65	4.77	5.36	14.16	13.75	9.17
1,000	0.0000	0.0001	0.0000	0.0001	0.0000	0.0000	18.46	17.61	18.17	38.42	38.24	25.06
	test			all			test			all		
marginal	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf
10	0.0077	0.0074	0.0063	0.0084	0.0077	0.0165	0.03	0.03	0.03	0.19	0.19	0.22
20	0.0040	0.0041	0.0031	0.0043	0.0041	0.0089	0.05	0.03	0.03	0.22	0.22	0.21
100	0.0010	0.0009	0.0007	0.0010	0.0009	0.0019	0.03	0.03	0.03	0.21	0.18	0.23
500	0.0003	0.0003	0.0002	0.0003	0.0002	0.0004	0.04	0.06	0.06	0.40	0.25	0.39
1,000	0.0002	0.0002	0.0001	0.0002	0.0001	0.0002	0.08	0.08	0.11	0.42	0.37	0.50
	test			all			test			all		
trapezium	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf	lgbm	xgb	rf
	0.0001	0.0001	0.0000	0.0000	0.0000	0.0000	0.07	0.04	0.05	0.37	0.41	0.55

4.2 New York City taxi fare prediction

We consider data about the taxi fares in New York (GoogleCloud, 2018). This data set consists of a train and test set of respectively 55,423,856 and 9,914 observations, representing taxi rides in New York City, and seven variables each. One of the variables is called `fare_amount`, which is a continuous variable indicating the fare amount (inclusive of tolls) for a taxi ride in New York City. The other six variables represent the pickup and drop off locations, the pickup time and the number of passengers. The related notebook "NYC Taxi Fare - Data Exploration" written by van Breemen (2018) uses 2,000,000 rows of the training data to construct a linear regression model in order to predict the variable `fare_amount`. The first step is cleaning the data, e.g. removing missing data, removing noisy data points with underwater locations and so on. This results into a data set consisting of 1,918,905 lines, of which 75% will be used to train the model and 25% to test the model. In the next step, some data exploration reveals that the important features will be the year and hour of the pickup time, the driven distance and the number of passengers. The latter variables are therefore used in the linear regression model to predict the fare amount for a taxi ride in New York City. Once again, the interest of this paper is not on how this model is constructed, but on the calculation of the concordance probability of the model once the predictions are available. Normally, this measure is only determined for the test set which consists here of 479,727 observations. Since we focus on large data sets, we also consider the 1,918,905 predictions of the entire cleaned data set. Note that the correlation between the predictions and the observations is 89.52% for the test set and 89.24% for the complete cleaned data set.

The goal is to predict the C-index for different values of ν. Similar to the simulation study, we therefore first determine the value of ν such that $x\%$ of the pairwise absolute differences of the observed values is smaller than ν, with $x \in \{0, 10, 20, 30, 40, 50\}$. A first possible way to determine these values is by considering all possible pairs between the observations in order to determine the absolute differences between observations belonging to the same pair. However, in case of 1,918,905 observations, this would result in 1,841,097,240,060 pairs and corresponding differences. A closer look to the data reveals that out of these almost two million observations, only 2,569 unique values for the fare amount for a taxi ride in NYC are denoted. These unique values are represented in $\mathbf{y}$ and the corresponding frequencies in $\mathbf{w}$. Applying the function `combn` in R on $\mathbf{y}$, results in all possible pairs of these unique values. The corresponding frequencies of these pairs are obtained by the strict upper triangle of the matrix $\mathbf{ww}^T$. However, do note that there are still $\frac{1}{2}\mathbf{w}^T(\mathbf{w} - 1)$ pairs possible that consist of two identical observations, and hence with a difference of zero between both. After summing up the frequencies of pairs with the same absolute difference between their observations, the empirical cumulative distribution function of those differences can be constructed. From this function, the ν values are determined and represented in the headings of Table 7.

In order to determine the bias of the concordance probability estimates, we first need to determine its exact value. Note that we cannot take advantage anymore of the small number of unique values in the observations, since their predictions can differ. Therefore, a for loop is used for all the observations. In each iteration, we select the rows with an observation strictly larger than the considered observation added up with ν. The number of selected rows is for each iteration stored in $\mathbf{u}$. In this selection, we count the number of predictions that are larger than the prediction of the considered element, and store this value in $\mathbf{v}$. Hence, the concordance probability can be obtained by the division of $\bar{\mathbf{v}}$ by $\bar{\mathbf{u}}$. For all considered values of ν, the concordance probability for the test set and the complete data set can be found in Table 7. Note that the run times to calculate the exact concordance probability on the complete cleaned data set are staggering.

Table 8 shows the bias and run time of the marginal approximation and the k-means approximation in this example. First of all, the bias of all approximations is low, especially for the marginal

Table 7: This table shows the exact concordance probabilities together with the computing times for different values for ν. The upper part focuses on the test set (test) and the lower part on the complete cleaned data set (all).

	ν - test					
	0	12.12	20.75	25.60	31.64	38.54
C	0.8583	0.9808	0.9817	0.9800	0.9773	0.9783
run time (s)	8,908	4,125	3,455	3,295	3,159	3,023
	ν - all					
	0	12.87	22.20	30.30	39.44	49.43
C	0.8577	0.9801	0.9799	0.9763	0.9772	0.9810
run time (s)	138,058	58,355	45,559	36,842	31,896	27,397

approximation when $\nu > 0$. Nevertheless, we still advise to use the k-means approximation in this continuous version due to the very small run times, only yielding a small bias. Moreover, the marginal algorithm is not always able to determine an approximation when ν is large and the number of boundary values is small. In these cases, the low number of regions makes it namely impossible to compare regions that satisfy the restriction of ν. Focusing for example on the complete data set with 100 boundary values and $\nu = 49.43$, the smallest boundary value τ_1 is 3.3 whereas the biggest boundary value τ_{100} is 52. Since the absolute difference between τ_{100} and τ_1 is smaller than ν, no valid region-to-region comparisons can be made. Despite the fact that the run times of the marginal algorithm are much higher than the ones of the k-means algorithm, it is worth mentioning that they are still much smaller than the original ones denoted in Table 7. Finally, general conclusions from the simulation study are confirmed in this example, e.g. the bias decreases when the number of boundaries increases, the run time increases when the sample size increases and so on.

5 Conclusion

The current existing algorithms to compute the concordance probability are only adapted to a discrete response variable in case of large data sets. Therefore, we proposed two computationally efficient algorithms to estimate the concordance probability in both the discrete and continuous setting: the k-means algorithm and the marginal algorithm. In the discrete setting, the marginal approximation is the fastest method and moreover, it achieves the same bias as the standard approximation based on the trapezium rule. However, in case of a continuous response variable, the k-means algorithm is the most precise and results in the smallest run time. These conclusions are based on an extensive simulation study, that also focuses on the variability of the estimates and the run times of the algorithms. The good performance is also illustrated on two real data applications. Further lines of research can consist of adapting these methods to different types of concordance probabilities. In survival analysis for example, it can happen that some observations are right censored. In order to have a comparable pair of two survival times with their predictions, one needs to be sure that the observation with the smallest observed survival time is not censored, see (Harrell et al., 1982; Gerds and Schumacher, 2007). For the k-means approximation, this can be obtained by adding in the indicator functions of Equation (6) the condition that y_j is not censored.

The implementations of the discussed approximations of the concordance probability are written in R and are available on github as an R -package [2].

Table 8: The bias of the concordance probability estimates for the taxi fare example, based on the *k*-means approximation and the marginal approximation. This is done for the test set (test) and the complete data set (all), for different values of ν.

bias

k-means

k-means	ν - test						ν - all					
	0	12.12	20.75	25.60	31.64	38.54	0	12.87	22.20	30.30	39.44	49.43
10	0.1405	0.0192	0.0183	0.0200	0.0227	0.0212	0.1413	0.0199	0.0201	0.0237	0.0228	—
20	0.0398	0.0147	0.0113	0.0200	0.0056	0.0163	0.0386	0.0196	0.0169	0.0237	0.0228	0.0190
100	0.0028	0.0099	0.0094	0.0100	0.0094	0.0142	0.0020	0.0055	0.0087	0.0067	0.0079	0.0190
500	-0.0069	0.0036	0.0042	0.0028	0.0068	0.0101	-0.0071	0.0026	0.0065	0.0082	0.0068	0.0188
1,000	-0.0076	0.0019	0.0015	0.0045	0.0029	0.0053	-0.0083	0.0021	0.0033	0.0028	0.0099	0.0149

marginal

marginal	ν - test						ν - all					
	0	12.12	20.75	25.60	31.64	38.54	0	12.87	22.20	30.30	39.44	49.43
10	0.0534	0.0052	0.0072	0.0147	—	—	0.0538	0.0035	0.0103	—	—	—
20	0.0319	0.0055	0.0065	0.0141	—	—	0.0325	0.0051	0.0090	—	—	—
100	0.0123	0.0024	0.0010	0.0005	0.0012	0.0044	0.0135	0.0022	0.0010	0.0006	0.0045	0.0042
500	0.0091	0.0011	0.0008	0.0007	0.0008	0.0012	0.0101	0.0010	0.0008	0.0007	0.0013	0.0026
1,000	0.0075	0.0008	0.0006	0.0006	0.0007	0.0010	0.0087	0.0007	0.0006	0.0007	0.0011	0.0026

run time (s)

k-means

k-means	ν - test						ν - all					
	0	12.12	20.75	25.60	31.64	38.54	0	12.87	22.20	30.30	39.44	49.43
10	1.10	1.14	1.89	1.83	1.72	1.30	5.14	3.57	6.19	5.69	2.24	9.12
20	1.74	3.15	4.63	2.52	3.19	2.15	2.40	3.01	7.02	6.75	7.02	11.31
100	1.22	0.97	1.70	2.01	2.06	0.69	5.75	5.06	5.04	3.55	10.48	3.45
500	4.07	2.47	3.91	3.38	2.33	2.51	11.86	8.46	10.41	9.18	8.28	7.99
1,000	9.46	5.31	6.50	4.20	6.45	4.79	25.00	14.58	14.64	14.29	13.36	13.81

marginal

marginal	ν - test						ν - all					
	0	12.12	20.75	25.60	31.64	38.54	0	12.87	22.20	30.30	39.44	49.43
10	2.66	3.16	3.17	2.99	3.03	4.18	11.81	13.49	14.18	13.19	13.63	13.11
20	4.58	6.95	6.02	6.20	5.68	6.09	18.33	25.71	27.26	24.25	26.41	24.90
100	14.38	20.92	20.17	19.08	19.06	18.97	58.09	82.01	79.48	79.64	81.29	84.61
500	29.00	37.63	38.85	36.17	36.06	35.78	115.20	152.52	152.51	145.28	142.08	150.61
1,000	38.86	47.19	43.99	44.92	43.51	44.14	150.41	173.61	174.67	179.13	179.27	179.15

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References

Animesh (2019). Predict click through rate (ctr) for a website.

Bamber, D. (1975). The area above the ordinal dominance graph and the area below the receiver operating characteristic graph. Journal of mathematical psychology, 12(4):387–415.

Bouckaert, R. R. (2006). Efficient auc learning curve calculation. In Australasian Joint Conference on Artificial Intelligence, pages 181–191. Springer.

Calders, T. and Jaroszewicz, S. (2007). Efficient auc optimization for classification. In European Conference on Principles of Data Mining and Knowledge Discovery, pages 42–53. Springer.

De Cnudde, S., Ramon, Y., Martens, D., and Provost, F. (2019). Deep learning on big, sparse, behavioral data. Big data, 7(4):286–307.

Eguchi, S. and Copas, J. (2002). A class of logistic-type discriminant functions. Biometrika, 89(1):1–22.

Fawcett, T. (2006). An introduction to roc analysis. Pattern recognition letters, 27(8):861–874.

Gerds, T. A. and Schumacher, M. (2007). Efron-type measures of prediction error for survival analysis. Biometrics, 63:1283–1287.

GoogleCloud (2018). New york city taxi fare prediction.

Harrell, F. E., Califf, R. M., Pryor, D. B., Lee, K. L., and Rosati, R. A. (1982). Evaluating the yield of medical tests. Journal of the American Medical Association, 247:2543–2546.

Heller, G. and Mo, Q. (2016). Estimating the concordance probability in a survival analysis with a discrete number of risk groups. Lifetime data analysis, 22(2):263–279.

Komori, O. (2011). A boosting method for maximization of the area under the roc curve. Annals of the Institute of Statistical Mathematics, 63(5):961–979.

Liu, X.-Y., Wu, J., and Zhou, Z.-H. (2008). Exploratory undersampling for class-imbalance learning. IEEE Transactions on Systems, Man, and Cybernetics, Part B (Cybernetics), 39(2):539–550.

Ma, S. and Huang, J. (2005). Regularized roc method for disease classification and biomarker selection with microarray data. Bioinformatics, 21(24):4356–4362.

Pencina, M. J. and D'Agostino, R. B. (2004). Overall c as a measure of discrimination in survival analysis: model specific population value and confidence interval estimation. Statistics in medicine, 23(13):2109–2123.

Razavian, N., Blecker, S., Schmidt, A. M., Smith-McLallen, A., Nigam, S., and Sontag, D. (2015). Population-level prediction of type 2 diabetes from claims data and analysis of risk factors. Big Data, 3(4):277–287.

Reddy, C. K. and Aggarwal, C. C. (2015). Healthcare data analytics, volume 36. CRC Press.

Steyerberg, E. W., Vickers, A. J., Cook, N. R., Gerds, T., Gonen, M., Obuchowski, N., Pencina, M. J., and Kattan, M. W. (2010). Assessing the performance of prediction models: a framework for some traditional and novel measures. Epidemiology (Cambridge, Mass.), 21(1):128.

van Breemen, A. (2018). Nyc taxi fare - data exploration.

Yan, G. and Greene, T. (2008). Investigating the effects of ties on measures of concordance. Statistics in medicine, 27(21):4190–4206.

Appendix A

Assume that X is a random variable following a beta-binomial distribution, e.g. $X \sim BB(\alpha, \beta, n)$, and denote the probability density function of the beta-binomial, beta and binomial distribution respectively as f_{BB}, f_{Beta} and f_{Bin}. Then the following calculations show the relation between these distributions as discussed in Section 3.1:

$$
\begin{aligned}
f_{BB}(x|\alpha, \beta, n) &= \int_0^1 f_{Bin}(x|p) f_{Beta}(p|\alpha, \beta) dp \\
&= \int_0^1 \binom{n}{x} p^x (1-p)^{n-x} \frac{p^{\alpha-1}(1-p)^{\beta-1}}{Beta(\alpha, \beta)} dp \\
&= \frac{\binom{n}{x}}{Beta(\alpha, \beta)} \int_0^1 p^{x+\alpha-1}(1-p)^{n-x+\beta-1} dp & \text{(A.1)} \\
&= \frac{\binom{n}{x}}{Beta(\alpha, \beta)} Beta(x+\alpha, n-k+\beta) & \text{(A.2)} \\
&= \frac{\Gamma(n+1)\Gamma(\alpha+\beta)\Gamma(x+\alpha)\Gamma(n-x+\beta)}{\Gamma(x+1)\Gamma(n-x+1)\Gamma(\alpha)\Gamma(\beta)\Gamma(n+\alpha+\beta)}. & \text{(A.3)}
\end{aligned}
$$

From Equation (1) to Equation (2), the definition of the beta function $Beta$ is used, and from Equation (2) to (3) the definition of the gamma function Γ together with its relation to the beta function.

Appendix B

In this appendix, the results of the simulation study in the discrete setting are shown.

Table B.1: This table considers the discrete simulation setting with $\mu = 0.50$ and $\kappa = 50$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This all is shown in function of the number of boundary values or clusters, for the k-means approximation, the marginal approximation and the one based on the trapezium rule. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0075	-0.0107	-0.0021	-0.0023	0.5167	0.5070	4.6971	4.6490
20	-0.0001	0.0002	0.0001	0.0002	0.6277	0.6065	4.6992	4.5465
100	0.0000	0.0000	0.0000	0.0000	0.8426	0.8810	6.3347	6.3110
500	0.0000	0.0000	0.0000	0.0000	4.9459	4.7380	19.7852	19.7825
1,000	0.0000	0.0000	0.0000	0.0000	16.5195	16.0410	40.8346	40.8205
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0191	0.0267	0.0193	0.0283	0.1101	0.1453	0.9143	1.1840
20	0.0051	0.0063	0.0045	0.0058	0.1812	0.2725	1.2505	1.5353
100	0.0008	0.0011	0.0004	0.0006	0.1479	0.2130	0.2409	0.1015
500	0.0008	0.0010	0.0003	0.0003	0.5301	0.6510	0.1321	0.1782
1,000	0.0008	0.0010	0.0003	0.0003	1.9919	3.0160	0.2073	0.2715
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0072	0.0072	0.0072	0.0072	0.1096	0.1090	1.2355	1.2310
20	0.0038	0.0038	0.0038	0.0038	0.1113	0.1110	1.2457	1.2360
100	0.0008	0.0008	0.0008	0.0008	0.1284	0.1280	1.3583	1.3540
500	0.0002	0.0002	0.0002	0.0002	0.1945	0.1940	1.8772	1.8780
1,000	0.0001	0.0001	0.0001	0.0001	0.2774	0.2750	2.5106	2.5050
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0009	0.0011	0.0003	0.0004	0.0039	0.0020	0.0207	0.0240
20	0.0008	0.0011	0.0003	0.0004	0.0036	0.0020	0.0256	0.0310
100	0.0008	0.0011	0.0003	0.0003	0.0052	0.0040	0.0273	0.0450
500	0.0008	0.0010	0.0003	0.0003	0.0067	0.0040	0.0320	0.0500
1,000	0.0008	0.0010	0.0003	0.0003	0.0105	0.0060	0.0454	0.0800
trapezium	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
	0.0000	0.0000	0.0000	0.0000	0.3087	0.3070	3.0455	3.0440
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
	0.0008	0.0010	0.0003	0.0003	0.0101	0.0060	0.0464	0.0630

Table B.2: This table considers the discrete simulation setting with $\mu = 0.10$ and $\kappa = 15$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This all is shown in function of the number of boundary values or clusters, for the k-means approximation, the marginal approximation and the one based on the trapezium rule. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0026	-0.0026	0.0003	0.0007	0.7010	0.7210	5.9778	5.4425
20	-0.0004	-0.0003	-0.0003	0.0000	0.5586	0.5295	4.4681	3.8385
100	-0.0002	-0.0002	-0.0002	-0.0002	0.8311	0.7720	6.3787	6.3190
500	-0.0002	-0.0002	-0.0001	-0.0001	4.6868	4.4250	19.9964	19.7895
1,000	-0.0002	-0.0002	-0.0001	-0.0001	14.1436	14.9040	42.1839	41.4760
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0116	0.0157	0.0123	0.0178	0.2456	0.3935	2.3443	4.0407
20	0.0037	0.0050	0.0036	0.0048	0.1951	0.2400	1.3723	1.2717
100	0.0011	0.0015	0.0005	0.0006	0.1530	0.1140	0.2567	0.1832
500	0.0011	0.0015	0.0004	0.0005	0.5078	1.0070	0.5364	0.3355
1,000	0.0011	0.0015	0.0004	0.0005	1.1389	2.0965	1.2206	2.3445
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0186	0.0186	0.0186	0.0186	0.1121	0.1120	1.2524	1.2470
20	0.0099	0.0099	0.0099	0.0099	0.1125	0.1120	1.2539	1.2460
100	0.0019	0.0019	0.0019	0.0019	0.1297	0.1290	1.3659	1.3610
500	0.0003	0.0002	0.0003	0.0003	0.1969	0.1960	1.8933	1.8940
1,000	0.0000	0.0000	0.0001	0.0001	0.2805	0.2780	2.5368	2.5300
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0012	0.0016	0.0004	0.0006	0.0045	0.0050	0.0252	0.0300
20	0.0012	0.0015	0.0004	0.0005	0.0034	0.0040	0.0258	0.0320
100	0.0011	0.0015	0.0004	0.0005	0.0055	0.0053	0.0292	0.0473
500	0.0011	0.0015	0.0004	0.0005	0.0079	0.0052	0.0362	0.0602
1,000	0.0011	0.0015	0.0004	0.0005	0.0109	0.0060	0.0499	0.0880
trapezium	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
	-0.0002	-0.0002	-0.0001	-0.0001	0.3131	0.3120	3.1069	3.1060
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
	0.0011	0.0015	0.0004	0.0005	0.0090	0.0080	0.0440	0.0580

Table B.3: This table considers the discrete simulation setting with $\mu = 0.10$ and $\kappa = 150$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This all is shown in function of the number of boundary values or clusters, for the k-means approximation, the marginal approximation and the one based on the trapezium rule. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0068	-0.0068	-0.0024	-0.0029	0.5268	0.4970	4.6623	4.6470
20	0.0001	0.0003	-0.0002	-0.0001	0.5864	0.5600	4.5954	3.9205
100	-0.0001	-0.0001	-0.0001	-0.0001	0.8301	0.7720	6.3045	6.2565
500	0.0000	0.0000	-0.0001	-0.0001	4.6777	4.4325	19.8896	19.6850
1,000	0.0000	0.0000	-0.0001	-0.0001	14.0217	13.1865	42.1063	41.3815
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0170	0.0241	0.0180	0.0237	0.1543	0.1932	1.2438	1.8035
20	0.0050	0.0062	0.0045	0.0059	0.2057	0.3150	1.4313	1.7775
100	0.0014	0.0019	0.0006	0.0007	0.1503	0.1068	0.2420	0.1345
500	0.0013	0.0018	0.0004	0.0006	0.5007	0.2217	0.5241	0.2482
1,000	0.0013	0.0018	0.0004	0.0006	1.1029	2.1043	1.2087	2.3322
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0069	0.0070	0.0069	0.0069	0.1100	0.1090	1.2676	1.2680
20	0.0036	0.0036	0.0036	0.0036	0.1100	0.1090	1.2665	1.2670
100	0.0007	0.0007	0.0007	0.0007	0.1163	0.1160	1.2906	1.2880
500	0.0001	0.0001	0.0001	0.0001	0.1511	0.1510	1.4895	1.4840
1,000	0.0000	0.0001	0.0000	0.0000	0.1907	0.1890	1.7298	1.7250
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0014	0.0020	0.0005	0.0007	0.0045	0.0020	0.0337	0.0280
20	0.0014	0.0019	0.0004	0.0006	0.0039	0.0030	0.0337	0.0280
100	0.0013	0.0018	0.0004	0.0006	0.0042	0.0040	0.0353	0.0340
500	0.0013	0.0018	0.0004	0.0006	0.0063	0.0050	0.0409	0.0540
1,000	0.0013	0.0018	0.0004	0.0006	0.0079	0.0050	0.0461	0.0630
trapezium	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
	0.0000	0.0000	-0.0001	-0.0001	0.3001	0.2990	2.9779	2.9770
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
	0.0013	0.0018	0.0004	0.0006	0.0089	0.0060	0.0370	0.0510

Table B.4: This table considers the discrete simulation setting with $\mu = 0.25$ and $\kappa = 50$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This all is shown in function of the number of boundary values or clusters, for the k-means approximation, the marginal approximation and the one based on the trapezium rule. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0109	-0.0136	-0.0029	-0.0022	0.5227	0.5020	4.6176	4.5790
20	0.0001	0.0003	0.0002	0.0003	0.6095	0.5700	4.6541	4.1635
100	0.0000	0.0000	0.0000	0.0000	0.8381	0.7950	6.3364	6.2920
500	0.0001	0.0000	0.0000	0.0000	5.1556	5.1110	19.8713	19.8500
1,000	0.0001	0.0000	0.0000	0.0000	16.2201	16.4855	40.8874	40.8250
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0198	0.0307	0.0196	0.0311	0.1284	0.1597	1.0836	1.4550
20	0.0051	0.0063	0.0044	0.0058	0.1896	0.2755	1.3292	1.6480
100	0.0010	0.0013	0.0004	0.0006	0.1489	0.1880	0.2969	0.1203
500	0.0009	0.0013	0.0003	0.0004	0.6278	0.9455	0.2888	0.1842
1,000	0.0009	0.0012	0.0003	0.0004	1.1688	1.6800	0.6113	0.2740
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0083	0.0083	0.0083	0.0083	0.1101	0.1090	1.2242	1.2270
20	0.0044	0.0044	0.0044	0.0043	0.1106	0.1100	1.2292	1.2320
100	0.0009	0.0009	0.0009	0.0009	0.1257	0.1250	1.3306	1.3260
500	0.0002	0.0002	0.0002	0.0002	0.1866	0.1850	1.7856	1.7770
1,000	0.0001	0.0001	0.0001	0.0001	0.2601	0.2580	2.3467	2.3430
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0010	0.0013	0.0003	0.0004	0.0043	0.0030	0.0297	0.0400
20	0.0010	0.0013	0.0003	0.0004	0.0027	0.0030	0.0273	0.0340
100	0.0009	0.0013	0.0003	0.0004	0.0050	0.0050	0.0342	0.0440
500	0.0009	0.0013	0.0003	0.0004	0.0078	0.0043	0.0430	0.0560
1,000	0.0009	0.0013	0.0003	0.0004	0.0098	0.0050	0.0526	0.0823
trapezium	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
	0.0001	0.0001	0.0000	0.0000	0.3053	0.3040	3.0089	3.0085
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
	0.0009	0.0013	0.0003	0.0004	0.0093	0.0050	0.0383	0.0530

Appendix C

In this appendix, the results of the simulation study in the continuous setting are shown.

Table C.1: This table considers the continuous simulation setting with $\rho = 0$ and $\nu = 0$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

k-means	bias				run time (s)			
	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	-0.0024	-0.0029	0.0022	0.0038	1.0263	0.9195	7.0400	5.5005
20	0.0005	0.0001	-0.0003	-0.0012	1.1580	0.9765	7.3263	5.9520
100	0.0000	0.0001	0.0000	0.0000	2.2384	1.6940	11.3656	10.3800
500	0.0000	0.0000	0.0000	0.0000	15.2763	15.6920	26.8637	26.4390
1,000	0.0000	0.0000	0.0000	0.0000	34.3116	35.2730	46.4865	46.1975
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0351	0.0491	0.0359	0.0493	0.4490	0.7553	2.4559	3.6705
20	0.0172	0.0223	0.0163	0.0215	0.6323	0.8053	2.4941	3.8607
100	0.0024	0.0032	0.0021	0.0029	1.4116	1.8070	2.5765	0.3045
500	0.0006	0.0008	0.0003	0.0004	9.6199	18.4325	2.8644	0.3145
1,000	0.0005	0.0007	0.0002	0.0003	17.0168	29.5770	2.8465	0.2853
marginal	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	0.0000	0.0000	0.0000	0.0000	2.0515	2.0520	26.7363	26.6895
20	0.0000	0.0000	0.0000	0.0000	3.6855	3.6870	49.0309	48.9470
100	0.0000	0.0000	0.0000	0.0000	18.6691	18.6560	250.4291	248.8755
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0006	0.0008	0.0002	0.0002	0.0523	0.0702	1.7858	2.5702
20	0.0005	0.0007	0.0002	0.0002	0.0425	0.0540	3.0504	4.2420
100	0.0005	0.0006	0.0002	0.0002	0.1459	0.2048	9.8668	14.0612

Table C.2: This table considers the continuous simulation setting with $\rho = 0$ and $\nu = 0.3583$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0024	-0.0021	0.0005	0.0018	1.0285	0.9245	7.0952	5.5435
20	0.0001	0.0001	-0.0001	0.0000	1.1580	0.9745	7.3927	6.0075
100	0.0000	0.0000	-0.0001	-0.0001	2.2287	1.6840	11.2822	10.2935
500	0.0000	-0.0001	-0.0001	-0.0001	15.1196	15.5025	26.7356	26.3135
1,000	-0.0001	-0.0001	-0.0001	-0.0001	33.6731	34.6105	45.9020	45.6100
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0320	0.0418	0.0332	0.0416	0.4474	0.7668	2.4760	3.7098
20	0.0167	0.0221	0.0161	0.0218	0.6322	0.8092	2.5068	3.9133
100	0.0026	0.0034	0.0022	0.0029	1.4119	1.8040	2.5677	0.3075
500	0.0007	0.0009	0.0003	0.0004	9.6294	18.4737	2.8580	0.3050
1,000	0.0006	0.0008	0.0002	0.0003	17.0606	29.6748	2.8474	0.3225
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0001	-0.0001	-0.0001	-0.0001	2.0994	2.1000	26.7484	26.7860
20	-0.0001	-0.0001	-0.0001	-0.0001	3.8516	3.8520	48.9944	49.0825
100	-0.0001	-0.0001	-0.0001	-0.0001	84.3169	84.3170	317.8971	315.8615
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0007	0.0010	0.0002	0.0003	0.0507	0.0772	1.8203	2.7230
20	0.0007	0.0009	0.0002	0.0003	0.0497	0.0650	3.0622	4.1202
100	0.0006	0.0008	0.0002	0.0002	0.6802	1.0220	9.8971	16.1810

Table C.3: This table considers the continuous simulation setting with $\rho = 0$ and $\nu = 0.7416$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0022	-0.0014	0.0003	0.0000	1.0246	0.9170	7.0611	5.5180
20	0.0008	0.0002	0.0003	0.0011	1.1522	0.9705	7.3847	6.0020
100	-0.0001	-0.0001	0.0001	0.0000	2.2238	1.6785	11.2907	10.2975
500	0.0000	-0.0001	-0.0001	-0.0001	14.9875	15.4265	26.5436	26.1240
1,000	-0.0001	-0.0001	-0.0001	-0.0001	33.0831	34.0690	45.2205	44.9320
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0423	0.0587	0.0439	0.0586	0.4471	0.7527	2.4578	3.6938
20	0.0254	0.0351	0.0223	0.0306	0.6308	0.8033	2.5044	3.8827
100	0.0028	0.0035	0.0025	0.0033	1.4142	1.8052	2.5722	0.2963
500	0.0008	0.0011	0.0004	0.0005	9.6469	18.4815	2.8590	0.3043
1,000	0.0007	0.0009	0.0003	0.0003	17.0871	29.7192	2.8452	0.3060
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0001	-0.0001	-0.0001	-0.0001	2.0833	2.0880	26.6854	26.7050
20	-0.0001	-0.0001	-0.0001	-0.0001	3.7804	3.7700	49.1028	48.9365
100	-0.0001	-0.0001	-0.0001	-0.0001	67.8759	67.9005	300.6183	298.5055
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0009	0.0012	0.0003	0.0004	0.0561	0.0903	1.7996	2.4957
20	0.0008	0.0010	0.0002	0.0003	0.0800	0.1218	2.9585	4.0628
100	0.0007	0.0009	0.0002	0.0003	0.5187	0.7805	10.0947	16.7948

Table C.4: This table considers the continuous simulation setting with $\rho = 0.25$ and $\nu = 0$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	0.0142	0.0174	0.0219	0.0239	1.0310	0.8880	6.8763	5.4495
20	0.0090	0.0095	0.0113	0.0108	1.1825	0.9810	7.4700	6.0335
100	0.0021	0.0021	0.0022	0.0022	2.2628	1.6840	11.4107	10.3405
500	0.0004	0.0005	0.0004	0.0004	14.5521	14.1795	26.7214	26.3120
1,000	0.0002	0.0003	0.0002	0.0002	33.7758	34.9045	46.2797	46.0320
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0378	0.0468	0.0347	0.0427	0.5111	0.6972	2.3339	3.6152
20	0.0179	0.0248	0.0163	0.0211	0.6767	0.8275	2.4550	3.9225
100	0.0025	0.0031	0.0020	0.0027	1.4298	1.8153	2.7002	0.3020
500	0.0006	0.0008	0.0003	0.0004	9.3448	18.3017	2.5973	0.3035
1,000	0.0005	0.0006	0.0002	0.0003	16.8166	29.3665	2.8414	0.3348
marginal	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	0.0155	0.0155	0.0155	0.0155	2.0485	2.0505	26.8095	26.8445
20	0.0080	0.0080	0.0080	0.0079	3.6768	3.6810	49.1431	49.0935
100	0.0016	0.0017	0.0016	0.0016	18.6833	18.6850	250.5547	249.9060
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0005	0.0007	0.0002	0.0002	0.0522	0.0690	1.8174	2.5452
20	0.0005	0.0006	0.0002	0.0002	0.0397	0.0540	3.1205	4.2248
100	0.0004	0.0006	0.0001	0.0002	0.2279	0.3653	8.8337	11.3668

Table C.5: This table considers the continuous simulation setting with $\rho = 0.25$ and $\nu = 0.7416$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	0.0093	0.0095	0.0172	0.0168	1.0316	0.8890	6.7590	5.3490
20	0.0059	0.0065	0.0089	0.0084	1.1796	0.9790	7.3514	5.9230
100	0.0020	0.0020	0.0020	0.0019	2.2526	1.6725	11.2988	10.2390
500	0.0005	0.0005	0.0004	0.0004	14.3184	13.9990	26.3693	25.9665
1,000	0.0003	0.0003	0.0002	0.0002	32.4910	33.7730	44.8315	44.5885
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0443	0.0607	0.0452	0.0599	0.5092	0.6895	2.3034	3.5803
20	0.0262	0.0366	0.0222	0.0300	0.6744	0.8155	2.4331	3.9035
100	0.0027	0.0034	0.0025	0.0033	1.4280	1.8105	2.6872	0.3048
500	0.0007	0.0009	0.0004	0.0005	9.4002	18.3627	2.5976	0.2850
1,000	0.0006	0.0009	0.0002	0.0003	16.8475	29.5138	2.8394	0.3052
marginal	500,000		5,000,000		500,000		5,000,000	
	mean	median	mean	median	mean	median	mean	median
10	0.0276	0.0276	0.0276	0.0276	2.0951	2.0935	26.6326	26.6720
20	0.0144	0.0144	0.0143	0.0143	3.8069	3.8020	49.1097	49.2280
100	0.0032	0.0032	0.0032	0.0032	68.0152	68.0225	298.9286	297.9795
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0008	0.0011	0.0003	0.0003	0.0545	0.0880	1.8056	2.4965
20	0.0007	0.0009	0.0002	0.0003	0.0688	0.0940	3.0020	4.1795
100	0.0006	0.0008	0.0002	0.0003	0.5745	0.8470	9.2107	12.8475

Table C.6: This table considers the continuous simulation setting with $\rho = 0.5$ and $\nu = 0$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0451	0.0426	0.0444	0.0426	1.3275	1.3760	11.0675	8.4615
20	0.0223	0.0216	0.0225	0.0228	1.2339	0.9960	7.6307	5.9180
100	0.0041	0.0043	0.0044	0.0044	2.3798	1.6730	11.2259	10.1895
500	0.0009	0.0008	0.0008	0.0008	13.9066	14.0420	26.2616	26.0010
1,000	0.0004	0.0004	0.0004	0.0004	33.5897	34.7080	45.4601	45.3240
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0304	0.0114	0.0310	0.0274	0.5886	0.9725	7.0572	11.9343
20	0.0161	0.0222	0.0150	0.0205	0.7020	0.9138	2.8837	4.0043
100	0.0025	0.0030	0.0020	0.0027	1.5403	2.1868	2.6976	0.2988
500	0.0005	0.0007	0.0003	0.0004	9.0546	16.7807	2.2227	0.3317
1,000	0.0004	0.0005	0.0002	0.0002	16.3951	29.0728	1.9932	0.2795
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0314	0.0314	0.0314	0.0314	2.3976	2.3970	26.8700	26.8700
20	0.0162	0.0162	0.0162	0.0162	4.3068	4.3100	49.2660	49.0730
100	0.0033	0.0033	0.0033	0.0033	21.5017	21.5230	249.1292	249.2600
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0005	0.0006	0.0002	0.0002	0.0702	0.0872	1.7800	2.6195
20	0.0004	0.0006	0.0001	0.0002	0.0845	0.1150	3.9106	4.5258
100	0.0004	0.0005	0.0001	0.0002	0.2957	0.4195	7.8842	10.0610

Table C.7: This table considers the continuous simulation setting with $\rho = 0.5$ and $\nu = 0.3583$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0562	0.0745	0.0482	0.0513	1.3331	1.3815	11.0709	8.4265
20	0.0144	0.0135	0.0151	0.0148	1.2388	1.0030	7.6560	5.9555
100	0.0029	0.0030	0.0030	0.0030	2.3889	1.6765	11.2417	10.2040
500	0.0006	0.0006	0.0006	0.0006	13.7362	13.8815	26.0416	25.7790
1,000	0.0003	0.0003	0.0003	0.0003	32.9581	34.1270	44.7975	44.6580
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0291	0.0383	0.0302	0.0496	0.5902	0.9797	7.0510	11.8870
20	0.0160	0.0225	0.0160	0.0209	0.7057	0.9110	2.8767	3.9880
100	0.0025	0.0030	0.0021	0.0028	1.5494	2.2068	2.7107	0.3110
500	0.0006	0.0007	0.0003	0.0004	9.0493	16.7798	2.2135	0.3003
1,000	0.0005	0.0006	0.0002	0.0002	16.4039	29.2357	2.0005	0.2762
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0499	0.0498	0.0498	0.0498	2.1031	2.1010	26.8011	26.8015
20	0.0233	0.0233	0.0233	0.0233	3.8852	3.8910	49.4683	49.5160
100	0.0055	0.0055	0.0055	0.0055	84.2894	84.2345	314.3510	314.2770
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0008	0.0008	0.0002	0.0003	0.0520	0.0850	1.8610	2.7732
20	0.0005	0.0007	0.0002	0.0002	0.0678	0.0783	3.1378	4.2897
100	0.0005	0.0006	0.0002	0.0002	0.7482	0.9652	8.2329	10.1155

Table C.8: This table considers the continuous simulation setting with $\rho = 0.5$ and $\nu = 0.7416$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

| | bias | | | | run time (s) | | | |
| | 500,000 | | 5,000,000 | | 500,000 | | 5,000,000 | |
k-means	mean	median	mean	median	mean	median	mean	median
10	0.0215	0.0084	0.0239	0.0082	1.3308	1.3740	11.1616	8.5590
20	0.0175	0.0171	0.0188	0.0196	1.2366	0.9975	7.7186	6.0010
100	0.0039	0.0038	0.0041	0.0040	2.3745	1.6655	11.2435	10.2005
500	0.0008	0.0008	0.0008	0.0008	13.5943	13.7045	25.9223	25.6600
1,000	0.0004	0.0004	0.0004	0.0004	32.4882	33.6255	44.2479	44.1040
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0360	0.0282	0.0391	0.0376	0.5895	0.9682	7.0922	11.9578
20	0.0210	0.0291	0.0198	0.0273	0.7036	0.9445	2.9005	4.0180
100	0.0024	0.0032	0.0024	0.0032	1.5438	2.2000	2.7082	0.3228
500	0.0006	0.0008	0.0003	0.0005	9.0637	16.8247	2.2149	0.3277
1,000	0.0005	0.0007	0.0002	0.0003	16.4881	29.0623	1.9988	0.3110
	500,000		5,000,000		500,000		5,000,000	
marginal	mean	median	mean	median	mean	median	mean	median
10	0.0492	0.0492	0.0492	0.0492	2.1101	2.1120	26.8251	26.7965
20	0.0263	0.0263	0.0263	0.0263	3.8448	3.8470	49.1135	49.1770
100	0.0060	0.0060	0.0060	0.0060	67.8301	67.8420	299.4398	299.2035
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0006	0.0008	0.0002	0.0003	0.0524	0.0810	1.8424	2.6905
20	0.0006	0.0008	0.0002	0.0003	0.0637	0.0840	3.0133	3.7787
100	0.0005	0.0007	0.0002	0.0002	0.5069	0.7445	8.4574	10.4945

Table C.9: This table considers the continuous simulation setting with $\rho = 0.75$ and $\nu = 0$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

| | bias | | | | run time (s) | | | |
| | 500,000 | | 5,000,000 | | 500,000 | | 5,000,000 | |
k-means	mean	median	mean	median	mean	median	mean	median
10	0.0335	0.0122	0.0478	0.0416	1.4215	1.4720	10.6566	8.5950
20	0.0292	0.0279	0.0319	0.0322	1.6224	1.3290	9.2174	8.9905
100	0.0066	0.0065	0.0066	0.0066	2.3701	1.6160	11.1091	9.9235
500	0.0013	0.0013	0.0012	0.0012	12.7239	12.2810	25.7784	25.2040
1,000	0.0006	0.0006	0.0006	0.0006	31.0945	31.4045	44.3241	44.0440
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0328	0.0420	0.0362	0.0676	0.5898	1.0290	5.9504	7.4762
20	0.0150	0.0216	0.0146	0.0200	0.9622	1.3867	4.3958	4.5757
100	0.0024	0.0029	0.0018	0.0024	1.6814	2.1835	3.0211	0.3210
500	0.0004	0.0006	0.0003	0.0003	8.1180	14.8922	3.1020	0.3502
1,000	0.0003	0.0004	0.0001	0.0002	15.2836	21.3305	2.7704	0.3103
	500,000		5,000,000		500,000		5,000,000	
marginal	mean	median	mean	median	mean	median	mean	median
10	0.0479	0.0479	0.0479	0.0479	2.0728	2.0720	26.8740	26.8965
20	0.0253	0.0253	0.0253	0.0253	3.6706	3.6660	49.1315	49.1400
100	0.0053	0.0053	0.0053	0.0053	18.6860	18.6460	250.4356	250.7675
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0004	0.0005	0.0001	0.0002	0.0561	0.0710	1.8541	2.7330
20	0.0003	0.0004	0.0001	0.0001	0.0307	0.0380	3.1078	3.9758
100	0.0003	0.0004	0.0001	0.0001	0.1644	0.1930	7.6044	9.2860

Table C.10: This table considers the continuous simulation setting with $\rho = 0.75$ and $\nu = 0.3583$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0519	0.0509	0.0483	0.0476	1.4156	1.4635	10.7063	8.6330
20	0.0179	0.0175	0.0185	0.0179	1.6191	1.3285	9.2981	9.0775
100	0.0046	0.0045	0.0043	0.0044	2.3733	1.6155	11.0899	9.9065
500	0.0008	0.0008	0.0008	0.0008	12.5908	12.1410	25.5900	25.0230
1,000	0.0004	0.0004	0.0004	0.0004	30.5345	30.8385	43.6687	43.3895
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0213	0.0160	0.0253	0.0278	0.5870	1.0292	5.9550	7.5243
20	0.0160	0.0222	0.0151	0.0192	0.9604	1.3900	4.4204	4.5732
100	0.0021	0.0029	0.0019	0.0027	1.6787	2.1740	3.0171	0.3262
500	0.0004	0.0006	0.0002	0.0003	8.1303	14.9240	3.1048	0.3433
1,000	0.0003	0.0005	0.0001	0.0002	15.3172	21.3845	2.7652	0.2862
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0645	0.0644	0.0644	0.0644	2.0915	2.0900	26.9187	26.9915
20	0.0320	0.0320	0.0320	0.0320	3.8855	3.8905	49.2526	49.4965
100	0.0080	0.0080	0.0079	0.0079	79.2247	79.2360	314.4613	314.6485
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0006	0.0005	0.0001	0.0002	0.0508	0.0823	1.8325	2.6225
20	0.0004	0.0005	0.0001	0.0002	0.0685	0.0773	3.1018	4.1240
100	0.0003	0.0005	0.0001	0.0002	0.6090	0.8910	7.6440	9.9490

Table C.11: This table considers the continuous simulation setting with $\rho = 0.75$ and $\nu = 0.7416$. It shows the mean and median bias and run time, but also the interquartile range and standard deviation over the estimates and over the run time. This is all shown in function of the number of boundary values for the marginal approximation, or the number of clusters for the k-means approximation. Two data set sizes are considered, namely 500,000 and 5,000,000.

	bias				run time (s)			
k-means	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	-0.0117	-0.0270	0.0104	0.0064	1.4151	1.4630	10.6875	8.6155
20	0.0320	0.0322	0.0314	0.0321	1.6175	1.3260	9.2665	9.0200
100	0.0047	0.0047	0.0050	0.0050	2.3635	1.6065	11.0586	9.8780
500	0.0010	0.0010	0.0011	0.0011	12.4493	12.0150	25.4325	24.8580
1,000	0.0005	0.0005	0.0005	0.0005	29.9562	30.2540	43.0638	42.7810
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0504	0.0846	0.0514	0.0797	0.5864	1.0292	5.9523	7.5095
20	0.0169	0.0213	0.0161	0.0223	0.9595	1.3813	4.4071	4.5825
100	0.0021	0.0029	0.0019	0.0024	1.6784	2.1730	3.0155	0.3260
500	0.0004	0.0006	0.0003	0.0003	8.1326	14.9302	3.1069	0.3225
1,000	0.0003	0.0005	0.0001	0.0002	15.3199	21.3508	2.7586	0.2720
marginal	**500,000**		**5,000,000**		**500,000**		**5,000,000**	
	mean	median	mean	median	mean	median	mean	median
10	0.0512	0.0512	0.0512	0.0512	2.0736	2.0785	26.9187	26.9545
20	0.0297	0.0296	0.0296	0.0296	3.8399	3.8440	49.2491	49.3375
100	0.0072	0.0072	0.0073	0.0073	63.6601	63.6515	297.8260	298.3230
	σ	IQR	σ	IQR	σ	IQR	σ	IQR
10	0.0003	0.0004	0.0001	0.0002	0.0548	0.0850	1.9506	2.6660
20	0.0004	0.0005	0.0001	0.0002	0.0782	0.1055	3.1387	4.0985
100	0.0003	0.0004	0.0001	0.0002	0.5359	0.7883	8.5080	11.3178