Robust prediction of failure time through unified Bayesian analysis of nonparametric transformation models

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Abstract

Nonparametric transformation models (NTMs) have sparked much interest in survival prediction owing to their flexibility with both transformations and error distributions unspecified. However, fitting these models has been hampered because they are unidentified. Existing approaches typically constrain the parameter space to ensure identifiability, but they incur intractable computation and cannot scale up to complex data; other approaches address the identifiability issue by making strong a priori assumptions on either of the nonparametric components, and thus are subject to misspecifications. Utilizing a Bayesian workflow, we address the challenge by constructing new weakly informative nonparametric priors for infinite-dimensional parameters so as to remedy flat likelihoods associated with unidentified models. To facilitate applicability of these new priors, we subtly impose an exponential transformation on top of NTMs, which compresses the space of infinite-dimensional parameters to positive quadrants while maintaining interpretability. We further develop a cutting-edge posterior modification technique for estimating the fully identified parametric component. Simulations reveal that our method is robust and outperforms the competing methods, and an application to a Veterans’ lung cancer dataset suggests that our method can predict survival time well and help develop clinically meaningful risk scores, based on patients’ demographic and clinical predictors.

Keywords: Identifiability; Posterior modification; Quantile-knots I-splines; Stan; Weakly informative priors.

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1 Introduction

The linear transformation model raised by Cheng, Wei and Ying is quite flexible including whilst not limited to three commonly used and highly interpretable survival models, proportional hazards (PH), proportional odds (PO) and accelerated failure time (AFT) (Cheng et al., 1995; Horowitz, 1996). It is known challenging for estimation of infinite-dimensional parameters in the nonparametric transformation model (NTM) in the sense that both functional forms of transformation and the error distribution are unspecified (Chen, 2002; Linton et al., 2008; Chiappori et al., 2015; among others). Particularly, to estimate such nonparametric components is essential for prediction of failure times and conditional hazards in the community of biostatistics (Song et al., 2007, pp. 207; Lin et al., 2017, pp. 980), name a few. Motivated by the flexibility and prediction capability of the nonparametric transformation model, we attempt to develop a robust Bayesian solution to address estimating the NTM within the Bayesian paradigm.

Model identifiability is the foremost concern to be addressed in estimation of NTMs (Härdle and Stoker, 1989; Ichimura, 1993; among others). Econometricians have sufficient discussions on conditions to obtain fully identified model. Their common outline is to do scale and location normalizations, where the former was generally imposed to the regression vector, and the latter may be imposed to either the transformation function or the distribution of random error (Horowitz, 1996; Ye and Duan, 1997; Görgens and Horowitz, 1999; Chen, 2002; Linton et al., 2008; Chiappori et al., 2015; among others). Under their normalization conditions, various estimators for two infinite-dimensional parameters were developed based on nonparametric techniques such as kernel smoothing and rank estimation. In summary, their contributions lie in establishing theoretical results such as \( \sqrt{n} \)-convergency and related inference, whereas they do not touch upon computational
feasibility and tractability in practice.

In the community of statistics and biostatistics, for NTMs, researchers cared about estimation of the regression vector owing to interpretability of the relative risk score but circumvented estimation of nonparametric components (Song et al., 2007; Liu et al., 2021; among others). Otherwise, to avoid model unidentifiability, there is wealth of literature which made strong a priori assumptions either about the transformation such as the AFT model (Walker and Mallick, 1999; Jin et al., 2003; Komárek and Lesaffre, 2008; among others), or about the error distribution functional such as PH and PO models (Chen et al., 2002; Zeng and Lin, 2006; Hanson and Yang, 2007; Zeng and Lin, 2007; Wang and Dunson, 2011b; Cai et al., 2011; de Castro et al., 2014; among others). However, designating the transformation function or the error distribution may be subject to misspecification, leading to inconsistent estimation, invalid statistical inference, and erroneous predictions.

Bayesian approaches appear to be preferable for survival analysis since available priori information may be difficult to be included in specific models under the frequentist paradigm (McKeague and Tighiouart, 2000). In Bayesian approaches, background knowledge expressed in prior is updated with information in observed data formed as the likelihood to determine the posterior distribution (van de Schoot et al., 2021). Existing Bayesian literature on NTMs is rare and mainly took the two-step strategy to estimate and select models sequentially. Mallick and Walker (2003) suggested to estimate the NTM first and then do model selection by comparing discrepancy measures between estimated and specific survival models. They built a Polya tree variant prior for the distribution of centred model error for the purpose of full identification, and modeled the transformation function by a noninformative prior which is a projection of incomplete beta functions. However, the use of the Polya tree prior might be troublesome to some extent since it is sensitive
to elicitation of the centering distribution, incurring pretty slow convergence of posterior (Müller et al., 2015, pp.39). Their effort provides an evidence that full identifiability may severely restrict computing tractability of Bayesian methods. Alternatively, Zhou and Hanson (2018) circumvented the issue of identifiability by estimating all models first based on a transformed Bernstein polynomial (TBP) prior for the baseline survival probability in each model, followed by selecting the “best” one through Bayesian criteria such as log pseudo marginal likelihood. Their corresponding R package spBayesSurv is computationally convenient and outperforms other existing Bayesian packages if correctly specifies the model. Nevertheless, Zhou and Hanson’s approach is subject to model misspecifications if the underlying model is none of PH, PO or AFT models.

Note that, unidentifiability causes no real difficulties in the Bayesian approach (Lindley, 1972, pp.46), because once the prior is proper, the posterior is also proper (Gelman et al., 2013, pp.52). That is why Andrew Gelman would prefer the so-called Bayesian identifiability, “..., a Bayesian model is identified if the posterior distribution is proper. Then one can do Bayesian inference..., all that’s needed is a finite integral of the probability distribution.” (Andrew’s blog). Particularly, if one’s interest falls into prediction, the posterior predictive distribution (PPD) of a future observation is always unique by integrating over the parameters although there are multiple solutions of the triplet parameter in the unidentified model. However, even theoretically it is reasonable to do prediction without fully identifying the model, sampling the posterior is still a big challenge because the posterior distribution cannot converge with flat likelihood (Gelman et al., 2013, pp.89), incurring meaningless final model results. The below insight inspires our methodology to address the problem that, in Bayesian analysis, priors play a defining role and have substantive impact to final model results by incorporating previous knowledge into estimation process.
We are motivated to assign weakly informative nonparametric priors for infinite-dimensional parameters to mitigate the lack of identifiability, achieving well converged and accurate final model results under the NTM.

Our Bayesian inference procedure is kicked off by imposing the exponential transformation to the NTM. Then we construct a new weakly informative nonparametric prior for the monotone transformation function, assign the Dirichlet process mixture (DPM) model for the model error distribution, and develop the cutting-edge posterior projection technique to estimate the fully identified parametric component. We also build the R package BuLTM interfacing with Stan to implement prediction and develop relative risk scores.

Novelties of our methodology are trifold. The first is that we transform the NTM to an equivalent working model to make it possible for robust prediction and efficient model fitting. There are two categories of priors for sign-varying monotone functions in literature. One is not applicable to modeling the transformation in the NTM as it encounters the possibly infinite intercept in its monotone functional form (Neelon and Dunson (2004); Shively et al. (2009); Bornkamp and Ickstadt (2009); Lenk and Choi (2017); among others); the other is nontrivial to be extended to censored observations since it adds response-based monotonicity shape restriction on squared Gaussian processes of the mean regression function (Riihimäki and Vehtari (2010); Lin and Dunson (2014); Wang and Berger (2016); among others). In contrast, once the transformation is confined to be a sign-invariant function, the modeling of which is relatively tractable (Gelman et al., 2013, pp.493).

The second novelty of our approach is that we construct a new manoeuvrable weakly informative prior for nonnegative differentiable monotone functions. There are two branches of methods to modeling nonnegative monotone functions, increments based models (Kalbfleisch,
1978; Hjort, 1990; Arjas and Gasbarra, 1994; McKeague and Tighiouart, 2000; among others), and I-splines type priors (Cai and Dunson, 2007; Wang and Dunson, 2011a; among others). The differentiability of the recast transformation makes it natural to assign an I-splines type prior, which used to be accompanied with a knots tuning procedure that is time consuming and yet unstable. We build the so-called quantile-knots I-splines prior, which borrows strength from empirical quantiles of the failure time to simplify specification of knots of spline basis, enjoying expedient computation without tuning procedure.

The third novelty is that we develop the state-of-the-art posterior modification to estimate the fully identified vector of coefficients under the NTM. The vector of coefficients is fully identified subject to a normalization constraint. There are two representative categories of priors for constrained vectors, one is the polar-system reparameterization (Park et al., 2005), and the other is built-in uniform distribution of Stan (Carpenter et al., 2017). However, in our Bayesian workflow, the assigned nonparametric priors have no constraints, and thus it does not make sense to directly assign a constrained prior for the parametric component. This motivates us to seek for posterior modification technique. We employ posterior projection onto Stiefel manifold (Sen et al., 2022) to estimate the fully identified parametric component, performing well in both point and interval estimation evaluated by frequentist operating characteristics, and bringing no extra computation burden to sampling.

Our work has contributions trifolds. The first is that we suggest a refined definition of Bayesian identifiability that, a Bayesian regression model is identified if the prior(s) for the unidentified infinite-dimensional parameter(s) is weakly informative. The weakly informative prior is a kind of “stronger” proper prior that is able to control prior variance moderately and thus make well-converged posterior sampling. We are not the daredevil to
claim since existing literature has had a few explorations in other environments to avoid burdensome computation for full identification of models. In biomedical studies, Branscum et al. (2008) and Müller and Mitra (2013) adopted centered and concentrated nonparametric priors for population distributions under the unidentified finite mixture model and for random effects distributions under the unidentified nonparametric random effects model, respectively. Both priors are actually weakly informative. Beyond this, even for the prevailing high-dimensional vector factor model, Berchuck et al. (2021) constructed a process with finite moments as the weakly informative nonparametric prior for the columns of the factor loadings matrix. The above work and our current one attempt to mitigate the loss of identifiability by weakly informative nonparametric priors rather than fully identify the model.

Next, the proposed quantile-knots I-splines prior is built originally for differentiable nonnegative monotone functions, while it can also model continuous but nondifferentiable ones. It can be viewed as a combination of several groups of nonnegative independent increment (NII) processes from inherence of the expression of I-spline basis functions (Ramsay, 1988). Consequently, by fixing smoothness order of I-spline basis functions to be one, the proposed prior reduces to the nondifferentiable piecewise exponential prior, a special case of NII processes (Ibrahim et al., 2001, pp.48). Finally, we supply a most robust and unified Bayesian solution for practitioners implemented by the R package BuLTM, which is computationally convenient and efficient to predict failure times and output estimates of predict survival probability, conditional hazards, and the relative risk score. In accuracy of predicting conditional survival probability, BuLTM outperforms spBayesSurv under the PH model and model misspecification situations, and is comparable to spBayesSurv under PO and AFT models.
The remainder of this article is organized as follows. Section 2 introduces the working model and highlight out methodology philosophy. Section 3 introduces the proposed quantile-knots I-splines prior for the recast transformation. Sections 4 and 5 introduce estimation of the parametric component and MCMC procedure, respectively. Sections 6 and 7 assess and demonstrate our method compared with existing work. Section 8 concludes the article with a brief discussion. Related details are collected in the supplementary materials and the R package BuLTM is available at GitHub https://github.com/LazyLaker.

2 Model and identifiability

2.1 Multiplicative relative risk model

Let $T$ be the censored failure time, and $Z$ and $\beta$ be the $p$-dim covariate vector and the coupled $p$-dim vector of regression coefficients, respectively. The traditional linear transformation model raised by Cheng et al. (1995) was formulated as

$$h(T) = \beta^T Z + \epsilon,$$

where $h(\cdot)$ is an unknown strictly increasing function and $\epsilon$ is the model error with distribution function $F_\epsilon = 1 - S_\epsilon$. Model (1) is called the nonparametric transformation model (NTM) when both $h$ and $S_\epsilon$ are unspecified, where the transformation $h(\cdot)$ may be sign varying on $\mathbb{R}^+$. 

We aim to build methodology to predict failure time and develop relative risk scores based on estimation of NTM (1). For this purpose, our first step is to impose the exponential transformation to NTM (1) and obtain

$$H(T) = \xi \exp(\beta^T Z),$$

where $\xi$ is a positive constant.
where the recast transformation $H(\cdot) = \exp\{h(\cdot)\}$ and the model error $\xi = \exp(\epsilon)$ with distribution function $F_\xi = 1 - S_\xi$. The nonparametric transformation model (2) with multiplicative relative risk is abbreviated as MTM thereafter, where $H$ is positive on $\mathbb{R}^+$ and the multiplicative random error $\xi$ is also positive. MTM (2) is equivalent to NTM (1) in the sense that they share common parametric component $\beta$, and strictly $S_\epsilon(\cdot) = S_\xi\{\exp(\cdot)\}$ and $h(\cdot) = \log H(\cdot)$.

The above monotonic transformation step plays the critical role in establishing our Bayesian methodology route. To estimate NTM (1) directly has long been challenging to proceed with while estimating the MTM is possibly doable in that, the monotonic transformation compresses the space of infinite-dimensional parameters, the transformation function and the survival probability functions of model error, from $\mathcal{M}_{\mathbb{R}} \times \mathcal{S}_{\mathbb{R}}$ to a reasonable subset of $\mathcal{M}_{\mathbb{R}^+} \times \mathcal{S}_{\mathbb{R}^+}$, where $\mathcal{M}_A$ denotes the space of monotone functions with range $A$, and $\mathcal{S}_A$ denotes the space of survival probability functions with support $A$. Particularly, under a mild condition (A3), we have $H(0) = 0$ directly in the MTM, removing many irrational transformation functions that are not suitable to the survival context. Consequently, the space of infinite-dimensional parameters is compressed to $\{(H, S_\xi)|H \in \mathcal{M}_{\mathbb{R}^+}, H(0) = 0, S_\xi \in \mathcal{S}_{\mathbb{R}^+}\}$ under MTM (2). Our spirit has allies in literature about the linear transformation model where they rewrote their transformation as the logarithm of a cumulative hazard function (Scheike, 2006; Zeng and Lin, 2006; among others).

Meanwhile, the recast MTM (2) still maintains analogous interpretability of NTM (1) although the regression kernel relocates from the survival probability function to the cumulative hazard function with the insight of relationship between transformed failure time and the relative risk, which is multiplicative (up to an exponential tilt) in the former and
additive in the latter, respectively. Let $\Lambda(\cdot)$ be the cumulative hazard function of a time variable. By some simple algebra, the counterpart of expression (1.3) that motivates linear transformation model (1) in Cheng et al. (1995) can be represented as

$$ G\{\Lambda_T|Z(t)\} = H(t) \exp(-\beta^T Z), \quad (3) $$

for MTM (2), where $G^{-1} = \Lambda_\zeta$ is the link working on the cumulative hazard of the failure time. Specifically, if the link functional forms of $G(\cdot)$ are identity and $\{\exp(\cdot) - 1\}$, or alternatively, the model error $\zeta$ is exponentially distributed with unit rate, and log-logistically distributed with unit shape and scale parameters, then model (2) reduces to PH and PO models, respectively.

### 2.2 Identifiability

In model (2), we target to estimate the triplet $(\beta, H, S_\zeta)$ jointly for the purpose of prediction of the survival time or mortality through survival probability or the cumulative hazard function. Note that nonparametric transformation models are unidentifiable or underidentified in that they generate flat likelihood. Take MTM (2) for instance, where the likelihood function is identical for collections of parameters, say, $\{\beta, H(t), S_\zeta(t)\}$, $\{\beta, c_1 H(t), S_\zeta(c_1^{-1}t)\}$ and $\{c_2 \beta, [H(t)]^{c_2}, S_\zeta(t^{1/c_2})\}$ with arbitrary positive constants $c_1$ and $c_2$.

Model unidentifiability is fatal to frequentist inference since there does not exist most likely estimator. The parametric component is readily to be fully identified by imposing scale normalization (Härdle and Stoker, 1989) and is discussed in details in section 4. To fully identify the NTM, in terms of nonparametric components, frequentists may impose location normalization to either error distributions by assuming zero median or mean (Ye and Duan, 1997; Linton et al., 2008; Chiappori et al., 2015; among others), or to the transformation by assuming zero value for a finite point (Horowitz (1996); Gørgens and
Horowitz (1999); Chen (2002); among others); in Bayesian analysis, Mallick and Walker (2003) strictly fully identifies the model by building a constrained Polya tree variant prior for the model error distribution to control both location and variance of the model error. Nonetheless, the choice of centering distribution of Polya trees is so tricky that may affect inference unduly and slow down convergence of the posterior severely (Hanson and Johnson, 2002). We tried to add constraints in line of Horowitz’s normalizations for $\beta$ and $H$ and unfortunately, the results are still computationally infeasible as predictable. Refer to Supplement S.4.1. In summary, to realize the traditional full identification is more meaningful in theory but subject to numerical intractability.

In Bayesian community, there has long been the voice that unidentifiability brings no conceptual difficulty to Bayesian approaches (Gustafson, 2009). The hazard of analyzing unidentified models is obvious such as the resulting inconsistent inference owing to poorly placed prior. However, the other side of the coin is that, one may design a prior to reach the tradeoff between full identification of the model and feasible posterior sampling. This drives us to pursue placing reasonable priors on the unconstrained space of infinite-dimensional parameters to play the role of confining posterior samples. The weakly informative prior distribution is an ideal weapon that compromises between sacrificing part of full identification and forfeiting purely objective sampling from noninformative priors. If we simply employ proper but noninformative priors, the posterior cannot converge but wanders all around the parameter space instead (Branscum et al., 2008). In contrast, the weakly informative prior prevents the sampler from running to highly implausible values that are far away from its center and therefore, assures well-converged and mixed posterior (McElreath, 2020, pp.262). In summary, the lack of identifiability is mitigated by weakly informative priors, escaping from the hurdle caused by sampling on complicated constrained space; con-
currently, the induced posterior variance is dominated by variance of weakly informative priors because of law of total variance, leading to efficient convergence.

In our explorations, although we admit that a few inner points of the posterior surface (percentage less than 0.5%) may exceed the maximum tree depth of No-U-Turn sampler (NUTS) (Hoffman and Gelman, 2014) in MCMC sampling, our method enjoys fast convergence and well mixing of MCMC chains with high effective sample size (ESS) in MCMC diagnosis, see Supplement S.6.4; and in prediction, our method performs robustly and accurately in many true model cases, compared with spBayesSurv (Zhou and Hanson, 2018); meantime, the posterior is neither sensitive to subjective choices of hyperparameters in the weakly informative priors nor similar to priors, referred to Supplements S.7 and S.9, respectively. Our findings are in line with results of existing literature about unidentified parametric models where the lack of identifiability is mitigated by weakly informative priors (McCulloch and Rossi (1994); Gutiérrez et al. (2014); McElreath (2020); Cole (2020); Burgette et al. (2021); among others).

Let us conclude discussion on Bayesian identifiability in this subsection. In Bayesian-specific workflow, prior plus likelihood with data generates the posterior, and the resulting inference starts a new research cycle. The influence of priors makes it possible that we request Bayesian identifiability rather than the restrictive full identifiability to do robust and efficient prediction of failure time successfully in the situation of loss of identifiability. In this sense, frequentists can establish ideal theoretical properties while our Bayesian perspective can offer good solution balancing methodology and practice.
3 Likelihood and prior

3.1 Likelihood

For the real survival time $T$ and the random censoring variable $C$, one denotes the observed time-to-event as $\tilde{T} = \min(T, C)$. The censoring indicator $\delta = I(T \leq C)$. Let $S_\xi$ and $f_\xi$ be the survival probability and density function of $\xi$, respectively. In this section, we consider the following assumptions.

(A1) The exp-transformation $H$ is differentiable.

(A2) The multiplicative random error $\xi$ is continuous.

(A3) The covariate $Z$ is independent of $\xi$.

(A4) The censoring variable $C$ is independent of $T$ given $Z$.

(A1) is required since there is $H'$ functional in the likelihood representation below; (A2) is mild; (A3) is general and can derive that $H(0) = 0$, referred to Supplement S.1; (A4) is the general noninformative censorship condition.

With independent triplets of observed data $\{(\tilde{T}_i, Z_i, \delta_i)\}_i^n$, one writes the complete data likelihood as

$$L(\beta, H, S_\xi, f_\xi | \tilde{T}, Z, \delta) = \prod_{i=1}^n \left[ f_\xi \{ H(\tilde{T}_i)e^{-\beta^T Z_i} \} H'(\tilde{T}_i)e^{-\beta^T Z_i} \delta_i [ S_\xi \{ H(\tilde{T}_i)e^{-\beta^T Z_i} \} ]^{1-\delta_i} \right].$$

(4)

Since $\xi$ is an arbitrary continuous positive random variable, the DPM model (Lo, 1984) is a natural choice of the prior for $S_\xi$ and $f_\xi$. Choices of kernel of the DPM for nonparametric survival probability is flexible (De Iorio et al., 2009). In this article, without loss of generality, we adopt the Weibull kernel such that

$$S_\xi = 1 - \sum_{l=1}^L p_l F_w(\psi_l, \nu_l), f_\xi = \sum_{l=1}^L p_l f_w(\psi_l, \nu_l),$$

(5)

where $F_w$ and $f_w$ denote the CDF and density function of Weibull distribution, respectively.

We refer details and justification of the DPM prior to Supplement S.2.
As shown in (4), $H$ should be differentiable on $\mathbb{R}^+$, or its subset. Most increments based models (Kalbfleisch, 1978; Arjas and Gasbarra, 1994; among others) are not differentiable everywhere, and those differentiable ones may induce complicated and intractable form of the derivative (Dykstra and Laud, 1981; Hjort, 1990; among others). In this article, we construct a quantile-knot I-splines type prior for $H$ and its derivative $H'$, which is computationally expedient. Details about the prior are discussed in the following subsection.

3.2 Quantile-knots I-splines prior

Suppose the survival outcome $T$ is observed on interval $D = (0, \tau]$, where $\tau$ is the largest survival time in the sample. Note that, $H$ is a nonnegative strictly increasing differentiable function on $D$ based on transformation model (2) and likelihood function (4). It is natural to model $H$ and $H'$ by monotone splines,

$$H(t) = \sum_{j=1}^{K} \alpha_j B_j(t), \quad H'(t) = \sum_{j=1}^{K} \alpha_j B'_j(t),$$

(6)

where $\{\alpha_j\}_{j=1}^{K}$ are positive coefficients to guarantee nondecreasing monotonicity, $\{B_j(t)\}_{j=1}^{K}$ are I-spline basis functions (Ramsay, 1988) on $D$ and $\{B'_j(t)\}_{j=1}^{K}$ are corresponding derivatives. The number of I-spline basis functions $K$ is the sum of number of interior knots and the order of smoothness $r$ with $(r - 1)$th order derivative existing. Empirically, $r$ may take value from 2 to 4 and we take the default value $r = 3$ in R package splines. Interior knots cut the time interval $D$ into $(K - r + 1)$ partitions. Then our concern lies in specifying the number and locations of interior knots for modeling the exp-transformation.

We construct an I-splines type prior based on representations (6) by selecting interior knots from empirical quantiles of survival times, namely quantile-knots I-splines prior. First we fix the initial number of interior knots $N_I$ which is much less than that in other typical I-splines type models coupled with the shrinkage prior. Our insight comes from the
advantage of quantiles that small number of quantiles quantify different “locations” of a
distribution and therefore they can be viewed as alternative measures of the shape of the
predictive distribution of $T$. Meanwhile, the corresponding posterior is not sensitive within
the range of small number of knots, indicating that the proposed prior is free of tuning,
referred to Supplement S.7.1. It is expedient in implementation compared to those priors
requiring tuning, referred to Supplement S.4.2.

Next, given the initial number of interior knots $N_I$, we propose a two-step data-driven
procedure to specify their locations using information of survival times and censoring states.

Let $\hat{F}_X(t) = n^{-1} \sum_{i=1}^{n} I(X_i \leq t)$ be the empirical CDF of $X$ and $\hat{Q}_X(p) = \hat{F}_X^{-1}(p) = \inf\{t : p \leq \hat{F}_X(t)\}$ be the corresponding empirical quantile function, where $X$ is the placeholder
for $T$ and $\tilde{T}$, uncensored and observed survival times, respectively. Let $j = 0, \ldots, N_I - 1$.

Step 1: Selects $N_I$ empirical quantiles of observed failure times as interior knots $0 < t_0 <
\cdots < t_{N_I - 1} \leq \tau$, where $t_j = \hat{Q}_T\{j/(N_I - 1)\}$.

Step 2: If $|\hat{F}_T(t_j) - \hat{F}_{\tilde{T}}(t_j)| > z_0 \geq 0.05$, then interpolate a new knot $t_j^* = \hat{Q}_{\tilde{T}}(j/(N_I - 1))$.

Output sorted series of $\{t_0, \ldots, t_j, t_j^*, \ldots, t_{N_I - 1}\}$ as final interior knots.

In step 1, we choose equally spaced percentiles of uncensored survival times since in-
formation about $H'$ is provided by uncensored survival times only. In step 2, we make
interpolation in case high censoring of survival times and insufficient uncensored observ-
ations.

Take 5 initial knots for instance i.e. it contains 3 quartiles and 2 endpoints of uncensored
survival times. In Figure 1, there are apparent deviations between uncensored and observed
curves on the first three interior knots. Therefore, we interpolate by three new knots
$t_j^* = Q_{\tilde{T}}(j/4)$, for $j = 0, 1, 2$. Finally, we obtain $(t_0^*, t_0, t_1^*, t_1, t_2^*, t_2, t_3, t_4 = \tau)$ as our interior
knots.
By the above operation, I-spline basis functions \( \{ B_j(t) \}_{j=1}^K \) are specified. We further assign an exponential prior for \( \{ \alpha_j \}_{j=1}^K \). Consequently, we have built our quantile-knots I-splines prior for \( H \), which is weakly informative by the fact that, given \( \alpha_j \sim \exp(\eta) \),

\[
E\{H(t)\} = \eta^{-1} \sum_{j=1}^K B_j(t) < \infty \quad \text{and} \quad \text{Var}\{H(t)\} = \sum_{j=1}^K \eta^{-2} B_j^2(t) < \infty \quad \text{for any } \eta > 0 \text{ and } t < \infty.
\]

**Remark 1.** The quantile-knots I-splines prior can also be applied to model non differentiable functions. The proposed prior can be viewed a combination of NII processes, referred to Supplement S.3. Particularly, when \( r = 1 \), I-spline function reduces to straight line on each partition, and the proposed prior reduces to the piecewise exponential prior.

### 4 Estimation of parametric component

Besides nonparametric estimation, estimation of the parametric component \( \beta \) is essential as well. On one hand, posterior samples of \( \beta \) are necessary to computing the PPD of a new observation if its posterior is proper; on the other, marginal posterior of fully identified \( \beta \) is crucial to interpretation of the relative risk score. Notice that no constraint is added to
any component of \((\beta, H, S_\xi)\) in likelihood (4). Thus a noninformative Gaussian prior on \(\mathbb{R}^p\) is a natural choice to model \(\beta\). Let \(\beta^* \in \mathbb{R}^p\) be the unconstrained counterpart of the parametric component \(\beta\). Therefore, posterior samples of the triple \((\beta^*, H, S_\xi)\) are jointly and unifiedly drawn by MCMC. One may compute the PPD of a new observation based on the resulting proper posterior of the triplet. Choices of prior for \(\beta^*\) do not impact its posterior too much since one may even consider improper priors. The following corollary tells very mild conditions such that the posterior of \(\beta^*\) is still proper with the improper uniform prior.

**Corollary 1.** The posterior distribution of \(\beta^*\) is proper under following conditions: (i) \(0 < \tilde{T}_i < \infty\), for \(i = 1, \ldots, n\), (ii) priors for \(\{\psi_l, \nu_l\}_{l=1}^{L-1}, \{p_l\}_{l=1}^L\) in model (5) and \(\{\alpha_j\}_{j=1}^K\) in model (6) are proper, (iii) \(0 < K, L < \infty\) in models (5) and (6), (iv) the kernel \(f_w\) in model (5) satisfies that \(xf_w(x) < \infty\) for all \(x > 0\), (v) let \(Z^*\) be the \(n_1 \times p\) matrix of the covariates of uncensored observations, where \(n_1 = \sum_{i=1}^n \delta_i\), and \(Z^*\) is of full rank \(p\).

The proof for conditions is referred to *Supplement S.5*.

Note that the triplet \((\beta^*, H, S_\xi)\) can be estimated jointly so that prediction of failure times is doable, while each parameter is not separately identified. That is, the offending \(\beta^*\) leads to a ridge on the likelihood in a certain direction of parameter space of \(\beta\). If interest focuses on relative risk scores, one still needs good estimate for fully identified \(\beta\). As we mention in literature review, scale normalization makes \(\beta\) identified. To obtain posterior of normalized \(\beta\), *Stan* provides a constrained prior while it is not applicable in our case. Alternatively, we consider modification of the posterior distribution of unconstrained \(\beta^*\) to obtain marginal posterior of fully identified \(\beta\).

Firstly, we adopt the norm-one normalization such that \(||\beta|| = 1\), where \(||\cdot||\) is the \(L_2\) norm. This makes \(A\), the constrained space of \(\beta\), a unit hyper-sphere in \(\mathbb{R}^p\), exactly the
Stiefel manifold St(1, p)

\[ \mathcal{A} = \{ x : ||x|| = 1 \} = \{ x \in \mathbb{R}^{1 \times p} : x^T x = I_1 \} = \text{St}(1, p), \]

where \( I_1 \) is the order one identity matrix. We define the metric projection operator into \( \mathcal{A} \) as the mapping \( m_{\mathcal{A}} : \mathbb{R}^p \to \mathcal{P}(\mathcal{A}) \), where \( \mathcal{P}(\mathcal{A}) \) is the power set of \( \mathcal{A} \). Let \( \text{dist}(x^*, \mathcal{A}) = \inf\{||x^* - x||, x \in \mathcal{A}\} \) be the distance between \( x^* \in \mathbb{R}^p \) and \( \mathcal{A} \). The metric projection operator \( m_{\mathcal{A}} \) is determined by

\[ m_{\mathcal{A}}(x^*) = \{ x \in \mathcal{A} : ||x - x^*|| = \text{dist}(x^*, \mathcal{A}) \}. \]

Then, the projection of \( x^* \) into \( \text{St}(1, p) \) is unique and is given by \( m_{\mathcal{A}}(x^*) = x^*/||x^*|| \) (Absil and Malick, 2012, Proposition 7).

Next, let \( \beta^{(i)*} \) be the \( i \)th posterior sample of \( \beta^* \) drawn from the MCMC. We get the \( i \)th projected posterior sample of fully identified \( \beta \), denoted as

\[ \beta^{(i)} = m_{\mathcal{A}}(\beta^{(i)*}). \]

Since the posterior of \( \beta^* \) is proper and absolutely continuous, projected posterior of \( \beta \) is always proper by proposition 6 in Sen et al. (2022). Posterior of fully identified \( \beta \) has excellent frequentist performance in terms of low bias and credible intervals that reach the nominal rate, reconciling the frequentist and Bayesian measures of uncertainty quantification.

**Remark 2.** *Neither the built-in uniform prior for unit vectors in Stan nor the polar-system reparameterization by Park et al. (2005) works for MTM (2). The modeling of unconstrained nonparametric components dominate the Bayesian inference.* Let the true fully identified parameter triplet be \( (\beta_0, H_0, S_{\xi_0}) \), where \( ||\beta_0|| = 1 \), and \( H_0 \in \mathcal{H}_D = \{ f | f(x) \geq 0, f'(x) > 0, f(0) = 0, x \in D \} \). *Since we assign a weakly informative prior for \( H \) in model (2), sample paths of \( H \) are located around their center \( E(H) \in \mathcal{H}_D \) and finally converge to*
\( H_0^q \), where \( q = \arg\min_q d(H_0^q, E(H)) \), and \( d(f_1, f_2) = \left\{ \int_D [f_1(s) - f_2(s)]^2 ds \right\}^{1/2} \) is the \( L_2 \) distance. Hence posterior sampling of \( \beta^* \) from the constrained prior falls around \( q\beta_0 \) out of \( A \), and thus hardly converges to \( \beta_0 \) since \( \{\beta_0, H_0(t)^q, S_\xi(t^{1/q})\} \) is not the correct triplet of parameters. In addition, another normalization of fixing \( \beta_1 = 1 \) is not applicable as well since the constrained space is not a Stiefel manifold.

5 MCMC and prediction

According to above prior settings, nonparametric parameters \( H \) and \( S_\xi \) in MTM (2) are encapsulated in elements of \( \alpha \) and \( (p, \phi, \nu) \), respectively, where \( \alpha = \{\alpha_j\}_{j=1}^K \), \( p = \{p_l\}_{l=1}^L \), \( \phi = \{\phi_l\}_{l=1}^L \), and \( \nu = \{\nu_l\}_{l=1}^L \). Recall that \( \beta^* \in \mathbb{R}^p \) is the unconstrained vector of regression coefficients in MTM (2). Let \( \Theta = (\alpha, \beta^*, p, \phi, \nu) \) be the vector of all parameters. Then the posterior density is

\[
\pi(\Theta|\tilde{T}, Z, \delta) \propto \mathcal{L}(\Theta|\tilde{T}, Z, \delta)p(\alpha)p(\beta^*) \prod_{l=1}^L G_0(\psi_l, \nu_l),
\]

where \( \mathcal{L} \) is the likelihood for \( \Theta \) which is equivalent to (4) and both \( p(\cdot) \) represent prior densities. For each parameter in the posterior density, we set their priors as

\[
\alpha_j \sim \exp(\eta), \beta^* \sim N(0, 10^6 I_p), G_0(\psi_l, \nu_l) = G(1, 1) \times G(1, 1),
\]

\[
p_l = q_l \prod_{L=1}^{l-1} (1 - q_l), q_l \sim \text{Beta}(1, c), l = 1, \ldots, L - 1; p_L = 1 - \sum_{l=1}^{L-1} p_l.
\]

Here \( \eta \) is the parameter of the prior for \( \alpha \). One may either assign a hyperprior for \( \eta \) or fix it to a constant, referred to Supplement S.7.2 for sensitivity analysis of \( \eta \). Parameters \( \{q_l\}_{l=1}^L \) are latent variables for stick breaking construction of the DPM, and \( G(\theta, v) \) is the Gamma distribution with parameters \( \theta \) and \( v \). We fix \( c = 1 \) as default total mass parameter in BuLTM. For the base measure \( G_0 \), we recommend to fix it as that in (8) rather than assign it another hyperprior, referred to Supplement S.2 for justification.
We implement the NUTS by Stan as our MCMC sampler since Θ is continuous. NUTS is a tuning free extension of Hamilton Monte Carlo, which is robust and efficient for continuous-variable models. Stan becomes popular in recent years and appealing since it provides clear automatic posterior sampling procedures that needs no particular justification. Therefore, users are released from complicated probabilistic deriving and implementation. Our R package BuLTM is developed based on Stan.

For prediction purpose, the posterior predictive survival probability of a future observation \( T_0 \) given covariates \( Z_0 \) is an average of conditional predictions over the posterior distribution of Θ (Gelman et al., 2013, pp.7). Mathematically, \( S_{T_0|Z_0}(t) \) is the integral of product of conditional survival probability given Θ and \( \pi(Θ|\tilde{T}, Z, δ) \),

\[
S_{T_0|Z_0}(t) = \int S_{T_0|Z_0}(t|Θ)\pi(Θ|\tilde{T}, Z, δ)dΘ = \int [S_ξ\{H(t)\exp(-β^*^TZ_0)\}]\pi(Θ|\tilde{T}, Z, δ)dΘ,
\]

where \( S_ξ \) and \( H \) are expressed by elements of Θ as in (5) and (6), respectively. As mentioned in subsection 2.2, unidentified MTM (2) means that collections of triplets \((β^*, H, S_ξ)\) generate unique likelihood (4), which has the same form as \( S_{T_0|Z_0}(t|Θ) \). The uniqueness of \( S_{T_0|Z_0}(t|Θ) \) determines the uniqueness of \( S_{T_0|Z_0}(t) \), the posterior predictive survival probability of \( T_0 \), if the posterior \( \pi(Θ|\tilde{T}, Z, δ) \) is proper. Numerically, this integral is approximated by averaging all posterior samples. Suppose that we have drawn \( N \) samples of unconstrained \( β^* \) and sample paths of \( H \) and \( S_ξ \), denoted by \( β^{(i)*}, H^{(i)} \) and \( S^{(i)}_ξ \) respectively, for \( i = 1, \ldots, N \). Then the conditional survival probability \( S_{T_0|Z_0} \) and the conditional cumulative hazard \( Λ_{T_0|Z_0} \) are estimated respectively by

\[
\hat{S}_{T_0|Z_0}(t) = N^{-1}\sum_{i=1}^{N} S^{(i)}_ξ\{H^{(i)}(t)\exp(β^{(i)*}^TZ_0)\}, \quad \hat{Λ}_{T_0|Z_0}(t) = -\log(\hat{S}_{T_0|Z_0}(t)).
\]
6 Simulations

Extensive simulations are conducted to evaluate robustness of prediction of failure times by the proposed BuLTM method and performance of the estimate of fully identified $\beta$ under the nonparametric transformation model setting. We compare BuLTM with spBayesSurv by Zhou and Hanson (2018), which provides a unified two-step Bayesian route for fitting and selecting main stream transformation models of PO, PH and AFT. Details about reproducibility and simulation results in highly-censored cases are put into Supplements S.6.1 and S.6.2.

Simulated failure times are generated following model (2). Under each setting we generate 300 Monte Carlo replicates, each with sample size $n = 200$. The vector of regression coefficients is $\beta = (\beta_1, \beta_2, \beta_3)^T = (\sqrt{3}/3, \sqrt{3}/3, \sqrt{3}/3)^T$ such that $||\beta|| = 1$. For covariates $Z = (z_1, z_2, z_3)$, $z_1 \sim \text{Bin}(0.5)$ indicating a discrete/categorical variable, $z_2, z_3 \sim N(0, 1)$ as continuous variables with correlation coefficient 0.2, and $z_1$ is independent of $(z_2, z_3)$.

We assess the performance of BuLTM under four true model cases including PH, PO, AFT models, and a case where none of them is the true model.

**Case 1.** Non-PH/PO/AFT : $\xi \sim 0.5\text{Log-Normal}(0, 0.5) + 0.5\text{Weibull}(1.5, 1)$,

$$H(t) = (0.6t + 0.78t^{1/2} + 0.745)(0.5\Phi_{0.5,1}(t) + 0.5\Phi_{4.0,5}(t) - c_1), C \sim U(2, 4.5);$$

**Case 2.** PH model : $\xi \sim \exp(1)$,

$$H(t) = (t + 1.213t^{1/2} + 1.5)(0.5\Phi_{0.5,1}(t) + 0.5\Phi_{4.5,0.3}(t) - c_2), C \sim U(1, 5);$$

**Case 3:** PO model : $\xi \sim \text{Log-Logistic}(0, 1)$,

$$H(t) = (t + 1.213t^{1/2} + 1.5)(0.5\Phi_{1.0,5}(t) + 0.5\Phi_{4.5,0.3}(t) - c_3), C \sim U(3.5, 5);$$

**Case 4:** AFT model : $\xi \sim \text{Log-Normal}(0, 1), H(t) = t, C \sim U(2.5, 5).$

Here $\Phi_{\mu,\sigma}$ denotes the CDF of $N(\mu, \sigma^2)$, and $c_k$ is the constant such that $H(0) = 0$, for $k = \ldots$
1, 2, 3. The censoring variable $C$ is generated independent of $Z$, leading to approximately 27%, 29%, 24%, and 25% censoring rates respectively.

6.1 Prediction of conditional survival probability

We assess the accuracy of prediction of failure times and visualize predictive survival probability and cumulative hazard functions. Following (9), BuLTM computes the PPD by posterior samples of triplet $(H, S_\xi, \beta^*)$. Accuracy of prediction is assessed by the $L_2$ distance between real conditional survival curves and the PPD. Numerically, the $L_2$ distance is approximated by root integrated square error (RISE) on the observed time interval. The smaller RISE, the better for prediction. For each prediction scenario, we compare PPDs of three new observations with different sets of covariates: $Z_1 = (0, 0, 0)^T$, $Z_2 = (1, 1, 1)^T$, and $Z_3 = (0, 1, 1)^T$, respectively.

Table 1 shows that, under these three sets of new observations, BuLTM overwhelmingly outruns spBayesSurv in performance of predicting conditional survival probability under non-PH/PO/AFT, PH, and PO models, and is comparable with spBayesSurv under the AFT model. It is reasonable that BuLTM is superior to spBayesSurv in Case 1 since the non-PH/PO/AFT model is beyond the application scope of spBayesSurv; BuLTM still outperforms spBayesSurv with smaller $L_2$ distance under Cases 2 and 3, where the true model is PH and PO, respectively. In addition, for the first three cases, even for estimating baseline survival probability that determines the approach of spBayesSurv, which corresponds to the prediction case where all covariates are zero, BuLTM still surprisingly outplays spBayesSurv. spBayesSurv becomes the competitor of BuLTM under the true AFT model, which is a special case of the transformation model with the transformation function known and fixed. This might be an evidence that estimation of the transformation function plays a dominating role for prediction through transformation regressions.
Figure 2: The predicted conditional survival probability curve \( S(t) \) and the conditional cumulative hazard function \( \Lambda(t) \) for \( Z = (0, 0, 0)^T \); row 1: survival probability; row 2: cumulative hazard functions; row 3: tails of survival probability; column 1: Case 1; column 2: Case 2; column 3: Case 3; column 4: Case 4.

Table 1: The RISEs between the conditional survival curves and true curves predicted by \texttt{BuLTM} (MTM) and \texttt{spBayesSurv} under Cases 1 to 4. Data size \( n = 200 \).

| \( Z \) | \( Z_1 \) | \( Z_2 \) | \( Z_3 \) |
|---|---|---|---|
| Case 1: Non- PH/PO/AFT | 0.063 | 0.086 | 0.136 |
| Case 2: PH | 0.068 | 0.148 | 0.245 |
| Case 3: PO | 0.071 | 0.097 | 0.163 |
| Case 4: AFT | 0.142 | 0.122 | 0.221 |

Next, Figure 2 displays the predicted baseline survival probability curves and corresponding baseline cumulative hazard curves for Cases 1-4.

As shown in the first row of Figure 2, \texttt{BuLTM} fits baseline survival probability curves pretty well. In terms of baseline cumulative hazard curves shown in the second row, we find some deviation at tails in Cases 1 and 2. This is reasonable by the zoomed-in tail analysis of survival probability curves shown in the third row of Figure 2. Despite negligible bias in the tail of the survival probability, the corresponding cumulative hazard function deviates...
significantly as its log-transformation.

6.2 Parametric estimation

We evaluate the performance of parametric estimation for fully identified $\beta$ by the BuLTM method. We evaluate point estimation by following frequentist operating characteristics, average bias of estimates (BIAS), the square root of the mean squared error of the estimator (RMSE), the average posterior standard error (PSD), the standard error of the estimated values (SDE), and the coverage probability of the 95% credible interval (CP), as usual. Bias of BuLTM should be computed in a different way from spBayesSurv. In each replication of simulations, BuLTM provides an estimate of a unit vector. Note that, repeated estimates of element-wise mean of unit vectors is not a unit vector since for $v_1, \ldots, v_n \in \text{St}(1,p)$, $\|n^{-1}\sum_{i=1}^n v_i\| \leq 1$ by triangle inequality. We thus need to re-scale the mean vector into unit norm before we compute the element-wise bias.

Results of parametric estimation are summarized in Table 2 for Cases 1-3. Results under the AFT model is put into Supplement S.6.3. Case 1 is out of application scope of the spBayesSurv where none of PH, PO and AFT models provides reasonable parametric estimation, and hence we leave the place of assessment results blank. We find that parametric estimation given by BuLTM has little bias and the PSD is quite close to the SDE, and the CP is close to the nominal level in all cases. When the true model is one of PH and PO models, BuLTM has lower bias for almost all parameters and has lower RMSE for all parameters than spBayesSurv. These results demonstrate that BuLTM estimates the fully identified $\beta$ quite well.
Table 2: The performance of parametric estimation of BuLTM and spBayesSurv under Cases 1-3.

| Parameter | Case 1: Non-PH/PO/AFT | BuLTM | spBayesSurv |
|-----------|-----------------------|-------|-------------|
|           | BIAS | RMSE | PSD | SDE | CP | BIAS | RMSE | PSD | SDE | CP |
| β₁        | 0.005 | 0.065 | 0.066 | 0.065 | 94.3 | 0.012 | 0.169 | 0.174 | 0.167 | 94.0 |
| β₂        | -0.008 | 0.051 | 0.050 | 0.050 | 95.3 | -0.008 | 0.130 | 0.123 | 0.123 | 92.3 |
| β₃        | -0.013 | 0.052 | 0.050 | 0.051 | 91.7 | -0.005 | 0.130 | 0.122 | 0.124 | 94.0 |

Case 2: PH

| Method | Parameter | BIAS | RMSE | PSD | SDE | CP | BIAS | RMSE | PSD | SDE | CP |
|--------|-----------|------|------|-----|-----|----|------|------|-----|-----|----|
| BuLTM  | β₁        | -0.013 | 0.123 | 0.123 | 0.121 | 94.7 | 0.012 | 0.169 | 0.174 | 0.167 | 94.0 |
|        | β₂        | 0.006 | 0.083 | 0.087 | 0.081 | 95.0 | -0.008 | 0.130 | 0.123 | 0.123 | 92.3 |
|        | β₃        | 0.006 | 0.086 | 0.088 | 0.085 | 95.0 | -0.005 | 0.130 | 0.122 | 0.124 | 94.0 |
| spBayesSurv | β₁ | -0.032 | 0.172 | 0.175 | 0.170 | 95.0 | 0.002 | 0.258 | 0.256 | 0.259 | 94.7 |
|        | β₂        | -0.026 | 0.088 | 0.095 | 0.084 | 95.3 | 0.010 | 0.142 | 0.136 | 0.142 | 94.7 |
|        | β₃        | -0.027 | 0.102 | 0.095 | 0.098 | 93.0 | 0.013 | 0.135 | 0.136 | 0.135 | 95.0 |

Case 3: PO

We visualize obtained coverage of credible intervals given credibility at 25%, 50%, 75%, 90%, and 95%. Figure 3 shows plots of obtained coverage in Cases 1-3.

![Figure 3](image)

Figure 3: Coverage of credible intervals given different credibility; (a), Case 1; (b), Case 2; (c), Case 3.

We find that for Non-PH/PO/AFT and PH models, coverage of all parameters is close to nominal rates given different credibility; while for the PO model, coverage of β₂ has deviation under credibility levels 50% and 75%. It implies that the posterior sampled by
BuLTM describes the true posterior well and thus interval estimation is precise under almost all credibility levels.

7 Application to lung cancer data

We apply the BuLTM to gain more biological knowledge by analyzing two data sets from R package survival, veterans lung cancer data and Stanford heart transplant data. We analyze the former here and put results of the latter to Supplement S.8 since both have similar performance. The veterans lung cancer data set contains 137 patients from a randomised trial receiving either a standard or a test form of chemotherapy. In the study, the failure time is one of the primary endpoints for the trial and 128 patients were followed to death. This data set is renown and used in many demonstration of methodology in survival analysis (Song et al. (2007); Li et al. (2019); among others).

Our goals include prediction of failure times and computing relative risk scores, together with assessment. Likewise, we include six covariates, the first five of which are $Z_1 = \text{karno}/10$ (karnofsky score), $Z_2 = \text{prior}/10$ (prior treatment, with 0 for no therapy and 10 otherwise), $Z_3 = \text{age}/100$ (years), $Z_4 = \text{diagtime}/100$ (time in months from diagnosis to randomization), and $Z_5 = I(\text{treatment} = \text{test form of chemotherapy})$. The remaining is the covariate of cell type which has four categories, adeno, squamous, small cell, and large cell. Thus we include indicator variables to associate with time-to-death, that is, $Z_6 = I(\text{cell type} = \text{squamous})$, $Z_7 = I(\text{celltype} = \text{small})$, and $Z_8 = I(\text{celltype} = \text{large})$.

**Prediction** We predict conditional survival probability by BuLTM and compare its predictive capability with spBayesSurv. Our method is implemented by R package BuLTM. Recall that spBayesSurv fits three survival models first and then selects one, and it selects the PO model in this case. We evaluate the predictive capability of two methods by areas under the
time-dependent ROC(t) curve (AUC) for censored failure time, implemented by R package \texttt{survivalROC} \citep{Heagerty:2000}, where the continuous diagnostic marker is posterior predicted survival probability given by two methods. Figure 4(a) demonstrates superiority of \texttt{BuLTM} approach in predictive capability since the AUC(t) curve under the MTM is higher than any other three semiparametric survival models fitted by \texttt{spBayesSurv} almost everywhere on the follow-up time interval. Meanwhile, the AUC(t) curve by PO model is higher than other two models except months between 5th and 15th month, supporting the selection of the PO model for targeted data. To further check prediction difference between these two methods, we compare predicted survival probability curves of \texttt{BuLTM} and \texttt{spBayesSurv} on two new observations. Let these two new observations share different cell types, adeno and squamous respectively, same binary covariates $Z_2 = Z_5 = 0$, and same continuous covariates taking mean values of the data set.

![Figure 4](image)

Figure 4: Prediction comparison between BuLTM and spBayesSurv; (a), corresponding time dependent AUC(t) curves using survival probability as predictors; (b), predicted conditional survival probability curves given cell types adeno and squamous; the PO model is selected.

Figure 4(b) displays that the predicted conditional survival probability curves of \texttt{BuLTM} and \texttt{spBayesSurv} have slight deviations for cell type of squamous, while is close to each other for cell type of adeno. We may conjecture that the true survival model is not exactly but close to the PO model so that \texttt{BuLTM} and \texttt{spBayesSurv} have similar posterior predicted baseline survival probability (survival of patient with adeno cell type) while for
other conditional probability, they have slight deviations.

**Parametric estimation** We add the smoothed partial rank (SPR) estimator for the regression coefficient under the nonparametric transformation model setting into our comparison (Song et al., 2007). Results of estimated $\beta$ are given in Table 3.

Table 3: Results of estimated $\beta$ for veterans administration lung cancer data. Credible intervals are given on 95% credibility. The confidence interval of SPR is Wald-type and at 95% confidence level.

| Coefficient | BuLTM Estimate | Credible interval | spBayesSurv Estimate | Credible interval | SPR Estimate | Confidence interval |
|-------------|----------------|------------------|-----------------------|------------------|--------------|--------------------|
| $\beta_1$   | 0.119          | (0.045, 0.246)   | 0.617                 | (0.449, 0.800)   | 1            | -                  |
| $\beta_2$   | -0.302         | (-0.951, 0.897)  | -1.391                | (-8.597, 6.028)  | -0.626       | (-1.831, 0.579)    |
| $\beta_3$   | **-0.006**     | (-0.700, 0.671)  | **1.426**             | (-1.643, 4.477)  | **0.827**    | (-3.071, 4.725)    |
| $\beta_4$   | 0.081          | (-0.693, 0.730)  | 0.033                 | (-3.533, 3.469)  | -0.752       | (-7.320, 5.826)    |
| $\beta_5$   | -0.044         | (-0.227, 0.117)  | -0.147                | (-0.739, 0.487)  | -0.839       | (-1.878, 0.200)    |
| $\beta_6$   | 0.350          | (0.093, 0.694)   | 1.387                 | (0.396, 2.334)   | 2.764        | (0.469, 5.060)     |
| $\beta_7$   | **-0.005**     | (-0.242, 0.205)  | **0.058**             | (-0.739, 0.916)  | **0.082**    | (-0.771, 0.935)    |
| $\beta_8$   | 0.274          | (0.053, 0.571)   | 1.367                 | (0.444, 2.308)   | 2.642        | (1.446, 3.838)     |

All three methods are competitive and consistent in detection of significance of covariates. However, BuLTM is able to detect reasonable signs of coefficients of $\beta_3$ and $\beta_7$, which correspond to covariates $Z_3 = \text{age}/100$ and $Z_7 = I(\text{celltype} = \text{small})$, respectively. In Figure 5, we tempt to provide evidence of rationale of negative effects of $Z_3$ and $Z_7$ from the perspective of the Kaplan-Meier (K-M) estimator. Figure 5(a) shows that survival rate of individuals elder than 60 years old is lower than that of younger than 60 from the second month of the trial on, coincided with the common sense that aged have higher risk in mortality of lung cancer. Similar results are found in Li et al. (2019), where the nonlinear effect of age estimated by them is almost zero before age 65 and significantly negative.
after 65. Figure 5(b) shows that patients with small cell type tumor have lower survival rate than that with adeno tumor from the third month of the trial on, coincided with the review published on *The Lancet* that prognosis in small cell lung cancer is poor compared to non-small cell (van Meerbeeck et al., 2011). The negative effect of small cell type is also reported in Section 4 by Li et al. (2019).

![Figure 5: (a), K-M estimators for individuals elder and younger than 60 years old; (b), K-M estimators for small cell and cell of adeno.](image)

**Relative risk score** Relative risk scores are important in many situations such as examining the estimated hazard ratio (Van Houwelingen, 2007). The relative risk score induced by *BuLTM* is superior if it is evaluated by the area under the time-dependent ROC(t) curve (AUC) for censored failure time while the estimated relative risk score acts as the diagnostic marker.

![Figure 6: Time dependent AUC(t) computed by relative risk scores (a), method “K-M”; (b), method “NNE”.](image)

Figure 6 displays the comparison of approaches *BuLTM*, *spBayesSurv*, and SPR, where *BuLTM* is superior to the other two methods evaluated by both dynamic AUC metrics of
the K-M estimator and the nearest neighbor estimator (NNE) presented by Heagerty et al. (2000).

8 Discussion

In this article, we revisit the concept of Bayesian identifiability since it has been an inconclusive debate in the past decade. Our success in robust prediction of failure time based on unidentified NTMs provides an evidence that we may relax full identifiability to lack of identifiability but still able to do estimation and prediction well enough within the Bayesian workflow. This investigation is worthy in the current data era that is demanding in computational feasibility and tractability. For a broad range of unidentified models in other research environments, if full model identification brings large obstacles to computation, one may try to meet with Bayesian identifiability by assigning appropriate weakly informative priors so that prediction and other research targets are doable. Also we use the word “unidentifiability” but avoid confusion with “nonidentifiability” in Gelfand and Sahu (1999), where the likelihood is free of some parameters that are not identifiable.

The coupled R package BuLTM is a good competitor of spBayesSurv, which is possibly the best Bayesian method in existing literature designed to cover main specials of NTMs, PH, PO, and AFT models. The two-step spBayesSurv method is remarkable in handling large scale survival data with sample size more than 45000. Nevertheless, for the finite sample situations like moderate sample size 100 and above, BuLTM outperforms in prediction and parametric estimation is most cases and is expedient to output results of conditional survival probability, cumulative hazards, and relative risk scores, not restricting applications to aforementioned three mainstay transformation models. The superiority might be explained from three aspects. The first is the influence due to nonparametric priors used in these
two methods. **BuLTM** combines two weakly informative priors, the newly proposed quantile-knots I-splines prior for $H$ and the DPM prior for $S_\xi$ to compute PPDs; and **spBayesSurv** employs the transformed Bernstein polynomial (TBP) prior for baseline survival probability and transfers it to PPDs. However, the quantile-knots I-splines prior may be more effective in catching majority shape information of the PPD than the TBP prior, since it aggregates more knots on the majority of time intervals (referred to Figure 1) rather than the spirit of equally spaced knots in the TBP prior. The more knots, the more information. Secondly, for estimation of the fully identified parametric component, **BuLTM** enjoys lower RMSE than **spBayesSurv** since it incorporates the information of $||\beta|| = 1$, which significantly reduces the posterior variance after posterior projection. Finally, the excellent performance of **BuLTM** may owe to the use of the state-of-the-art NUTS algorithm, which is purely designed for sampling of continuous parameters, besides automatic “black-box” inference on top; whilst **spBayesSurv** has to design adaptive Metropolis samplers for discrete parameters to incorporate spatially referenced data.

A natural next step work may use the spirit of solving estimation of the NTM to estimation of single index models from the Bayesian perspective; another natural extension is to study random effects models where the nonparametric transformation acts as the functional random effect.

**SUPPLEMENTARY MATERIAL**

**Title:** Supplementary material for “Robust prediction of failure time through unified Bayesian analysis of nonparametric transformation models”. (PDF file)

**R-package:** The R package **BuLTM** is available in GitHub [https://github.com/LazyLaker](https://github.com/LazyLaker).

The code and real data for real world data analysis is uploaded.
S.1 Deriving $H(0) = 0$ from assumption (A3)

**Proof.** Suppose $H(0) = a > 0$ for a positive constant $a$. Then we have $Pr\{T > 0|Z\} = Pr\{H(T) > a|Z\} = Pr\{\xi \exp(\beta^T Z) > a\} = Pr\{\xi > a \exp(-\beta^T Z)\} = 1$. As a counterexample, we suppose $Z \sim N(0, 1)$, $\xi \sim \exp(1)$, $\beta = -1$. Let $Y = \exp(Z) \sim \text{Log-normal}(0, 1)$. Since $\xi$ and $Z$ are independent, we have $Pr\{\xi > a \exp(-\beta^T Z)\} = Pr\{\xi > aY\} = \int_0^{+\infty} \int_a^{\infty} \text{Log-normal}(y; 0, 1) \exp(-x)dydx < 1$, which contradicts the assumption that $\xi$ is independent of $Z$. Therefore, $H(0) = 0$. 

S.2 The DPM model for $S_\xi$

A regular Dirichlet process mixture (DPM) model (Lo, 1984) is assigned for $S_\xi$, the survival probability function of the positive random variable $\xi$. The DPM is a kernel convolution to the Dirichlet process (DP). We use the stick breaking representation for $G \sim \text{DP}(c, G_0)$ (Sethuraman, 1994)

$$G(\cdot) = \sum_{l=1}^{\infty} p_l \delta_{\theta_l}(\cdot), \theta_l \sim G_0, p_l \sim \text{SB}(1, c)$$

where $\delta(\cdot)$ is the point mass function, and SB is the stick-breaking representation. We call $G_0$ as the base measure and $c$ as the total mass parameter, acting as the center and precision of the DP, respectively.

Following the above stick-breaking representation, we construct the truncated DPM
priors for $S_\xi$ and $f_\xi$ with the Weibull kernel such that

$$S_\xi = 1 - \sum_{l=1}^{L} p_l F_w(\psi_l, \nu_l), f_\xi = \sum_{l=1}^{L} p_l f_w(\psi_l, \nu_l), p_l \sim \text{SB}(1, c), (\psi_l, \nu_l) \sim G_0,$$

where $L$ is the truncation number, and $F_w$ and $f_w$ denote CDF and density of Weibull distribution, respectively. We fix the truncation number $L$ rather than sampling it to simplify computation as a common strategy (Rodriguez et al., 2008). The truncation number $L$ is generally selected such that $e = 1 - \sum_{l=1}^{L-1} p_l$ is as small as possible. Ohlsson et al. (2007) suggests to use $L > 5c + 2$ since $e < 0.01$ under this truncation. We set $c = 1$ and thus the truncation number $L$ wouldn’t be too large. In our numerical studies we find an $L$ in the range of $10 - 15$ is appropriate to approximate the DPM model well. We also find the performance of model estimation is stable to the change of $L$ and $c$, so we fix these two parameters without any prior on them, which simplifies the posterior computation.

Let $G_0$ be the base measure for $(\psi_l, \nu_l)$. We recommend to choose $G_0 = G(1, 1) \times G(1, 1)$ as the specified base measure without any hyperprior for it. The setting of $G_0$ in our approach implies that $E\{F_\xi(t)\} = 1 - \exp(-t)$ i.e the nonparametric transformation model is centering around the PH model. Such elicitation of the DPM model is a weakly informative prior for $S_\xi$ since the variance of the DP is finite (Nieto-Barajas et al., 2012). Note that it is nontrivial to select the hyperprior for $G_0$. For the base measure in the DPM with Weibull kernel, Kottas (2006) proposed a Uniform-Pareto (Upar) prior and Shi et al. (2019) proposed a low information omnibus (LIO) prior, while neither of them is applicable to our method. The Upar prior is not applicable to our unidentified models since the Upar prior is noninformative to $(\psi, \nu)$; otherwise the MCMC algorithm can hardly converge. The LIO prior is a kind of hierarchical specification, which is too complicated to be incorporated into our method with heavy computation burden.
S.3 Relationship between the quantile-knots I-splines prior and the NII process

We summarize the relationship between the quantile-knots I-splines prior and the nonnegative independent increment process here. Let $s_0 = 0 < s_1 < s_2 < \cdots < s_J = \tau$ and we get $J$ disjoint partitions $[0, s_1], (s_1, s_2], \cdots, (s_{J-1}, s_J]$ of $D$. Note that each I-spline function starts at 0 in an initial flat region, increases in the mid region, and then reaches 1 at the end (Wang and Dunson, 2011b). Therefore, the range of all I-spline functions is $[0, 1]$. Then we determine the I-spline basis functions with knots $s_0 = 0 < s_1 < s_2 < \cdots < s_J = \tau$ and smoothness order $r > 1$ as \{\(B_j(t)\)\}_{j=1}^{K=J+r}$. We call two I-spline functions $B_{j_1}(t)$ and $B_{j_2}(t)$ are “joint” on a certain interval $D_i$ for $i = 1, \cdots, J$, if $\exists t' \in D_i$ such that $B_{j_1}(t'), B_{j_2}(t') \in (0, 1)$. Otherwise, they are “disjoint” on $D_i$. We also call an I-spline function $B_j(t)$ “crosses” an interval $D_i$ if $\exists t' \in D_i$ such that $0 < I_j(t_0) < 1$.

We divide all $K$ I-spline basis functions into $r$ groups. Among the $r$ groups, for $\iota = 1, \ldots, r$, the $\iota$th group consists of $B_{\iota}, B_{\iota+r}, B_{\iota+2r}, \ldots$ such that all I-spline functions in this group are disjoint. That is, for any $D_i$, only one of the I-spline functions within the $\iota$th group crosses the interval $D_i$. We define the combination of I-spline functions within the $\iota$th group as

$$H_\iota(t) = \sum_{k \geq 1} \alpha_{\iota+kr} B_{\iota+kr}(t).$$

Then $H_\iota(t)$ has independent increments among all knots $s_0 = 0 < s_1 < s_2 < \cdots < s_J = \tau$, if the coefficients \{\(\alpha_{\iota+kr}\)\}_{k \geq 1} are independent positive variables. Therefore, $H_\iota$, the combination of I-splines functions within the $\iota$th group is an NII process with independent increment on fixed locations (Phadia, 2015, pp.129). Then we rewrite the equation (6) in
the manuscript, the I-splines model into sum of $H_i$

$$H(t) = \sum_{j=1}^{K=J+r} \alpha_j B_j(t) = \sum_{i=1}^{r} H_i(t).$$

This equation clearly shows that the quantile-knots I-splines prior is combination of $r$ groups of NII processes. Specifically, when $r = 1$, all I-spline functions are disjoint and therefore, the combination of them reduces to the piecewise exponential model if $\alpha_j \sim \exp(\eta)$ independently. Actually, the first step of determining the initial knots in the quantile-knots I-splines prior is similar to the construction of the piecewise exponential prior in survival models, where partitions of time axis are often taken on empirical quantiles of observed failure times (de Castro et al., 2014).

S.4 Alternative I-splines priors for $H$

One may consider other alternative choices of parametric and nonparametric priors for the triplet $(\beta, H, S_\xi)$. Here we introduce some alternative choices of priors. It includes how to choose an identified priors such that the multiplicative transformation model frequency type identified. Another construction of I-splines prior with shrinkage prior for $H$ is also given here.

S.4.1 Fully identified priors

In this subsection we discuss the construction of identified priors. Our spirit is from Horowitz’s normalization conditions. Like the manuscript, we use the unit scale condition that $||\beta|| = 1$ as an equivalent condition of Horowitz’s scale normalization. Rather than applying posterior projection, we assign the uniform distribution on the $p$-dim unit hypersphere as the prior for the fully identified $\beta$. It is conducted by following transfor-
\[ \beta_\ast \sim N(0, I), \beta = \beta_\ast/||\beta_\ast||^{1/2}. \]

Still we need the location normalization, which assumes that the the \( H(t_0) = 1 \) or \( h(t_0) = 0 \) for some finite \( t_0 \) (Horowitz, 1996). We adopt the I-spline priors as our initial. We formulate \( H \) by
\[ H(t) = \sum_{j=1}^{K} \alpha_j I_j(t), \]
where \( K = J + r \) is the number of I-spline functions (see Section S.3). By the characteristic of I-spline functions on interval \( D = (0, \tau] \), if \( \sum_{j=1}^{K} \alpha_j = 1 \), \( H \) will surely pass the point \((\tau, 1)\). That is, for \( h = \log H \), we have \( h(\tau) = 0 \). Therefore, the location normalization condition is transferred to a sum-to-one restriction, that is, \((\alpha_1, \ldots, \alpha_K)\) is a \( K \)-dim simplex.

We consider two choices of priors for the \( p \)-dim simplex. The first one is the Dirichlet prior
\[ (\alpha_1, \ldots, \alpha_K) \sim \text{Dir}(a_1, \ldots, a_K), \]
where \( \{a_j\}_{j=1}^{K} \) are hyperparameters of Dirichlet distribution. Alternatively, we may consider a kind of transformed prior. For \( j = 1, \ldots, K \),
\[ \alpha_j^* \sim \exp(\eta), \alpha_j = \alpha_j^*/\sum_{j=1}^{K} \alpha_j^*. \]
Both these two priors normalize the location of \( H \) and therefore, fully identify the transformation function.

The above priors make the transformation model fully identified. However, with these priors, we find that the MCMC procedure by NUTS converges very slowly and suffers from poor mixing. What’s worse, the prediction accuracy is poor. These two drawbacks force us to not to work on a fully identified model.
S.4.2 The shrinkage prior and comparison

We here introduce the commonly used shrinkage priors for I-spline functions as an alternative of the proposed quantile-knots I-splines prior for $H$. All I-splines variant priors for $H$ and $H'$ has the same shell

$$H(t) = \sum_{j=1}^{K} \alpha_j B_j(t), \quad H'(t) = \sum_{j=1}^{K} \alpha_j B'_j(t).$$

However, unlike the proposed prior which selects knots from empirical quantiles of observed failure times, the traditional I-splines prior selects sufficiently many (usually from 10 to 30) equally spaced knots from the observed time interval (Cai et al. (2011); Wang and Dunson (2011b); among others). Then, to avoid overfitting due to using too many knots, one has to incorporate a shrinkage prior for the coefficients $\alpha_j$ to select appropriate I-spline functions. We here consider the truncated generalized double Pareto prior:

$$\alpha_j \sim N^+(0, \sigma_j^2), \quad \sigma_j \sim \exp(\eta_j), \quad \eta_j \sim \text{Ga}(\theta, \zeta),$$

where $N^+$ denotes the truncated Gaussian distribution such that $\alpha_j > 0$. This is a truncated form of the widely used generalized double Pareto prior as shrinkage prior for coefficients of basis functions (Gelman et al., 2013). In general, $\theta = \zeta = 1$ are typical default hyperparameters. In BuLTM, we further simplify this prior as $\sigma_j \sim \exp(1)$. The use of shrinkage prior for I-splines functions may be sensitive to the number of knots (Perperoglou et al., 2019). In our experience, as the number of knots increases, the computation burden of the shrinkage prior becomes heavier while it may not improve the accuracy of final model results. Therefore, the use of shrinkage priors may be accompanied with a time consuming tuning procedure to determine the best number of equally spaced knots. We compare the shrinkage prior using 15 equally spaced knots and the proposed quantile-knots I-splines prior under model setting Case 1 in the manuscript. Table 4 shows the parametric
estimation and root integrated square error (RISE) of estimated baseline survival probability functions using these two nonparametric priors in 100 Monte Carlo replications. We find that both priors provide similar estimation results whereas the proposed quantile-knots I-splines prior performs slightly better.

Table 4: Parametric estimation results employing two nonparametric priors for $H$ (standard deviation in bracket) and RISE of estimated baseline survival probability functions.

|          | Quantile-knots | Shrinkage  |
|----------|----------------|------------|
| $\beta_1 = 0.577$ | 0.579(0.070) | 0.581(0.069) |
| $\beta_2 = 0.577$ | 0.578(0.050) | 0.576(0.049) |
| $\beta_3 = 0.577$ | 0.575(0.050) | 0.574(0.050) |
| RISE      | 0.063          | 0.064      |

S.5 Proof of Corollary 1

Conditions required for Corollary 1 are quite mild. Conditions (i) is a general setting for right censored data. Conditions (ii) and (iii) are general settings for Bayesian analysis. Condition (iv) is satisfied in BuLTM by using the Weibull kernel in the DPM model. It is easily to show that both log-logistic and log-normal kernels fulfill this condition. Condition (v) is similar to condition (ii) in de Castro et al. (2014), which is a common condition within the survival context.

Proof. Let $\Theta = (\alpha, \beta^*, p, \phi, \nu)$ and $p(\Theta)$ be the product of priors of elements in $\Theta$. To show the posterior $\pi(\Theta)$ is proper is equivalent to show that $\int_{D_{\Theta}} \pi(\Theta)d\Theta < \infty$, where $D_{\Theta}$ is the domain of $\Theta$.

By condition (v), let $n_1$ be the number of uncensored observations and $n_0$ be the number
of censored observations such that \( n = n_1 + n_0 \), and then we have

\[
\mathcal{L}(\Theta) < \mathcal{L}^*(\Theta) \equiv \prod_{i=1}^{n_1} f_x \{ H(T_i) \exp(-\beta^*T_i) \} H'(T_i) \exp(-\beta^*T_i)
\]

\[
= \prod_{i=1}^{n_1} \sum_{j=1}^{K} \alpha_j B'_j(T_i) \exp(-\beta^*T_i) \sum_{i=1}^{L} p_j f_w \{ \exp(-\beta^*T_i) \sum_{j=1}^{K} \alpha_j B_j(T_i); \phi_i, \nu_i \}.
\]

By condition \((ii)\), we first integrate out all \( p_l \) and it remains to show that

\[
\mathcal{A}_i = \int_{D_{\Theta|\neg p_l}} \left\{ \prod_{i=1}^{n_1} \left[ \prod_{i=1}^{K} \alpha_j B'_j(T_i) \sum_{j=1}^{K} \alpha_j B_j(T_i) \right] \exp(-\beta^*T_i) \right\} d(\Theta - p_l) < \infty,
\]

for all \( l \), where \( \Theta - p_l \) denotes all parameters except \( p_l \) and \( D_{\Theta|\neg p_l} \) denotes corresponding domains.

By condition \((v)\), we can find \( p \) uncensored observations such that the \( p \times p \) matrix of their covariates, with each row being the vector of covariates of one observation, is full rank. Let \( Z^* \) denote that matrix and therefore \( Z^* \) is a one-on-one linear operation. Let \( \gamma = -Z^* \beta^* = (\gamma_1, \ldots, \gamma_p)^T \). Then we have

\[
\mathcal{A}_i \leq M_1 \int_{D_{\Theta|\neg p_l, \beta^*}} p(\Theta - p_l) \prod_{i=1}^{n_1} \exp(-\gamma_i) f_w \{ \exp(-\gamma_i) \sum_{j=1}^{K} \alpha_j B_j(T_i); \phi_i, \nu_i \} \]

\[
\times \sum_{j=1}^{K} \alpha_j \gamma_j'(T_i) \exp(-\gamma_i) \exp(-\gamma_i) \sum_{j=1}^{K} \alpha_j B_j(T_i); \phi_i, \nu_i \]

\[
\leq M_1 \int_{D_{\Theta|\neg p_l, \beta^*}} p(\Theta - p_l) \prod_{i=1}^{n_1} \int_{R^p} \exp(-\gamma_i) f_w \{ \exp(-\gamma_i) \sum_{j=1}^{K} \alpha_j B_j(T_i); \phi_i, \nu_i \} \]

\[
\times \sum_{j=1}^{K} \alpha_j B'_j(T_i) \exp(-\gamma_i) \exp(-\gamma_i) \sum_{j=1}^{K} \alpha_j B_j(T_i); \phi_i, \nu_i \}
\]

where \( M_1 \) is a constant. The first inequality is by condition \((iv)\) and the second inequality is by Cauchy–Schwarz inequality.

Let \( \alpha = (\alpha_1, \ldots, \alpha_K)^T, \phi_i = (B'_1(T_i), \ldots, B'_K(T_i))^T \) and \( \Phi_i = (B_1(T_i), \ldots, B_K(T_i))^T \).

For any \( T_i \) satisfying condition \((i)\), both \( ||\phi_i|| \) and \( ||\Phi_i|| \) are finite and if \( B_j(T_i) = 0, \)
$B_j'(T_i) = 0$. Therefore, under condition (i), $\alpha^T \phi_i / \alpha^T \Phi_i$ is a finite function of $\alpha \in R_+^K$. Since $\int_{-\infty}^{+\infty} \exp(-\gamma_i) f_w \{ \exp(-\gamma_i) \} d\gamma_i = 1$, hence,

$$B_i \leq M_2 \int_{D(\Theta|-p_l,\beta^*)} p(\Theta|-p_i) d(\Theta|-p_i) < \infty.$$

Therefore, the posterior is proper.

### S.6 Additional simulation results

We report additional simulations here. We first introduce the reproducibility of all simulations, and report results of simulations in highly-censored cases, results of parametric estimation under AFT models, results of effective sample size (ESS) given by BuLTM in simulations, and results of prediction and estimation on data sets with size 100.

#### S.6.1 Reproducibility of simulations

This subsection is about details for reproducibility of our simulation results. In all simulations, we run four independent parallel chains in BuLTM as the default setting in Stan. The length of each chain is 2500 with the first 500 iterations burn-in and we aggregate four chains to obtain totally 8000 posterior samples without any thinning. The MCMC procedure in spBayesSurv draws the same number of samples as ours. In all simulations we set $L = 12$ for the truncation number of DPM $v = 1$ for the total mass parameter, and $r = 3$ for the order of smoothness of I-spline functions. In case the censoring rate is higher than 50%, we use 5 initial knots; when the censoring rate is less than 50% we use 6 initial knots in constructing the quantile-knots I-splines prior. The coefficients $\{\alpha_j\}_{j=1}^K$ are assigned exponential prior with parameter 1. The credible interval of estimates given by BuLTM is the default central posterior interval in Stan; the credible interval of estimates...
given by \texttt{spBayesSurv} is the highest posterior density interval computed by \texttt{R} package \texttt{HDIInterval}. All numerical studies are realized in \texttt{R} 4.1.0 with \texttt{rstan} version 2.26.4.

S.6.2 Highly censored cases

We assess \texttt{BuLTM} under four cases with high censoring rates. These model settings are similar to the model settings used in the manuscript while the censoring rates are all higher 50%.

\textbf{HCase 1.} Non- PH/PO/AFT : $\xi \sim 0.55\text{LogNormal}(0, 0.5) + 0.45\text{Weibull}(1.5, 1)$,

$$H(t) = (0.8t + t^{1/2} + 0.825)(0.5\Phi_{0.5,0.2}(t) + 0.5\Phi_{3,0.5}(t) - c_1), C \sim \text{U}(2, 4.5);$$

\textbf{HCase 2.} PH model : $\xi \sim \text{exp}(1)$,

$$H(t) = (0.8t + t^{1/2} + 0.825)(0.5\Phi_{0.5,0.2}(t) + 0.5\Phi_{2.5,0.3}(t) - c_2), C \sim \text{min}(\text{exp}(1), 2.5);$$

\textbf{HCase 3:} PO model : $\xi \sim \text{log-logistic}(0, 1)$,

$$H(t) = H(t) = (0.8t + t^{1/2} + 0.825)(0.5\Phi_{0.5,0.2}(t) + 0.5\Phi_{2.5,0.3}(t) - c_3), C \sim \text{min}(\text{exp}(3/4), 3.5);$$

\textbf{HCase 4:} AFT model : $\xi \sim \text{log-normal}(0, 1), H(t) = t, C \sim \text{min}(\text{exp}(3/4), 5).$

Here $\Phi_{\mu,\sigma}$ denotes the CDF of $N(\mu, \sigma^2)$, and $c_k$ is the constant such that $H(0) = 0$, for $k = 1, 2, 3$. The censoring variable $C$ is generated independent of $Z$, leading to approximately 63%, 58%, 59%, and 61% censoring rates, respectively. For each prediction scenario, we compare PPDs of three new observations with sets of covariates: $Z_1 = (0, 0, 0)^T, Z_2 = (1, 1, 1)^T$ and $Z_3 = (0, 1, 1)^T$, respectively.

Table 5 shows that \texttt{BuLTM} still works well when the censoring rate goes high. We find that when the censoring rate is higher than 50%, \texttt{BuLTM} outperforms \texttt{spBayesSurv} under Non-PH/PO/AFT and PH models, is comparable under the PO model, and is slightly worse than \texttt{spBayesSurv} under the AFT model. This result is inline with results we report in the manuscript. Readers may wonder why \texttt{BuLTM} does not works well under the PO model. We
Table 5: The RISE between true conditional survival functions and functions predicted by BuLTm and spBayesSurv under HCases 1 to 4.

|       | HCase 1: Non- PH/PO/AFT | HCase 2: PH | HCase 3: PO | HCase 4: AFT |
|-------|-------------------------|-------------|-------------|--------------|
|       | BuLTm PH PO AFT         | BuLTm PH    | BuLTm PO    | BuLTm AFT    |
| $Z_1$ | 0.068 0.078 0.070 0.120 | 0.074 0.080 | 0.010 0.098 | 0.079        |
| $Z_2$ | 0.105 0.142 0.117 0.197 | 0.077 0.084 | 0.125 0.126 | 0.158 0.125 |
| $Z_3$ | 0.152 0.208 0.164 0.241 | 0.100 0.110 | 0.139 0.135 | 0.178 0.132 |

conjecture a possible reason is that the log-logistic distribution is heavy tailed and may be hard to approximated by the DPM. One future work is to model the distribution of model error $\xi$ though a more complicated nonparametric prior.

Results of parametric estimation are summarized in Table 6 for HCases 1-3. Case 1 is out of application scope of the spBayesSurv where none of PH, PO and AFT models provides reasonable parametric estimation, and hence we omit results of spBayesSurv. We find that parametric estimation given by BuLTm has little bias and the PSD is quite close to the SDE, and the CP is close to the nominal level in all cases. When the true model is one of PH and PO models, BuLTm has lower bias for almost all parameters and has lower RMSE for all parameters than spBayesSurv. These results demonstrate that BuLTm estimates the fully identified $\beta$ quite well.
Table 6: Results of estimation of $\beta$ by BuLTM and spBayesSurv in HCases 1 to 3.

| Parameter | BIASCUPEDCP | BIASCUPEDCP |
|-----------|-------------|-------------|
| $\beta_1$ | 0.003 0.098 0.092 0.097 94.0 | 0.003 0.072 0.067 0.071 92.0 |
| $\beta_2$ | 0.009 0.072 0.067 0.068 94.0 | 0.009 0.072 0.067 0.068 94.0 |

HCase2: PH

| Method | Parameters | BIASCUPEDCP | BIASCUPEDCP |
|--------|------------|-------------|-------------|
| BuLTM  | $\beta_1$  | 0.005 0.159 0.152 0.158 93.7 | 0.011 0.218 0.211 0.214 92.7 |
| spBayesSurv | $\beta_1$  | 0.018 0.240 0.227 0.240 92.0 | 0.000 0.335 0.315 0.335 94.7 |

S.6.3 Parametric estimation under AFT models

Results of parametric estimation are given by Table 7, where we find BuLTM has lower RMSE than spBayesSurv for all parameters. In terms of BIAS, BuLTM outperforms spBayesSurv in the highly-censored case and is comparable in the case with the lower censoring rate. This result as well as results of prediction demonstrate that BuLTM performs robustly under the AFT model.
Table 7: Results of estimation of $\beta$ under AFT models.

| Method    | Parameter | Case4: AFT1, 25% Censored |              | HCase4: AFT2, 61% Censored |
|-----------|-----------|---------------------------|--------------|---------------------------|
|           |           | BIAS          | RMSE         | PSD          | SDE          | CP          | BIAS          | RMSE         | PSD          | SDE          | CP          |
| BuLTM     | $\beta_1$ | 0.017         | 0.107        | 0.102        | 0.107        | 92.3        | 0.011         | 0.138        | 0.130        | 0.138        | 94.0        |
|           | $\beta_2$ | -0.009        | 0.079        | 0.076        | 0.076        | 92.3        | -0.004        | 0.101        | 0.095        | 0.098        | 93.0        |
|           | $\beta_3$ | -0.008        | 0.079        | 0.077        | 0.081        | 92.7        | -0.007        | 0.101        | 0.094        | 0.093        | 95.0        |
| spBayesSurv | $\beta_1$ | 0.000         | 0.159        | 0.150        | 0.159        | 90.3        | 0.016         | 0.207        | 0.194        | 0.206        | 92.0        |
|           | $\beta_2$ | 0.002         | 0.078        | 0.079        | 0.078        | 92.3        | 0.016         | 0.105        | 0.103        | 0.104        | 91.0        |
|           | $\beta_3$ | 0.003         | 0.084        | 0.079        | 0.084        | 92.0        | 0.014         | 0.101        | 0.103        | 0.100        | 93.7        |

S.6.4 Effective sample size of $\beta$

The effective sample size (ESS) is useful as first level checks when analyzing reliability of inference. It measures how many independent draws contain the same amount of information as the dependent posterior samples obtained by the MCMC procedure. ESS is usually accompanied with $\hat{R}$, the diagnostics of convergence of MCMC. In an MCMC procedure, especially the case where multiple chains are used, very low ESS may be caused by divergent chains or poor mixing and hence, large $\hat{R}$. If one obtains sufficient ESS (ESS that is greater then 400 is considered to be sufficient by Vehtari et al. (2021)) after sampling, it is highly possible that all chains are converged and well mixed. Therefore, we report ESS of $\beta$ in our simulation studies here as the diagnosis of MCMC.

Results of average estimated ESS of $\beta$ in all the simulation studies in the manuscript are given by Table 8, from which we find in each simulation the ESS of $\beta$ is sufficiently large. This is owed to the NUTS used by Stan, which is more possible to sample nearly independent draws (Hoffman and Gelman, 2014). In terms of other parameters, only a
few parameters suffer from low ESS in sporadic Monte Carlo replications as a drawback of analysis of unidentified models. Even so, the MCMC algorithm is still well converged and mixed examined by \( \hat{R} \) in \texttt{Stan} and thus the final model results are reasonable. Therefore, when using \texttt{BuLTM}, one can simply increase the length of MCMC chains to obtain sufficient ESS for all parameters in any situations regardless of the lack of identifiability. Particularly, if one’s interest falls on estimating \( \beta \), the vector of regression parameters, the length of chains needed is quite small, and the required computation burden is mild.

Table 8: The average estimated ESS of \( \beta = (\beta_1, \beta_2, \beta_3)^T \) in simulation studies.

|       | Case 1 | HCase 1 | Case 2 | HCase 2 | Case 3 | HCase 3 | Case 4 | HCase 4 |
|-------|--------|---------|--------|---------|--------|---------|--------|---------|
| \( \beta_1 \) | 5935.29 | 6201.22 | 6697.80 | 6187.15 | 6026.63 | 5744.58 | 7014.90 | 6431.38 |
| \( \beta_2 \) | 5573.79 | 6243.93 | 7305.17 | 6800.33 | 6697.69 | 6302.88 | 7497.02 | 6900.31 |
| \( \beta_3 \) | 5591.05 | 6193.69 | 7307.38 | 6757.07 | 6689.56 | 6263.12 | 7487.56 | 7053.08 |

**S.6.5 Simulations on data sets with size 100**

Additional simulations on data sets with size 100 are conducted to evaluate the performance of \texttt{BuLTM} on moderate data size. We considers the same setting of Case 1-4 in the manuscript for true models.

**Prediction** Table 9 summaries results of prediction performance, where we find \texttt{BuLTM} outperforms \texttt{spBayesSurv} in prediction when the true model is one of non-PH/PO/AFT, PH, and PO models with small data size, and is comparable with \texttt{spBayesSurv} when the true model is the AFT model. These results are consistent with that on data size of 200. It demonstrates that \texttt{BuLTM} still performs well on small data sets in prediction.
Table 9: The RISE between the true conditional survival functions and functions predicted by BuLTM (MTM) and spBayesSurv under Cases 1 to 4. Data size $n = 100$.

| Z         | MTM | PH  | PO  | AFT |
|-----------|-----|-----|-----|-----|
| $Z_1$     | 0.068 | 0.068 | 0.069 | 0.120 |
| $Z_2$     | 0.102 | 0.148 | 0.118 | 0.199 |
| $Z_3$     | 0.149 | 0.245 | 0.164 | 0.240 |

Table 10: The performance of parametric estimation of BuLTM and spBayesSurv under Cases 1-3 with size 100. spBayesSurv cannot provide reasonable estimation in Case 1 and we omit it.

| Case 1: Non-PH/PO/AFT | BuLTM | spBayesSurv |
|-----------------------|-------|-------------|
| Parameter             | BIAS  | RMSE        | PSD | SDE | CP  | BIAS  | RMSE        | PSD | SDE | CP  |
| $\beta_1$             | -0.006 | 0.098       | 0.095 | 0.097 | 93.7 | 0.022 | 0.238       | 0.250 | 0.237 | 97.3 |
| $\beta_2$             | -0.010 | 0.074       | 0.069 | 0.071 | 94.3 | 0.008 | 0.135       | 0.136 | 0.135 | 95.7 |
| $\beta_3$             | 0.016  | 0.074       | 0.068 | 0.069 | 93.7 | 0.011 | 0.143       | 0.138 | 0.143 | 95.7 |

Parametric estimation Table 10 summarizes results of parametric estimation on data sets with size $n = 100$ under model settings of non-PH/PO/AFT, PH, and PO, where we find the BIAS and RMSE are low, the PSD is close to SDE, and the CP is close to the
nominal rate of credibility. Compared to spBayesSurv, BuLTM has lower BIAS under the PH model, and is comparable under the PO model.

S.7 Sensitivity analysis

We analyze sensitivity of the proposed quantile-knots I-splines prior for $H$ in this section. There are two pre-specified hyperparameters in the prior, the hyperparameter $\eta$ for the exponential prior, and the number of initial knots. Here we show that the final prediction results is not sensitive to either the initial number of initial knots or the hyperparameter $\eta$.

S.7.1 Sensitivity of number of initial knots in the quantile-knots I-splines prior

Sensitivity analysis of the choice of initial number of basic knots ($N_I$) in the quantile-knots I-splines prior is conducted by 100 Monte Carlo studies under Case1 setting in the manuscript. Candidates for the number of initial knots are taken from range 5 to 11, where we display results of using 5, 6 and 11 initial knots here for comparison. Results of parametric estimation and the RISE of estimated baseline survival probability curves among different number of initial knots are shown in Table 11, where we find with different choices of $N_I$, both results of parametric estimation and RISE of estimated survival probability curves have very mild variation. Figure 7 displays plots of average estimated baseline survival probability curves under three choices of number of initial knots, where we find they are close to each other. This sensitivity analysis numerically demonstrates that the quantile-knots I-splines prior is not sensitive to its choice of number of knots. And therefore, it is generally tuning-free and computationally expedient.
Table 11: Parametric estimation results (standard deviation in bracket) and RISE of estimated baseline survival probability functions under different choices of $\eta$.

|         | $N_I = 5$       | $N_I = 6$       | $N_I = 11$       |
|---------|-----------------|-----------------|-----------------|
| $\beta_1 = 0.577$ | 0.578(0.070) | 0.580(0.070) | 0.586(0.069) |
| $\beta_2 = 0.577$ | 0.575(0.051) | 0.575(0.051) | 0.572(0.052) |
| $\beta_3 = 0.577$ | 0.561(0.058) | 0.560(0.058) | 0.557(0.058) |
| RISE    | 0.063           | 0.063           | 0.066           |

Figure 7: Pointwise mean estimated baseline survival probability curves under 100 replications. Real line, $N_I = 5$; dash line, $N_I = 6$; dotted line, $N_I = 11$.

S.7.2 Sensitivity of $\eta$ in the quantile-knots I-splines prior

Let $\eta$ be the hyperparameter of exponential prior for coefficients of the quantile-knots I-splines prior in equation (8) in the manuscript. Sensitivity analysis of $\eta$ is conducted under the setting Case1 in the manuscript. For the sensitivity of $\eta$, among 100 Monte Carlo replications, we choose $\eta$ from three candidates of $\eta = 1, 5, 0.2$, corresponding to three levels of informative priors. Notice that we should avoid using too small $\eta$ since it implies too large prior variance, then the prior is not sufficiently informative anymore. Similarly, too large $\eta$ induces too small variance, which is too informative to provide sufficient uncertainty.
Results of parametric estimation and RISE of estimated baseline survival curves are given in Table 12. From the table we find that estimation to the parametric component varies quite little among all choices of $\eta$ and the RISE of estimated baseline survival curves is almost the same with different values of $\eta$. For visualization, plots of estimated survival curves given different values of $\eta$ are shown in Fig 8, where we find all estimated curves are close to each other. This sensitivity analysis numerically demonstrates that the quantile-knots I-splines prior is not sensitive to the choice of $\eta$ within the range 0.2 to 5. Therefore, it is safe to fix $\eta$ rather than to assign hyperprior for it.

Table 12: Parametric estimation results (standard deviation in bracket) and RISE of estimated baseline survival probability functions under different choices of $\eta$.

|       | $\eta = 1$ | $\eta = 5$ | $\eta = 0.2$ |
|-------|-------------|-------------|---------------|
| $\beta_1 = 0.577$ | 0.580(0.070) | 0.571(0.071) | 0.592(0.068) |
| $\beta_2 = 0.577$ | 0.575(0.052) | 0.578(0.051) | 0.569(0.052) |
| $\beta_3 = 0.577$ | 0.560(0.058) | 0.564(0.057) | 0.553(0.059) |
| RISE   | 0.063       | 0.064       | 0.065         |

Figure 8: Pointwise mean estimated baseline survival probability curves in 100 replications. Real line, $\eta = 1$; dash line, $\eta = 5$; dotted line, $\eta = 0.2$. 
S.8 Application to Stanford heart transplant data

We apply BuLTM to analyse the Stanford heart transplant data included in R package survival. The data set records patients on the waiting list for the Stanford heart transplant program. In this example, we study the time-to-death of patients who did not receive heart transplant and remove those who received heart transplant, which are considered as left truncated observations. Finally, we have $n = 103$ patients, and 73 of them are censored. We include two covaraites previously processed by R, which are $Z_1 =$ age $- 48$ (age-48 years) and $Z_2 = I$(prior) (prior surgery).

**Prediction** Similarly, we predict conditional survival probability by BuLTM and compare its predictive capability with spBayesSurv. In this case, spBayesSurv selects the AFT model. We evaluate the predictive capability of two methods by areas under the time-dependent ROC($t$) curve (AUC) for censored failure time, where the continuous diagnostic marker is posterior predicted survival probability given by two methods. Figure 9(a) demonstrates superiority of BuLTM approach in predictive capability in this case because of the higher AUC($t$) curve. Meanwhile, we don’t find clear difference between the three semiparametric models fitted by spBayesSurv in prediction. To further check their prediction results, we compare posterior predicted survival probability of BuLTM and spBayesSurv on two new observations, one accepted prior surgery while the other not. Let the two new observations have the same age of the mean age of the data set. Figure 9(b) displays that the predicted conditional survival probability curves of BuLTM and spBayesSurv have deviations in prediction of two new observations. We conjecture the true model might not be any one of PH, PO or AFT models. We will further check results of parametric estimation.
Figure 9: Prediction comparison between BuLTM and spBayesSurv; (a), corresponding time dependent AUC(t) curves using survival probability as predictors; (b), predicted conditional survival probability curves with and without prior surgery; the AFT model is selected.

Table 13: Results of estimated $\beta$ for the analysis to Stanford heart transplant data.

| Parameter | BuLTM      | 95%CI       | spBayesSurv | 95%CI       |
|-----------|------------|-------------|-------------|-------------|
| $\beta_1$ | -0.052     | (-0.433, 0.032) | -0.028     | (-0.085, 0.029) |
| $\beta_2$ | 0.816      | (-0.998, 0.999) | 0.704      | (-1.110, 2.871) |

**Parametric estimation** Table 13 shows results of estimated $\beta$ by BuLTM and spBayesSurv. Both estimates and detection of significance are similar by these two methods. One may wonder that the marginal posterior mean of BuLTM is not centering at the posterior interval. Owing to the posterior projection, the marginal projected posterior of $\beta$ is not normal anymore, but rather, skewed.

**Relative risk score** We assess relative risk scores by areas under time-dependent $ROC(t)$ curves (AUC) for censored failure time. Figure 10 displays the comparison of approaches BuLTM and spBayesSurv, where BuLTM is superior by both dynamic AUC merits. Mean-
while, we find that under the NNE method, the AUC($t$) curve given by the AFT model is higher than the other two models, and all three models have comparable AUC($t$) curves, supporting the selection of the AFT model.

![Graph](image)

**Figure 10:** time dependent AUC($t$) computed by relative risk scores (a), method “K-M”; (b), method “NNE”.

### S.9 Posterior checking

We mitigate unidentifiability of the NTM by assigning weakly informative priors for both $H$ and $S_\xi$, which are not fully objective priors. One may worry whether these priors are so informative that the prior-to-posterior updating is not driven by data. We conduct posterior checking on simulation studies and application examples to check difference between priors and marginal posterior and obtain similar results. Here we take our application to veterans lung cancer data set as an example. We take $\alpha_j \sim \exp(1)$ for $j = 1, \ldots, K$ as weakly informative priors and $p(\beta^*) \propto 1$ as flat priors. Figure 11 compares priors and marginal posterior of first eight coefficients of I-spline functions. For all $\{\alpha_j\}_{j=1}^8$, their variance is controlled by the weakly informative prior, demonstrating the fact that impact of priors remedies the flat likelihood. In addition, most of I-splines coefficients vary significantly.
from the prior, evidencing that the prior-to-posterior updating is driven by data.

Figure 11: Comparison between the marginal posterior density and priors of $\alpha_1, \ldots, \alpha_8$. Shaded region, marginal posterior density; Wide line, prior density of $\exp(1)$.

Note that comparing prior and posterior of the fully identified parameter $\beta$ is meaningless since the projected posterior of $\beta$ is certainly different from priors of $\beta^*$. Therefore, in terms of the parametric component, we compare with priors and marginal posterior of $\beta^*$, the unconstrained parameter sampled from MCMC. Fig 12 shows apparent difference between flat priors and marginal posterior of $\beta^*$, which also demonstrates the data driven procedure. An interesting finding is that, although $\beta^*$ is unidentified, some of parameters such as $\beta_1$ and $\beta_5$ have low posterior variance and posterior intervals that are short enough. This supports the fact that we mitigate unidentifiability through weakly informative non-parametric priors. Meanwhile, we are aware of the necessity of posterior modification by checking marginal posterior of $\beta^*$, since posterior of $\beta_2$ and $\beta_4$ has long tails and wide posterior interval, which is not reliable (Gelman et al., 2013, pp.221).
Figure 12: Comparison between the the marginal posterior density of $\beta^*$ without posterior projection and corresponding priors. Shaded region, posterior density; Wide line, flat prior.

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