Fitting Semiparametric Cumulative Probability Models for Big Data

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Abstract

Cumulative probability models (CPMs) are a robust alternative to linear models for continuous outcomes. However, they are not feasible for very large datasets due to elevated running time and memory usage, which depend on the sample size, the number of predictors, and the number of distinct outcomes. We describe three approaches to address this problem. In the divide-and-combine approach, we divide the data into subsets, fit a CPM to each subset, and then aggregate the information. In the binning and rounding approaches, the outcome variable is redefined to have a greatly reduced number of distinct values. We consider rounding to a decimal place and rounding to significant digits, both with a refinement step to help achieve the desired number of distinct outcomes. We show with simulations that these approaches perform well and their parameter estimates are consistent. We investigate how running time and peak memory usage are influenced by the sample size, the number of distinct outcomes, and the number of predictors. As an illustration, we apply the approaches to a large publicly available dataset investigating matrix multiplication runtime with nearly one million observations.

Keywords: Cumulative probability models; semiparametric; big data
1 Introduction

Continuous outcomes often require a transformation prior to fitting linear models. The choice of transformation is not always clear, and different transformations may result in different conclusions. Semiparametric linear transformation models (Zeng and Lin, 2007) assume a linear model after a monotonic transformation which is nonparametrically estimated. The outcome and predictor variables are linked through an unobserved latent variable, where the latent variable is connected to the predictors as in a traditional linear model and to the outcome through an unknown monotonic transformation. These models are desirable because they require neither an explicit transformation of the outcome nor a model for the conditional expectation. Instead, the conditional distribution given covariate values is modeled, from which conditional expectations, quantiles, and other quantities can be derived.

Recently, Liu et al. (2017) showed that semiparametric linear transformation models can be fit using cumulative probability models (CPMs). CPMs have typically been reserved for the analysis of ordered categorical response variables; e.g., proportional odds and other “cumulative link models” (McCullagh 1980; Agresti 2010). With CPMs, the continuous outcome variable is effectively treated as if it were ordinal because what matters is the order of the outcome values, not the values themselves. Liu et al. (2017) showed that the multinomial likelihood used for CPMs is the likelihood of a semiparametric linear transformation model. Using computer simulations, they showed that CPMs perform well in many scenarios. Under mild conditions, CPMs yield estimates that are consistent and asymptotically normal (Li et al. 2021).

Because the transformation between the outcome and the latent variable is modeled nonparametrically, CPMs can be slow to fit with large samples, especially when there are many unique outcome values (Liu et al., 2017). The sparse nature of the score and Hessian matrices of CPMs can be exploited to make computation feasible for sample sizes in the thousands (Harrell, 2020). However, even when employing computationally efficient algorithms, CPMs are not able to handle larger sample sizes. For example, we cannot fit a CPM to a simulated dataset with 50,000
distinct outcomes on a server with 48 cores and 192 gigabytes of memory. The robustness and flexibility of CPMs make them desirable for analyses of large datasets; however, current big data implementations are not feasible.

The purpose of this paper is to describe and evaluate methods for fitting CPMs for big data, either by reducing the sample size through dividing the data into subsets or by reducing the number of distinct outcomes via binning or rounding. In Section 2, we introduce three approaches to fitting a CPM for a large dataset. In the divide-and-combine approach, the sample size of each individual CPM is greatly reduced. In the binning and rounding approaches, the outcome variable is redefined to have a greatly reduced number of distinct values. We carry out computer simulations to evaluate and compare these approaches in Section 3, and apply them to a real data example in Section 4. Section 5 contains a discussion.

2 Methods
2.1 Cumulative probability models

In this subsection we briefly describe cumulative probability models (CPMs) and relevant notation; details can be found in Liu et al. (2017). One way to motivate CPMs for a countinuous outcome $Y$ is through a linear transformation model,

$$Y = H(\beta^T X + \epsilon),$$

(1)

where $X$ is a vector of $p$ predictors, $\epsilon \sim F_\epsilon$ with $F_\epsilon$ known, and the transformation $H(\cdot)$ is assumed to be non-decreasing and otherwise unknown. It is easy to show that for any $y$,

$$\Pr(Y \leq y|X) = \Pr\{\epsilon \leq H^{-1}(y) - \beta^T X\} = F_\epsilon\{H^{-1}(y) - \beta^T X\}.$$ 

Let $G = F_\epsilon^{-1}$ and $\alpha = H^{-1}$. Then model (1) becomes a CPM,

$$G\{\Pr(Y \leq y|X)\} = \alpha(y) - \beta^T X, \text{ for any } y,$$

(2)

where $G(\cdot)$ is a link function. The “intercept” $\alpha(y)$ in the CPM has a nice interpretation: It is a transformation of the outcome such that the transformed value is related to the predictors linearly. This is because model (1) can be alternatively expressed as $\alpha(Y) = \beta^T X + \epsilon$. 

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Now consider a dataset \( \{(y_i, x_i) : i = 1, \ldots, N\} \), where \( N \) is the sample size. We first consider the scenario where there are no ties in the outcomes. The CPM in (2) becomes

\[
G\{\Pr(Y \leq y_i | X) \} = \alpha_i - \beta^T x_i, \quad \text{for every } y_i,
\]

where \( \alpha_i = \alpha(y_i) \). Without loss of generality, we assume \( y_1 < y_2 < \cdots < y_N \); then \( \alpha_1 < \alpha_2 < \cdots < \alpha_N \). Model (3) is identical to some models for ordered categorical outcomes: for example, proportional odds model (when \( F \) is the logistic distribution) and probit model (when \( F \) is the normal distribution). It becomes the proportional hazards model when \( F \) is the left-skewed Gumbel distribution.

As described in Liu et al. (2017), the nonparametric likelihood for the model is

\[
L^* (\beta, \alpha) = \prod_{i=1}^{N} \{G^{-1}(\alpha_i - \beta^T x_i) - G^{-1}(\alpha_{i-1} - \beta^T x_i)\}.
\]

Here \( \alpha_0 \) is an auxiliary parameter and \( \alpha_0 < \alpha_1 \). Because \( L^*(\beta, \alpha) \) is maximized when \( \hat{\alpha}_0 = -\infty \) and \( \hat{\alpha}_N = +\infty \), it can be simplified as

\[
\{G^{-1}(\alpha_1 - \beta^T x_1)\} \{G^{-1}(\alpha_2 - \beta^T x_2) - G^{-1}(\alpha_1 - \beta^T x_2)\} \cdots \{1 - G^{-1}(\alpha_{N-1} - \beta^T x_N)\}.
\]

This is the same as the likelihood when the outcomes are treated as if they were ordered categorical. We can obtain the nonparametric maximum likelihood estimates (NPMLE) \((\hat{\alpha}, \hat{\beta})\) from this likelihood. Then the NPMLE of the transformation function \( \alpha(y) \) is \( \hat{\alpha} = \{\hat{\alpha}_1, \ldots, \hat{\alpha}_{N-1}\} \). It is an increasing step function, with a step for each of the \( N - 1 \) intervals between adjacent outcome values from \( y_1 \) to \( y_N \).

When there are ties in the outcomes, the above derivations still apply with a slight modification. Here model (3) is applicable for every distinct outcome value, and for each such value, there is a corresponding \( \alpha \) value. Let \( M \) be the number of distinct outcome values. The NPMLE of \( \alpha(y) \) becomes \( \hat{\alpha} = \{\hat{\alpha}_1, \ldots, \hat{\alpha}_{M-1}\} \), an increasing step function with a step for each of the \( M - 1 \) intervals between adjacent distinct outcome values.

Using modern empirical process theory and under mild regularity conditions, Li et al. (2021) showed the consistency and asymptotic normality of the NPMLEs, \((\hat{\alpha}, \hat{\beta})\). Asymptotic theory
relies on compactness of the estimator of $\alpha(\cdot)$, which does not hold if $Y$ is unbounded. Hence, Li et al (2021) specify lower and upper bounds for $Y$, $L$ and $U$ respectively, such that any observation outside the the interval $(L, U)$ is censored. The corresponding censored data likelihood is equivalent to a likelihood that treats these values as belonging to the lowest / highest ordered categories. Under this censoring, $(\widehat{\alpha}, \widehat{\beta})$ is consistent for $(\alpha(y), \beta)$ for $y \in [L, U]$. In addition, $\sqrt{N}(\widehat{\alpha} - \alpha(y), \widehat{\beta} - \beta)$ converges weakly to a tight Gaussian process whose variance can be estimated as the inverse of the Hessian matrix. Furthermore, the asymptotic variance of $\sqrt{N}(\widehat{\beta} - \beta)$ attains the semiparametric efficiency bound. Details are in Li et al. (2021).

The Hessian matrix has dimensions $(M - 1 + p) \times (M - 1 + p)$. Because of the special structure of the likelihood function (4), the portion of the Hessian matrix with respect to the alpha parameters is tridiagonal. This allows matrix inversion efficiently through Cholesky decomposition (Sall 1991).

Taking advantage of these facts, Harrell implemented a computationally efficient algorithm in the `orm()` function in the `rms` R package (Harrell 2020) to fit CPMs. However, as the number of parameters increases with the number of distinct outcome values, the function eventually fails for very large datasets due to heavy demand on computation time and memory usage. The next three subsections describe approaches to fit CPMs for very large datasets.

### 2.2 Divide and combine

In the divide-and-combine approach, the data are evenly divided into subsets, a CPM is fit to each subset, followed by a final step to aggregate all the information. The goal is to make the sample sizes of the subsets small enough to fit CPMs relatively quickly with a reasonable amount of computer resources. Let $K$ be a target number of subsets, and $n_k$ be the size of subset $k$ ($k = 1, \cdots, K$). If $N$ is a multiple of $K$ then $n_1 = \cdots = n_K = N/K$. If not, our implementation ensures that $\max|n_k - n_{k'}| \leq 1$ for any two subsets. Let $m_k$ be the number of unique outcome values in subset $k$. Let $c(k) = (\widehat{\alpha}^{(k)}, \widehat{\beta}^{(k)})$ be the vector of parameter estimates from subset $k$, where $\widehat{\alpha}^{(k)}$ has length $m_k - 1$ and $\widehat{\beta}^{(k)}$ has length $p$. Let $c_j^{(k)}$ be the $j$-th element of $c^{(k)}$.

As $\hat{\alpha}(y)$ is estimated nonparametrically, it is defined only over the range of outcomes in the
data used to fit a CPM. To ensure that $\hat{\alpha}(y)$ is available over the widest range of outcomes from all the subsets, in the partition step, we randomly assign the $K$ observations that have the smallest outcome values one to each subset, and similarly, randomly assign the $K$ observations that have the largest outcome values one to each subset. The rest are allocated to the subsets randomly. This way, $\hat{\alpha}(y)$ will be available from all the subsets over the interval $[y(K), y(N-K)]$, spanning from the $K$-th smallest to the $K$-th largest outcome values.

After fitting individual CPMs to subsets, we compute the estimates of $\alpha$ (an $(M - 1)$-vector) and $\beta$ (a $p$-vector). The estimates of the beta parameters are straightforward to compute as they are the average of the corresponding beta estimates from the subsets. However for a parameter in $\alpha$, due to random partitioning, the corresponding alpha estimates in the subsets can be at different index positions; we thus define a $K$-vector for each parameter to indicate which estimate from the individual models will be used in the computation. Figure 1 illustrates the definition. For example, a $K$-vector of $(3, 6, \ldots, 1)$ indicates that the corresponding estimate is an average of $c^{(1)}_3, c^{(2)}_6, \ldots, c^{(K)}_1$. The first and last several parameters in $\alpha$ will not have estimates available from all the subsets; in the $K$-vector, we use 0 to indicate that the corresponding model is not contributing. There are at most $K - 1$ such alpha parameters at each end. $K$-vectors can also be defined for the beta parameters: $(m_1, \ldots, m_K)$ for $\beta_1$, $(m_1 + 1, \ldots, m_K + 1)$ for $\beta_2$, etc.

Once we have defined all the $K$-vectors, we can compute the final parameter estimates. Given a $K$-vector $a = (a_1, a_2, \ldots, a_K)$, the corresponding parameter estimate is an average,

$$\sum_k c^{(k)}_{a_k} I(a_k > 0) / \sum_k I(a_k > 0).$$

When $y \in [y(K), y(N-K)]$, the average is always over $K$ values. Since $\hat{\alpha}^{(k)}$ is non-decreasing for every $k$, the final alpha estimates over $y \in [y(K), y(N-K)]$ are also non-decreasing. This monotonicity is not guaranteed at the ends. To ensure monotonicity at the ends, we apply the following constraints sequentially: Backwardly for $i = K - 1, \ldots, 1$, if $\alpha_i > \alpha_{i+1}$ then set $\alpha_i = \alpha_{i+1}$; forwardly for $i = M - K + 1, \ldots, M - 1$, if $\alpha_i < \alpha_{i-1}$ then set $\alpha_i = \alpha_{i-1}$.

The estimates of $(\alpha, \beta)$ using this divide and combine approach for a fixed $K$ are consistent
Figure 1: Illustration of alpha estimation in the divide-and-combine approach. Consider a hypothetical dataset with 15 observations, divided into three subsets. Each subset has 5 observations and 4 alpha estimates; they are shown in red, green, and blue for subsets 1, 2, and 3, respectively. The goal is to compute the 14 alpha estimates in the combine step. The $K$-vector for the outcome $y = 13.8$ (indicated by the first vertical dotted line) is $(2, 1, 3)$ as it corresponds to the 2nd interval in subset 1, 1st in subset 2, and 3rd in subset 3. The $K$-vector for $y = 18.5$ (the second dotted line) is $(0, 4, 4)$ as it has no contribution from subset 1 and corresponds to the 4th interval in subsets 2 and 3. The black horizontal lines are the alpha estimates in the combine step, and the dashed black lines at the ends are the values before imposing the monotonicity constraint.

and asymptotically normal under the same conditions that are required for consistency and asymptotic normality of the standard CPM estimators. In short, under these conditions, each of the estimates in the $K$ separate analyses is consistent and asymptotically normal, and as the analyses are independent, their average is also consistent and asymptotically normal.

Because of the independence between the $K$ separate analyses, the variance-covariance matrix for $(\hat{\alpha}, \hat{\beta})$ can be computed easily with $K$-vectors. Let $V^{(k)}$ be the variance-covariance matrix of $(\hat{\alpha}^{(k)}, \hat{\beta}^{(k)})$, and $v_{i,j}^{(k)}$ be its element at $(i, j)$. The variance of a parameter in $(\hat{\alpha}, \hat{\beta})$ with $K$-vector $a = (a_1, a_2, \ldots, a_K)$ is estimated as

$$ \sum_k v_{a_k,a_k}^{(k)} I(a_k > 0) / \{ \sum_k I(a_k > 0) \}^2. $$

The covariance between a parameter with $K$-vector $a = (a_1, a_2, \ldots, a_K)$ and another with $K$-vector...
$b = (b_1, b_2, \ldots, b_K)$ is estimated as

$$\sum_k v_{a_k, b_k}^{(k)} I(a_k > 0) I(b_k > 0) / \sum_k I(a_k > 0) \cdot \sum_k I(b_k > 0).$$

We note that the variance estimates for the alpha parameters at the ends may be slightly overestimated because the monotonicity constraints would likely reduce the variation of the final estimates. The whole variance-covariance matrix has dimensions $(M - 1 + p) \times (M - 1 + p)$, which can be very large. For example, when $M = 100,000$ and $p = 100$, the matrix has more than 10 billion numbers. This is a challenge in both computation and storage. In our implementation, we calculate the diagonal values (i.e., the variances) for the alpha portion and the full $p \times p$ variance-covariance matrix for the beta portion. One consequence of this choice is that the conditional mean or median given covariate values would not have an estimated standard error as they require covariances in the computation.

### 2.3 Equal-quantile binning

In equal-quantile binning, we first group the outcomes into equal-quantile bins and then assign a new outcome value to the observations in each bin. Specifically, we define a new outcome variable, $Y_b$, which for each bin $B$, takes the value median of all the observations in the bin.

When there are not many ties in the original outcome, the number of distinct values in $Y_b$ is often the number of bins, $M_b$, which can be predetermined. We then fit a CPM of $Y_b$ on the predictor variables.

To ensure that the $N$ observations are divided to $M_b$ bins as evenly as possible, we implement the following algorithm: Express $N$ as

$$N = M_b q + r = (M_b - r)q + r(q + 1),$$

where $q = \lfloor NM_b^{-1} \rfloor$ is the floor of $NM_b^{-1}$ (i.e., the quotient) and $r$ is the remainder (i.e., $r = N \mod M_b$); $r = 0$ when $N$ is a multiple of $M_b$. There will be $M_b - r$ bins, each with $q$ observations, and $r$ bins, each with $q + 1$ observations. To achieve this, we first generate a random list of length $M_b$, in which the value $q$ occurs $M_b - r$ times and $q + 1$ occurs $r$ times. We then sort the observations
by the outcome, and group them according to the values in the random list. For example, if the
list is \((q+1, q, \cdots)\), those with the smallest \(q+1\) outcome values are in the first bin, the next set
of \(q\) observations are in the second bin, etc.

One advantage of binning is that it is scale-independent with respect to the outcome, a feature
shared by the CPM itself. Another advantage is that it allows us to control the refinement in
the new outcome variable \(Y_b\) because the number of bins can be predetermined. Note that in the
binning approach, \(\alpha(y)\) extends only to the median values of the first and last bins instead of the
ends of the original outcome.

It is well-known that with ordinal data, CPMs estimate the same beta parameter if one combines
adjacent ordinal categories [REF]. Similarly, with continuous data, when one bins outcomes, one
estimates the same beta parameter as if one had fit a CPM to the continuous data. Specifically, let
\(Y_b = g_b(Y)\), where \(g_b(\cdot)\) is the binning function. From (1), \(Y_b = g_b(H(\beta^T X + \epsilon)) = H_b(\beta^T X + \epsilon)\)
where \(H_b(\cdot) = g_b(H(\cdot))\) is the resultant transformation from the latent variable scale to the binned
observed outcome scale. Because \(g_b(\cdot)\) is monotonic, then \(H_b(\cdot)\) is monotonic, although the inverse
transformation, \(\alpha_b(Y) = H_b^{-1}(Y)\), is not one-to-one because of the binned nature of the data. The
estimator for \(\beta\), \(\hat{\beta}\), remains consistent and asymptotically normal. The estimator, \(\hat{\alpha}_b\) is consistent
for \(\alpha_b(y)\) which is a discretized version of \(\alpha(y)\). As the binning becomes finer, i.e., \(M_b \rightarrow N\),
\(\alpha_b(y) \rightarrow \alpha(y)\). Hence, as one would expect, the accuracy of \(\hat{\alpha}_b\) for estimating \(\alpha(y)\) depends on
the fineness of the binning. With that said, with large sample sizes and continuous data, any bias
in \(\hat{\alpha}_b\) due to binning except in the tails of the distribution, is often negligible, as will be seen in
Section 3.

2.4 Rounding with refinement

Rounding can also reduce the number of distinct outcomes. While binning can substantially redef-
fine the outcomes at the extreme ends, rounding often keeps those values nearly unchanged. For
example, suppose the largest five values of a dataset are \(\{50.3, 79.7, 130.3, 203.8, 310.7\}\), and bins
are chosen to be of size 5. Then binning would collapse these values to their median, 130.3. In con-
trast, rounding to integers would keep these values largely unchanged with little loss of information. However, rounding to a decimal place can be a poor choice for skewed outcomes. For example, suppose the smallest five observations from that same dataset are \{0.002, 0.009, 0.019, 0.035, 0.041\}. Then rounding to the integer could result in a substantial loss of information at the lower end. For this reason we consider two general rounding strategies: rounding to decimals and rounding to significant digits. We also describe a refinement step, which allows both rounding strategies to approximately result in a target number of distinct values.

Let \(s\) be an integer, and \(\lfloor a \rceil_s\) be the result of rounding a number \(a\) to decimal place \(s\) (when \(s > 0\)), to an integer (when \(s = 0\)), or to \(10^{-s}\) (when \(s < 0\)). For example, \(\lfloor 12.34 \rceil_1 = 12.3\), \(\lfloor 12.34 \rceil_0 = 12\), and \(\lfloor 12.34 \rceil_{-1} = 10\). When \(s = 0\), we omit the subscript and write \(\lfloor a \rceil\). Let \(\lfloor a \rceil^{(s)}\) (\(s > 0\)) be the result of rounding \(a\) to \(s\) significant digits. Let \(p(a) = \lfloor \log_{10} a \rfloor\) be the place of the first significant digit of \(a\). Then \(\lfloor a \rceil^{(s)} = \lfloor a \rceil_{s-1-p(a)}\). For example, \(\lfloor 12.34 \rceil^{(2)} = \lfloor 12.34 \rceil_0 = 12\).

We now refine these two types of rounding. When we round \(a\) to an integer, \(\lfloor a \rceil\) is the integer that is closest to \(a\). We could refine this by rounding \(a\) to the closest multiple of 0.5, which is effectively \(\lfloor 2a \rceil / 2\). Similarly, \(\lfloor 3a \rceil / 3\) is to round \(a\) to the closest multiple of 1/3. In general, for any real number \(t \in [1, 10]\), \(\lfloor ta \rceil / t\) is to round \(a\) to the closest multiple of \(1/t\). As \(t\) increases from 1 to 10, more refined rounding is achieved; when \(t = 10\), we reach \(\lfloor a \rceil_1\). For any integer \(s\) and any number \(t \in [1, 10]\), we define

\[
\lfloor a \rceil_{s,t} = \lfloor ta \rceil_s / t
\]

as the value after rounding \(a\) to place \(s\) at refinement level \(t\). When \(t = 1\), \(\lfloor a \rceil_{s,1} = \lfloor a \rceil_s\); as \(t\) increases, \(\lfloor a \rceil_{s,t}\) becomes more refined and \(\lfloor a \rceil_{s,10} = \lfloor a \rceil_{s+1}\). Similarly, for any integer \(s > 0\) and any number \(t \in [1, 10]\), we define

\[
\lfloor a \rceil^{(s,t)} = \lfloor a \rceil_{s-1-p(a),t}
\]

as the value after rounding \(a\) to \(s\) significant digits at refinement level \(t\). When \(t = 1\), \(\lfloor a \rceil^{(s,1)} = \lfloor a \rceil^{(s)}\); as \(t\) increases, \(\lfloor a \rceil^{(s,t)}\) becomes more refined and \(\lfloor a \rceil^{(s,10)} = \lfloor a \rceil^{(s+1)}\).

We now describe the two rounding algorithms for a given dataset. Let \(m_{s,t}\) be the number of
distinct values after rounding the outcomes to place \( s \) at refinement level \( t \). Similarly, let \( m^{(s,t)} \) be that after rounding to \( s \) significant digits at refinement level \( t \). Let \( M_r \) be a target number of distinct outcomes after rounding. Our two rounding algorithms are:

**Decimal place rounding with refinement:**

(Ia) Identify \( s \) such that \( m_{s,1} \leq M_r < m_{s+1,1} \);

(Ib) If \( m_{s,1} = M_r \), set \( t = 1 \). Otherwise, search over a grid in \([1, 10] \) to identify \( t \) such that \( m_{s,t} \) is closest to \( M_r \), as measured by the smallest \(| \log m_{s,t} - \log M_r | \);

(Ic) Define a new outcome variable \( Y_r \) such that its value is \( \lceil y_i \rceil_{s,t} \) for observation \( i \).

**Significant digit rounding with refinement:**

(IIa) Identify \( s \) such that \( m^{(s,1)} \leq M_r < m^{(s+1,1)} \);

(IIb) If \( m^{(s,1)} = M_r \), set \( t = 1 \). Otherwise, search over a grid in \([1, 10] \) to identify \( t \) such that \( m^{(s,t)} \) is closest to \( M_r \), as measured by the smallest \(| \log m^{(s,t)} - \log M_r | \);

(IIc) Define a new outcome variable \( Y_r \) such that its value is \( \lceil y_i \rceil^{(s,t)} \) for observation \( i \).

In our implementation of these rounding algorithms, the grid for \( t \) has increment of 0.1, and the resulting numbers of distinct values in \( Y_r \) have been always <1% different from the target number \( M_r \). Compared to the binning approach, these rounding approaches do not require sorting of the outcomes, but they are scale-dependent with respect to the outcome.

The theoretical justification for rounding is identical to that for binning because they both merge adjacent values in discretized categories.

### 3 Simulations and Results

#### 3.1 Simulation setup

We simulated datasets with various sample sizes and with \( p = 50 \) predictor variables. Half of the predictors are binary with success probabilities ranging from 0.05 to 0.5, and half are continuous
Table 1: Evaluation set-up of simulated data

| $N$  | $p$ | Truth | Whole data | Divide-and-combine                             | Binning | Rounding |
|------|-----|-------|------------|-----------------------------------------------|---------|----------|
| $10^4$ | 50 | ✓     | ✓          | ✓ ($K = 10$)                                  | ✓ ($M_b = 10^4$) | ✓ ($M_r \sim 10^4$) |
| $4 \times 10^4$ | 50 | ✓     | ✓          | ✓ ($K = 40$)                                  | ✓ ($M_b = 10^4$) | ✓ ($M_r \sim 10^4$) |
| $10^6$ | 50 | ✓     | ✓          | ✓ ($K = 100$)                                 | ✓ ($M_b = 10^4$) | ✓ ($M_r \sim 10^4$) |

from normal distributions with mean ranging from 0 to 2.4 and variance 1. The beta coefficients for half of the predictors were specified in the range $[-1, 1]$ and those for the other predictors were set as zero. We then generated $y^* = \beta^T x + \epsilon$, where $\epsilon \sim F_\epsilon$, and $y = H(y^*)$. We considered six scenarios, corresponding to the combinations of three options for $H(\cdot)$ and two options for $F_\epsilon$. The three options for $H(\cdot)$ are: (1) $y = y^*$, for which the inverse is $\alpha(y) = y$; (2) $y = \exp(y^*)$, for which $\alpha(y) = \log(y)$; and (3) $y = \log(y^* + y_0^*)$, where $y_0^*$ is added to ensure $y^* + y_0^* > 0$ for all the simulated $y^*$; for this transformation, $\alpha(y) = e^y - y_0^*$. The two options of $F_\epsilon$ are: (i) the logistic distribution $F_\epsilon(u) = e^u/(1 + e^u)$; (ii) the Gumbel distribution $F_\epsilon(u) = \exp(-e^{-u})$.

We simulated datasets with sample size $N = 10^4$, $4 \times 10^4$ and $10^6$. The smaller sample sizes allow us to compare the three new approaches with the “gold standard” approach of fitting a single CPM to the original data. We also compared the parameter estimates with the true parameters used in data generation. In the divide-and-combine approach, the data were partitioned into $K = 10$ subsets when $N = 10^4$, 40 when $N = 4 \times 10^4$, and 100 when $N = 10^6$. In the binning approach, the outcomes were grouped into $M_b = 1,000$ bins when $N = 10^4$, and 10,000 bins otherwise. In the rounding approach, the outcomes were rounded with a target number of $M_r = 1,000$ when $N = 10^4$, and 10,000 otherwise. These settings are displayed in Table 1.

The endpoints we evaluated include: (1) the estimates of the parameters in $\alpha$ and $\beta$, and their standard errors; (2) estimates of conditional mean and median at 10 sets of $x_0$ randomly selected from the simulated datasets. Specifically, let $y_{(j)}$ $(j = 1, \ldots, M)$ be the $j$-th smallest distinct outcome value. Given $X = x_0$, the cumulative distribution function of $Y$ is estimated as $\hat{P}_j = \Pr(Y \leq y_{(j)}|x_0) = F_\epsilon(\hat{\alpha}_j - \hat{\beta}^T x_0)$ when $j < M$, and $\hat{P}_M = \Pr(Y \leq y_{(M)}|x_0) = 1$ when $j = M$. The corresponding probability mass function is estimated as $\hat{p}_j = \Pr(Y = y_{(j)}|x_0) = \hat{P}_j - \hat{P}_{j-1}$.
\(j = 1, \cdots, M\), where \(\hat{P}_0 = 0\). We then computed the conditional mean, \(\sum_{j=1}^{M} \hat{p}_j y(j)\); and the conditional median as the average of the two adjacent \(y(j)\) and \(y(j+1)\) for which \(\hat{P}_j < 0.5\) and \(\hat{P}_{j+1} > 0.5\). The true conditional mean and median at \(X = x_0\) were empirically obtained by first generating 10,000 values of \(\epsilon \sim F_\epsilon\) and corresponding \(H(\beta^T x_0 + \epsilon)\), and then computing their mean and median.

### 3.2 Simulation results

Figure 2 shows the parameter estimates and their standard errors from the three new approaches for the simulation scenario with logistic residual distribution, identity transformation \(y = H(y^*) = y^*\), and \(N = 10^4\). The results of the “gold standard” approach of fitting a CPM with the whole dataset are also shown.

The \(\hat{\alpha}(y)\) from all the approaches agreed very well with the true \(\alpha(y)\) over a wide range of \(y\) from \(<0.5\) percentile to \(>99.5\) percentile. The standard error for \(\hat{\alpha}(y)\) was also relatively low in this range due to the high data density. There was some departure of \(\hat{\alpha}(y)\) from the truth at the ends, with relatively high standard errors, probably due to a lack of information as a result of data sparcity.

In the divide-and-combine approach, \(\hat{\alpha}(y)\) started to nearly flatten out at \(y(K)\) and \(y(N-K)\). This approach also yielded slightly higher standard errors than the other approaches. In the binning approach, by definition, \(\hat{\alpha}(y)\) extends only to the median values of the first and last bins. The rounding to decimal place approach had nearly identical estimates of the alpha parameters and their standard errors as the “gold standard” approach. This is because the outcome in this simulation scenario had a relatively symmetric distribution, for which rounding to a decimal place tends to have little effect at the ends where the values are relatively large. In comparison, rounding to significant digits tends to have a slightly larger effect at the ends.

The estimates of the beta parameters were also quite accurate for all approaches. The binning and rounding approaches and the “gold standard” approach had nearly identical estimates of the beta parameters and their standard errors. In comparison, the divide-and-combine approach yielded
Figure 2: Estimation of parameters and their standard errors under the scenario of logistic residual distribution, \( y = H(y^*) = y^*, \) \( N = 10^4 \). Left panel: alpha estimates as functions of the outcome (top) and their standard errors (bottom). The gray line is the truth: \( \alpha(y) = y \). The rounding approaches and the CPM on the original data had nearly identical results. Right panel: beta estimates (top) and their standard errors (bottom). Gray diagonal lines \( y = x \) are added for reference. The binning and rounding approaches and the CPM on the original data had nearly identical results.

slightly different parameter estimates and slightly higher standard errors.

The results for the other transformations and for the Gumbel residual distribution showed similar patterns (Supplemental Material). Note that for very skewed outcomes, the rounding to
Figure 3: Estimation of conditional mean (top) and conditional median (bottom) for 10 sets of $x$. The columns are for the three simulation scenarios with outcome transformations $y = y^*$, $y = \exp(y^*)$, and $y = \log(y^* + y_0^*)$, respectively, all with logistic residual distribution and $N = 10^4$. The significant digits approach had nearly identical estimates of all the parameters and their standard errors as the “gold standard” approach, while rounding to a certain decimal place rounded many values at the lower end to a single value, which is undesirable.

Figure 3 shows the estimated conditional mean and median for 10 sets of $x$ randomly selected from the simulated datasets. When the conditional distribution is relatively symmetric, as in the scenarios with $y = y^*$ and $y = \log(y^* + y_0^*)$, the estimation of conditional mean performed well. When the conditional distribution is very skewed, as in the scenario with $y = \exp(y^*)$, the estimation of conditional mean performed poorly. We repeated the simulations under the latter scenario with multiple replicates and found a high variation in the results, presumable due to high variation in the alpha estimates at the high end of the outcomes. The pattern we observed seems
Figure 4: Estimation of parameters for large sample sizes under the scenario of logistic residual distribution and $y = H(y^*) = y^*$. Top row: $N = 4 \times 10^4$. Bottom row: $N = 10^6$. It was impossible to fit a single CPM on the original data with $N = 10^6$. Left: alpha estimates as functions of the outcome. The gray line is the truth: $\alpha(y) = y$. Right: beta estimates. Gray diagonal lines $y = x$ are added for reference.

to be overestimation from the divide-and-combine approach and underestimation from the other approaches including the “gold standard” CPM on the original data. In contrast, the conditional medians performed quite well for all the approaches in all the scenarios. The results for the Gumbel residual distribution have similar patterns (Supplemental Material).
Figure 4 shows the estimates of the parameters for sample sizes $4 \times 10^4$ and $10^6$ with logistic residual distribution and $y = H(y^*) = y^*$. In comparison to the results for $N = 10^4$ in Figure 2, a larger sample size clearly led to a smaller difference between the estimates and the truth, illustrating that the approaches yield consistent parameter estimates. The standard error estimates also became smaller as the sample size increased (Supplemental Material).

The divide-and-combine approach introduces variation due to random partitioning. However, the variation due to random partitioning is minor relative to that from random sampling (see details in Supplemental Material).

### 3.3 Time and peak memory usage

To help determine the number of subsets in the divide-and-combine approach and the target number of distinct values in the binning and rounding approaches, we evaluate the running time and peak memory usage when fitting a single CPM with respect to the sample size, the number of distinct outcome values, and the number of predictors. We generated datasets with various values of $N$ (sample size: $N = 5000, 10000, 20000, 30000, 40000$), $M$ (number of distinct outcome values: $M = 1000, 5000, 10000, 20000, 40000$), and $p$ (number of predictors: $p = 10, 25, 50, 100$). All variables were continuous. When $M < N$, equal-quantile binning was used to achieve the desired $M$. There are 18 combinations of $N$ and $M$ for each value of $p$, and there are a total of 72 datasets. We fit `orm()` to each dataset and recorded the running time and peak memory usage.

The top row in Figure 5 shows the time usage with respect to changes in $N$ and $M$ when $p = 50$ (left), and with respect to changes in $N$ and $p$ when $M = 1000$ (right). The patterns are similar for other values of $p$ and $M$. The results indicate a log-log linear relationship of time on $N$, $M$, and $p$. We therefore fit a log-log linear model, which is multiplicative on the time scale: 

$$
time = 4.13 \times 10^{-7} \cdot N^{0.92}M^{1.01}p^{0.98}; \quad \text{this model had } R^2 = 0.998.
$$

Thus time is approximately proportional to $NMp$; we found that time $= 2 \times 10^{-7} \cdot NMp$ seems to fit well to our results. The left panel of Figure 6 shows the comparison of the observed running time and the fitted values from these two models. Note that the constant factor $2 \times 10^{-7}$ depends on our server configuration and
Figure 5: Time and peak memory usage for fitting orm() to datasets with various $N$, $M$, and $p$. The axes are drawn on the log scale.

may vary greatly across hardware configurations.

The bottom row in Figure 5 shows the peak memory usage under the same settings as in the top row; again, the results for other values of $p$ and $M$ have similar patterns. The results suggest that peak memory usage is influenced heavily by $M$, to a much less degree by $p$, and almost ignorably by $N$. An examination of the log-log plot of peak memory usage versus $M - 1 + p$ (in Supplemental Material) suggested that the peak memory usages for datasets with $M \geq 5000$
fall along a line while those for $M = 1000$ are far above that line, presumably due to overhead operations that can dominate memory usage for a relatively small $M$. We thus fit a log-log linear model to the results with $M \geq 5000$, which led to: $\text{memory} = 1.60 \times 10^{-7} \cdot (M - 1 + p)^{1.92}$, with $R^2 = 0.999$. This model suggests that peak memory usage is approximately proportional to $(M - 1 + p)^2$, at least for $M \geq 5000$. This makes sense as the memory usage is probably devoted mostly to the Hessian matrix, which has dimensions $(M - 1 + p) \times (M - 1 + p)$. For our data, $\text{memory} = 7.5 \times 10^{-8} \cdot (M - 1 + p)^2$ seems to fit well. The right panel of Figure 6 shows the peak memory usage versus $M - 1 + p$, and the curves of these two models.

The results that the running time of a single CPM is approximately proportional to $NMP$ and that the peak memory usage is approximately proportional to $(M - 1 + p)^2$ is helpful when determining the number of subsets in the divide-and-combine approach and the target number of distinct values in the binning and rounding approaches. In the divide-and-combine approach, a subset has much smaller $N$ and $M$ than those in the original data, and the individual jobs take much less time and memory to run. This also allows simultaneous model fitting for multiple subsets, further speeding up the process. In the binning and rounding approaches, $M_b$ and $M_r$ are typically

Figure 6: Fitted models for time and peak memory usage. Left: Observed running time vs. fitted values from two models. Right: Peak memory usage vs. $M - 1 + p$, and curves from two models.
Table 2: Outcome categorization after rounding in the SGEMM dataset

| range               | # obs  | # distinct values |
|---------------------|--------|-------------------|
|                     | $y_i$  | $\lfloor y_i \rfloor$ | $\lceil y_i \rceil$ | $\lfloor y_i \rfloor$ | $\lceil y_i \rceil$ | $\lfloor y_i \rfloor$ | $\lceil y_i \rceil$ |
| $[10, 100)$         | 563831 | 8453              | 88               | 862              | 862               | 8453              | 4424             |
| $[100, 1000)$       | 368366 | 70217             | 900              | 8855             | 900               | 8855              | 4635             |
| $>1000$             | 34203  | 28129             | 1875             | 12356            | 207               | 1875              | 1009             |
| Total               | 966400 | 106799            | 2863             | 22073            | 1969              | 19183             | 10068            |

much smaller than $M$ in the original data. As a result, these approaches also take much less time and memory, making it feasible to fit a CPM even with a large sample size.

4 A Data Example

We applied our approaches to a publicly available dataset, in which an algorithm for multiplying two matrices of dimensions $2048 \times 2048$ was evaluated for its running time on a parameterizable SGEMM GPU kernel (Nugteren and Codreanu 2015; Ballester-Ripoll et al. 2017). The algorithm has 14 parameters, and 241,600 parameter combinations were feasible due to various kernel constraints. For each combination, 4 runs were performed and the running time was recorded in milliseconds. For this dataset, $N = 966,400$ and $p = 14$, and there are $M = 106,799$ distinct outcome values. More details can be found at the University of California Irvine Machine Learning Repository (http://archive.ics.uci.edu/ml/datasets/SGEMM+GPU+kernel+performance).

The outcome variable, the algorithm running time, is very skewed, with skewness 3.93 and a range from 13.25 to 3397.08 milliseconds. One could apply a transformation (e.g., logarithm) on the outcome and then fit a linear model, not knowing if the transformation would be a good choice. The CPM instead allows us to obtain a suitable transformation empirically.

We fit CPMs of the outcome on the 14 predictor variables with the three methods described in Section 2. In the divide-and-combine approach the data were divided into $K = 48$ subsets of size 20,133 or 20,134. In binning and rounding, the target number of distinct outcome values was set as 10,000, and the final numbers of distinct outcome values were 9,067 and 10,068, respectively. For rounding, we chose to round to significant digits. The rationale behind this decision can be seen in
Table 2 where we divide the outcomes into three regions: [10, 100), [100, 1000), and those >1000. The 2nd and 3rd columns display the number of observations and the number of distinct outcome values in these regions. For this dataset, rounding to a decimal place (columns 4–5) would result in very few distinct values representing the 563,831 outcomes in [10, 100), but a lot more distinct values representing the 34,203 outcomes that are >1000. In contrast, rounding to a certain number of significant digits (columns 6–8) gives more balanced categorizations of the outcome. The selected rounding scheme was rounding to 3 significant digits at refinement level 5.2 (column 8), resulted in a fairly good balance and \( M_r \approx 10,000 \). The divide-and-combine approach took 2 hours 37 minutes on our server while the binning and rounding approaches each took 7 hours 12 minutes.

The results are summarized in Figure 7. The top left plot shows the alpha estimates as functions of the outcome. The outcome range was [13.25, 3397.08] in the original data, [15.15, 3268.00] after binning, and [13.25, 3396.15] after rounding. The three alpha estimates agreed remarkably well with each other from the 0.01 percentile to the 99.99 percentile of the outcome [15.41, 3248.05]. Note that \( \hat{\alpha}(y) \) is an estimated transformation of the outcome such that the transformed value would relate to the predictors linearly. Here all three \( \hat{\alpha}(y) \) are very different from a log transformation, which would be a straight line on this plot as the x-axis is on the log scale. This indicates that the true transformation must be very different from logarithm, which would often be used to transform a skewed outcome in a traditional analysis. The bottom left plot shows the standard errors of the alpha estimates, which are also very similar from 0.01 to 99.99 percentiles. The top right plot of Figure 3 shows comparisons of the beta estimates from the three methods, with the results of rounding on the x-axis and those of the other two methods on the y-axis. Again, the three methods’ beta estimates and standard errors (bottom right plot) agree remarkably well.

5 Discussion

Cumulative probability models (CPMs) are a robust alternative to linear models. However they are not feasible for very large datasets as the running time and memory usage increase with the sample size, the number of distinct outcomes, and the number of predictors. In this paper, we addressed
Figure 7: Results of the three approaches on the SGEMM dataset. Left: Estimates of $\alpha(y)$ (top) and their standard errors (bottom). The 0.01 and 99.99 percentiles of the outcome are marked by the gray vertical lines. Right: Estimates of beta parameters (top) and their standard errors (bottom). Gray diagonal lines $y = x$ are added for reference.

This problem can be addressed with three approaches. The divide-and-combine approach focuses on reducing the sample size of individual CPMs, and the binning and rounding approaches focus on reducing the number of distinct outcome values. With computer simulations, we showed that these approaches perform quite well, with estimates of parameters and their standard errors very similar to those from a single CPM on the whole dataset (when the latter is feasible), and with consistent parameter...
estimates. The rounding approach has two algorithms, rounding to a decimal place (for not-too-skewed outcomes) and rounding to significant digits (for skewed outcomes). Both algorithms have a refinement step to achieve the desired number of distinct outcomes. All three approaches yielded comparable results when applied to a large dataset with nearly one million observations.

We also studied the running time and peak memory usage in relation to the sample size $N$, the number of distinct outcomes $M$, and the number of predictors $p$. We showed that the running time is approximately proportional to $NMP$, and that the peak memory usage is approximately proportional to $(M - 1 + p)^2$. These results can help plan the analysis by determining the number of subsets in the divide-and-combine approach and the number of target distinct outcomes in the binning and rounding approaches. There is a trade-off between speed and accuracy. Therefore, for the divide-and-combine approach, we recommend as few subsets as allowed by computer resources, and for the binning and rounding approaches, we recommend as large target number of distinct outcomes as allowed by computer resources.

There are some limitations in the divide-and-combine approach. When the sample size is very large, computation of the covariances in the variance-covariance matrix will be infeasible as it requires a large amount of storage space. In addition, when a predictor variable has a vast majority of the observations having one value and only a few observations having a different value, a subset may have all its observations having the same value in the variable. In this case, there would be no estimate for the corresponding coefficient. Similarly, a categorical predictor variable having a rare category may also cause a problem. Therefore it might be necessary to pre-screen and remove such predictor variables, or consider the predictor variables when dividing the data in a manner to ensure feasible estimation in each subset. Given these limitations of the divide-and-combine approach and the simplicity of binning and rounding, one might prefer one of the latter approaches.

We focused on generic binning and rounding algorithms: equal-quantile binning, rounding to a decimal place, and rounding to significant digits. Alternative, and probably more ad hoc, binning and rounding approaches might be desirable in certain applications. For example, one might bin the outcome with more convenient or interpretable cutoff values, or transform the outcome to a
different scale and then round it, or round the outcome differently in different regions.

In summary, we have provided three approaches to the problem of fitting CPMs to big data. They perform quite well and take a reasonable amount of time and computer resources to finish. These approaches have been implemented in our cpmBigData R package.

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