KL-divergence Based Deep Learning for Discrete Time Model

Li Liu, Xiangeng Fang, Di Wang, Weijing Tang, Kevin He

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Abstract

Neural Network (Deep Learning) is a modern model in Artificial Intelligence and it has been exploited in Survival Analysis. Although several improvements have been shown by previous works, training an excellent deep learning model requires a huge amount of data, which may not hold in practice. To address this challenge, we develop a Kullback-Leibler-based (KL) deep learning procedure to integrate external survival prediction models with newly collected time-to-event data. Time-dependent KL discrimination information is utilized to measure the discrepancy between the external and internal data. This is the first work considering using prior information to deal with short data problem in Survival Analysis for deep learning. Simulation and real data results show that the proposed model achieves better performance and higher robustness compared with previous works.
1 Introduction

Survival Analysis, or Time-to-Event Analysis, is an important subject in Statistics, where statistical and machine learning models are proposed to analyze survival data, whose outcome of interest is the time until one event happens (event time), such as the time when one patient dies during the clinical study. In general two reasons make survival analysis necessary for analyzing survival data. Firstly, researchers are interested in the distribution of the time for the event, not only the status of the event at one given time point. Secondly, in most times, we cannot record the event time for one individual due to the missing follow-up time or the limited time range for one study. We can only record a censored time (such as the last follow-up or diagnosing time) for the individual. These two reasons motivate many modern algorithms to deal with survival data, and methodologies proposed in survival analysis have been extended to other fields, such as fraud detection used in Finance.

Discrete time model is one branch of survival analysis, where the observed time is recorded as a discrete value. It is widely used when the event time is recorded based on a given time unit, such as day or month, or we want to model the grouped time, where each discrete time value can be understood as the index of a continuous time interval. Note that although our model focuses on discrete time model, we borrow ideas a lot from literature researching on continuous time model, [20] provides a unified form of continuous and discrete time model, we refer that book for readers who are interested in the connection.

Statisticians have developed various statistical models in survival analysis with rich theoretical properties to analyze survival data, such as Kaplan-Meier estimator [21] and Cox model [7]. However, the assumptions for these models usually do not hold in many real datasets, especially when the size of data is large. For instance, in SUPPORT (stands for Study to Understand Prognoses Preferences Outcomes and Risks of Treatment, [24]) data, most of the covariates are biological levels that have non-linear relationship with risk score, while Cox model assumes the relationship to be linear. Additionally, [11] uses a graph and one categorical feature (whether the patient has cancer or not) to show that proportional hazard assumption does not hold in SUPPORT, either, which is another important assumption made in Cox model. Since in real cases either one or both of the assumptions (linear, proportional hazard) will be violated, more flexible models are required for survival data analysis, such as machine learning algorithms, which emphasize not on the form of the model, but on what to learn from the data.

In machine learning field, deep learning (also known as neural network training) is renowned for its strong performance on several supervised learning problems, such as image classification. Deep learning methods have been proposed in Survival Analysis recently in the sense that neural network possesses high flexibility to model data and do feature transformations. Although the theoretical principles of deep learning are still unclear, many deep learning experiments and works show the superiority of deep learning compared with other traditional statistical or machine learning algorithms when the size of survival data is large. Notably, several works have been proposed to apply deep learning into survival analysis ([10, 22, 6, 30, 35, 11, 27, 26, 39, 35, 42]) and most of the works have shown that deep learning can achieve better performances compared with other statistical survival models or machine learning methods designed for Survival Analysis and we provide an overview of most these methods in Section 2.

Although deep learning is famous for its ability to achieve an extraordinary performance when the size of data is large, this may not be the case in many real datasets. For example, due to the privacy, we may not be able to obtain a large amount of data for a clinical study, but only obtain partial information such as the parameters of some estimated statistical models or those of a pre-trained deep learning model. However, the strict assumptions required by many statistical models still do not hold for some datasets even though their size of data is short. Take SUPPORT as an example, it is obvious that the non-linear property of the covariates is independent with the size of data. In these cases, we have a small size of data, but we still...
require a flexible and satisfactory model.

In this paper, we provide two approaches for training neural network on a small size of data. One approach is still training a model on a small size of data, but exploits information from other sources, such as an estimated model (prior model). To integrate other information, we propose a model that combines the prior information into our loss function for deep learning. Generally, we use Kullback-Leibler (KL) divergence \[25\] to calculate the similarity between local model (model that is trained with the accessible small dataset and the information from prior data) and prior model (model that has been estimated before, such as published statistical model or trained model from other data sources) and select a hyperparameter to determine the weight for local information and prior information. High weight for local data means the model tends not to use much prior information, while low weight means the model tends to believe that prior information is good enough for the model. We also extend this method to competing risk problem with a slight (but useful) modification.

As for the other approach, we follow \[11\], but specially design the neural network structure, with two structures that used for modeling proportional and non-proportional data, and also commonly-seen three link functions that used in discrete time model \[20\] (altogether six options). For proportional version, the new design is useful in data suitable for using these 3 link functions, but also reduces the number of nodes in the neural network, which will relieve the overparameterization problem \[4\], meaning the number of parameters is too large compared with the size of data. For non-proportional version, we do not restrict the activation function used in the output layer to be only sigmoid function (simulating logit link), but also the log and log-log link functions.

Based on our experiences in dealing with survival data with deep learning, we also provide with a comprehensive software combining all the contributions proposed in this paper and other necessary components for deep learning in survival analysis with the aid of prior model. This software is written by Python and deep learning process is completed by Pytorch, a well-designed package for training neural network. We design this software to not only show the novelty and comprehensiveness of our work, but also make it super convenient for users who are interested in this topic but would like to apply these methods into their own problems, such as combining a Cox model with local model a grouped relative risk model to model a clinical dataset with time values grouped by a series of time intervals \[41\].

As a recap, we summarize our work as follows:

- We provide two approaches to alleviate small data problems in deep learning. One is applying KL divergence to integrate data or model from other sources. The other one is specially design six neural network structures to adapt to datasets with various statistical properties.

- We extend our likelihood function and KL divergence to competing risk setting, which provides a novel approach solving competing risk problems.

- We provide a software which is comprehensive and user-friendly.

The organization of this paper is as follows. Section 2 recaps related works and their connections with our paper. Section 3 provides the details of discrete time model and the loss function used in our deep learning model, we have also provided details on how to parameterize the loss function by modeling hazard function with deep learning and how to extend it into competing risk problems. Section 4 provides some simulation studies, showing the proposed two approaches in our paper are useful when data has desired properties. Section 5 shows the results for real data analysis. We show the trend of our results compared with other models when we increase the size of local data and also run our model with hyperparameter tuning on a complicated EHR dataset. Section 6 concludes our work and proposes some future extensions for this paper.
2 Related Work

There has been a large body of models dealing with survival data. Cox proportional hazard model \([7]\) may be the most commonly used model in current survival analysis problems and also is a starting point of the future works. The formula of Cox model can be written as

\[
\lambda(t; Z) = \lambda_0(t) \exp(Z^\top \beta)
\]

(1)

where \( Z = [Z_1, \ldots, Z_p]^\top \) is the derived covariate vector obtained from the basic covariates \( x \). \( \beta = (\beta_1, \ldots, \beta_p)^\top \) is a vector of unknown parameters requiring estimation. It has two assumptions, where the first one is linear assumption, meaning the log risk of the hazard function is a linear function of derived features \( Z^\top \beta \), while the second one is proportional hazard assumption, which means the ratio of hazard function is constant over time \( \frac{\lambda(t_0; x)}{\lambda_0(t_0)} = \exp(Z^\top \beta) \) is constant for any \( t_0 \). Since either one or both of the assumptions will be violated in real cases, many alternative models are proposed, such as \([1]\), \([13]\) and \([43]\), but still suffer from restrictions brought by improper assumptions.

As mentioned in Section 1, machine learning algorithms are favored with researchers due to free of strict statistical assumptions. Random Survival Forest (RSF)\([16]\) uses only observed time and status to create a forest which ensures each node of the tree to be populated by individuals with similar survival. It achieves improvement in several survival datasets and is a benchmark for survival analysis in machine learning algorithms, but it does not consider the information of covariates for each individual, which may lead to inaccurate results.

Deep learning is shown to be empirically promising in many previous works compared with other machine learning algorithms. To the best of our knowledge, \([10]\) is the first paper proposing neural network to tackle with survival analysis problems and Deepsurv \([22]\) is the first paper that shows empirically that deep learning can provide improvement in results for survival analysis. For Deepsurv, it relieves the log risk term of the Cox proportional hazard model, from \( Z^T \beta \) to a general function \( g(\theta; Z) \) and this function is modeled by a neural network, with \( \theta \) the set of unknown parameters required estimation. However, Deepsurv still keeps the proportional hazard assumption even if it provides opportunity to model non-linear relation between covariates and log risk. Additionally, it chooses partial likelihood \([8]\) as the loss function, which prevents the usage of stochastic gradient descent (SGD) or mini-batch gradient descent due to the existence of at-risk set. Although \([27]\) proposes a case-control sampling method to approximate partial likelihood empirically by restricting the size of at-risk set into a small number (and even 1 in that paper), there is still no theoretical guarantee that restricting the size of at-risk set is reasonable.

Nnet-survival \([11]\), LogisticHazard \([26]\) and Deephit \([30]\) are three main papers that regard loss function the discrete likelihood function. Nnet-survival models the hazard value at different time points for one individual using neural network, Deephit models the probability mass functions (PMF), and LogisticHazard experiments both ways. Nnet-survival provides two versions of model structures, with proportional version same as using log-log link function in the last hidden layer. It also exploits the fact well known in survival analysis that discrete time survival data can be expressed as a Bernoulli log-likelihood of the hazard values (data expansion). Nevertheless it neither provides justification on the design, nor gives thorough consideration on other extensions, which are complemented in our paper.

Deephit focuses on modeling PMF with competing risk setting, and it adds a penalization term, making the model focuses more on the discrimination loss and provides advantages to have satisfactory result when

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1. \( Z \) can be understood as a feature transformation of \( x \), which means the covariates used in the model can be raw features (\( x \)) or processed features (such as adding on interaction terms or higher-order terms for \( x \)).

2. we refer LogisticHazard as a name of \([26]\), but LogisticHazard is actually one (but the most important) of the models proposed in that paper.
the metric is chosen to be Concordance-index. For competing risk setting, our paper instead models cause-specific hazard function (the hazard function for a given time point and also a given cause leading to the event) instead of PMF, and we are the first group using neural network to model hazard function for competing risk problems.

LogisticHazard provides a numerical stable implementation of flexible version model in Nnet-survival, it also provides comparison experiments on modeling PMF and hazard function and two ways of interpolation, making it possible to provide with a smooth survival function for discrete time model. In our paper, we take these two ways of interpolation as two tuning options and we can offer fair and comprehensive experiment result on a data with continuous time value, unifying both continuous and discrete time model. Moreover, our software follows pycox, an existing Python software for deep learning in survival analysis and LogisticHazard, we also show in our paper that due to the similarity of old and new loss functions, we can smoothly transfer all the techniques that used in pycox into our software, but not coding from scratch.

3 Methodology

This section is divided into 2 parts, in the first part we provide with a comprehensive introduction of discrete time model. In the second part we show the details to parameterize our model with a neural network.

3.1 Discrete Time Model: An Introduction

3.1.1 Probability Definitions and Data Structure

To capture the random behavior of the event and censored time, we define the probability density functions of them and further use likelihood function to estimate the parameters based on the given data. Define $T^*$ and $C$ to be event time and censored time (we will define $T$ as the observed time for each individual, so here we use $T^*$ instead), and define $\tau_1 < \tau_2 < \ldots < \tau_K$ for $K$ values that $T^*$ and $C$ take, then for event time variable $T^*$, we define

$$f(\tau_k|\mathbf{Z}) = P(T^* = \tau_k \mid \mathbf{Z}), k = 1, 2, \ldots, K$$

as the probability of $T^* = \tau_k$ given the derived covariates $\mathbf{Z}$. Define $F(t|\mathbf{Z}) = P(T^* \leq t \mid \mathbf{Z})$ as the cumulative density function of $T^*$. $S(t|\mathbf{Z}) = P(T > t \mid \mathbf{Z}) = \sum_{j \mid \tau_j > t} f(\tau_j) = 1 - F(t|\mathbf{Z})$ as the survival function. We also define a hazard function

$$\lambda(\tau_k|\mathbf{Z}) = P(T^* = \tau_k \mid T^* \geq \tau_k, \mathbf{Z}), k = 1, \ldots, K$$

(2)

which describes the instant death rate at time $t$ given the individual still survives at time $t$.

One interesting property in discrete time model is that we can uniformly express the survival function and density function by hazard function. Note that

$$\lambda(\tau_k|\mathbf{Z}) = P(T^* = \tau_k \mid T^* \geq \tau_k, \mathbf{Z}) = \frac{P(T^* = \tau_k \mid \mathbf{Z})}{P(T^* \geq \tau_k \mid \mathbf{Z})} = \frac{f(\tau_k|\mathbf{Z})}{S(\tau_k|\mathbf{Z})} = \frac{S(\tau_{k-1}|\mathbf{Z}) - S(\tau_k|\mathbf{Z})}{S(\tau_{k-1}|\mathbf{Z})}$$

We can get $S(\tau_k|\mathbf{Z}) = [1 - \lambda(\tau_k|\mathbf{Z})]S(\tau_{k-1}|\mathbf{Z})$ and $f(\tau_k|\mathbf{Z}) = \lambda(\tau_k|\mathbf{Z})S(\tau_{k-1}|\mathbf{Z})$. So the final expression is

$$S(\tau_k|\mathbf{Z}) = \prod_{i=1}^{k} [1 - \lambda(\tau_i|\mathbf{Z})]$$

(3)

and

$$f(\tau_k|\mathbf{Z}) = \prod_{i=1}^{k-1} [1 - \lambda(\tau_i|\mathbf{Z})]\lambda(\tau_k|\mathbf{Z})$$

(4)
For censoring time $C$, we can similarly define the probabilistic functions as

$$f_C(\tau_k | Z) = P(C = \tau_k | Z)$$

$$F_C(t | Z) = P(C \leq t | Z)$$

$$S_C(t | Z) = P(C > t | Z) = \sum_{j \mid \tau_j > t} f_C(\tau_j) = 1 - F_C(t | Z)$$

And finally we define the observed time and status as

$$T = \min(T^*, C), \Delta = I(T^* \leq C)$$

(5)

where $T$ is the random value for observed time, which is the minimum of event and censored time. $\Delta$ is the status indicator, where $\Delta = 1$ means the event time for individual is observed and known, $\Delta = 0$ means it is missing and censored time is used as the alternative. $I(\cdot)$ is the indicator function. Note that we also require $T^*$ and $C$ and independent conditional on the derived covariates $Z$, which is a common assumption in survival analysis.

Given the necessary probabilistic definitions, we can understand the data as the samples drawn from the population described by the distributions for each random variable. Suppose we have gotten the data \{Z_i, t_i, \delta_i\}_{i=1}^n with $n$ the number of observations. Then $Z_i$ is the derived covariates vector for individual $i$, $t_i \in \{\tau_1, \tau_2, \ldots, \tau_K\}$ is the observed discrete time and $\delta_i$ is the status indicator. $\delta_i = 1$ means the event time for this patient is known, then $t_i$ is the event time. $\delta_i = 0$ means the event time for this patient is unknown, then $t_i$ is the censored time.

### 3.1.2 Likelihood Function

Note that given the observed time $T = \tau_k$ with $k \in \{1, \ldots, K\}$ and the status $\Delta = \delta$ with $\delta \in \{0, 1\}$, we have

$$P(T = \tau_k, \Delta = \delta) = P(T^* = \tau_k, C \geq \tau_k)^\delta P(T^* > \tau_k, C = \tau_k)^{1-\delta}$$

$$= P(T^* = \tau_k)^\delta P(C \geq \tau_k)^\delta P(T^* > \tau_k)^{1-\delta} P(C = \tau_k)^{1-\delta}$$

$$= f(\tau_k)^\delta S(\tau_k)^{1-\delta} P(C \geq \tau_k)^\delta P(C = \tau_k)^{1-\delta}$$

(We omit the covariates $Z$ for simplicity) We want to model the event time distribution, so we delete the term $P(C \geq \tau_k)^\delta P(C = \tau_k)^{1-\delta}$ (due to random censoring) and we can write out the likelihood contribution for one individual as $f(\tau_k)^\delta S(\tau_k)^{1-\delta}$. More rigorously, suppose \{Z_i, t_i, \delta_i\} is the information for the $i$-th observation, then we can get the likelihood contribution

$$L_i = f(t_i | Z_i)^\delta S(t_i | Z_i)^{1-\delta_i}$$

And the final likelihood function for the observed data can be written as

$$L = \prod_{i=1}^n L_i = \prod_{i=1}^n f(t_i | Z_i)^{\delta_i} S(t_i | Z_i)^{1-\delta_i}$$

(6)

and the log-likelihood is

$$l = \log L = \sum_{i=1}^n \delta_i \log f(t_i | Z_i) + (1 - \delta_i) \log S(t_i | Z_i)$$

(7)

Following survival literatures, we note (6) as discrete time log-likelihood.
Moreover, combining (4) and (3) into (7), define \( T_i = \tau_j \), we can get

\[
l = \sum_{i=1}^{n} \delta_i \left( \sum_{k=1}^{j-1} \log(1 - \lambda(\tau_k | Z_i)) + \log \lambda(\tau_j | Z_i) \right) + (1 - \delta_i) \sum_{k=1}^{j} \log(1 - \lambda(\tau_k | Z_i))
\]

\[
= \sum_{i=1}^{n} \left\{ \sum_{k=1}^{j} \log(1 - \lambda(\tau_k | Z_i)) \right\} + \delta_i \log \left( \frac{\lambda(\tau_j | Z_i)}{1 - \lambda(\tau_j | Z_i)} \right)
\]

\[
= \sum_{i=1}^{n} \sum_{k=1}^{K} I(T_i \geq \tau_k) \left[ \log(1 - \lambda(\tau_k | Z_i)) + I(T_i = \tau_j, \Delta_i = 1) \log \left( \frac{\lambda(\tau_j | Z_i)}{1 - \lambda(\tau_j | Z_i)} \right) \right]
\]

where \( I(T_i = \tau_j, \Delta_i = 1) = 1 \) if \( T_i = \tau_j \) and \( \Delta_i = 1 \) both hold. In other words, this term equals to zero at any time point as long as this individual is censored (only has censored time but not event time).

At last, define \( Y_i(k) = I(T_i \geq \tau_k) \) and \( \delta_i(j) = I(T_i = \tau_j, \Delta_i = 1) \), we have the final log-likelihood function

\[
l = \sum_{i=1}^{n} \sum_{k=1}^{K} Y_i(k) \left[ \log(1 - \lambda(\tau_k | Z_i)) + \delta_i(j) \log \left( \frac{\lambda(\tau_j | Z_i)}{1 - \lambda(\tau_j | Z_i)} \right) \right]
\]

\[
(9)
\]

### 3.1.3 Likelihood Function with Prior

The likelihood function introduced above paves the way for exploiting deep learning methods to estimate unknown parameters. However, they suffer the shortage of data in many cases, which motivates us to use prior information, the information from external sources, to improve the performance of the model. In this section we introduce the likelihood function with prior that firstly proposed by [41], which is also used as the main loss function in our deep learning model. For the second way of relieving small data problem (six special designs of neural networks), see Section

Kullback-Leibler (KL) divergence is one common metric used for measuring the similarity between two probabilistic distributions. [17] mentioned firstly the connection between linear models and life tables and [17] applies the KL divergence in the Generalized Linear Model. Note that hazard function is a conditional probability in discrete time survival model, we can exploit it to compute the similarity between hazard functions for local and prior models for a given individual at a given time point. After that we can summarize over time points and observations to get an overall KL divergence. Note that we only show required formulas for support of our deep learning method and put additional explanations in the appendix, for people who are interested in more theoretical details, we refer [41] as the reference. Also, we will frequently exchange word **local** with **internal** and **prior** with **external** in this paper, we mention it here for unambiguity.

Let \( \tilde{\lambda}(\cdot) \in \mathbb{R}^{n \times K} \) be the hazard function for external model and \( \lambda(\cdot) \in \mathbb{R}^{n \times K} \) be that for internal model. They define

\[
d_k \left( \tilde{\lambda}, \lambda; Z_i \right) = \tilde{\lambda}(\tau_k | Z_i) \log \left( \frac{\tilde{\lambda}(\tau_k | Z_i)}{\lambda(\tau_k | Z_i)} \right) + \left( 1 - \tilde{\lambda}(\tau_k | Z_i) \right) \log \left( \frac{1 - \tilde{\lambda}(\tau_k | Z_i)}{1 - \lambda(\tau_k | Z_i)} \right)
\]

to be the KL divergence between two hazard functions for individual \( i \) at time \( \tau_k \), and they define the overall KL divergence to be

\[
D_{KL}(\tilde{\lambda}, \lambda) = \sum_{i=1}^{n} \sum_{k=1}^{K} Y_i(k) d_k \left( \tilde{\lambda}, \lambda; Z_i \right)
\]

By simple calculations, we can obtain

\[
D_{KL} \left( \tilde{\lambda}, \lambda \right) = -\sum_{i=1}^{n} \sum_{k=1}^{K} Y_i(k) \left[ \tilde{\lambda}(\tau_k | Z_i) \log \left( \frac{\lambda(\tau_k | Z_i)}{1 - \lambda(\tau_k | Z_i)} \right) + \log \left( 1 - \lambda(\tau_k | Z_i) \right) \right] + C
\]

7
To be more clear, $\lambda(\tau_k|Z_i)$ is the estimated hazard function with internal dataset based on external prior model at time $\tau_k$ for individual $i$. Here $C$ is the term not related to $\lambda(\tau_k|Z_i), \forall i, k$, we do not need to write out this part since only $\lambda(\cdot)$ is unknown and need to be estimated by training a neural network.

To balance the trade-off between internal and external model, we can use a hyperparameter $\eta \geq 0$ to balance the weights. More specifically, we define a penalized log-likelihood as

$$l_\eta = \frac{l - \eta D_{KL}(\tilde{\lambda}, \lambda)}{1 + \eta}$$

(10)

And our goal is to maximize it. Larger $\eta$ means more weights on minimizing $D_{KL}(\tilde{\lambda}, \lambda)$, and lower value means less difference between $\tilde{\lambda}$ and $\lambda$. In that case model will tend to believe more on prior information and similarly, smaller $\eta$ means model will put more weights on the discrete time log-likelihood.

Note that (10) can be rewritten as

$$l_\eta = \sum_{i=1}^{n} \sum_{k=1}^{K} Y_l(k) \left[ \frac{\delta_l(j) + \eta \tilde{\lambda}(\tau_k|Z_i)}{1 + \eta} \log \left\{ \frac{\lambda(\tau_k|Z_i)}{1 - \lambda(\tau_k|Z_i)} \right\} + \log \{1 - \lambda(\tau_k|Z_i)\} \right]$$

(11)

which is the final loss function used for training our deep learning model. Note that $\lambda(\tau_k|Z_i)$, the hazard value at time $k$ for the $i$-th individual, is the parameter that required estimation. So there are altogether $nK$ unknown values in this function.

In our model, the negative likelihood function ($-l$) is taken as the loss function and our goal is to optimize the loss function with deep learning. More details will be introduced later.

### 3.1.4 Computational Advantage in Implementation

Although our model training procedure described above seems hard to implement in practice due to the requirement of using chain rule to compute the gradient, we can apply one computational advantage, which makes it much easier for us to implement this algorithm. In details, we can use the same form of log-likelihood function to unify formula (9) and (11). Define

$$l_{all}(\theta, p) = \sum_{i=1}^{n} \sum_{k=1}^{K} Y_l(k) \left\{ \{p(\tau_k|Z_i) \log \{\lambda(\tau_k|Z_i)\}\} + (1 - p(\tau_k|Z_i)) \log \{1 - \lambda(\tau_k|Z_i)\} \right\}$$

be the form of the log-likelihood functions introduced before with $\theta$ all unknown parameters in the model and $p = \{p(\tau_k|Z_i)\}_{i,k} \in \mathbb{R}^{n \times K}$. It is easy to see that $l(\theta) = l_{all}(\theta, \delta)$ and $l_\eta(\theta) = l_{all}(\theta, \delta + \eta \tilde{\lambda})$, where $\delta = \{\delta_l(k)\}_{i,k} \in \mathbb{R}^{n \times K}$. Since $p$ has no unknown values in both loss functions, for each batch-training step, we can pre-compute $p$ and pass the results into the loss function. Due to this finding, we only need to add one new class for our loss function and pass one additional input parameter matrix $(p(k|x_i), \forall i, k)$ into the loss function method, holding other modules unchanged. In this way all computational advantages mentioned in LogisticHazard [20] (pycox) can be smoothly transplanted into our model instead of coding from scratch, with a minor additional memory occupation.

### 3.1.5 Discussion: What is Prior Information?

#### 3.2 Deep Learning: What and How?

##### 3.2.1 What is Deep Learning?

Although the idea for combining prior information in loss function comes from [41], it still assumes a statistical assumption for the hazard function, which is $\lambda(t_k; Z_i) = g(\gamma_k + Z_i^T \beta)$ with $g(u) = h^{-1}(u)$ and
h(u) being our interest, a monotonically increasing and twice differentiable link function. The linear form of \( \beta, \gamma \) and \( Z \) can be too restrictive in many cases, and deep learning is a natural way of modeling non-linear relationships between the covariates and the outcome of interest.

Deep learning is also named as neural network training, which is renowned for its ability to approximate a large amount of functions. Mathematically, a neural network is to find a functional approximation between input and output. The inner architecture of a neural network (also known as computational graph) can simulate basic mathematical operations such as add, multiply, nesting of functions and non-linear transformations, leading to really complex functions by combining these elements. For example:

- A one-layer neural network with an identity activation function can be used to simulate a linear model
  \[
y = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p.
\]
- A one-layer neural network with a sigmoid activation function can be used to simulate a GLM with logistic link: \( \logit(y) = \beta_0 + \beta_1 x_1 + \ldots + \beta_p x_p \).
- A three-layer neural network is equivalent to defining \( \lambda(\cdot; \phi) = f_3(f_2(f_1(\cdot))) \) with \( f_1, f_2, f_3 \) three arbitrary and learnable functions [22].

The first two examples show that linear models and GLM with logistic link function can be covered by a one-layer fully-connected feedforward neural network with or without sigmoid activation function added into the final layer, respectively. For the structure of neural network, the first layer takes the input value, and the output of each layer will be used as the input of the next layer. Mathematically, suppose that we have a \( l \)-layer fully-connected feed-forward neural network with \( \{h_1, h_2, \ldots, h_{l-1}\} \) pre-defined numbers of nodes for each hidden layer (The number of nodes for input layer and output layer are fixed and they depend on the data and the value of interest, we define them as \( h_0 \) and \( h_l \), respectively, for unification) and \( \{s^{(1)}, s^{(2)}, \ldots, s^{(l)}\} \) activation functions for each layer, then the formula for the \( i \)-th individual can be written as

\[
\begin{align*}
Z_i^{(1)} &= f^{(1)}(Z_i) = s^{(1)}(W^{(1)}Z_i + b^{(1)}) \\
Z_i^{(2)} &= f^{(2)}(Z_i^{(1)}) = s^{(2)}(W^{(2)}Z_i^{(1)} + b^{(2)}) \\
Z_i^{(3)} &= f^{(3)}(Z_i^{(2)}) = s^{(3)}(W^{(3)}Z_i^{(2)} + b^{(3)}) \\
& \quad \ldots \\
Z_i^{(l)} &= f^{(l)}(Z_i^{(l-1)}) = s^{(l)}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \\
l_i &= r(Z_i^{(l)})
\end{align*}
\]

where \( Z_i^{(m)} \in \mathbb{R}^{h_m}, m = 0, 1, \ldots, l \) is the input of the \( m \)-th layer with \( h_m \) defined as the number of dimensions for the input of the \( m \)-th layer. We also assume \( Z_i^{(0)} = Z_i \) and \( h_0 = p \) the dimension of \( Z_i \) without loss of generality. \( f^{(m)} : \mathbb{R}^{h_{m-1}} \rightarrow \mathbb{R}^{h_m} \) is the transformation function for the \( m \)-th layer. \( W^{(m)}Z^{(m)} + b^{(m)} \) is the linear combination term with \( W^{(m)} \in \mathbb{R}^{h_m \times h_{m-1}}, b^{(m)} \in \mathbb{R}^{h_m} \) as the unknown parameters require learning, \( s^{(m)} \) is the activation function such as identity, sigmoid or ReLU function operating element-wise (the function will be operated on each element of the input vector and give an output vector with the same size, same for below). \( r(Z_i^{(l)}) \) is a function of \( Z_i^{(l)} \) and \( l_i \) is the final value and usually the loss function. For this model, \( \{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \ldots, W^{(l)}, b^{(l)}\} \) are unknown parameters requiring estimation and there are altogether \( \sum_{k=1}^l h_k(h_{k-1} + 1) \) unknown values, a linear function with respect to \( h_i, i = 0, 1, \ldots, l \).

In our paper, we model the hazard function \( \lambda_i, i = 1, 2, \ldots, n \) by a neural network, which means for the \( i \)-th observation, we will take its derived covariates \( Z_i \) as input, and take the output vector of the neural network as the estimated hazard value. Mathematically, we want to use neural network to model a function \( g(\theta) : \mathbb{R}^p \rightarrow \mathbb{R}^K \) where \( p \) is the dimension of \( Z_i \) and \( K \) means the number of time intervals, \( \theta \) is the set of
unknown parameters \( \{W^{(1)}, b^{(1)}, W^{(2)}, b^{(2)}, \ldots\} \) require learning. If we want to use fully-connected neural network, then the formula can be written as (12) but with the last two equations changing as

\[
\begin{align*}
\lambda_i &= f^{(l)}(Z_i^{(l-1)}) = s^{(l)}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \\
l_i &= r(\lambda_i)
\end{align*}
\]

and it has a one-to-one correlation with the series of pre-defined hyperparameters, such as number of layers, number of hidden units for each layer, activation function and so on.

**Remark** As a side note, fully-connected feedforward neural network is flexible enough to model structured data such as clinical data. Nevertheless, it is inconvenient to model unstructured data (image, text) using this structure. In that case, the linear combination term \( W^{(l)}Z_i^{(l)} + b^{(l)} \) can also be changed to adapt to different data structures. For example, in Convolutional Neural Network (CNN), the connection between input and weight is not fully-connected, but focusing on a 'local patch' of the data. This is mainly used in image data, where the 'local patch' structure is extremely significant for data analysis. Although the combination of \( W, Z_i \) and \( b \) will be slightly different for other structures such as CNN, fully-connected feedforward neural network is flexible enough to tackle with the survival data. Moreover, as we will also see later, this has little effect on the training process of neural network, so we will assume our model of interested to be fully-connected feed-forward neural network except for extra mentioning.

### 3.2.2 How to Use Deep Learning

The way for training a neural network is the same as machine learning, which lies in the field of optimization, minimizing/maximizing a loss function computed by data by iteratively computing the value and gradient (for some algorithms, Hessian is also required) of the loss function and then updating the unknown parameters by optimization algorithms such as gradient descent or Newton method until convergence. In Deep Learning, computing the value and gradient can be done by forward and backward propagation efficiently and exactly [28], especially at the time when Graphical Processing Unit (GPU) can be used for dramatically accelerating of the deep learning model by parallel computing. We only introduce the main ideas of forward and backward propagation in the main part, but leave some technical details into Appendix.

For forward propagation, it means passing the input vector of each individual \( Z_i \) to get the values of each layer \( \{Z_i^{(1)}, Z_i^{(2)}, \ldots, Z_i^{(l)}\} \) and the value of loss function \( l_i \) following (12) given the values of \( \{W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}\} \). In this step we can get all necessary values for each layer. For backward propagation, we use the values computed by forward propagation to obtain the gradients with respect to unknown parameters \( \{W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}\} \). Note that for forward propagation, we will firstly use \( W^{(1)}, b^{(1)} \) for calculation and then use \( W^{(2)}, b^{(2)} \) until \( W^{(l)}, b^{(l)} \). But for backward propagation, the gradient with respect to \( W^{(l)}, b^{(l)} \) will be firstly obtained, and then \( W^{(l-1)}, b^{(l-1)} \) until \( W^{(1)}, b^{(1)} \). On a computational graph, the backward propagation behaves like computing from the output layer to the input layer, just the opposite direction of the forward propagation. Therefore for the calculation of gradients in a neural network, it is also called "backward" propagation.

After obtaining the function values and gradients, neural network can obtain the next update for each unknown parameter by gradient descent based optimization algorithms. In our model, we would like to use Mini-batch method as the optimization algorithm, which means we only need to compute the function values (obtained by forward propagation) and the gradients of each parameter (obtained by backward propagation) for a small batch of training set. Mathematically, suppose that \( \alpha \) is the parameter we would like to update, \( b \) is the batch size, \( \{l_1, l_2, \ldots, l_b\} \) are the loss functions obtained by \( b \) individuals in that batch.

---

3 To be more clear, we give another set of indices for the observations of that batch sampled from the original dataset, which means they do not necessarily need to be the first \( b \) samples.
each step, we can write the update formula as

$$\alpha' = \text{Optim}(\alpha, \frac{1}{b} \sum_{k=1}^{b} \frac{\partial l_k}{\partial \alpha})$$

and usually $b$ is the hyperparameter requires tuning. Optim can be SGD [36], Adam, AdamW [23] and RMS-Prop [40]. In implementation, we only provide the last 3 advanced optimizers for options in hyperparameter tuning since SGD will provide much inferior result compared with the other three optimizers.

The reason for using Mini-batch training is twofold: Firstly, it is difficult to fit the large dataset into the memory, making the normal gradient descent infeasible. Even if the data can be fit into the memory, this method can also fall into local minima easily [5] for deep learning. Secondly, SGD suffers from a high variance, which leads to a high fluctuation especially when the algorithm is close to the convergence. Mini-batch training can reduce the variance and relieve this situation.

In summary, the training procedure for our model can be described as follows:

**Algorithm 1 Training Procedure of Neural Network**

**Require:** Dataset ($\{Z_1, \ldots, Z_n\}$), Neural Network with Initial Value $\{W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}\}$, Batch Size $b$

while Stopping criteria meets do

Sample out $b$ individuals.

**Forward Propagation:** Compute $\{l_1, \ldots, l_b\}$ with $\{W^{(1)}, b^{(1)}, \ldots, W^{(l)}, b^{(l)}\}$ following (12).

**Backward Propagation:** Compute $\frac{\partial l_i}{\partial W_j}$ and $\frac{\partial l_i}{\partial b_j}$ for each $i = 1, 2, \ldots, b$ and $j = 1, 2, \ldots, l$.

Update the parameters $W_j$ with $W_j'$ and approximated gradient $\frac{1}{b} \sum_{i=1}^{b} \frac{\partial l_i}{\partial W_j}$, similarly for $b_j$. This means

$$W_j' = \text{Optim}(W_j, \frac{1}{b} \sum_{i=1}^{b} \frac{\partial l_i}{\partial W_j}), b_j' = \text{Optim}(b_j, \frac{1}{b} \sum_{i=1}^{b} \frac{\partial l_i}{\partial b_j})$$

with Optim be Adam, AdamW or RMSProp.

$W_j = W_j', b_j = b_j', \forall j = 1, \ldots, l$

end while

Note that in our simulation and real data experiments, we stop the algorithm based on early stopping, which means we will split the training data into 'true' training data used for model training and validation data. After each iteration, we will compute the loss based on validation data and if the loss does not decrease after several iterations, we stop the algorithm. It is called early stopping since the model may not meet the convergence criteria, but it is one really common trick in machine learning community and its goal is to prevent overfitting.

Last but not least, hyperparameter tuning is required in deep learning since each set of hyperparameters uniquely define a structure of neural network and there is no theoretical guarantee that which set of hyperparameters is the best for different tasks (similar as 'no free lunch theorem' [37]). For saving time we narrow down the range of tuning for each hyperparameter based on our experiments and we put the main technical details and results in the Appendix. Here are some take-away recommendations.

1. Batch size $b$ should be tuned in the range of 0.1% to 5% of the data size.

2. No significant difference in three optimizers (RMSProp, Adam, AdamW) with default values of parameters recommended in Pytorch.

3. Dropout Rate can be chosen between 0 and 0.25.
4. Learning Rate can be chosen from 0.0001 to 0.05.

We also put them into our software for the sake of users.

3.2.3 Six Designs for Proportional Hazards Assumption and Three Link Functions

Deep learning is renowned for its extraordinary results in many tasks, including survival data analysis. However, this may lead to over-parameterization problem, which means the number of unknown parameters is too high compared with the size of data. In that case, training with neural network with few restrictions may provide in contrast worse results compared with other statistical or machine learning algorithms. Also, when the data is observed to have some desired statistical properties, it is also not wise to directly use deep learning for model training, but not consider mature statistical models.

In this part, we design 6 neural networks adapting to different demands. We provide options for modeling proportional and non-proportional data\(^4\) and also three link functions, combining them to get altogether 6 designs.

In general, discrete time model can be unified as

\[
h[\lambda(t|Z)] = h[\lambda_0(t)] + Z'\beta
\]

where \(h\) is a monotone-increasing and twice-differentiable function mapping \([0, 1]\) into \([-\infty, \infty]\) with \(h(0) = -\infty\). Then if \(h(u) = \log(-\log(1-u))\), we have the grouped relative risk model \([19]\). If \(h(u) = \log u\), we have the discrete relative risk model \([34]\). If \(h(u) = \log u/(1-u)\), we have the discrete logistic model \([7]\). Thanks to \([13]\) we can specially define the last layer and simply change the form of function \(h(\cdot)\). To be more clear, for proportional version, the second last hidden layer will be fully connected with the final hidden layer, which is a scalar and shows the total effect of derived covariates. Then the final hidden layer will be fully connected with the output layer, with edges the baseline hazard values for each time point and the connection for the last two layer is specially defined, depending on \(h(\cdot)\). The formula of neural network for proportional data follows \([12]\) but with the last two equations changing as

\[
Z^{(l)}_i = f^{(l)}(Z^{(l-1)}_i) = w^{(l)} Z^{(l-1)}_i
\]

\[
h(\lambda_i) = h(\sigma(w^{(l+1)})) + Z^{(l)}_i
\]

\[
l_i = r(\lambda_i)
\]

and \(w^{(l)} \in \mathbb{R}^{h_{l-1}}\), \(w^{(l+1)} \in \mathbb{R}^K\) and \(\sigma(x) = \frac{1}{1+e^{-x}}\) is the sigmoid activation function, \(Z^{(l)}_i \in \mathbb{R}^K\) is the vector with all values the same as \(Z^{(l)}_i\). Note that \(\sigma(w^{(l+1)})\) simulates the baseline hazard value at each time point. We put on a sigmoid function on the initial weights \(w^{(l+1)}\) since the baseline hazard value belongs in the range \([0, 1]\) and sigmoid function is a one-to-one mapping, which means each distinct value of \(w^{(l+1)}\) will lead to one unique value of baseline hazard for each time point.

For modeling non-proportional data, the structure does not require special design. Figure \([1]\) provides a comparison. For the normal design (which is also model designed for non-proportional model), the edges between the final hidden layer and the output layer are different for hazard values at different time points, which means the weights between the last two layers are time-dependent. Mathematically, we can write the formula for the last two layers as

\[
\lambda_i(\tau_k) = w^{(l+1)}(\tau_k)_i Z^{(l-1)}_i, k = 1, \ldots, K
\]

\(^4\)Actually, the proportional design will not simulate a model that follows proportional hazard assumption when the derived covariates for one patient are time-dependent.
where $\lambda_i = (\lambda_i(t_1), \ldots, \lambda_i(t_K))^\top$ and $W^{(l)} = (w(t_1), \ldots, w(t_K))^\top$. It is obvious that $w(t_k)$ is a time-dependent coefficients operating on $Z_i^{(l-1)}$ and this ensures that the model itself will be non-proportional.

3.3 Extension: Competing Risk Setting

Competing Risk Problem focuses on the case when we not only want to model the event time, but also the cause that lead to the event. For example, people suffering from cancers usually have co-morbidities, such as cardiovascular disease. Although the competing risk problem is regarded really challenging in survival analysis, our model can solve the discrete competing risk problem just by a simple extension of the activation function. We noticed that [30] is the first paper using deep learning to solve competing risk problem in discrete time model to the best of our knowledge. However, it models the PMF for each cause at each time point, but not the hazard function. In other words, our model is the first to model hazard function with neural network for solving competing risk problem in discrete time model. We also included the option for solving competing risk problem in our software.

In this section, we will introduce the theoretical guarantees for our extension. Since some of the formulas can be transferred directly from previous sections, we only introduce new notations and refer readers to the previous equations for old ones.

3.3.1 Notations

Compared with single-risk (simpler case that introduced in Section 3.1) case, here we define the cause-specific hazard function resulting from cause $r$ as

$$\lambda_r(t_k|Z) = P(T^* = t_k, R = r | T^* \geq t_k, Z)$$

where $r \in \{1, 2, \ldots, q\}$ means the number of causes for the event and we assume there are altogether $q$ causes. The overall hazard function is defined as

$$\lambda(t_k|Z) = \sum_{r=1}^{q} \lambda_r(t_k|Z) = P(T^* = t_k | T^* \geq t_k, Z)$$

Figure 1: Comparison between proportional and non-proportional designs
and the formula for the survival function $S(t|\mathbf{Z})$ and the probability density function $f(\tau_k|\mathbf{Z})$ can be obtained with the same expression but different meaning of $\lambda(\tau_k|\mathbf{Z})$. One difference is

$$f_r(\tau_k|\mathbf{Z}) = P(T^* = \tau_k, R = r \mid \mathbf{Z}) = \lambda_r(\tau_k|\mathbf{Z}) \prod_{i=1}^{k-1} (1 - \lambda(\tau_i|\mathbf{Z}))$$  \hspace{1cm} (16)$$

As for the likelihood function, suppose for the $i$-th individual, we have $\{\mathbf{Z}_i, t_i, r_i, \delta_i\}$ as the information and $t_i = \tau_k$, then similarly we can define the likelihood contribution from individual $i$ as

$$L_i = P(T^*_i = t_i, R_i = r_i)^{\delta_i} P(T^*_i > t_i)^{1-\delta_i} P(C_i \geq t_i)^{\delta_i} P(C_i = t_i)^{1-\delta_i}$$

$$= f_{r_i}(t_i)^{\delta_i} S(t_i)^{1-\delta_i} = \lambda_{r_i} (\tau_k|\mathbf{Z}_i)^{\delta_i} (1 - \lambda(\tau_k|\mathbf{Z}_i))^{1-\delta_i} \prod_{j=1}^{k-1} (1 - \lambda(\tau_j|\mathbf{Z}_i))$$  \hspace{1cm} (17)$$

Take the logarithm and combining the log-likelihood for each observation, define $t_i = \tau_j$ we can get the final log-likelihood function

$$l = \sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{q} \mathcal{Y}_i(k) \left[ \log(1 - \lambda(\tau_k|\mathbf{Z}_i)) + \delta_i(j) \log \frac{\lambda_{r_i}(\tau_j|\mathbf{Z}_i)}{1 - \lambda(\tau_j|\mathbf{Z}_i)} \right]$$

$$= \sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{q} \mathcal{Y}_i(k) \left[ \log(1 - \lambda(\tau_k|\mathbf{Z}_i)) + \sum_{r=1}^{q} \delta_i^r(j) \log \frac{\lambda_r(\tau_j|\mathbf{Z}_i)}{1 - \lambda(\tau_j|\mathbf{Z}_i)} \right]$$  \hspace{1cm} (18)$$

where we define $\delta_i^r(j) = I(T_i = j, R_i = r, \Delta_i = 1)$.

For the KL divergence, we follow [41] but make the extension from single-risk to competing risk, we define

$$d_k(\tilde{\lambda}, \lambda; \mathbf{Z}_i) = \sum_{r=1}^{q} \lambda_r(\tau_k|\mathbf{Z}_i) \log \left\{ \frac{\tilde{\lambda}_r(\tau_k|\mathbf{Z}_i)}{\lambda_r(\tau_k|\mathbf{Z}_i)} \right\} + \left\{ 1 - \tilde{\lambda}(\tau_k|\mathbf{Z}_i) \right\} \log \left\{ \frac{1 - \tilde{\lambda}(\tau_k|\mathbf{Z}_i)}{1 - \lambda(\tau_k|\mathbf{Z}_i)} \right\}$$

Then we can get

$$D_{KL}(\tilde{\lambda}, \lambda) = -\sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{q} \mathcal{Y}_i(k) \left[ \sum_{r=1}^{q} \lambda_r(\tau_k|\mathbf{Z}_i) \log \left\{ \lambda_r(\tau_k|\mathbf{Z}_i) \right\} + (1 - \tilde{\lambda}(\tau_k|\mathbf{Z}_i)) \log \left\{ 1 - \lambda(\tau_k|\mathbf{Z}_i) \right\} \right] + C$$

$$= -\sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{q} \mathcal{Y}_i(k) \left[ \sum_{r=1}^{q} \lambda_r(\tau_k|\mathbf{Z}_i) \log \left\{ \frac{\lambda_r(\tau_k|\mathbf{Z}_i)}{1 - \lambda(\tau_k|\mathbf{Z}_i)} \right\} + \log \left\{ 1 - \lambda(\tau_k|\mathbf{Z}_i) \right\} \right] + C$$

by noting that $\sum_{r=1}^{q} \lambda_r(\tau_k|\mathbf{Z}_i) = \tilde{\lambda}(\tau_k|\mathbf{Z}_i)$. Define $l_\eta = \frac{l - \eta D_{KL}(\tilde{\lambda}, \lambda)}{1 + \eta}$, we have

$$l_\eta = \sum_{i=1}^{n} \sum_{k=1}^{K} \sum_{r=1}^{q} \mathcal{Y}_i(k) \left[ \log(1 - \lambda(\tau_k|\mathbf{Z}_i)) + \sum_{r=1}^{q} \delta_i^r(j) \log \frac{\lambda_r(\tau_j|\mathbf{Z}_i)}{1 - \lambda(\tau_j|\mathbf{Z}_i)} \right]$$  \hspace{1cm} (19)$$

One question is to get $\tilde{\lambda}_r(\tau_k|\mathbf{Z}_i), \forall r$ at time point $k$ for the individual $i$. However this can be implemented easily by setting the activation function of the output layer as softmax function. More detailedly, instead of providing one node for each time point $k$ and individual $i$, we provide $q$ nodes and each node value is an estimation of cause-specific hazard value. The formula can also be written as [12] but with the last two equations changing as

$$\mathbf{\lambda}_i = f^{(l)}(\mathbf{Z}_i^{(l-1)}) = \text{MarginalSoftmax}(W^{(l)} \mathbf{Z}_i^{(l-1)} + b^{(l)})$$

$$l_i = r(\mathbf{\lambda}_i)$$
where the dimension of $\lambda_i$ will be changed from $K$ to $qK$ (which means $W^{(l)} \in \mathbb{R}^{qK \times h_{l-1}}$ and $b^{(l)} \in \mathbb{R}^{qK}$), and MarginalSoftmax will provide a transformation from $W^{(l)}Z_i^{(l-1)} + b^{(l)} \in \mathbb{R}^{qK}$ to $\lambda_i' \in \mathbb{R}^{K \times q}$ with each row of the new matrix the values for cause-specific hazard function. Then a softmax function will be operated on each row to get the final results. Mathematically, suppose $\lambda_{ki} \in \mathbb{R}^q$ is the $k$-th row for $\lambda_i$, then

$$
\lambda_{kij} = \frac{e^{\lambda_{ki}^j}}{\sum_{j=1}^q e^{\lambda_{ki}^j}}, \quad j = 1, 2, \ldots, q
$$

which is the formula of softmax function and $\lambda_{kij}$ and $\lambda_{ki}^j$ mean the $j$-th element of $\lambda_{ki}$, $\lambda_i$, respectively. After that the matrix will be changed back to a vector with dimension $qK$ without changing of meaning for each coordinate.

In summary, changing from sigmoid to softmax function means a generalization from binomial model to multinomial model, and softmax function corresponds to a multinomial logit function.

4 Simulations

In this section, we design various simulation settings for different goals. Firstly, we want to show that our model can perform better than other models when the quality of prior information is high, while when the quality of prior information is low, our model can at least obtain similar results compared with other models, since in this case, prior information can barely help improve the performance and robustness of the model. Secondly, we want to show that properties of deep learning still preserve and our model can obtain better results with the aid of suitable prior information. This can be done by simulating a non-linear and non-proportional dataset for the experiment. Our third goal is an extension, we observed that in real clinical cases, images are really important for experts to find out potential diseases. Based on this observation, we use MNIST [29], a fundamental imaging dataset in Artificial Intelligence, to design a clinical trial dataset for training, our goal is to show that Convolutional Neural Network (CNN) can be successfully applied in our model, demonstrating that our model has a huge potential to apply on unstructured data.

4.1 Simulation Settings

4.1.1 Simulation 1

In this experiment, we generate data with non-linear relationship between covariates and targets. Moreover, Part of the covariates are function of time, which means the proportional hazard assumption does not hold in this dataset. The goal for this simulation is to show that the ability for modeling non-linear and non-proportional data still exists in our model.

The form of the hazard function in this setting is given as

$$
h(t|x) = h_0(x) \exp(g(t, x))
$$

where $g(t, x) = a(x) + b(x)t$ and

$$
a(x) = \text{sign}(x_2) + 0.44x_0 + 0.66x_1 + 0.88x_2 + \frac{2}{3}(x_0^2 + x_2^2 + x_0x_1 + 2x_1x_2)
$$
$$
b(x) = |0.2(x_0 + x_1) + 0.5x_0x_1|
$$

In this simulation, we experiment with 3 models (Maybe 4 will be better): Cox model with proportional hazard assumption, LogisticHazard and our model. The event time is grouped with 20 time intervals and We want to show that LogisticHazard can achieve much better result compared with Cox model due to the
flexibility of deep learning model, and our model can still get a better result compared with LogisticHazard when using prior information.

Additionally, we will generate 10000 observations with given model assumptions, where 95% of the data will be used as external data and the remaining 5% will be used as internal data. For the existing models, only internal data will be available. While for our models, we will use LogisticHazard to train prior model (i.e. to get \( \hat{\lambda}(t_k, Z_i), \forall i, k \)) and apply the prior information into the local data in our model.

### 4.1.2 Simulation 3

In this experiment, we use MNIST, a well-known imaging dataset, to simulate the time and event status. We want to show that more advanced structures, such as Convolutional Neural Network (CNN), can also be used in our model for extracting information from imaging data. This is meaningful since there exist many real applications relying on imaging data, such as using using deep learning for tumor detection and so on.

MNIST is an imaging dataset with each image a \( 28 \times 28 \) handwritten-digit, which has a training set of 60000 examples and a test set of 10000 examples. Each image represents a digit and the event time will be generated based on the digit. More specifically, we define the event time to follow an exponential distribution \( t \sim \exp(\alpha) \) (which means the density function is \( f(x; \alpha) = \frac{1}{\alpha} e^{-x/\alpha} \)) with \( \alpha \) given as

\[
\alpha(\text{digit}) = \frac{365 \cdot \exp(-0.6 \cdot \text{digit})}{\log(1.2)}
\]

And the data is right-censored with a manually set threshold, which means the individual whose survival time is greater than the given threshold will be marked as censored and the event of time will be changed to that threshold.

In this setting, we sample 30000 images from the training dataset for saving time. The model training procedure is the same as what in simulation 2-1.

In summary, for each individual, the covariates are pixels of the image, the event time is generated by an exponential distribution defined above, and observations will be marked as censored when the time is greater than a given threshold.

### 4.2 Evaluation Metrics

Three metrics are used for evaluating discrete time survival model and each of them focuses on slightly different aspects of the model.

**Time Dependent Concordance Index** Concordance Index (C-index) [14] is a discriminative evaluation metric used in survival analysis and it comes from the concept of Area Under Curve (AUC), the metric used in machine learning for measuring discriminative ability of the model. Since deep learning is mainly proposed for modeling non-proportional data, C-index measured at a given time point may not provide an overall picture of the discriminative ability of the survival model, so in this experiment, we use the version of C-index in [3], to use the inverse probability weighted time dependent C-index combining the C-index measured at all possible event time points, which is

\[
C^{td} = \frac{\sum_{i: \Delta_i=1} \sum_{j: t_i < t_j} I \left( \hat{S}_{Z_i}(t_i) < \hat{S}_{Z_j}(t_j) \right) / \hat{G}^2(t_i)}{\sum_{i: \delta_i=1} \sum_{j: t_i < t_j} 1 / \hat{G}^2(t_i)} \tag{23}
\]

where \( Z_i, t_i, \delta_i \) are covariates, observed time and the indicator of event/censoring for observation \( i \). \( \hat{S}_{Z_i}(t_i) \) is the predicted survival function and \( \hat{G}(t) \) is the Kaplan-Meier (KM) estimator for the survival function of the censoring time. Note that under the independence assumption of censoring and event time, we have \( C^{td} \sim P(S_{Z_i}(T) < S_{Z_j}(T) \mid T_i < T_j) \) and higher \( C^{td} \) means better model.
**Integrated Brier Score**  Brier Score (BS) measures calibration and discriminative performance simultaneously since it can be decomposed into two terms measuring these two aspects respectively. It follows the idea of Mean Squared Error (MSE) and the formula for BS is defined as

\[
BS(t) = \frac{1}{n} \sum_{i=1}^{n} \left\{ \left( \frac{\hat{S}_{Z_i}(t)}{\hat{G}(t_i)} \right)^2 I(t_i \leq t, \delta_i = 1) + \left( \frac{1 - \hat{S}_{Z_i}(t)}{\hat{G}(t)} \right)^2 I(t_i > t) \right\}
\]

(24)

where \( n \) is the number of observations and the other notations are the same as (23). The Integrated Brier Score (IBS) \[12\] is defined as an integration of the Brier Score in the time interval, which is defined as

\[
IBS = \frac{1}{t_{\text{max}} - t_{\text{min}}} \int_{t_{\text{min}}}^{t_{\text{max}}} BS(t) \, dt
\]

(25)

And for IBS, we will firstly use the two interpolation schemes (CDI, CHI \[26\]) to transfer the survival function trained for discrete time model to continuous time and then define a fine grid of time points to compute the IBS. The integral will be approximated by numerical integration. Lower IBS means better result.

**Integrated Binomial Log Likelihood** This metric is also proposed in \[12\] and is very similar to IBS, which also focuses both calibration and discriminative performance of the model. The definition of Binomial Log Likelihood (BLL) is

\[
BLL(t) = \frac{1}{n} \sum_{i=1}^{n} \left\{ \log \left( \frac{1 - \hat{S}_{Z_i}(t)}{\hat{G}(t_i)} \right) I(t_i \leq t, \delta_i = 1) + \log \left( \frac{\hat{S}_{Z_i}(t)}{\hat{G}(t)} \right) I(t_i > t) \right\}
\]

(26)

and Integrated Negative Binomial Log Likelihood (INBLL) is defined as

\[
\text{INBLL} = -\frac{1}{t_{\text{max}} - t_{\text{min}}} \int_{t_{\text{min}}}^{t_{\text{max}}} BLL(t) \, dt
\]

(27)

and the notations are the same as what in IBS. Note that compared with IBS, it penalizes the error with the scale \(-\log(1 - x)\), which will lead to more penalization for larger magnitude of error. Lower INBLL means better model.

### 4.3 Results

#### 4.3.1 Simulation 1

In our project, we compete with LogisticHazard \[11\] \[26\]. 50 sets of internal data and 1 set of external data are generated in our model, which means all sets of internal data share the same prior information. The hyperparameter \( \eta \) for our model is tuned by 5-fold cross validation, where for each fold, 80% of the data will be sampled out for training and 20% for validation, with IBS as the selection criteria. After \( \eta \) is determined, we compute the prior information and both models will be trained with only local data, where 20% of the data is sampled as test data, and in the remaining 80% of the data, 80% will be used for training model and 20% is used for validation. Early Stopping is adopted with patience 5 and the stopping criteria is the loss function (??)

For neural network structures, we set a fully-connected neural network with two hidden layers. Each layer has 32 hidden nodes equipped with ReLU \[2\] activation function to prevent gradient vanishing, the dropout rate is set to be 0.1 and batch normalization \[15\] is used in each layer. The optimizer is chosen to
be Adam [23] with two parameters set for two momentum values default as 0.9 and 0.999. The learning rate is set to be 0.01 and the batch size for training is set to be 20 due to the small size of training data. Note that for both models, the parameters are set to be the same for fairness.

Figure 2 to 6 have shown the results for different schemes when using 3 different metrics, where for IBS and IBLL, we divide the time as 100 time intervals with equal length. Significant improvement in average performance and robustness is shown in experiment results. Note that for figure 4 and figure 5 (scheme 3 and scheme 5), our model does not perform better than existing model, it is reasonable because in these 2 cases, the external data has information that far different from local and true model (with correct day effects and 10 covariate effects), leading to $\eta$ be near 0. Note that for figure 5 (scheme 4), our model performs really well, this is because the magnitude of loss does not differ a lot compared with scheme 5, which means the noise does not corrupt the prior data too much. In real cases this is significant since this shows that our model can not only behave better with high quality of prior information, but also can be used to identify the quality of prior data when we would like to apply prior information with unknown quality.

![Figure 2: Results for Scheme 1](image1)

![Figure 3: Results for Scheme 2](image2)

4.3.2 Simulation 2-1

For this experiment, we compete our model with Cox model and LogisticHazard. For our model, the hyperparameter tuning procedure, the model parameters and the data splitting rules are the same as what in Simulation 1.

Figure 7 has shown the comparison results with respect to 3 different metrics. For Cox model, it does not perform really well compared with the other two models since Cox model cannot deal with non-linear and non-proportional data really well, which is one advantage of Deep Learning. For the other two models, our
Figure 4: Results for Scheme 3

Figure 5: Results for Scheme 4

Figure 6: Results for Scheme 5
model performs slightly better than LogisticHazard, which makes sense due to the aid of prior information in our model.

Figure 7: Results for Simulation 2-1

4.3.3 Simulation 2

In this experiment, we compare our models with LogisticHazard, but with varied ratio of local data. We try 3 ratios, \{2\%, 5\%, 10\%\} (which means a given ratio of data will be sampled out as internal data) and run 50 experiments with hyperparameter tuning and data splitting the same as what applied in Simulation 1. The model structures are summarized in figure 7. We train with Adam optimizer with two parameters for moments fixed as default values (0.9 and 0.999 described before), the learning rate is set as constant 0.005. We also apply early stopping with patience 10. The maximum number of training epoch is set to be 100 for saving time. We also use GPU in this model for accelerating training of Convolutional Neural Network, which can be easily done with torch.tuple.

| Layer | Name          | Kernel Size | Stride | # of Channels | Input Size  | Output Size   |
|-------|---------------|-------------|--------|---------------|-------------|---------------|
| 1     | Conv2d        | 5 × 5       | 1 × 1  | 16            | 1 × 28 × 28 | 16 × 24 × 24  |
| 2     | MaxPool2d     | 2 × 2       | 2      |               | 16 × 24 × 24| 16 × 12 × 12  |
| 3     | Conv2d        | 5 × 5       | 1 × 1  | 16            | 16 × 12 × 12| 16 × 8 × 8    |
| 4     | AdaAvgPool2d  | 8 × 8       | 8      |               | 16 × 8 × 8  | 16 × 1 × 1    |
|       | Flatten       |             |        |               | 16 × 1 × 1  | 16            |
| 5     | Linear        |             |        |               | 16           | 16            |
| 6     | Linear        |             |        |               | 16           | 20            |

Table 1: Neural Network Structure Used in Simulation 3

The results are shown below and the stability is significantly improved with the amount of internal data increasing. Meanwhile, our model performs better when IBS is used as the evaluation criteria.

5 Real Data Analysis

In this section, we apply our method on 3 real datasets, which are the Study to Understand Prognoses Preferences Outcomes and Risks of Treatment (SUPPORT), the Molecular Taxonomy of Breast Cancer International Consortium (METABRIC) and Medical Information Mart for Intensive Care III (MIMIC-III). Note that the covariates of each dataset have different properties that require processing by neural network, which provides with space for us to demonstrate some advanced usages of neural network architectures in our model.
5.1 Information of the datasets

**SUPPORT** SUPPORT dataset is a large study focusing on the survival time of seriously ill hospitalized patients [24]. Around 68.1% people died during the study with median time 58 days. The original data consists of 9105 patients and 14 features, for which all features are indices observed or diagnosed by patients (age, sex, race, number of comorbidities, presence of diabetes, presence of dementia, presence of cancer, mean arterial blood pressure, heart rate, respiration rate, temperature, white blood cell count, serum’s sodium, and serum’s creatinine). The data we use in our experiment follows [22], where missing data are dropped and altogether 8873 patients are kept in the dataset.

Note that in this dataset, we have continuous, binary and nominal features. Therefore we apply embedding techniques to specially do data-preprocessing for nominal features, which is a common trick used in deep learning for nominal features. Figure 9 shows the meaning of embedding. This shows the easy-to-use essence of deep learning since if we would like to use traditional statistical models such as GLM, we need to carefully learn the knowledge in the dataset, which is not necessary for deep learning.

**METABRIC** METABRIC [9] is one dataset that focuses on studying the relationship between gene and clinical features and breast cancer. Following [22], we drop some missing data and 1904 patients are preserved with 9 features, where 4 are gene features and 5 are clinical features. This dataset has only binary and continuous features, so no other additional data-preprocessing steps are required.

**MIMIC-III** MIMIC-III [33], [18], is a deidentified dataset associated with over 40k patients who stayed in critical care units of the Beth Israel Deaconess Medical Center between 2001 and 2012. Compared with other datasets, this is an electronic health record (EHR) data, which means real-time features that observed in a routine basis can be accessible. In other words, the size of this dataset is much larger and features are more complicated than the other two datasets. The goal for using this dataset is to show that with proper tuning of some common parameters for deep learning, our model can achieve a satisfactory result with only part of this dataset accessible. We do not use SUPPORT or METABRIC for this aim due to the reason that the size of these two datasets is not so large, which means other models may not be able to train a reasonable result.
Figure 9: Illustration of Embedding. Suppose the dimensionality of all nominal features is $m$ and the desired embedding layer is $n$, essentially this is a one-layer fully connected neural network and this can be understood as a linear projection from $\mathbb{R}^m$ to $\mathbb{R}^n$. After getting the embedding layer with $n$ dimensions, we combine the values with other features (suppose the dimensionality of all other features is $p$) to get the input layer with dimensionality $n + p$. This is the input layer used for model training.

5.2 Results

**SUPPORT** For this dataset, we have subsampled 5%, 10% and 20% of the data as internal data, and then for each ratio, we have 50 groups of data for experiments and $\eta$ is tuned with 5-fold cross validation, where the data splitting procedure and evaluation metrics are the same as what in Simulation 1. Due to the existence of categorical covariates in SUPPORT, we create an additional embedding layer to deal with them and then combine the embedded features with other features to be the input of the 3-layer fully-connected neural network. ReLU is used as the activation function for each layer, Batch Normalization is also equipped for better training of the neural network in each layer with momentum 0.1. Dropout rate is set to be 0.2 for each layer. For the optimization, AdamWR [31] is applied with decoupled weight decay rate to be 0.01 and learning rate is set to be the constant 0.01, holding other parameters default. Early Stopping is used with patience 10.

Figure 10: Results (left: SUPPORT, right: METABRIC)
The left graph in Figure 10 shows the trend of changing sample size. Similar as what has shown in Simulation 3, the stability of the model improves when the sample size of local data increases. Additionally, for LogisticHazard, the results improve with more local data, while for our model, the improvement is not so straightforward. We guess this is because when the size of training data is large enough, deep learning can model well enough and in such case, prior information is not a significant factor for prediction accuracy.

**METABRIC** For this dataset, we follow similar data splitting rules as SUPPORT, except for the change of ratio of internal data. We sampled out 10%, 20% and 30% of the data as internal since the size of data for METABRIC is much smaller than SUPPORT. Since we require no data-preprocessing tricks for this dataset, we use the same model parameters as what used in simulation 1, as the data structures for these two experiments are essentially equivalent. The goal for this experiment is the same as SUPPORT, which means we want to show the trend of our comparison result with the size of internal data increasing.

The right graph in Figure 10 shows the results for METABRIC, similar trends appear and the conclusion is the same, we do not repeat that due to the length limit.

**MIMIC-III**

6 Conclusion and Future Work

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A  Appendix

A.1 How to Apply KL Divergence on Hazard Function?

The reason for the validity of using KL Divergence on hazard function is that hazard function can be understood as a conditional probability, which has a distribution \[ P \] and \[ Q \]. In discrete case, suppose \( P = (p_1, p_2, \ldots, p_m)^\top \) and \( Q = (q_1, q_2, \ldots, q_m)^\top \) are two probability distributions with \( \sum_{i=1}^{m} p_i = 1 \) and \( \sum_{i=1}^{m} q_i = 1 \), then the KL Divergence is defined as

\[
D_{KL}(P, Q) = \sum_{i=1}^{m} p_i \log \frac{p_i}{q_i}
\]

In single-risk case, we can consider the hazard value for a given individual \( i \) at time point \( \tau_k \) as the probability of event happens at \( \tau_k \) conditioning on this individual is still at risk at \( \tau_k \). So we can define two complementary events (binomial distribution): Event happens and does not happen conditioning on the derived covariates and individual is at risk at time point \( \tau_k \). We can define the distribution as \( P = (p_1, p_2)^\top \), where

\[
p_1 = \lambda(\tau_k | Z_i) = P(T_i = \tau_k | T_i \geq \tau_k, Z_i) \\
p_2 = 1 - \lambda(\tau_k | Z_i) = P(T_i > \tau_k | T_i \geq \tau_k, Z_i)
\]

Suppose \( P \) is the distribution for hazard value of external model and \( Q \) being that of internal model, then the definition of the time-dependent KL Divergence for single risk is actually the KL Divergence between \( P \) and \( Q \), which leads to the definition

\[
d_k(\lambda, \lambda; Z_i) = \tilde{\lambda}(\tau_k | Z_i) \log \left\{ \frac{\lambda(\tau_k | Z_i)}{\lambda(\tau_k | Z_i)} \right\} + \left\{ 1 - \tilde{\lambda}(\tau_k | Z_i) \right\} \log \left\{ \frac{1 - \tilde{\lambda}(\tau_k | Z_i)}{1 - \lambda(\tau_k | Z_i)} \right\}
\]

For Competing Risk case, the number of events for the distribution will change from 2 to \( q + 1 \), with \( q \) the number of causes leading to the event. Mathematically, we can define the distribution as \( P = (p_1, \ldots, p_q, p_{q+1})^\top \), where

\[
p_r = \lambda_r(\tau_k | Z_i) = P(T_i = \tau_k, R_i = r | T_i \geq \tau_k, Z_i), r = 1, 2, \ldots, q \\
p_{q+1} = 1 - \sum_{r=1}^{q} \lambda_r(\tau_k | Z_i) = P(T_i > \tau_k | T_i \geq \tau_k, Z_i)
\]

and the computation of time-dependent KL Divergence for competing risk setting follows the same principle, yielding

\[
d_k(\lambda, \lambda; Z_i) = \sum_{r=1}^{q} \tilde{\lambda}_r(\tau_k | Z_i) \log \left\{ \frac{\lambda_r(\tau_k | Z_i)}{\lambda_r(\tau_k | Z_i)} \right\} + \left\{ 1 - \tilde{\lambda}(\tau_k | Z_i) \right\} \log \left\{ \frac{1 - \tilde{\lambda}(\tau_k | Z_i)}{1 - \lambda(\tau_k | Z_i)} \right\}
\]

A.2 Mathematical Formulas for Backward Propagation

Backward Propagation is the way of computing gradient for a neural network, and the essential rule is chain’s rule. To be more clear we repeat the formula of fully-connected feed-forward neural network and shows the
details for gradient calculation.

\[ Z_i^{(1)} = f^{(1)}(Z_i) = s^{(1)}(W^{(1)}Z_i + b^{(1)}) \]
\[ Z_i^{(2)} = f^{(2)}(Z_i^{(1)}) = s^{(2)}(W^{(2)}Z_i^{(1)} + b^{(2)}) \]
\[ Z_i^{(3)} = f^{(3)}(Z_i^{(2)}) = s^{(3)}(W^{(3)}Z_i^{(2)} + b^{(3)}) \]
\[ \cdots \]
\[ Z_i^{(l)} = f^{(l)}(Z_i^{(l-1)}) = s^{(l)}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \]

Then we have

\[
\frac{\partial l_i}{\partial Z_i^{(l)}} = \nabla r(Z_i^{(l)})
\]
\[
\frac{\partial l_i}{\partial Z_i^{(l-1)}} = \frac{\partial Z_i^{(l)}}{\partial Z_i^{(l-1)}} \nabla r(Z_i^{(l)}) = W^{(l)^\top}[s^{(l)'}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \odot \nabla r(Z_i^{(l)})]
\]
\[
\frac{\partial l_i}{\partial W^{(l)}} = \frac{\partial Z_i^{(l)}}{\partial W^{(l)}} \nabla r(Z_i^{(l)}) = [s^{(l)'}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \odot \nabla r(Z_i^{(l)})]Z_i^{(l-1)^\top}
\]
\[
\frac{\partial l_i}{\partial b^{(l)}} = s^{(l)'}(W^{(l)}Z_i^{(l-1)} + b^{(l)}) \odot \nabla r(Z_i^{(l)})
\]

where \(\odot\) means the element-wise product, which means \((p_1, \ldots, p_m) \odot (q_1, \ldots, q_m) = (p_1q_1, \ldots, p_mq_m)\). From the results we can find that after knowing the values of \(W^{(l)}, Z_i^{(l-1)}, b^{(l)}\), the gradient of \(s^{(l)}(W^{(l)}Z_i^{(l-1)} + b^{(l)})\) (which is the connection between \(l-1\)-th and \(l\)-th layer) and the gradient of \(l_i\) with respect to \(Z_i^{(l)}\) (which is \(\nabla r(Z_i^{(l)})\) since it is just the loss function), we can obtain the gradients with respect to \(W^{(l)}\) and \(b^{(l)}\).

As for those with respect to \(\{W^{(k)}, b^{(k)}\}, k = 1, 2, \ldots, l-1\), these can be obtained reversely by chain’s rule. For a given \(k\), suppose that the values of \(W^{(k)}, Z_i^{(k-1)}, b^{(k)}\), the gradient of \(s^{(k)}(W^{(k)}Z_i^{(k-1)} + b^{(k)})\) and the gradient of \(l_i\) with respect to \(Z_i^{(k)}\), then the gradients with respect to \(W^{(k)}, b^{(k)}\) can be obtained by chain’s rule, which means

\[
\frac{\partial l_i}{\partial W^{(k)}} = \frac{\partial Z_i^{(k)}}{\partial W^{(k)}} \frac{\partial l_i}{\partial Z_i^{(k)}}
\]
\[
\frac{\partial l_i}{\partial b^{(k)}} = \frac{\partial Z_i^{(k)}}{\partial b^{(k)}} \frac{\partial l_i}{\partial Z_i^{(k)}}
\]

and \(\frac{\partial Z_i^{(k)}}{\partial W^{(k)}}\) and \(\frac{\partial Z_i^{(k)}}{\partial b^{(k)}}\) can be obtained by knowing that \(Z_i^{(k)} = s^{(k)}(W^{(k)}Z_i^{(k-1)} + b^{(k)})\), \(\frac{\partial l_i}{\partial Z_i^{(k)}}\) is known due to the assumption, so we can know that by chain’s rule and induction, the gradients for each unknown variables can be obtained reversely (from \(W_i^{(l)}, b_i^{(l)}\) to \(W_i^{(1)}, b_i^{(1)}\) and after forward propagation finishes (otherwise we will not know \(Z_i^{(k)}, k = 1, 2, \ldots, l\)).

Fortunately due to the huge progress of deep learning community, advanced softwares have developed mature solutions for computing gradients in neural network. For our simulations and real data experiments, we use Pytorch as the bedrock of our neural network training, which uses Jacobian matrices and automatic differentiation for gradient calculation. For people who are more interested, see [32] for more details.

### A.3 Hyperparameter Tuning Recommendations for Deep Learning

Neural network training will be affected by a series of hyperparameters, and usually there is no uniform choice that will permanently be the best option for getting the best result. For this reason we provide with extra experiments that support our choices for several mostly common tuned hyperparameters, we also set our choices as the default option for our software.
**Batch Size**  Figure 14 shows the comparison result. From left to right, we have generated 30000, 5000 and 500 data points following the 3rd scheme of the simulation 1 and also a real dataset SUPPORT. We have found that about 5% of the size is a maximum boundary for the mini-batch training. For the minimum, it is a little hard to determine, but 0.1 - 1% of the size is a safe range, which means that if you have a data size of 10000, then we recommend tuning the batch size from 10 to 500.

![Batch Size Result](image)

Figure 11: Batch Size Result, for batch size that out of the range showing on the graph, the convergence loss is so high that the scale of the graph will be demolished, which means those options should not be considered in the hyperparameter tuning process. Same as below.

**Learning Rate**  We have taken a series of values for potential learning rate, which ranges from 0.00001 to 0.1, we have observed that the values from 0.0001 to 0.05 can be a proper range, so this will be our range for tuning.

![Learning Rate Result](image)

Figure 12: Learning Rate Result

**Optimizers**  We have tried 4 optimizers (SGD, Adam, RMSProp, AdamW) and 3 are comparable, the other one is inferior. So these three optimizers will be used.

![Optimizers Result](image)

Figure 13: Optimizers Result
**Dropout Rate** We take \([0, 0.1, 0.25, 0.5]\) as potential values for tuning and for the first three values, there are no significant difference but they all behave better than the 0.50.5 case. This is reason that for default hyperparameter tuning recommendation, we will use \([0, 0.1, 0.25]\) as 3 potential options.

![Figure 14: Dropout Rate Result](image)