Better Approximate Inference for Partial Likelihood Models with a Latent Structure

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Abstract

Temporal Point Processes (TPP) with partial likelihoods involving a latent structure often entail an intractable marginalization, thus making inference hard. We propose a novel approach to Maximum Likelihood Estimation (MLE) involving approximate inference over the latent variables by minimizing a tight upper bound on the approximation gap. Given a discrete latent variable $Z$, the proposed approximation reduces inference complexity from $O(|Z|^c)$ to $O(|Z|)$. We use convex conjugates to determine this upper bound in a closed form and show that its addition to the optimization objective results in improved results for models assuming proportional hazards as in Survival Analysis.

1 Introduction

Temporal Point Processes (TPPs) provide a formal framework to model the occurrences of discrete events in time (like failures or financial transactions). Recent work ([Linderman and Adams, 2014] [Snoek et al., 2013]) on modelling TPPs with latent factors have showcased their ability to capture correlations such as inhibitory relationships & a dichotomy of classes of neurons in neural spike recordings. Although, there have been several advances in non-parametric Bayesian inference ([Samo and Roberts, 2015]) most models are parametric ([Cox, 1955]) where parameter estimation is done by maximizing the likelihood of observed point values. Survival analysis is the problem of estimating survival times for entities (like nodes in a machine) and it has largely relied on TPPs to estimate survival times in the presence of censored observations. Semi-parametric methods like the Cox Proportional Hazards (CPH) [Cox, 1955] allow parametric estimation using a partial likelihood objective without estimating the baseline hazard. Therefore, we propose an approximate inference strategy for latent variable models with a partial likelihood objective. We introduce an inference method for models where the normalization factor includes interactions over log-linear factors. Such models are common in TPPs assuming proportional hazards ([Rosen and Tanner, 1999]) or in latent Conditional Random Fields (CRFs) where the normalization involves a sum over finite potential functions ([Sutton et al., 2012]). [Rosen and Tanner, 1999] introduce an inference strategy for CPH which is similar to our proposed method, but they fail to identify cases where the approximation fails. Although our inference strategy is applicable to all likelihood in a TPP, we focus on its impact in the case of partial likelihoods since the objective there is closely related to the MLE objectives observed in latent CRFs, thus making our work applicable to a broader class of problems.

Inspired by [Jebara and Choromanska, 2012] we introduce a distribution agnostic closed form tight upper bound on likelihood estimations for TPPs resembling [Diggle, 2005]. The upper bound can be minimized via standard gradient descent based iterative methods [Ruder, 2016]. Finally, we prove a tight upper bound on the Jensen inequality for strictly convex polynomial functions on $\mathbb{R}_{++}$.

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2 The Inference Problem

Given a compact set $S$ equipped with Borel $\sigma$-algebra $\mathbb{B}(S)$, $X(t) : \Omega \rightarrow \Gamma$ is a TPP if $X(t)$ is a measurable transform from the probability space $(\Omega, \mathcal{F}, \mathbb{P})$ to the space of counting measures $\Gamma$ on $S$. Given a series of events $\{ (\delta_i, x_i, t_i) \}_{i=1}^{N}$; for a given event $x_i$ the event of interest occurred $(\delta_i = 1)$ at time $t_i$ or the observation was censored $(\delta_i = 0)$. The risk set for $x_i$ is given by $R(t_i) = \{ x_j : t_j \geq t_i \}$. Under a Poisson TPP with intensity $\lambda(x)$, the likelihood of the event $\delta_i = 1$ for $x_i$ at $t_i$ given that the event hasn’t occurred till $t_i$ is given by $\mathbb{P}(\delta_i = 1) = \frac{\lambda(x_t)}{\int_B \lambda(x)dx}$. Once again we use the Taylor series approximation to eq. 3 to a finite set of factors from $R(t_i)$ (closely resembling latent CRFs [Quattrom et al., 2007] in likelihood estimation).

We modify the formulation by adding latent variables $z$ (see Figure 1) and now the intensity function in the TPP is function of parameters $\beta$, input $x_i$ and latent variable $z_i \sim p(z_i, \theta)$. [Rosen and Tanner, 1999] and [Diggle, 2005] used partial likelihood models to efficiently compute the MLE estimates for the parameters in an inhomogenous Poisson process. Partial likelihood was first introduced by [Cox, 1955] with the aim of identifying variables that impact survival analysis without worrying about the baseline hazard. For the same reasons, we choose to maximize the partial likelihood of an event $(\delta_i, x_i, t_i)$ conditioned on the risk set $R(t_i)$. Thus the denominator in eq. 1 now involves a sum over a finite set of factors from $R(t_i)$ (closely resembling latent CRFs [Quattrom et al., 2007] in likelihood estimation).

![Diagram](image)

\[ \mathbb{P}(\delta_i | x_i, R(t_i), \beta) = \mathbb{E}_{z_i \sim p(z_i|x_i)} \left[ \frac{\exp \beta x_i^T}{\sum_{j \in R(t_i)} \exp \beta z_j^T x_j} \right] \] (1)

3 Approximate Inference Solution

In this section we provide a computationally tractable approximation for the maximum-likelihood estimation of the semi-parametric latent variable model defined in section 2 and in section 4 we show the conditions under which the approximation is tight. Assuming $z_i \perp z_{j \neq i} | x_i, x_j$ we can define positive random variables (R.V.) $\alpha_{z_i}$ and $\eta_{z_i}$, which are functions of $\beta$, $R(t_i)$ & $z$. This assumption implies that $\alpha_{z_i} \perp \eta_{z_{j \neq i}} | x_i, x_j$. In the rest of the paper (unless stated otherwise), the expectation $\mathbb{E}$ is over the distribution $z_i \sim p(z_i | \theta, x_i)$. Using this re-formulation and the Taylor series expansion we can re-write eq. 1 as,

\[ \alpha_{z_i} = \exp \beta x_i^T, \quad \eta_{z_{j \neq i}} = \sum_{j \in R(t_i)} \exp \beta x_j^T \] (2)

\[ \mathbb{E} \left[ \frac{(\alpha_{z_i} + \eta_{z_{j \neq i}})}{\alpha_{z_i}} \right]^{-1} = \mathbb{E} \left[ \sum_{p=1}^{\infty} (-1)^p \mathbb{E}(\eta_{z_{j \neq i}})^p \mathbb{E}(\alpha_{z_i}^{-p}) \right] \approx \left[ \sum_{p=1}^{K} (-1)^p \mathbb{E}(\eta_{z_{j \neq i}})^p \mathbb{E}(\alpha_{z_i}^{-p}) \right] \] (3)

**Lemma 1.** If we assume $\alpha_{z_i}, \eta_{z_{j \neq i}}$ to have moments of order $\mathcal{H}_{\alpha_{z_i}}, \mathcal{H}_{\eta_{z_{j \neq i}}}$ respectively, then their ratio distribution will have moments of order $\mathcal{H}_{\alpha_{z_i}} + \mathcal{H}_{\eta_{z_{j \neq i}}}$, [Cedilnik et al., 2006]

Using the Mellin Transform theory for ratio distributions of positive independent random variables (R.V.); we have $\mathbb{E}(X/Y)^p = \mathbb{E}(X^p) \mathbb{E}(Y^{-p})$. Based on lemma 1 we limit the expansion in eq. 3 to a finite $K$. At this point, we are computing expectations over convex functions $x^p$ and $x^{-p}$ with $p > 0$ (defined on $\mathbb{R}_{++}$). Since for a convex $f$, $E(f(x)) \geq f(E(x))$ (Jensen inequality) we can further approximate eq. 3 with eq. 4. Once again we use the Taylor series approximation to finally arrive at a tractable maximum-likelihood objective (eq. 5). For each data point the inference complexity under the original objective is $\mathcal{O}(|z|^{1|R(t_i)|})$ whereas under the proposed marginalization the complexity reduces to $\mathcal{O}(|z|)$.

\[ \mathbb{E} \left[ \frac{(\alpha_{z_i} + \eta_{z_{j \neq i}})}{\alpha_{z_i}} \right]^{-1} \approx \sum_{p=1}^{K} \mathbb{E}(\eta_{z_{j \neq i}})^p \mathbb{E}(\alpha_{z_i})^{-p} \] (4)
\[
P(\delta_i | x_i, R(t_i), \beta) = \left[ \frac{\mathbb{E}_{z_i \sim p(\cdot | \theta, x_i)}(\exp \beta_{z_i}^T x_i)}{\sum_{j \in R(t_i)} \mathbb{E}_{z_j \sim p(\cdot | \theta, x_j)}(\exp \beta_{z_j}^T x_j)} \right]^{\delta_i}
\]

(5)

The crux of the approximation lies in the Jensen inequality. Therefore, we spend the following section on identifying a tight distribution independent bound on the inequality gap. If this inequality gap is reduced then we know that 5 is a good approximation for 1.

4 Bounding the Approximation [Analysis]

We identify the conditions under which the approximation 3 is feasible and provide a closed form bound for it. In order to simplify the statements in the rest of the paper, we introduce some notations and assumptions here. We assume that the R.V. \( z_i \sim p_0 (\cdot | x_i) \) has mean \( \mu(x_i) \) and \( z_i - \mu(x_i) \) is sub-Gaussian with parameter \( \sigma(x_i) \). This assumption is fairly common in latent variable models where the true posterior \( p(z_i | x_i) \) is approximated by a Gaussian distribution \( N(\mu(x_i), \sigma(x_i)) \).

For a continuous function \( \beta_{z_i} = \beta(z_i) \), with \( z_i \) lying in a closed, bounded set (with probability \( \delta \)), one can bound the values attained by \( \exp \beta_{z_i}^T x_i \). Thus for a R.V. \( z_i \) we obtain reasonable probabilistic bounds on \( \alpha_{z_i}, \eta_{z_i} \), formalized by the following statement: \( \alpha_{z_i} \in [\mathcal{L}(\alpha_{z_i}), \mathcal{U}(\alpha_{z_i})], \eta_{z_i} \in [\mathcal{L}(\eta_{z_i}), \mathcal{U}(\eta_{z_i})] \) with probability \( \delta \) (defined in theorem 1).

**Theorem 1.** Although this is stated for \( \alpha_{z_i} \), the statement for \( \eta_{z_i} \) is similar.

With probability \( \delta = \operatorname{erf} \left( \frac{1}{2} \frac{\mathcal{U}(\alpha_{z_i}) - \exp \beta_{z_i}^T \mu(x_i)}{\sqrt{2} \sigma(x_i) (\exp \beta_{z_i}^T \mu(\cdot)) \| \beta_{z_i} \|_2} \right) - \operatorname{erf} \left( \frac{1}{2} \frac{-\mathcal{L}(\alpha_{z_i}) - \exp \beta_{z_i}^T \mu(x_i)}{\sqrt{2} \sigma(x_i) (\exp \beta_{z_i}^T \mu(\cdot)) \| \beta_{z_i} \|_2} \right) \),

\[
\mathbb{E}(\phi_p(\alpha_{z_i})) - \phi_p(\mathcal{E}(\alpha_{z_i})) \leq \kappa \phi_p(\mathcal{U}(\alpha_{z_i})) + (1 - \kappa) \phi_p(\mathcal{L}(\alpha_{z_i})) - \phi_p(\kappa \mathcal{U}(\alpha_{z_i}) + (1 - \kappa) \mathcal{L}(\alpha_{z_i}))
\]

(6)

\[
\kappa = \nabla \phi \star \left[ \frac{\phi_p(\mathcal{U}(\alpha_{z_i})) - \phi_p(\mathcal{L}(\alpha_{z_i}))}{\mathcal{U}(\alpha_{z_i}) - \mathcal{L}(\alpha_{z_i})} \right]
\]

(7)

The conjugate \( \phi_p^*(y) = \sup_x y^T x - \phi_p(x), \nabla \phi_p^*(y) = \{ x : y^T x - \phi_p(x) = \phi_p^*(y) \} \), is a singleton set for strictly convex functions.

5 Joint Objective Function

Since gradients for conjugate functions \( \phi_p^*(x) \) are well defined in our case (see Appendix A.2), we can show that the approximation in eq. 5 is good when the joint objective is minimized (eq. 8). The joint objective enforces the model to find optimal \( (\theta^*, \beta^*) \) that maximizes the likelihood in eq. 1, while ensuring proximity to the true objective. Eq. 8 can also be viewed from the perspective of a regularized objective where the model learns to enforce additional constraints on the variance of \( \alpha_{z_i}, \eta_{z_i} \), and thus ends up with distributions of \( z_i \) with rapidly decaying Gaussian tails.

\[
(\beta^*, \theta^*) = \arg \min_{\beta, \theta} \sum_{i=1}^{N} \left[ \frac{\mathbb{E}_{z_i \sim p(\cdot | \theta, x_i)}(\exp \beta_{z_i}^T x_i)}{\sum_{j \in R(t_i)} \mathbb{E}_{z_j \sim p(\cdot | \theta, x_j)}(\exp \beta_{z_j}^T x_j)} + \sum_{j \in R(t_i)} L(x_j, \kappa_j, \theta, \beta) \right]
\]

(8)

Here \( L(x_j, \kappa_j, \theta, \beta) \) is obtained by using theorem 1 which bounds the Jensen’s inequality for each data point \( (\delta_i, x_i, t_i) \), via a sum over gradients computed for the functions \( \phi_p^* \).

6 Results

We analyze two types of results: (1) we evaluate our combined objective (eq. 8) on a proportional hazards (CPH) model and show an improvement in the concordance-index (table 1), (2) we compare our proposed distribution agnostic bound against a standard bound for the Jensen inequality [Dragomir, 1999].

6.1 Survival Analysis

Given a discrete \( z \) model the distribution \( z_i \sim p(\cdot | \theta, x_i) \) to be a multinomial. The final layer of the input encoder network is a softmax operation ensuring that the distribution over the latent
space of $z$ is a valid one. We compare our models: Latent Variable CPH via Hard/Soft Gating (LV-CPH-HG/LV-CPH-SG) against three popular baselines: CPH [Cox, 1955], RSF [Ishwaran and Lu, 2007], DEEPSURV [Katzman et al., 2016] on common datasets in survival analysis: METABRIC [Yao, 2014], ROTTERDAM-GBSG [Schumacher et al., 1994], SUPPORT [Knaus et al., 1995]. For the discrete case, it is easy to see that the regularizer $L(x_i, \kappa_i, \theta, \beta)$ in eq. 8 is minimized when $z_i$ has low variance (or entropy). We enforce a low entropy distribution by gating (soft/hard) the predictions $p(\cdot | \theta, x_i)$ obtained from the softmax layer. Since for the discrete case, low entropy ($H_{z_i}$) on $z_i \iff |L(\alpha_{z_i}) - U(\alpha_{z_i})| + |L(\eta_{z_i}) - U(\eta_{z_i})| < C$ and $C \to 0$ as $H_{z_i} \to 0$, one can instead minimize $H_{z_i}$ to effectively reduce the upper bound in theorem 1. Therefore, we conclude that optimizing for the joint objective function in eq. 8 instead of the mere approximation in eq. 5 leads to an improved concordance-index for CPH models.

6.2 Tightness of the proposed bound

Figure 2 compares the bound computed by [Dragomir, 1999] [baseline] (Appendix A.1) against our tight bound (Appendix A.2), by sampling $U(\alpha_{z_i}), U(\eta_{z_i}), L(\alpha_{z_i}), L(\eta_{z_i})$ from distinct fixed normal distributions. Our bound is much tighter for smaller values of $p$, and it converges to the baseline’s value for large $p$. Looking at figure 3 it is easy to verify that the bound we propose on Jensen’s inequality is stronger than the baseline.

| MODEL       | METABRIC     | ROTTERDAM-GBSG | SUPPORT          |
|-------------|--------------|----------------|-----------------|
| CPH         | 0.6306 ± 0.004 | 0.6578 ± 0.004 | 0.5828 ± 0.002  |
| DEEPSURV    | 0.6434 ± 0.004 | 0.6684 ± 0.003 | 0.6183 ± 0.002  |
| RSF         | 0.6243 ± 0.004 | 0.6512 ± 0.003 | 0.6130 ± 0.002  |
| LV-CPH-SG   | 0.6585 ± 0.003 | 0.6752 ± 0.002 | 0.6196 ± 0.001  |
| LV-CPH-HG   | 0.6349 ± 0.003 | 0.6866 ± 0.002 | 0.5706 ± 0.001  |

Table 1: Results of hard and soft linear gating networks and their comparison with relevant baselines (95% bootstrap CI ). [Nagpal et al., 2019]

7 Discussion

We propose an approximation for the MLE objective in TPPs involving a partial likelihood function with latent factors. We also show that the MLE approximation can be bounded by minimizing a joint objective which includes an upper bound on the approximation gap. We have shown this to be theoretically and empirically better for the partial likelihood estimation (in survival analysis). Future work on this inference method would be to further exploit the tractable closed form approximation gap by directly optimizing for it with iterative methods like ADAM. Yet another direction would be to extend this work to latent variable models for semi-parametric models like Gaussian processes for survival analysis [Fernández et al., 2016].
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A Appendix

A.1 Bounding Jensen’s Inequality [Dragomir – Loose Bound]

[Simic, 2009] propose multiple distribution agnostic upper bounds for Jensen’s inequality in the case of generic continuous convex functions defined on a compact set \([\mathcal{L}, \mathcal{U}]\). One of the popular bounds in this regime is the Dragomir’s inequality proposed in [Dragomir, 1999]. Given \(z_i\) is bounded with probability \(\delta\), section 4 bounds \(\alpha_z, \eta_{z_i}\) with \((\alpha_z \in [\mathcal{L}(\alpha_{z_i}), \mathcal{U}(\alpha_{z_i})], \eta_{z_i} \in [\mathcal{L}(\eta_{z_i}), \mathcal{U}(\eta_{z_i})])\). By Dragomir’s [Dragomir, 1999] inequality for a convex function \(f\),

\[
E[f(\alpha_z)] - f(E(\alpha_z)) \leq \frac{1}{4}(\mathcal{U}(\alpha_z) - \mathcal{L}(\alpha_z))(f'(\mathcal{U}(\alpha_z)) - f'(\mathcal{L}(\alpha_z)))
\]

(9)

For \(f \in \{f_\delta\}^\infty_{\delta=2}, f_\delta(x) = x^p\) and \(f \in \{f_\delta\}^\infty_{\delta=2}, f_\delta(x) = x^{-p}\), the bounds are given by eq. 10 and eq. 11 respectively.

\[
P \frac{1}{4}(\mathcal{U}(\eta_{z_{-1}}) - \mathcal{L}(\eta_{z_{-1}}))(\mathcal{U}(\eta_{z_{-1}})^{p-1} - \mathcal{L}(\eta_{z_{-1}})^{p-1})
\]

(10)

\[
P \frac{1}{4}(\mathcal{U}(\alpha_z) - \mathcal{L}(\alpha_z))(\mathcal{L}(\alpha_z)^{(p+1)} - \mathcal{U}(\alpha_z)^{(p+1)})
\]

(11)

This bound is easy to compute and can be visualized via the gap shown in figure 3. This is also quite naive and generic since it only uses the first order conditions for convex functions to arrive at an upper bound. In the following section we provide a tighter upper bound under the stronger assumptions of strict convexity.

A.2 Bounding Jensen’s Inequality [Convex Conjugate – Tight Bound]

This section provides the proof for theorem 1 in the main paper. We investigate bounds under the special case of strictly convex functions \(\{\phi_p\}^\infty_{p=2}\) with \(\phi_p : \mathbb{R}^+ \to \mathbb{R}^+\) and \(\phi_p(x) = x^p\). We also show visually (figure 3) that our bound is the tightest possible distribution agnostic bound for the given set of functions. With \(\mathcal{G}(\alpha_z, \phi_p)\) as the bound of interest,

\[
\mathcal{G}(\alpha_z, \phi_p) \leq \max_{\kappa \in [0,1]} \kappa \phi_p(\mathcal{U}(\alpha_z)) + (1 - \kappa)\phi_p(\mathcal{L}(\alpha_z)) - \phi_p(r \mathcal{U}(\alpha_z) + (1 - \kappa)\mathcal{L}(\alpha_z))
\]

(12)

Figure 3 depicts geometrically the maximization problem in the RHS of eq. 12 which we solve via the convex conjugate of \(\phi_p\). The optimization problem in eq. 12 involves identifying \(\alpha_{z_i} \in [\mathcal{L}(\alpha_{z_i}), \mathcal{U}(\alpha_{z_i})]\), such that the line in figure 3 denoted by \(y = \phi'(\alpha_{z_i})x + c\) where \(\alpha_{z_i}\) is farthest away from \(\phi(\alpha_{z_i})\) at the optimal point.

Given that \(\phi_p(x) = (1/x^p)\) is a closed proper strict convex function on \([\mathcal{L}(\alpha_{z_i}), \mathcal{U}(\alpha_{z_i})]\), (the case when we consider \(\phi_p(x) = x^p\) on \([\mathcal{L}(\eta_{z_{-1}}), \mathcal{U}(\eta_{z_{-1}})]\) is similar) we can define the convex conjugate of \(\phi_p(x)\). The form in eq. 13 is similar to what we need (distance between \(\phi_p(x)\) and a line with slope defined by 

\[
\phi_p^*(y) = \sup_x yx - \phi_p(x) \quad \partial \phi_p^*(y) = \{x : yx - \phi_p(x) = \phi_p^*(y)\}
\]

(13)

\[
\partial \phi_p(\phi_p(\mathcal{U}(\alpha_z)) - \phi_p(\mathcal{L}(\alpha_z))) = \arg\max_{w \in [\mathcal{L}(\alpha_z), \mathcal{U}(\alpha_z)]} \frac{\phi_p(\mathcal{U}(\alpha_z)) - \phi_p(\mathcal{L}(\alpha_z))}{\mathcal{U}(\alpha_z) - \mathcal{L}(\alpha_z)} - \phi_p(w).
\]

(14)

Since \((1/x^p)\) is strictly convex the subgradient of \(\phi_p^*\) at \(y\) is a singleton set and is exactly equal to the \(\partial \phi_p^*(y)\), giving us a unique maximizer \(w^*\) in eq. 14.

\[
\partial \phi_p^*(y) = \left(\frac{-p}{y}\right)^{-\frac{1}{p-1}} \quad w^* = \left(\frac{p}{\mathcal{L}(\alpha_z)^-p + \mathcal{U}(\alpha_z)^-p}\right)^{-\frac{1}{p-1}}
\]

(15)

Eq. 15 tells us that \(w^*\) (and thus the bound in Eq. 12) for a given sample \((x_i, t_i, R(t_i))\) is a function of \(\beta, x_i & x_k \in R(t_i)\). Given \(w^*\) it is easy to compute \(\mathcal{G}(\alpha_z, \phi_p)\) by,

\[
w^* = \kappa^* \mathcal{U}(\alpha_z) + (1 - \kappa^*)\mathcal{L}(\alpha_z)
\]

(16)

\[
\kappa^* = \frac{w^* - \mathcal{L}(\alpha_z)}{\mathcal{U}(\alpha_z) - \mathcal{L}(\alpha_z)}
\]

(17)

\[
\mathcal{G}(\alpha_z, \phi_p) = \kappa^* \phi_p(\mathcal{U}(\alpha_z)) + (1 - \kappa^*)\phi_p(\mathcal{L}(\alpha_z)) - \phi_p(\kappa^* \mathcal{U}(\alpha_z) + (1 - \kappa^*)\mathcal{L}(\alpha_z))
\]

(18)

In section 6 we empirically compared this bound with eqs. 10, 11 from appendix A.1.