

Insurance loss modelling with gradient tree-boosted mixture models

Yanxi Hou*

Jiahong Li[†]

Guangyuan Gao[‡]

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Abstract

In actuarial practice, mixture models [\[mixture models or mixture of models? both appear in the paper\]](#) is one widely applied statistical method to model the insurance loss data. Although the Expectation-Maximization (EM) algorithm usually plays an important tool for the parameter estimation of mixture models, it suffers from other issues which cause unstable predictions. For example, the feature engineering and variable selection are two important modelling issues, which are challenging for mixture models due to several component models involving. Moreover, to avoid overfitting is another technical concern of the modelling method for prediction of future losses. To address those issues, we propose an Expectation-Boosting (EB) algorithm, which replaces the maximization step in the EM algorithm by gradient boosting machines with regression trees. Our proposed EB algorithm can estimate the component regression functions non-parametrically and overfitting-sensitively, as well as perform automated feature engineering, model fitting and variable selection simultaneously, which fully explores the predictive power of feature space. We also conduct two simulation studies to show the good performance of the proposed algorithm and an empirical analysis of the claims amounts data for illustration.

Keywords: Insurance loss; Mixture models; EM algorithm; Gradient boosting; Parallel computing; Finite mixture of regressions; Zero-inflated Poisson model.

1 Introduction

It is well known that insurance loss data sometimes cannot be well modeled by a single distribution due to its complex data structures. For claim count data, a Poisson distribution may not be the best choice to model an excess of zero claims. For claim amount data, it usually exhibits multimodal or heavy-tailed phenomena, so a gamma distribution is not sufficient to address these data features. In the literature, one alternative way is to apply a mixture of distributions for univariate loss data. When the individual risk factors are available, a mixture of regressions is then used instead to model the risk heterogeneity, which is an extension to the mixture of distributions. In the literature, mixture models are proposed by Goldfeld and Quandt (1973). We refer to Lindsay (1995) and MacLahlan and Peel (2000) for a detailed review of mixture

*School of Data Science, Fudan University, 200433 Shanghai, China.

[†]School of Mathematical Sciences, Peking University, 100871 Beijing, China.

[‡]Center for Applied Statistics and School of Statistics, Renmin University of China, 100872 Beijing, China.

models. In the field of machine learning research, mixture models are also called as mixture of experts models (Jacobs et al., 1991; Jiang and Tanner, 1999).

We summarize some studies on mixture models for insurance loss modelling. Zhang et al. (2020, 2022) developed a multivariate zero-inflated hurdle model to describe multivariate count data with extra zeros. Delong et al. (2021) proposed a mixture of neural networks with gamma loss to model insurance claim amounts. Lee and Lin (2010) and Verbelen et al. (2015) used a mixture of Erlangs to model insurance claim amounts including censored and truncated data. Lee and Lin (2012) developed the multivariate version of mixture of Erlangs. Fung et al. (2019a), Fung et al. (2019b) and Tseung et al. (2021) proposed a so called logit-weighted reduced mixture of experts models for multivariate claim frequencies or severities distributions. To the best of our knowledge, the existing studies always impose a linearity constraint on the regression function, i.e., under a generalized linear model (GLM) framework. In this paper, we will relax this constraint by estimating regression functions non-parametrically.

Several aspects of modelling are very noteworthy in research. It is challenging to estimate parameters in mixture models, since the parameters in component models are related to each other. To overcome it, Dempster et al. (1977) proposed the Expectation-Maximization (EM) algorithm, which is an iterative method to estimate the component parameters and the latent component indicator variables. In addition, the variable selection and the feature engineering in mixture models are also challenging since the dependence between the covariate and response variables varies from one component to another. Khalili and Chen (2007) introduced a penalized likelihood approach for the variable selection. Huang and Yao (2012) and Huang et al. (2013) proposed a non-parametric mixture of regressions to relax the linearity assumption on the regression function. Moreover, the selection of the number of the components is another challenging problem. Naik et al. (2007) derived a new information criterion for the selection of the component number and variables. Kasahara and Shimotsu (2015) proposed a likelihood-based test to contrast the mixture models with different numbers of components. In this paper, we assume that the number of components is known, and we will address variable selection and feature engineering in the proposed method.

We propose an Expectation-Boosting (EB) algorithm for mixture models, which replaces the maximization step by a boosting step. It is well known that the boosting algorithm is an iterative method to estimate the regression function non-parametrically, where weak learners are calibrated step-wisely and added together. We roughly categorize some commonly used boosting algorithms into three groups: (a) Binary classification: AdaBoost, LogitBoost (real, discrete, gentle AdaBoost), AdaBoost.M1; (b) Multinomial classification: Stagewise Additive Modelling using a Multi-class Exponential loss (SAMME), SAMME.R (multi-class real AdaBoost); (c) Gradient based: gradient boosting machine/model (GBM), Newton boosting, gradient boosting decision tree (GBDT), eXtreme Gradient Boosting (XGBoost), light gradient boosting machine (LightGBM). The last type is based on gradient of loss function and Friedman (2001) has studied this type of boosting from a statistical perspective as an additive model. Our EB algorithm follows the GBDT algorithm in the boosting step. With the negative log-likelihood as the loss function for boosting, the boosting step increases the likelihood at each iteration of the EB algorithm. There are several advantages of the EB algorithm over the EM algorithm. First, the boosting algorithm is a flexible non-parametric regression method, which facilitates both non-linear effects and interaction. Thus, the variable selection and feature engineering are

performed automatically during the model fitting. Second, it is well known that the boosting algorithm is overfitting-sensitive (Bühlmann and Yu, 2003). This property is very useful since the ultimate goal of insurance loss modelling is to predict the future loss. Therefore, the out-of-sample prediction is more important than the goodness-of-fitting in our applications.

The rest of paper is structured as follows. Section 2 reviews mixture models and the EM algorithm. Section 3 presents the EB algorithm. We also discuss initialization, tuning parameters and parallel computing in detail. Section 4 studies two simulated data and a real data to illustrate the proposed methodology. Section 5 concludes the paper with several important findings. The R code of our work is publicly available on the github (<https://github.com/sxpyggy/boosting-mixture-code>).

2 Review: mixture models and the EM algorithm

In this section, we first review mixture models, particularly finite mixture of regressions (MacLahlan and Peel, 2000), and discuss different mixture structure. Then we review the EM algorithm which is the foundation of the proposed EB algorithm. In this paper, we focus on the exponential distribution family with an expectation parameter μ and a dispersion parameter ϕ . The exponential distributions form a general family of parametric distributions, which are fitting for different types of insurance loss data.

2.1 Mixture models

Suppose a random variable y follows a finite mixture of distributions with the k -th *component distribution* from a finite collection of distributions

$$\{f_1(y; \mu_1, \phi_1), \dots, f_K(y; \mu_K, \phi_K)\}$$

and *mixing probability* $p_k, k = 1, \dots, K (K \geq 1)$. The probability density function for y is given by a weighted sum of component distributions such that

$$f(y) = \sum_{k=1}^K p_k f_k(y; \mu_k, \phi_k).$$

If the *individual features* \mathbf{x}_i are available and have a systematic effect on the response variable y_i , then we can establish a finite mixture of regressions:

$$f(y|\mathbf{x}) = \sum_{k=1}^K p_k(\mathbf{x}) f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi_k(\mathbf{x})). \quad (2.1)$$

Note that (2.1) is a general representation for a finite mixture of regressions, i.e., both mixing probabilities and component parameters depend on \mathbf{x} .

In real applications, based on the features of data and the goal of modelling, we can make specific assumptions on (2.1). For example,

- The mixing probabilities are not related to \mathbf{x}

$$f(y|\mathbf{x}) = \sum_{k=1}^K p_k f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi_k(\mathbf{x}));$$

- Both mixing probabilities and dispersions are not related to \mathbf{x}

$$f(y|\mathbf{x}) = \sum_{k=1}^K p_k f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi_k);$$

- If the component distributions are from the same distribution family, we might assume that different component distributions have the same dispersion ϕ

$$f(y|\mathbf{x}) = \sum_{k=1}^K p_k f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi);$$

- The covariates \mathbf{x} are only related to the mixing probabilities:

$$f(y|\mathbf{x}) = \sum_{k=1}^K p_k(\mathbf{x}) f_k(y; \mu_k, \phi_k).$$

Selection among the above model alternatives can be viewed as imposing suitable constraints on the general form (2.1), which accelerates and stabilizes model fitting without compromising predictive performance. It actually provides practical flexibility according to different data structures and the goals of study.

2.2 The EM algorithm

Suppose that for a single sample y , we know exactly which component distribution it comes from, that is, we know the *full information* $(Y, \mathbf{Z}, \mathbf{x})$, where

$$\mathbf{Z} = (Z_1, \dots, Z_K) = (\mathbb{1}_1(k), \dots, \mathbb{1}_K(k))$$

is the one-hot encoding vector of *component indicator variable* k . Then the joint distribution function of (Y, \mathbf{Z}) given \mathbf{x} is given by

$$f(y, \mathbf{z}|\mathbf{x}) = \prod_{k=1}^K [p_k(\mathbf{x}) f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi_k(\mathbf{x}))]^{z_k}.$$

Equivalently, the complete log-likelihood function is

$$l(p, \mu, \phi|y, \mathbf{z}, \mathbf{x}) = \sum_{k=1}^K z_k [\log p_k(\mathbf{x}) + \log f_k(y|\mathbf{x}; \mu_k(\mathbf{x}), \phi_k(\mathbf{x}))]. \quad (2.2)$$

Given a data set $\{(y_i, \mathbf{z}_i, \mathbf{x}_i)\}_{i=1:n}$, we assume the parametric models of $p = (p_1, \dots, p_K)$, μ_k, ϕ_k such that $p(\mathbf{x}) = (p_1(\mathbf{x}; \theta_p), \dots, p_K(\mathbf{x}; \theta_p))$, $\mu_k(\mathbf{x}) = \mu_k(\mathbf{x}; \theta_\mu^{(k)})$ and $\phi_k(\mathbf{x}) = \phi_k(\mathbf{x}; \theta_\phi^{(k)})$, where $\theta_p, (\theta_\mu^{(k)})_{k=1:K}, (\theta_\phi^{(k)})_{k=1:K}$ are the unknown parameters. Note that θ_p does not have a superscript since it corresponds to the coefficients in a multinomial logistic classification while $\theta_\mu^{(k)}, \theta_\phi^{(k)}$ can be considered in separate component models; see below.

The regression coefficients can be estimated by the following $K+1$ independent optimizations:

$$\hat{\theta}_p = \arg \max_{\theta_p} \sum_{i=1}^n \sum_{k=1}^K z_{i,k} \log p_k(\mathbf{x}_i; \theta_p) \quad (2.3)$$

and

$$\left(\hat{\theta}_{\mu}^{(k)}, \hat{\theta}_{\phi}^{(k)}\right) = \arg \max_{\theta_{\mu}^{(k)}, \theta_{\phi}^{(k)}} \sum_{i=1}^n \sum_{k=1}^K z_{i,k} \log f_k \left(y_i; \mu_k \left(\mathbf{x}_i; \theta_{\mu}^{(k)} \right), \phi_k \left(\mathbf{x}_i; \theta_{\phi}^{(k)} \right) \right), \text{ for } k = 1, \dots, K. \quad (2.4)$$

Those optimizations are corresponding to a *multinomial logistic classification* and *K regressions*. The multinomial logistic classification (2.3) are fitted to all samples, while the k -th regression in (2.4) is fitted to partial samples with $\{i : z_{i,k} = 1\}$. In practice we do not have the full information $(Y, \mathbf{Z}, \mathbf{x})$, but only the incomplete information (Y, \mathbf{x}) . The EM algorithm is inspired by the above discussion.

Expectation step. With iterated $\hat{p}, \hat{\mu}, \hat{\phi}$, calculate the *conditional expectation* of \mathbf{z} :

$$\hat{z}_{i,k} = \hat{z}_k(\mathbf{x}_i) = \frac{\hat{p}_{i,k} f_k(y_i; \hat{\mu}_{i,k}, \hat{\phi}_{i,k})}{\sum_{l=1}^K \hat{p}_{i,l} f_l(y_i; \hat{\mu}_{i,l}, \hat{\phi}_{i,l})},$$

where $\hat{p}_{i,k} = \hat{p}_k(\mathbf{x}_i) = p_k(\mathbf{x}_i; \hat{\theta}_p)$, $\hat{\mu}_{i,k} = \hat{\mu}_k(\mathbf{x}_i) = \mu_k(\mathbf{x}_i; \hat{\theta}_{\mu}^{(k)})$, $\hat{\phi}_{i,k} = \hat{\phi}_k(\mathbf{x}_i) = \phi_k(\mathbf{x}_i; \hat{\theta}_{\phi}^{(k)})$.

Maximization step. Based on the log-likelihood function for full information

$$\begin{aligned} & l \left(\theta_p, (\theta_{\mu}^{(k)})_{k=1:K}, (\theta_{\phi}^{(k)})_{k=1:K} | \mathbf{y}, \hat{\mathbf{z}}, \mathbf{x} \right) \\ &= \sum_{i=1}^n \sum_{k=1}^K \hat{z}_{i,k} \left[\log p_k(\mathbf{x}_i; \theta_p) + \log f_k \left(y_i; \mu_k \left(\mathbf{x}_i; \theta_{\mu}^{(k)} \right), \phi_k \left(\mathbf{x}_i; \theta_{\phi}^{(k)} \right) \right) \right] \\ &= \sum_{i=1}^n \sum_{k=1}^K \hat{z}_{i,k} \log p_k(\mathbf{x}_i; \theta_p) + \sum_{i=1}^n \sum_{k=1}^K \hat{z}_{i,k} \log f_k \left(y_i; \mu_k \left(\mathbf{x}_i; \theta_{\mu}^{(k)} \right), \phi_k \left(\mathbf{x}_i; \theta_{\phi}^{(k)} \right) \right), \end{aligned} \quad (2.5)$$

calculate the MLE of regression coefficients by the following $K + 1$ independent optimizations:

$$\hat{\theta}_p = \arg \max_{\theta_p} \sum_{i=1}^n \sum_{k=1}^K \hat{z}_{i,k} \log p_k(\mathbf{x}_i; \theta_p) \quad (2.6)$$

and

$$\left(\hat{\theta}_{\mu}^{(k)}, \hat{\theta}_{\phi}^{(k)}\right) = \arg \max_{\theta_{\mu}^{(k)}, \theta_{\phi}^{(k)}} \sum_{i=1}^n \sum_{k=1}^K \hat{z}_{i,k} \log f_k \left(y_i; \mu_k \left(\mathbf{x}_i; \theta_{\mu}^{(k)} \right), \phi_k \left(\mathbf{x}_i; \theta_{\phi}^{(k)} \right) \right), \text{ for } k = 1, \dots, K. \quad (2.7)$$

[why using bold $\mathbf{p}, \mathbf{\mu}, \mathbf{\phi}, \mathbf{y}$? Need to define some new notions above?] These optimizations are similar to those in (2.3) and (2.4). The only difference is that $z_{i,k} \in \{0, 1\}$ in (2.3) and (2.4) while $\hat{z}_{i,k} \in (0, 1)$ in (2.6) and (2.7). Therefore, in the maximization step we perform a multinomial logistic classification with *fractional* response $\hat{z}_{i,k}$ [No illustration for a fractional response] and K weighted-regressions [No illustration as well] fitted to *all* samples with weights $\hat{z}_{i,k}$.

3 Expectation-Boosting algorithm

In the EM algorithm, the functions $p(\mathbf{x}), \mu_k(\mathbf{x}), \phi_k(\mathbf{x})$ are always assumed to be parametric functions. To make component models more flexible, we replace the maximization step in

the EM algorithm by a boosting step. Boosting algorithm estimates the regression functions non-parametrically and facilitates more flexible shapes of regression function. With negative log-likelihood function as the loss function in boosting algorithm, the boosting step increases the likelihood at each iteration, but overfitting-sensitively. The boosting step follows a generic functional gradient descent algorithm. We first describe generic functional gradient descent algorithm, then propose the EB algorithm, finally discuss interpretation, hyperparameter tuning and initialization in the EB algorithm. [\[why not put the review of generic functional gradient descent algorithm in Section 2.\]](#)

3.1 Generic functional gradient descent algorithm

Suppose a to-be-boosted non-parametric regression function as $F : \mathbb{R}^P \rightarrow \mathbb{R}$. In boosting algorithm, the goal is to estimate F to minimize the expected loss

$$\hat{F} = \arg \min_F \mathbb{E}[C(Y, F(\mathbf{x}))],$$

where $C : \mathbb{R} \times \mathbb{R} \rightarrow \mathbb{R}_+$ is the *loss function*. The expected loss is always replaced by sample average loss:

$$\hat{F} = \arg \min_F \frac{1}{n} \sum_{i=1}^n C(y_i, F(\mathbf{x}_i)).$$

In our setting of statistical modeling, the loss function depends on the corresponding likelihood function. We choose the *negative log-likelihood* function for the loss function. Hence, minimizing the loss function is equivalent to maximizing the likelihood. For example, in LogitBoost the loss function is negative binomial log-likelihood

$$C(y, F) = \log(1 + \exp(-2yF)), \quad y \in \{-1, 1\},$$

where

$$F(\mathbf{x}) = \frac{1}{2} \log \left(\frac{\Pr[Y = 1|\mathbf{x}]}{\Pr[Y = -1|\mathbf{x}]} \right). \quad (3.1)$$

In L_2 Boost, the loss function is negative normal log-likelihood

$$C(y, F) = (y - F)^2/2, \quad y \in \mathbb{R}, \quad (3.2)$$

where $F(\mathbf{x}) = \mathbb{E}(Y|\mathbf{x})$.

In the GLM framework, the link function connects the linear predictor with the parameters of interest such as mean, probability odds, etc. Here, we apply the same terminology where the link function connects the non-parametric regression function F with the parameters of interest. In LogitBoost, equation (3.1) implies a half logged probability odds link function $g : \mathbb{R}_+ \rightarrow \mathbb{R}$

$$g(\text{odds}) = \frac{1}{2} \log(\text{odds}) = \frac{1}{2} \log \left(\frac{\Pr[Y = 1|\mathbf{x}]}{\Pr[Y = -1|\mathbf{x}]} \right) = F(\mathbf{x}).$$

In L_2 Boost, we have an identify link function $g : \mathbb{R} \rightarrow \mathbb{R}$

$$g(\text{mean}) = \text{mean} = \mathbb{E}(Y|\mathbf{x}) = F(\mathbf{x}).$$

Remark that in our setting of statistical modeling, we first specify the likelihood function and the link function, then we derive the cost function. [\[The link function is not defined and not pointed to. It is better to give some descriptions for both loss and link functions\].](#)

We follow Bühlmann and Yu (2003) to briefly describe the generic functional gradient decent algorithm in Algorithm 1, which will be used as building blocks in the proposed EB algorithm. The algorithm estimates F in an additive form

$$\hat{F}(\mathbf{x}) = \hat{F}^{[0]}(\mathbf{x}) + \sum_{m=1}^M \hat{f}^{[m]}(\mathbf{x}),$$

where $\hat{F}^{[0]}$ is the initial value and $\hat{f}^{[m]}$ is called the m -th weak learner which involves only a small number of covariates. [\[Consider using algorithm package here\]](#)

Algorithm 1 The generic functional gradient decent algorithm.

- 1: Initialization. Set a suitable initial value $\hat{F}^{[0]}(\mathbf{x})$.
- 2: **for** $m = 1$ to M **do**
- 3: Projection of gradient to weak learner. Calculate *negative gradient*

$$u_i = -\frac{\partial C(y_i, F)}{\partial F} \Big|_{F=\hat{F}^{[m-1]}(\mathbf{x}_i)}, i = 1, \dots, n.$$

Data $(u_i, \mathbf{x}_i)_{i=1:n}$ is used to calibrate a weak learner $\hat{f}^{[m]}(\mathbf{x}; \hat{\theta}^{[m]})$ with *loss function* L_2 (3.2).[\[The weaker learner is not defined or described, and appear in the algorithm at the first time. It is better to put this sentence in the article and give this step a straightforward description.\]](#)

- 4: One-dimensional optimization and update. Solve a one-dimensional optimization to find *expansion coefficient* $\hat{\omega}^{[m]}$:

$$\hat{\omega}^{[m]} = \arg \min_{\omega} \sum_{i=1}^n C(y_i, \hat{F}^{[m-1]}(\mathbf{x}_i) + \omega \hat{f}^{[m]}(\mathbf{x}_i))$$

Update

$$\hat{F}^{[m]} = \hat{F}^{[m-1]} + s \hat{\omega}^{[m]} \hat{f}^{[m]},$$

where s is *shrinkage factor* (learning rate).

- 5: **end for**
 - 6: **return** $\hat{F}(\mathbf{x}) = \hat{F}^{[M]}$.
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In the algorithm, weak learners are fitted to negative gradient U rather than Y . Loss function in weak learners is always L_2 , independently with model loss function C . If decision trees (Breiman et al., 1984) are used as weak learners, the algorithm is called *gradient boosting decision tree (GBDT)*, where calibration of decision trees and variable selection are performed simultaneously. Please refer to Hastie et al. (2009) for decision trees and the recursive partitioning algorithm. Bühlmann and Hothorn (2007) argue that step 4 of one-dimensional optimization seems unnecessary given learning rate s is sufficiently small according to some empirical experiments.

3.2 Expectation-Boosting algorithm

In the EB algorithm, we follow the exact same expectation step as in the EM algorithm and replace the maximization step by boosting. The boosting algorithm is applied to estimate mixing

probabilities and component parameters given the conditional expectation of latent component indicator variables $\hat{z}_{i,k}$. To apply a boosting algorithm, we need to specify the likelihood function and the link function. In mixture models, the log-likelihood function is already given by (2.5). Therefore, we only need to specify the link functions for mixing probabilities, component means and component dispersions, respectively.

For mixing probabilities, we connect the mixing probabilities $p_1(\mathbf{x}), \dots, p_K(\mathbf{x})$ with the to-be-boosted regression functions $F_1(\mathbf{x}), \dots, F_K(\mathbf{x})$ by the multiple logistic link function $g_k : (0, 1)^K \rightarrow \mathbb{R}$: [\[Using \$p\(\mathbf{x}; F\(\mathbf{x}\)\)\$ or \$p\(F\(\mathbf{x}\)\)\$? They are different. Similarly for other functions.\]](#)

$$g_k(p_1(\mathbf{x}), \dots, p_K(\mathbf{x})) = \log p_k(\mathbf{x}) - \frac{1}{K} \sum_{l=1}^K \log p_l(\mathbf{x}) = F_k(\mathbf{x}), \quad k = 1, \dots, K. \quad (3.3)$$

or equivalently

$$g_k^{-1}(F_1(\mathbf{x}), \dots, F_K(\mathbf{x})) = \frac{\exp(F_k(\mathbf{x}))}{\sum_{l=1}^K \exp(F_l(\mathbf{x}))} = p_k(\mathbf{x}), \quad k = 1, \dots, K. \quad (3.4)$$

[\[It is not clear the difference between \$p\$ or \$p_k\$, \$F\$ and \$F_k\$. Similarly for other functions. Need definition of notions?\]](#) $[p_k(\mathbf{x})$ appears. The notions are not consistent. Similarly for other functions] With the negative log-likelihood function (2.6) of multinomial distribution, we derive the loss function as

$$C_Z((Z_k, F_k(\mathbf{x}))_{k=1:K}) = - \sum_{k=1}^K Z_k \log p_k(\mathbf{x}). \quad (3.5)$$

The negative gradient of the loss function w.r.t. F_k is given by

$$U_k((Z_k, F_k(\mathbf{x}))_{k=1:K}) = - \frac{\partial C_Z((Z_k, F_k(\mathbf{x}))_{k=1:K})}{\partial F_k(\mathbf{x})} = Z_k - p_k(\mathbf{x}), \quad k = 1, \dots, K. \quad (3.6)$$

For component parameters μ and ϕ , we denote the to-be-boosted regression functions by $G(\mathbf{x})$ and $H(\mathbf{x})$, respectively. The link functions depend on the component models. For example, in component Gaussian model we assume $\mu_k(\mathbf{x}) = G_k(\mathbf{x}), \log \phi_k(\mathbf{x}) = H_k(\mathbf{x})$; in component Poisson model $\log \mu_k(\mathbf{x}) = G_k(\mathbf{x})$; in component gamma model $G_k(\mathbf{x}) = \log \mu_k(\mathbf{x}), H_k(\mathbf{x}) = \log \phi_k(\mathbf{x})$. With the negative log-likelihood function (2.7), we derive the loss function as

$$C_k(Y, Z_k, G_k(\mathbf{x})) = -Z_k \log f_k(Y; \mu_k(\mathbf{x}), \phi_k), \quad k = 1, \dots, K, \quad (3.7)$$

where Z_k is treated as a weight multiplied to the usual negative log-likelihood function $-\log f_k$. The negative gradient of C_k w.r.t. G_k is given by

$$V_k(Y, Z_k, G_k(\mathbf{x})) = - \frac{\partial C_k(Y, Z_k, G_k(\mathbf{x}))}{\partial G_k(\mathbf{x})}. \quad (3.8)$$

Note that we have assumed that dispersion ϕ_k is fixed among samples (not related to \mathbf{x}). Upon the above defined notations, we are ready to introduce the proposed EB algorithm. We first summarize the proposed EB algorithm in Algorithm 2. [\[Consider using `algorithm` package here. It is better to write it into two loops as described in the following\]](#)

In this algorithm we have a hierarchical loop: the outer EB iteration 2-23 and the inner boosting iteration 5-11 and 14-20. The loop of inner boosting iteration following Algorithm 1 is nested into the loop of outer EB iteration. Hence, the EB algorithm takes much more time

Algorithm 2 The Expectation-Boosting algorithm.

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1: Initialization. Set  $\hat{p}_k^{[0]}(\mathbf{x}), \hat{\mu}_k^{[0]}(\mathbf{x}), \hat{\phi}_k^{[0]}$ ,  $k = 1, \dots, K$ .
2: for  $t = 1$  to  $T$  do
3:   Expectation. Calculate  $(\hat{z}_{i,k}^{[t]})_{i=1:n, k=1:K}$  given  $\hat{p}_k^{[t-1]}(\mathbf{x}), \hat{\mu}_k^{[t-1]}(\mathbf{x}), \hat{\phi}_k^{[t-1]}$ ,  $k = 1, \dots, K$ .
4:   Initialization of mixing probabilities. Set  $\hat{p}_k^{[t,0]}(\mathbf{x}), \hat{F}_k^{[t,0]}(\mathbf{x})$ ,  $k = 1, \dots, K$ .
5:   for  $m = 1$  to  $M_p$  do
6:     for  $k = 1$  to  $K$  do
7:       Projection of gradient to weak learner. Calibrate a weak learner  $\hat{f}_k^{[t,m]}$ .
8:       One dimensional optimization and update. Update  $\hat{F}_k^{[t,m]}$  using  $\hat{F}_k^{[t,m-1]}$  and  $\hat{f}_k^{[t,m]}$ .
9:     end for
10:    return  $\hat{p}_k^{[t,m]}$  according to (3.4),  $k = 1, \dots, K$ .
11:  end for
12:  return  $\hat{F}_k^{[t]} = \hat{F}_k^{[t,M_p]}, \hat{p}_k^{[t]} = \hat{p}_k^{[t,M_p]}$ ,  $k = 1, \dots, K$ .
13:  Initialization of component means. Set  $\hat{\mu}_k^{[t,0]}(\mathbf{x}), \hat{G}_k^{[t,0]}(\mathbf{x})$ ,  $k = 1, \dots, K$ .
14:  for  $m = 1$  to  $M_\mu$  do
15:    for  $k = 1$  to  $K$  do
16:      Projection of gradient to weak learner. Calibrate a weak learner  $\hat{g}_k^{[t,m]}$ .
17:      One dimensional optimization and update. Update  $\hat{G}_k^{[t,m]}$  using  $\hat{G}_k^{[t,m-1]}$  and  $\hat{g}_k^{[t,m]}$ .
18:    end for
19:    return  $\hat{\mu}_k^{[t,m]}$  according to corresponding link functions.
20:  end for
21:  return  $\hat{G}_k^{[t]} = \hat{G}_k^{[t,M_\mu]}, \hat{\mu}_k^{[t]} = \hat{\mu}_k^{[t,M_\mu]}$ ,  $k = 1, \dots, K$ .
22:  Estimation of dispersion. Calculate the MLE  $\hat{\phi}_k^{[t]}$  given  $\hat{\mu}_k^{[t]}(\mathbf{x})$  and  $\hat{z}_k^{[t]}(\mathbf{x})$ ,  $k = 1, \dots, K$ .
23: end for
24: return  $\hat{p}_k^{[T]}(\mathbf{x}), \hat{\mu}_k^{[T]}(\mathbf{x}), \hat{\phi}_k^{[T]}$ ,  $k = 1, \dots, K$ .

```

than the EM algorithm which contains only one loop. The EB algorithm can be accelerated by parallel computing. In the loop 6-9, the functions $(F_k)_{k=1:K}$ are boosted independently. In the loop 14-20, the component means are boosted independently. Thus, those boostings can be conducted simultaneously to reduce the running time; see Table 2. Remark that the loop 14-20 and the loop 15-18 are exchangeable since $\hat{\mu}_k^{[t,m]}$ only depends on $\hat{G}_k^{[t,m]}$. However, the loop 5-11 and the loop 6-9 are not exchangeable since $\hat{p}_k^{[t,m]}$ depends on all $(\hat{F}_k^{[t,m]})_{k=1:K}$ via equation (3.4). [\[Would it imply a parallel computation approach?\]](#)

Note that in the algorithm we have assumed that dispersion ϕ_k is fixed among samples (not related to \mathbf{x}). The extension to joint modelling of both mean and dispersion is not straightforward since they are not independent; please refer to Jorgensen (1997) for dispersion modelling. Joint modelling both mean and dispersion is not considered in this paper.

We now detail each step of the EB algorithm.

1. Initialization of EB algorithm. We initialize the following quantities:

1.1 Initialize $\hat{p}_1^{[0]}, \dots, \hat{p}_K^{[0]}$ and $\hat{F}_1^{[0]}, \dots, \hat{F}_K^{[0]}$:

- $\hat{p}_k^{[0]} = \frac{1}{K}$, $k = 1, \dots, K$,
- $\hat{F}_1^{[0]}, \dots, \hat{F}_K^{[0]}$ are obtained by (3.3).

1.2 Initialize $\hat{\mu}_1^{[0]}, \dots, \hat{\mu}_K^{[0]}$ and $\hat{G}_1^{[0]}, \dots, \hat{G}_K^{[0]}$:

- $\hat{\mu}_k^{[0]} = \frac{\sum_{i=1}^n Y_i}{n}$, $k = 1, \dots, K$,
- $\hat{G}_k^{[0]} = \mu_k^{-1}(\hat{\mu}_k^{[0]})$, $k = 1, \dots, K$,

where μ_k^{-1} denotes the link function in the component model k .

1.3 Initialize $\hat{\phi}_1^{[0]}, \dots, \hat{\phi}_K^{[0]}$ as the sample variance.

3. Expectation. Calculate the conditional expectation of latent component indicator variable given $\hat{p}_k^{[t-1]}(\mathbf{x}), \hat{\mu}_k^{[t-1]}(\mathbf{x}), \hat{\phi}_k^{[t-1]}$, $k = 1, \dots, K$:

$$\hat{z}_{i,k}^{[t]} = \frac{\hat{p}_k^{[t-1]}(\mathbf{x}_i) f_k(y_i; \hat{\mu}_k^{[t-1]}(\mathbf{x}_i), \hat{\phi}_k^{[t-1]})}{\sum_{l=1}^K \hat{p}_l^{[t-1]}(\mathbf{x}_i) f_l(y_i; \hat{\mu}_l^{[t-1]}(\mathbf{x}_i), \hat{\phi}_l^{[t-1]})}, \quad i = 1, \dots, n, k = 1, \dots, K.$$

Note that the conditional expectation carries the information obtained from last EB iteration $t - 1$. Although the initialization steps 4 and 13 reset the boosting at each EB iteration, the conditional expectations $\hat{z}_{i,k}^{[t]}$ interact with the boosting via the negative gradients (3.6) and (3.8) and the loss functions (3.5) and (3.7).

The steps 4-12 are a typical K -class logistic gradient boosting.

4. Initialization of mixing probabilities. Set $\hat{p}_k^{[t,0]}(\mathbf{x}), \hat{F}_k^{[t,0]}(\mathbf{x})$, $k = 1, \dots, K$ as

$$\begin{aligned} \hat{p}_k^{[t,0]} &= \frac{1}{K}, \quad k = 1, \dots, K, \\ \hat{F}_k^{[t,0]} &= \log \hat{p}_k^{[t,0]} - \frac{1}{K} \sum_{l=1}^K \log \hat{p}_l^{[t,0]}, \quad k = 1, \dots, K. \end{aligned} \tag{3.9}$$

In contrast to step 1, this initialization will be repeated at each outer EB iteration t . Later we will discuss another initialization strategy which considers the boosted values at the previous EB iteration.

7. Projection of gradient to weak learner. Compute the negative gradient for each data point $i = 1, \dots, n$ as

$$u_{i,k}^{[t,m]} = U_k \left(\left(\hat{z}_{i,k}^{[t]}, \hat{F}_k^{[t,m-1]}(\mathbf{x}_i) \right)_{k=1:K} \right) = \hat{z}_{i,k}^{[t]} - \hat{p}_{i,k}^{[t,m-1]}.$$

The data $(u_{i,k}^{[t,m]}, \mathbf{x}_i)_{i=1:n}$ is used to calibrate a L -terminal node regression tree with L_2 loss

$$\hat{f}_k^{[t,m]} \left(\mathbf{x}; R_{k,l=1:L}^{[t,m]}, \bar{u}_{k,l=1:L}^{[t,m]} \right),$$

where $R_{k,l=1:L}^{[t,m]}$ is the partition of covariate space and $\bar{u}_{k,l=1:L}^{[t,m]}$ contains the average gradient in each terminal node.

8. One dimensional optimization and update. It turns out that the one-dimensional optimization for expansion coefficient leads to the following update:

$$\hat{F}_k^{[t,m]}(\mathbf{x}_i) = \hat{F}_k^{[t,m-1]}(\mathbf{x}_i) + s_p \sum_{l=1}^L \gamma_{k,l}^{[t,m]} \mathbb{1}_{R_{k,l}^{[t,m]}}(\mathbf{x}_i),$$

where s_p is the learning rate and

$$\gamma_{k,l}^{[t,m]} = \frac{K-1}{K} \frac{\sum_{\{i: \mathbf{x}_i \in R_{k,l}^{[t,m]}\}} u_{i,k}^{[t,m]}}{\sum_{\{i: \mathbf{x}_i \in R_{k,l}^{[t,m]}\}} \left| u_{i,k}^{[t,m]} \right| \left(1 - \left| u_{i,k}^{[t,m]} \right| \right)}, \quad l = 1, \dots, L.$$

Please refer to equation (32) in Friedman (2001).

10. Return $\hat{p}_k^{[t,m]}$ according to (3.4), $k = 1, \dots, K$. The mixing probabilities are updated as

$$\hat{p}_k^{[t,m]} = \frac{\exp \left(\hat{F}_k^{[t,m]}(\mathbf{x}) \right)}{\sum_{l=1}^K \exp \left(\hat{F}_l^{[t,m]}(\mathbf{x}) \right)}, \quad k = 1, \dots, K.$$

In the loop 6-9, K independent boostings are performed for $F_k, k = 1, \dots, K$. Hence, we can accelerate the loop 6-9 by parallel computing. To the best of our knowledge, there is no available R package supporting a multinomial logistic boosting with fractional response \hat{z}_i . So we code steps 4-12 from bottom. Only the R package `rpart` is called to apply the recursive partition algorithm to calibrate the weak learner $\hat{f}_k^{[t,m]}$ in step 7.

The steps 13-21 implement K independent gradient boosting for each component mean.

13. Initialization of component means. Set $\hat{\mu}_k^{[t,0]}(\mathbf{x}), \hat{G}_k^{[t,0]}(\mathbf{x}), k = 1, \dots, K$ as:

$$\hat{\mu}_k^{[t,0]} = \frac{\sum_{i=1}^n y_i}{n}, \quad \hat{G}_k^{[t,0]} = \mu_k^{-1}(\hat{\mu}_k^{[t,0]}), \quad (3.10)$$

where μ_k^{-1} denotes the link function in the component model k . Similar to step 4, this initialization will be repeated at each outer EB iteration t . Later we will discuss another initialization strategy which considers the boosted values at the previous EB iteration.

16. Projection of gradient to learner. Compute the negative gradient for each data point $i = 1, \dots, n$ as

$$v_{i,k}^{[t,m]} = V_k(y_i, \hat{z}_{i,k}^{[t]}, \hat{G}_k^{[t,m-1]}(\mathbf{x}_i)).$$

The data $(v_{i,k}^{[t,m]}, \mathbf{x}_i)_{i=1:n}$ is used to calibrate a L -terminal node regression trees with L_2 loss

$$\hat{g}_k^{[t,m]} \left(\mathbf{x}; S_{k,l=1:L}^{[t,m]}, \bar{v}_{k,l=1:L}^{[t,m]} \right),$$

where $S_{k,l=1:L}^{[t,m]}$ is the partition of covariate space and $\bar{v}_{k,l=1:L}^{[t,m]}$ contains the average gradient in each terminal node.

17. One dimensional optimization and update. Conduct the following one-dimensional optimizations to find the best expansion coefficients:

$$\hat{w}_k^{[t,m]} = \arg \min_w \sum_{i=1}^n C_k(y_i, \hat{z}_{i,k}^{[t]}, \hat{G}_k^{[t,m-1]}(\mathbf{x}_i) + w \hat{g}_k^{[t,m]}(\mathbf{x}_i)).$$

Updates

$$\hat{G}_k^{[t,m]}(\mathbf{x}_i) = \hat{G}_k^{[t,m-1]}(\mathbf{x}_i) + s_\mu \hat{w}_k^{[t,m]} \hat{g}_k^{[t,m]}(\mathbf{x}_i),$$

where s_μ is the learning rate.

19. Return $\hat{\mu}_k^{[t,m]}$ according to corresponding link functions. The component means are updated as

$$\hat{\mu}_k^{[t,m]}(\mathbf{x}_i) = \mu_k(\hat{G}_k^{[t,m]}(\mathbf{x}_i)),$$

where μ_k denotes the inverse link function in component model k .

In the loop 14-20, K independent weighted boostings with weights $\hat{z}_{i,k}^{[t]}$ are implemented, we can accelerate this loop by parallel computing. We rely on the R packages `gbm` and `mboost` to perform the boosting in this loop. Those two packages can facilitate boosting with additional weights.

22. Estimation of dispersion. The MLE $\hat{\phi}_k^{[t]}$ is derived given the conditional expectation $\hat{z}_{i,k}^{[t]}$ and the component mean $\hat{\mu}_k^{[t]}(\mathbf{x}_i)$:

$$\hat{\phi}_k^{[t]} = \arg \max_{\phi_k} \sum_{i=1}^n -\hat{z}_{i,k}^{[t]} \log f_k(y_i; \hat{\mu}_k^{[t]}(\mathbf{x}_i), \phi_k), \quad k = 1, \dots, K. \quad (3.11)$$

In summary, a total of $(M_p + M_\mu) \times K \times T$ weak learners are calibrated in the EB algorithm. In the loop 6-9 the K weak learners can be calibrated simultaneously at each m , and in the loop 14-20 the K boosting algorithms can be conducted simultaneously at each t . Such a parallel computing will accelerate the EB algorithm significantly; see Table 2.

Gradient boosting with regression trees inherit the desirable features of trees. One of the advantages is automated feature engineering with regard to non-linearity, variable transformation and interaction. First, a tree produces a piecewise constant function facilitating non-linear effects of covariate. Second, trees are invariant under monotone transformations of the individual covariate. For example, using $x_j, \log x_j, \exp x_j$ as the j -th covariate leads to the same result. So there is no need for considering individual variable transformation. Third, a tree with L terminal nodes produces a function with interaction order at most $L - 1$. Another advantage of trees is internal variable selection. Trees tend to be robust against irrelevant covariates.

Moreover, trees are overfitting-sensitive given a suitable complexity parameter, i.e., any split not sufficiently improving the fit will not be attempted.

The boosting also mitigates many undesirable features of single tree model. For small trees, they are inaccurate due to the coarse nature of the piecewise constant functions. While for large trees, they are not stable due to high-order interaction involved. All of these are mitigated by boosting, which produces much finer piecewise constant functions and enhances stability by using small trees and by the effect of averaging over many of them. One remarkable feature of boosting is the resistance to overfitting, which owes to overfitting-sensitive split in trees and two regularization hyperparameters of the learning rate s and the number of iterations M . We normally specify a large M and early stop iterating by minimizing the validation loss before reaching M . For a sufficiently small learning rate, we usually do not observe a typical tick shape of validation loss but a leveling-off pattern; see Figure 1 in Friedman (2001).

3.3 Interpretation, hyperparameters tuning and initialization in the EB algorithm

A particular useful interpretative tool for boosting is relative importance proposed by Breiman et al. (1984). In mixture models, we consider the relative importance of covariates in each component and the overall relative importance. In the weak learner of tree $\hat{f}_k^{[T,m]}$, the relative importance of covariate x_j is

$$I_j(\hat{f}_k^{[T,m]}) = \sum_{l=1}^{L-1} e_l \mathbb{1}_{d_l}(j), \quad (3.12)$$

where the summation is over the nonterminal nodes l of the L -terminal node tree $\hat{f}_k^{[T,m]}$, d_l is the splitting variable associated with node l , and e_l is the corresponding empirical improvement in squared error as a result of the split given by

$$e_l = \frac{c_l c_r}{c_l + c_r} (\bar{a}_l - \bar{a}_r)^2.$$

Here, \bar{a}_l, \bar{a}_r are the left and right split gradient means respectively, and c_l and c_r are the corresponding sums of the weights. For a collection of trees $(\hat{f}_k^{[T,m]})_{m=1:M_p}$ for the k -th component, (3.12) can be generalized by its average over all of the trees

$$IP_{j,k} = \frac{1}{M_p} \sum_{m=1}^{M_p} I_j(\hat{f}_k^{[T,m]}), \quad (3.13)$$

which is interpreted as the relative importance of x_j in separating component k from the other components. The overall relative importance of x_j is obtained by averaging over all components:

$$IP_j = \frac{1}{K} \sum_{k=1}^K IP_{j,k}.$$

The above formulae are about relative importance of covariates in mixing probabilities. Similarly, we can obtain the relative importance of covariates in each component mean as

$$IM_{j,k} = \frac{1}{M_\mu} \sum_{m=1}^{M_\mu} I_j(\hat{g}_k^{[T,m]}), \quad k = 1, \dots, K, \quad (3.14)$$

and the overall relative importance of covariates in means as

$$IM_j = \frac{1}{K} \sum_{k=1}^K IM_{j,k}.$$

The EB algorithms have four types of hyperparameters: number of EB iterations T , numbers of boosting iterations M_p and M_μ , learning rates s_p and s_μ , and hyperparameters in weak learners. We denote the index of training data by $\mathcal{I}_{\text{train}} = \{1, \dots, n\}$, the index of validation data by \mathcal{I}_{val} and the index of test data by $\mathcal{I}_{\text{test}}$. They are mutually exclusive. The number of EB iterations T can be determined by screening the trace plot of the likelihood on the learning data $\mathcal{I}_{\text{learn}} = \mathcal{I}_{\text{train}} \cup \mathcal{I}_{\text{val}}$ at each iteration t :

$$\prod_{i \in \mathcal{I}_{\text{learn}}} \sum_{k=1}^K \hat{p}_k^{[t]}(\mathbf{x}_i) f_k(y_i; \hat{\mu}_k^{[t]}(\mathbf{x}_i), \phi_k^{[t]}).$$

If no obvious improvement is observed, the EB algorithm converges. For the numbers of boosting iterations M_p, M_μ , we specify a sufficiently large M_p, M_μ and calculate the validation loss on \mathcal{I}_{val} at each iteration m :

$$\sum_{i \in \mathcal{I}_{\text{val}}} \sum_{k=1}^K \hat{z}_{i,k}^{[t]} \log \hat{p}_k^{[t,m]}(\mathbf{x}_i), \quad (3.15)$$

$$\sum_{i \in \mathcal{I}_{\text{val}}} \hat{z}_{i,k}^{[t]} \log f_k(y_i; \hat{\mu}_k^{[t,m]}(\mathbf{x}_i), \phi_k^{[t]}), \quad k = 1, \dots, K. \quad (3.16)$$

If there is no obvious improvement of the validation loss, the corresponding boosting can be early stopped before reaching M_p or M_μ . For the learning rates s_p and s_μ , smaller learning rates tend to lead to a better fitting and predictive performance but requiring more boosting iterations. We adjust the learning rates by monitoring the validation loss (3.15) and (3.16), respectively. Note that we can specify different learning rates s_μ for different component means. The hyperparameters in weak learners of regression trees include complexity parameter, maximum depth, number of terminal nodes, etc. Those hyperparameters can be tuned as in typical regression trees. Please refer to Hastie et al. (2009) for more details. Although there are methods to systematically tune hyperparameters such as grid research, Bayesian optimization, etc. In many cases, hyperparameter tuning is more of an art than a science.

In steps 4 and 13 for the initialization of boosting, we initialize parameters at iteration t independently with the previously boosted estimates $\hat{p}_k^{[t-1]}, \hat{\mu}_k^{[t-1]}$; see equations (3.9) and (3.10). We call this as uncorrelated boosting. However, please note that boosting at iteration t is not independent with boosting at iteration $t-1$ since boosting at iteration t is based on $\hat{z}_i^{[t]}$ which depends on the boosted results at iteration $t-1$. The gains from the boosting at iteration $t-1$ are passed to the boosting at iteration t via the conditional expectation $\hat{z}_i^{[t]}$.

We might initialize parameters at iteration t as the previously boosted estimates

$$\hat{p}_k^{[t,0]} = \hat{p}_k^{[t-1]}, \hat{\mu}_k^{[t,0]} = \hat{\mu}_k^{[t-1]}.$$

This would lead a smaller required inner boosting iterations (i.e., an earlier stop on the validation loss) since the boosting starts from better initial values. We call this as forward boosting. However, with forward boosting, it is difficult to predict for new data due to the iterative

initialization. One solution is to apply an additional boosting step with default initialization (3.9) and (3.10) given the last conditional expectations of the latent variables $\hat{\mathbf{z}}_i^{[T]}$. In the following applications, we only implement the uncorrelated boosting.

[As mentioned in the introduction, boosting algorithms possess good properties to deal with some issues like variable selection, feature engineering and overfitting problems. Currently there is no discussion about these topics in this section and no illustration in the next simulation or real data analysis. It is better to address these aspects of EB algorithm and add some results in the next section. For example, variable importance plots and partial dependence plots. These are very useful for the interpretation of real data analyses.]

4 Applications

We conduct two simulated data analysis and a real data analysis. The first simulated data follows a zero-inflated Poisson model, which mimics claim count data with excess of zeros. We use this example to illustrate the advantages of the EB algorithm over the EM algorithm. The second simulated data follows a mixture of Gaussian models. We discuss constraints on mixing structure and parallel computing in this example. The real data contains the claims amount data of an insurance company. This example demonstrates how to choose component models and mixing structure in practice.

4.1 First simulated example: zero-inflated Poisson model

We consider a simulated data which is generated from a zero-inflated Poisson (ZIP) model. This simulated data mimics number of claims with excess of zeros. The underlying model is given by:

$$f_{\text{ZIP}}(N; \lambda, \pi_0) = \begin{cases} \pi_0 + (1 - \pi_0)e^{-\lambda} & \text{for } N = 0 \\ (1 - \pi_0)\frac{e^{-\lambda}\lambda^N}{N!} & \text{for } N \in \mathbb{N}_+. \end{cases} \quad (4.1)$$

The ZIP model is a mixture of a probability mass of 1 at 0 and a Poisson distribution. The mixing probability is π_0 and $1 - \pi_0$. The probability density function can be written as

$$f_{\text{ZIP}}(N; \lambda, \pi_0) = \pi_0 \mathbb{1}_0(N) + (1 - \pi_0) \frac{e^{-\lambda}\lambda^N}{N!}.$$

Suppose that five covariates $\mathbf{x} = (x_1, \dots, x_5)$ have systematic effects on both π_0 and λ : [It is better to give brackets for the exp function. Similarly for those in the rest of paper]

$$\pi_0(\mathbf{x}) = \frac{\exp(F(\mathbf{x}))}{1 + \exp(F(\mathbf{x}))}, \quad \lambda(\mathbf{x}) = \exp(G(\mathbf{x})), \quad (4.2)$$

where

$$F(\mathbf{x}) = 0.3 - 2x_2^2 + x_2 + 0.2x_5, \quad G(\mathbf{x}) = \log 0.5 + x_1^2 + 0.2 \log x_3 - 0.2x_1x_4. \quad (4.3)$$

The covariates are generated from the following distributions:

$$\begin{aligned}x_1 &\sim N(0, 0.5^2), \\x_2 &\sim U(0, 1), \\x_3 &\sim \Gamma(2, 0.5), \\x_4 &\sim \text{Bernulli}(0.5), \\x_5 &\sim \text{Bernulli}(0.2).\end{aligned}$$

Note that we use shape-rate parameters for gamma distribution Γ . We generate for $n = 10,000$ samples $(N_i, \mathbf{x}_i)_{i=1:n}$, which are partitioned into a learning data $i \in \mathcal{I}_{\text{learn}}$ of sample size 8,000 and a test data $i \in \mathcal{I}_{\text{test}}$ of sample size 2,000. If a Poisson distribution is fitted to the learning data, the MLE of Poisson mean is $1/|\mathcal{I}_{\text{learn}}| \sum_{i \in \mathcal{I}_{\text{learn}}} N_i = 0.2136$, implying the estimated proportion of zero claims as $\exp(-0.2136) = 80.77\%$ less than the empirical proportion 83.10% for the test data.

We will compare different models in terms of test loss defined as the average negative log-likelihood on the test data:

$$-\frac{1}{|\mathcal{I}_{\text{test}}|} \sum_{i \in \mathcal{I}_{\text{test}}} \log \left(\hat{\pi}_0(\mathbf{x}_i) \mathbb{1}_0(N_i) + (1 - \hat{\pi}_0(\mathbf{x}_i)) \frac{e^{-\hat{\lambda}(\mathbf{x}_i)} \hat{\lambda}(\mathbf{x}_i)^{N_i}}{N_i!} \right), \quad (4.4)$$

where $\hat{\pi}_0$ and $\hat{\lambda}$ are estimated on the learning data. Since we know the underlying $\pi_0(\mathbf{x})$ and $\lambda(\mathbf{x})$, we define another two test metrics based on F and G :

$$e_\pi = \frac{1}{|\mathcal{I}_{\text{test}}|} \sum_{i \in \mathcal{I}_{\text{test}}} (\hat{F}(\mathbf{x}_i) - F(\mathbf{x}_i))^2, \quad (4.5)$$

$$e_\lambda = \frac{1}{|\mathcal{I}_{\text{test}}|} \sum_{i \in \mathcal{I}_{\text{test}}} (\hat{G}(\mathbf{x}_i) - G(\mathbf{x}_i))^2. \quad (4.6)$$

We start with a null ZIP model without any covariates:

$$F(\mathbf{x}) = \alpha_0, \quad G(\mathbf{x}) = \beta_0 \quad (4.7)$$

The MLE can be obtained as $\bar{\pi}_0 = 0.5604$, $\bar{\lambda} = 0.4860$ via the EM algorithm on the learning data. The test loss is calculated as 0.5299. The estimated proportion of zero claims for the test data is calculated as

$$\frac{1}{|\mathcal{I}_T|} \sum_{i \in \mathcal{I}_T} \left(\bar{\pi}_0 + (1 - \bar{\pi}_0) e^{-\bar{\lambda}} \right) = \bar{\pi}_0 + (1 - \bar{\pi}_0) e^{-\bar{\lambda}} = 0.8308,$$

which is quite close the empirical proportion of 83.10%. Since we know the underlying $\pi_0(\mathbf{x})$ and $\lambda(\mathbf{x})$, we can calculate the true test loss as

$$-\frac{1}{|\mathcal{I}_{\text{test}}|} \sum_{i \in \mathcal{I}_{\text{test}}} \log \left(\pi_0(\mathbf{x}_i) \mathbb{1}_0(N_i) + (1 - \pi_0(\mathbf{x}_i)) \frac{e^{-\lambda(\mathbf{x}_i)} \lambda(\mathbf{x}_i)^{N_i}}{N_i!} \right) = 0.5150, \quad (4.8)$$

which is (surely) smaller than 0.5299 from the null model. The test metrics (4.5) and (4.6) are calculated as $e_\pi = 0.1151$, $e_\lambda = 0.1795$.

Next ZIP models with linear predictors are fitted, where $F(x)$ and $G(x)$ are assumed to be linear functions of \mathbf{x} . One component model is degenerated into a probability mass 1 at $N = 0$, so there is no coefficient in this component model. We consider three different mixture models, heterogeneous Poisson parameters only (4.9), heterogeneous mixing probabilities only (4.10) and both heterogeneous mixing probabilities and Poisson parameters (4.11):

$$F(\mathbf{x}) = \alpha_0, \quad G(\mathbf{x}) = \langle \boldsymbol{\beta}, \mathbf{x} \rangle, \quad (4.9)$$

$$F(\mathbf{x}) = \langle \boldsymbol{\alpha}, \mathbf{x} \rangle, \quad G(\mathbf{x}) = \beta_0, \quad (4.10)$$

$$F(\mathbf{x}) = \langle \boldsymbol{\alpha}, \mathbf{x} \rangle, \quad G(\mathbf{x}) = \langle \boldsymbol{\beta}, \mathbf{x} \rangle, \quad (4.11)$$

where $\langle \boldsymbol{\beta}, \mathbf{x} \rangle$ denotes the dot product of two vectors $\boldsymbol{\beta}, \mathbf{x}$. [\[Define inner product?\]](#) The MLE of regression coefficients $\boldsymbol{\alpha}$ and $\boldsymbol{\beta}$ can be obtained by the EM algorithm. We have summarized the results in Table 1. Model (4.11) has the best out-of-sample performance followed by Model (4.9), while Model (4.10) has the worst out-of-sample performance. All the three models are better than the null model (4.7). Note that those models ignore the potential non-linearity and interactions in covariates.

Finally we estimate F and G non-parametrically via the proposed EB algorithm. We also consider three different mixing structures, heterogeneous Poisson parameters only (4.12), heterogeneous mixing probabilities only (4.13) and both heterogeneous mixing probabilities and Poisson parameters (4.14):

$$F(\mathbf{x}) = \alpha_0, \quad G(\mathbf{x}) = G_0(\mathbf{x}) + \sum_{m=1}^{M_\lambda} s_\lambda \omega_\lambda^{[m]} g^{[m]}(\mathbf{x}), \quad (4.12)$$

$$F(\mathbf{x}) = F_0(\mathbf{x}) + \sum_{m=1}^{M_\pi} s_\pi \omega_\pi^{[m]} f^{[m]}(\mathbf{x}), \quad G(\mathbf{x}) = \beta_0, \quad (4.13)$$

$$F(\mathbf{x}) = F_0(\mathbf{x}) + \sum_{m=1}^{M_\pi} s_\pi \omega_\pi^{[m]} f^{[m]}(\mathbf{x}), \quad G(\mathbf{x}) = G_0(\mathbf{x}) + \sum_{m=1}^{M_\lambda} s_\lambda \omega_\lambda^{[m]} g^{[m]}(\mathbf{x}). \quad (4.14)$$

The results are listed in Table 1. Although the test losses change slightly among different models, we can clearly order the considered models according to the two metrics e_π and e_λ . We observe that Model (4.14) has the best out-of-sample performance in terms of all the metrics. Furthermore, all the models can address the excess of zeros since they are all based on the ZIP distribution. We conclude that when there is a complicated effect of covariate on parameters, the EB algorithm is more appropriate than the EM algorithm since more flexible regression functions are allowed in the EB algorithm.

Remarks. In the case of $K = 2$, there is only one to-be-boosted function F in mixing probabilities. We replace the boosting loop 5-12 of Algorithm 2 by Algorithm 5 L_2 -TreeBoost in Friedman (2001). However, one can still implement the original boosting in Algorithm 2, where F_1 and F_2 are boosted. They are related to F of the underlying model by $F_1 - F_2 = F$. The running time in this example takes only several seconds since there are only two regression functions F and G to be estimated. When mixture models contain $K > 2$ components, the boosting of mixing probabilities takes much more time since K functions are to be boosted. This will be discussed in the next example.

Table 1: Comparison of different ZIP models on the test data. Note that Models (4.7), (4.9), (4.10) and (4.11) are estimated via the EM algorithm, while Models (4.12), (4.13) and (4.14) are estimated via the EB algorithm.

model	test loss (4.4)	e_π (4.5)	e_λ (4.6)	proportion of zero claims
Null (4.7)	0.5299	0.1151	0.1795	0.8308
Varying λ (4.9)	0.5258	0.1112	0.1654	0.8305
Varying π (4.10)	0.5265	0.0959	0.182	0.8304
Varying π and λ (4.11)	0.5257	0.1159	0.1776	0.8304
Varying λ (4.12)	0.5234	0.1114	0.0928	0.8316
Varying π (4.13)	0.5256	0.0579	0.1738	0.8293
Varying π and λ (4.14)	0.5199	0.0687	0.0588	0.8336
True	0.5150	0.0000	0.0000	0.8310

4.2 Second simulated example: mixture of Gaussians

The underlying model is a mixture of three Gaussians. The mixing probabilities are related to covariates, while the parameters of component Gaussians are homogeneous among all samples. The probability density function is given by

$$f(y|\mathbf{x}; \mu, \sigma, p) = p_1(\mathbf{x})f_N(y; \mu_1, \sigma_1) + p_2(\mathbf{x})f_N(y; \mu_2, \sigma_2) + p_3(\mathbf{x})f_N(y; \mu_3, \sigma_3), \quad (4.15)$$

where $f_N(\cdot; \mu, \sigma)$ is the probability density function of a Gaussian distribution with mean μ and standard deviation σ . We assume that the mixing probabilities depend on the covariates vector $\mathbf{x} = (x_1, x_2, x_3, x_4)$ via the following equations

$$p_k(\mathbf{x}) = \frac{\exp(F_k(\mathbf{x}))}{\sum_{l=1}^3 \exp(F_l(\mathbf{x}))}, \text{ for } k = 1, 2, 3, \quad (4.16)$$

where

$$\begin{aligned} F_1(\mathbf{x}) &= x_1 + \log x_2, \\ F_2(\mathbf{x}) &= 1 - 0.5x_1 - x_1x_2 + 2x_3, \\ F_3(\mathbf{x}) &= 2 \sin x_1 + \log x_2 + x_1x_3. \end{aligned}$$

Note that covariate x_4 is a redundant variable. We specify $\mu_1 = -5, \mu_2 = 0, \mu_3 = 5, \sigma_1 = \sigma_2 = \sigma_3 = 1$. We generate the four covariates from the following distribution independently:

$$\begin{aligned} x_1 &\sim N(2, 1), \\ x_2 &\sim \text{Exp}(2), \\ x_3 &\sim \text{Bernulli}(0.5), \\ x_4 &\sim \Gamma(0.5, 0.5). \end{aligned}$$

Note that we use shape-rate parameters for gamma distribution Γ . We generate $n = 12,000$ samples, among which 10,000 samples are learning data and 2,000 samples are test data.

We first consider the parametric mixture models calibrated by the EM algorithm. The following mixtures of three linear regressions (or distributions) are fitted:

- Mixture of three distributions with homogeneous mixing probabilities (homogeneous null model without any covariates):

$$f(y|\mathbf{x}; \mu, \sigma, p) = p_1 f_N(y; \mu_1, \sigma_1) + p_2 f_N(y; \mu_2, \sigma_2) + p_3 f_N(y; \mu_3, \sigma_3). \quad (4.17)$$

- Mixture of three linear regressions with homogeneous mixing probabilities:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1 f_N(y; \mu_1(\mathbf{x}), \sigma_1) + p_2 f_N(y; \mu_2(\mathbf{x}), \sigma_2) + p_3 f_N(y; \mu_3(\mathbf{x}), \sigma_3), \quad (4.18)$$

where

$$\mu_1(\mathbf{x}) = \langle \boldsymbol{\alpha}, \mathbf{x} \rangle, \mu_2(\mathbf{x}) = \langle \boldsymbol{\beta}, \mathbf{x} \rangle, \mu_3(\mathbf{x}) = \langle \boldsymbol{\gamma}, \mathbf{x} \rangle. \quad (4.19)$$

- Mixture of three distributions with heterogeneous mixing probabilities modeled by a multiclass logistic regression:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1(\mathbf{x}) f_N(y; \mu_1, \sigma_1) + p_2(\mathbf{x}) f_N(y; \mu_2, \sigma_2) + p_3(\mathbf{x}) f_N(y; \mu_3, \sigma_3) \quad (4.20)$$

where

$$p_k(\mathbf{x}) = \frac{\exp(F_k(\mathbf{x}))}{\sum_{l=1}^3 \exp(F_l(\mathbf{x}))}, \text{ for } k = 1, 2, 3, \quad (4.21)$$

and

$$F_1(\mathbf{x}) = \langle \mathbf{a}, \mathbf{x} \rangle, F_2(\mathbf{x}) = \langle \mathbf{b}, \mathbf{x} \rangle, F_3(\mathbf{x}) = \langle \mathbf{c}, \mathbf{x} \rangle. \quad (4.22)$$

Note that this model follows the underlying mixture model. However, this model cannot address non-linear effects of covariates and their interactions on the mixing probabilities.

- Mixture of three linear regressions with both heterogeneous mean and heterogeneous mixing probabilities:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1(\mathbf{x}) f_N(y; \mu_1(\mathbf{x}), \sigma_1) + p_2(\mathbf{x}) f_N(y; \mu_2(\mathbf{x}), \sigma_2) + p_3(\mathbf{x}) f_N(y; \mu_3(\mathbf{x}), \sigma_3) \quad (4.23)$$

where the means and mixing probabilities follow equations (4.19), (4.21) and (4.22).

Next, we consider non-parametric mixture models calibrated by the proposed EB algorithm. The following mixture models are fitted:

- Mixture model with heterogeneous mean and homogeneous mixing probabilities:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1 f_N(y; \mu_1(\mathbf{x}), \sigma_1) + p_2 f_N(y; \mu_2(\mathbf{x}), \sigma_2) + p_3 f_N(y; \mu_3(\mathbf{x}), \sigma_3), \quad (4.24)$$

where μ_1, μ_2, μ_3 are estimated non-parametrically via the boosting algorithm. This model is comparable to model (4.18).

- Mixture model with heterogeneous mixing probabilities:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1(\mathbf{x}) f_N(y; \mu_1, \sigma_1) + p_2(\mathbf{x}) f_N(y; \mu_2, \sigma_2) + p_3(\mathbf{x}) f_N(y; \mu_3, \sigma_3) \quad (4.25)$$

where

$$p_k(\mathbf{x}) = \frac{\exp(F_k(\mathbf{x}))}{\sum_{l=1}^3 \exp(F_l(\mathbf{x}))}, \text{ for } k = 1, 2, 3. \quad (4.26)$$

Here F_1, F_2, F_3 are estimated non-parametrically via boosting algorithm. This model is comparable to model (4.20).

- Mixture model with both heterogeneous mean and heterogeneous mixing probabilities:

$$f(y|\mathbf{x}; p, \mu, \sigma) = p_1(\mathbf{x})f_N(y; \mu_1(\mathbf{x}), \sigma_1) + p_2(\mathbf{x})f_N(y; \mu_2(\mathbf{x}), \sigma_2) + p_3(\mathbf{x})f_N(y; \mu_3(\mathbf{x}), \sigma_3) \quad (4.27)$$

where both means and mixing probabilities are estimated non-parametrically via boosting algorithm. This model is comparable to model (4.23).

We summarize the results of the seven models in Table 2 including average negative log-likelihood on the test data, and the running time of the EM algorithm or the EB algorithm. Note that the true negative log-likelihood is calculated based on the simulated parameters $p(\mathbf{x}), \mu, \sigma$. All three models with linear predictors (4.18), (4.20) and (4.23) have a larger test loss than their counterpart boosted models (4.24), (4.25) and (4.27) since they cannot capture non-linear effects and interactions of covariates. The two models with both heterogeneous means and mixing probabilities (4.23) and (4.27) have no obvious better out-of-sample performance than the two models with only heterogeneous probabilities (4.20) and (4.25), respectively. It seems that the component means are not related to covariates.

For Model (4.27), we draw the trace plot of the loss during the EB iterations $t = 1, \dots, T$ in Figure 1. It shows that the EB algorithm converges after around 10 iterations. At the last EB iteration T , we draw the trace plot of the loss during the boosting iterations $m = 1, \dots, M_p$ for mixing probabilities in Figure 1. It shows that the boosting is robust against overfitting. At the last EB iteration T , we also draw the trace plot of the loss during the boosting iterations $m = 1, \dots, M_\mu$ for each component mean in Figure 2. It shows that the boosting cannot find heterogeneity in component means and the boosting stops early at very beginning. We calculate the overall relative importance of x_1, x_2, x_3, x_4 in mixing probabilities as 48.23, 34.51, 17.00, 0.25, which is align to the underlying model.

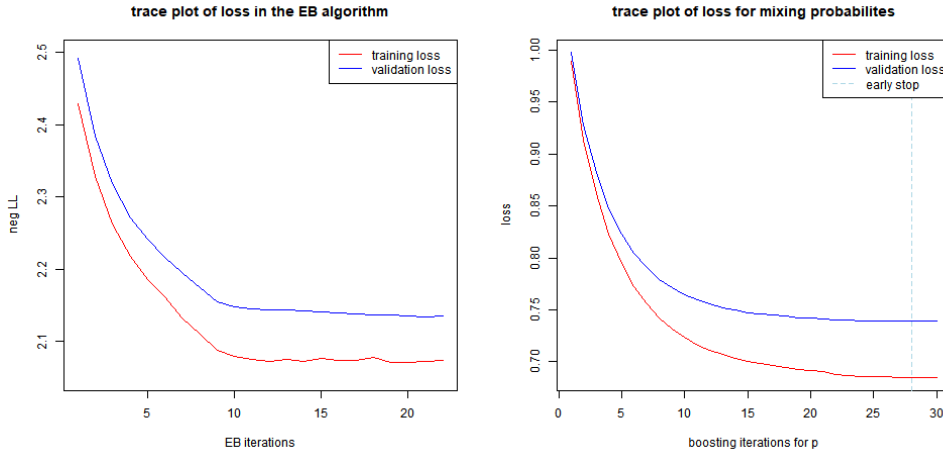


Figure 1: Left: The trace plot of loss during the EB iterations. Right: The trace plot of loss during the boosting iterations for mixing probabilities at last EB iteration T .

Comparison of the running times without parallel computing for models (4.24) and (4.25) implies that the boosting of mixing probabilities takes much more time than the boosting of component means does. Indeed, the boosting iteration of component means stop early while the boosting iteration of mixing probabilities takes more time to discover the heterogeneity; see the

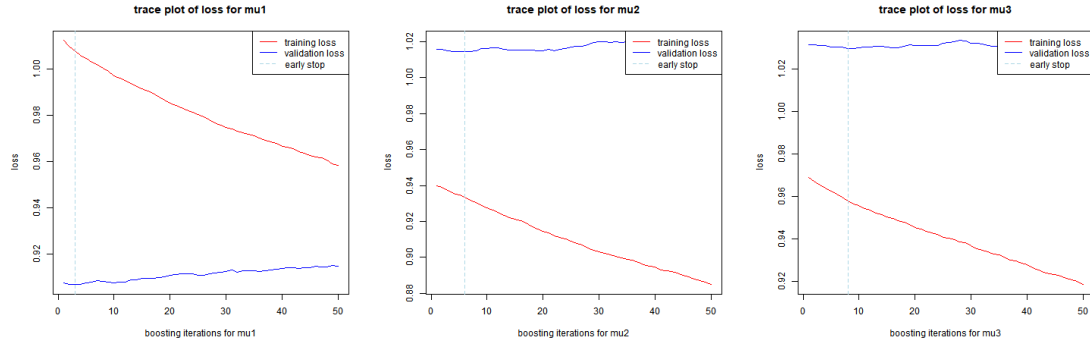


Figure 2: The trace plot of loss during the boosting iterations for component means at last EB iteration T .

Table 2: Comparison of different models in terms of test loss and running time. Note that Models (4.17), (4.18), (4.20) and (4.23) are estimated via the EM algorithm, while Models (4.24), (4.25) and (4.27) are estimated via the EB algorithm. [\[Not easy to distinguish the results between EM and EB\]](#)

model	test	running time	
	loss	without parallel computing	with parallel computing
Null (4.17)	2.4821	< 10 seconds	NA
Varying μ (4.18)	2.4779	< 10 seconds	NA
Varying p (4.20)	2.2016	< 10 seconds	NA
Varying μ and p (4.23)	2.2011	< 10 seconds	NA
Varying μ (4.24)	2.4139	< 10 seconds	NA
Varying p (4.25)	2.1330	650 seconds	381 seconds
Varying μ and p (4.27)	2.1320	1054 seconds	597 seconds
True	2.1231	NA	NA

underlying model (4.15). We accelerate the EB algorithm by applying parallel computing for the boosting of mixing probabilities, i.e., in loop 6-9 of Algorithm 2 we fit K trees simultaneously. It shows that parallel computing accelerates the EB algorithm significantly.

4.3 Real data example: claims severity modelling

[Is it necessary to separate the simulation and real data analysis into two subsections? Instead of saying the real data analysis the third example] In this example, we study the claims amount data `freMTPL2sev` from R package *CASdatasets*, which contains risk features and claim amounts from $n = 24,938$ motor third-party liabilities policies (after data cleaning). We plot the histogram and the cumulative distribution function of logged average claim amount in Figure 3, which shows three peaks and a heavy tail. An intuitive choice of component distributions is that three

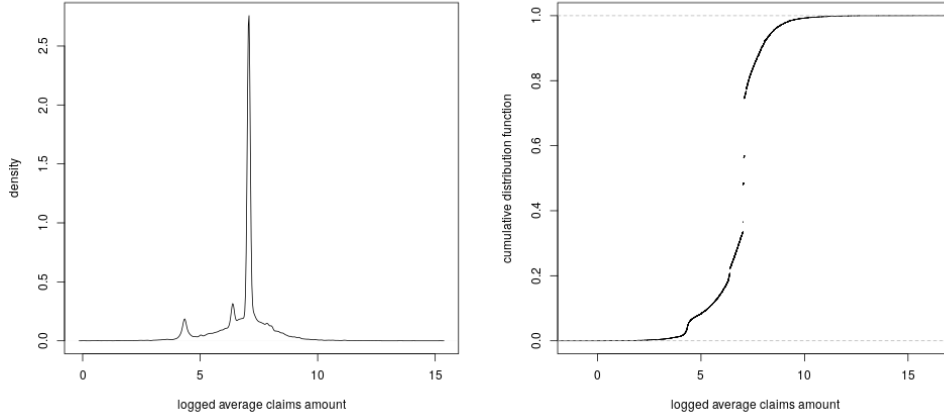


Figure 3: Histogram and the cumulative distribution function of logged average claims.

peaks are modeled by three gamma distributions, respectively, the resting non-tail part by a fourth gamma distribution, and the tail part by a Pareto distribution. Therefore, the probability density function (of the null model) is given by

$$f(y|\mathbf{x}; p, \mu, \phi, \alpha) = \sum_{k=1}^4 p_k f_G(y; \mu_k, \phi_k) + p_5 f_P(y; \alpha, M), \quad (4.28)$$

where μ, ϕ are mean and dispersion parameter of gamma distribution, and α, M are tail index and threshold of Pareto distribution. The logged survival function for logged average claims as shown in Figure 4 indicates a regularly varying tail at infinity (Embrechts et al., 1997). The threshold of Pareto distribution is selected as $M = 8158.13$ according to the Hill plot (Resnick, 1997) as shown in Figure 4. Please refer to Wüthrich and Merz (2022) for more discussions on this data.

The three peaks as shown in Figure 3 imply a way of initialization through the hidden component indicator variable:

$$\begin{aligned} \hat{\mathbf{z}}_i^{[0]} &= (\hat{z}_{i,1}^{[0]}, \hat{z}_{i,2}^{[0]}, \hat{z}_{i,3}^{[0]}, \hat{z}_{i,4}^{[0]}, \hat{z}_{i,5}^{[0]}) \\ &= (\mathbb{1}_{(0,500]} y_i, \mathbb{1}_{(500,1000]} y_i, \mathbb{1}_{(1000,1200]} y_i, \mathbb{1}_{(1200,8158.13]} y_i, \mathbb{1}_{(8158.13,\infty)} y_i). \end{aligned} \quad (4.29)$$

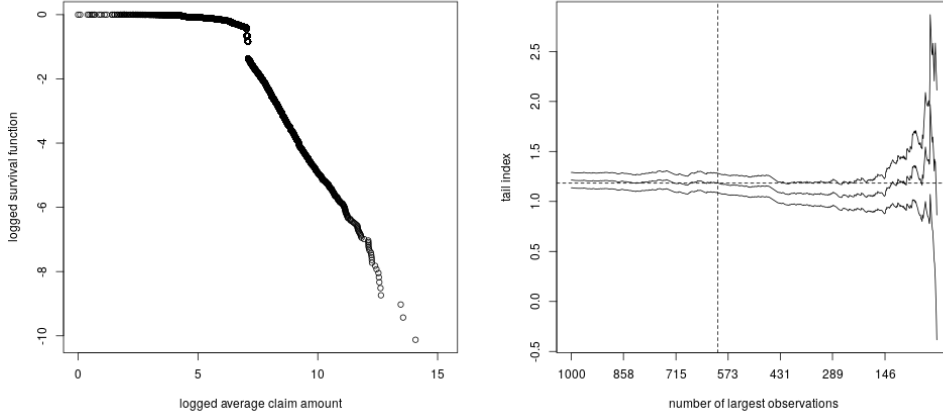


Figure 4: The logged survival function and the Hill plot for logged average claims.

Component parameters μ, ϕ, α can be initialized as the MLEs in a homogeneous model for the full information $(y_i, \hat{z}_i^{[0]}, \mathbf{x}_i)_{i=1:n}$, i.e., the MLEs of parameters in gamma/Pareto distribution fitted to the partial samples in five intervals $(0, 500], (500, 1000], (1000, 1200], (1200, 8158.13], (8158.13, \infty)$, respectively.

We first fit a mixture of distributions (4.28) to the data via the EM algorithm. The trace of learning loss is shown in Figure 5, implying a convergence after 80 iterations. The estimated

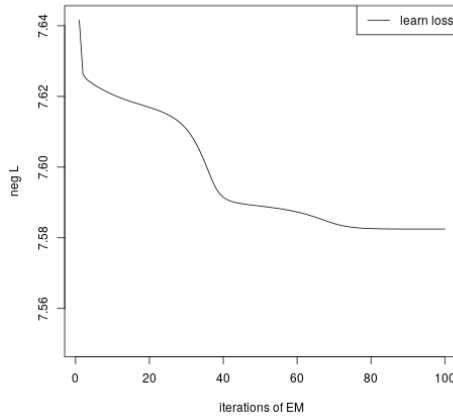


Figure 5: The trace plot the learning loss for the homogeneous model (4.28) during the EM iterations.

component parameters are listed in Table 3. We observe that the three peaks are captured by the first three component gamma distributions. The first three large shape parameters (small dispersion) imply the difficulties with mean modelling in the first three component models. The test loss is calculated as 7.5815. The mixing probabilities are estimated as $\hat{p}_1 = 0.0409$, $\hat{p}_2 = 0.0300$, $\hat{p}_3 = 0.4100$, $\hat{p}_4 = 0.4973$ and $\hat{p}_5 = 0.0218$.

Next we fit a mixture of distributions with heterogeneous mixing probabilities by the pro-

Table 3: The MLEs of component parameters in the homogeneous model (4.28). Tail index is estimated as $\hat{\alpha} = 1.0773$.

component k	μ_k	shape ($1/\phi_k$)	scale	rate
1	76.8727	105.556	0.7283	1.3731
2	592.5909	653.539	0.9067	1.1029
3	1171.3811	999.999	1.1714	0.8537
4	1534.5143	1.0377	1478.7768	7e-04

posed EB algorithm:

$$f(y|\mathbf{x}; p, \mu, \phi, \alpha) = \sum_{k=1}^4 p_k(\mathbf{x}) f_G(y; \mu_k, \phi_k) + p_5(\mathbf{x}) f_P(y; \alpha, M). \quad (4.30)$$

We draw the boxplot of the mixing probabilities in Figure 6. We observe that the mixing probabilities for the third and forth components p_3 and p_4 are more related with the covariates. The test loss is calculated as 7.5588 smaller than the null model.

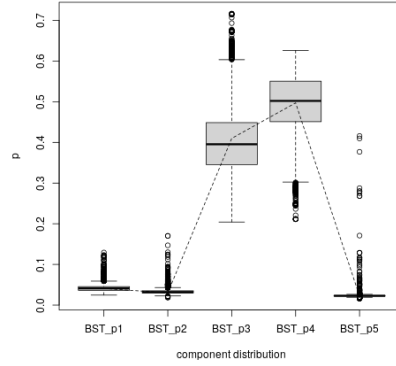


Figure 6: The boxplot of the estimated mixing probabilities in Model (4.30).

Finally, the small shape parameter of the forth component as shown in Table 3 indicates a possible improvement by boosting the forth component mean. Therefore, we fit the following mixture model:

$$f(y|\mathbf{x}; p, \mu, \phi, \alpha) = \sum_{k=1}^3 p_k(\mathbf{x}) f_G(y; \mu_k, \phi_k) + p_4(\mathbf{x}) f_G(y|\mathbf{x}; \mu_4(\mathbf{x}), \phi_4) + p_5(\mathbf{x}) f_P(y; \alpha, M).$$

The test loss is calculated as 7.5573 slightly smaller than that for model (4.30).

5 Conclusions

Insurance loss data sometimes cannot be sufficiently modeled by a single distribution, so a mixture of models is usually more preferred. Since there are multiple component models in a mixture of models, the parameter estimation problems is one key issue for data analysis. Thus,

the EM algorithm is one critical estimation method for mixture models in the literature. However, the EM algorithm usually requires parametric form of the component models, which limits the practical flexibility of mixture models. In this paper, we propose an Expectation-Boosting (EB) algorithm for mixture models, where both the mixing probabilities and the component models can be modeled non-parametrically. The core of the proposed algorithm is to replace the maximization step of the EM algorithm with a generic functional gradient descent algorithm. There are several advantages of the EB algorithm over the EM algorithm. First, boosting algorithm is a flexible non-parametric regression facilitating both non-linear effects and interaction. There is no need for specifying the form of component regression functions. Automated feature engineering is performed during the EB algorithm. Second, boosting algorithm is overfitting-sensitive, and variable selection is conducted simultaneously during the EB algorithm. The cost of more flexibility is more computing time than the EM algorithm since there are several inner boosting loops in each EB iteration.[\[I don't understand this sentence\]](#) We can accelerate the EB algorithm by conducting all the inner boosting loops simultaneously since they are independent given the component indicator variable z .

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