Neural Temporal Point Processes
For Modelling Electronic Health Records

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Abstract

The modelling of Electronic Health Records (EHRs) has the potential to drive more efficient allocation of healthcare resources, enabling early intervention strategies and advancing personalised healthcare. However, EHRs are challenging to model due to their realisation as noisy, multi-modal data occurring at irregular time intervals. To address their temporal nature, we treat EHRs as samples generated by a Temporal Point Process (TPP), enabling us to model what happened in an event with when it happened in a principled way. We gather and propose neural network parameterisations of TPPs, collectively referred to as Neural TPPs. We perform evaluations on synthetic EHRs as well as on a set of established benchmarks. We show that TPPs significantly outperform their non-TPP counterparts on EHRs. We also show that an assumption of many Neural TPPs, that the class distribution is conditionally independent of time, reduces performance on EHRs. Finally, our proposed attention-based Neural TPP performs favourably compared to existing models, and provides insight into how it models the EHR, an important step towards a component of clinical decision support systems.

1 Introduction

Healthcare systems today are under intense pressure. Costs of care are increasing, resources are constrained, and outcomes are worsening (Topol, 2019). Clinician diagnostic error is estimated at 10-15% (Graber, 2013) and Electronic Health Record (EHR) data suffers from poor coding and incompleteness which affects downstream tasks (Jetley and Zhang, 2019).

Given these intense challenges, healthcare stands as one of the most promising applications of Machine Learning (ML). In particular, interest in modelling EHRs has recently increased (Islam et al., 2017; Shickel et al., 2018; Darabi et al., 2019; Li et al., 2019; Rodrigues-Jr et al., 2019). However, facets of health evolve at differing rates, and EHRs are typically realised as noisy, multi-modal data occurring at irregular time intervals. This makes EHRs difficult to model using common ML methods.

We propose to address the temporal nature of EHRs by treating them as samples generated by a Temporal Point Process (TPP), a probabilistic framework which can deal with data occurring at irregular time intervals. Specifically, we use a Neural Network (NN) to approximate its density, which

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∗Equal contribution. Joseph Enguehard and Dan Busbridge led the research, implemented the models and performed the experiments. Adam Bozson created the synthetic EHR datasets and provided insights during project inception. Claire Woodcock strategically guided the project and contributed the broader impact statement. Nils Y. Hammerla provided technical guidance throughout.

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specifies the probability of the next event happening at a given time. We call these models Neural TPPs. We propose jointly modelling times and labels to capture the varying evolution rates within EHRs. To the best of our knowledge, we are the first to apply Neural TPPs to longitudinal EHR data.

To test this, aware of the need for transparency in research (Pineau et al., 2020) and for sensitive handling of health data (Kalkman et al., 2019), we perform an extensive study on synthetic EHR datasets generated using the open source Synthea simulator (Walonski et al., 2018). For completeness, we also perform evaluations on benchmark datasets commonly used in the TPP literature. We find that:

- Our proposed Neural TPPs, where labels are jointly modelled with time, significantly outperform on synthetic EHRs those that treat them as conditionally independent; a common simplification in the TPP literature,
- Particularly in the case of TPPs, using a single metric does not adequately capture how well a given model performs,
- Some datasets used for benchmarking TPPs are easily solved by a time-independent model.

On other datasets, including synthetic EHRs, TPPs outperform their non-TPP counterparts.

Finally, we present a Neural TPP whose attention-based mechanism provides interpretable information without compromising on performance. This is an essential contribution in the development of research for clinical applications.

2 Background

2.1 Temporal point processes

A TPP is a random process that generates a sequence of $N$ events $\mathcal{H} = \{t^m_i\}_{i=1}^N$ within a given observation window $t_i \in [w_-, w_+]$. Each event consists of labels $m \in \{1, \ldots, M\}$ localised at times $t_i - 1 < t_i$. Labels may be independent or mutually exclusive, depending on the task.

A TPP is fully characterised through its conditional intensity $\lambda^*_m(t)$:

$$\lambda^*_m(t) dt = \lambda_m(t|\mathcal{H}_t) dt = \Pr(t^m_i \in [t, t + dt] | \mathcal{H}_t), \quad t_{i-1} < t \leq t_i,$$  \hspace{1cm} (1)

which specifies the probability that a label $m$ occurs in the infinitesimal time interval $[t, t + dt]$ given past events $\mathcal{H}_t = \{t^m_i \in \mathcal{H} | t_i < t\}$. We follow Daley and Vere-Jones (2003) in using the shorthand $\lambda^*_m(t) = \lambda_m(t|\mathcal{H}_t)$ where the * indicates that $\lambda_m(t)$ is conditioned on past events. Given a specified conditional intensity $\lambda_m(t)$, the conditional density $p^*_m(t)$ is

$$p^*_m(t) = p_m(t|\mathcal{H}_t) = \lambda^*_m(t) \exp \left[ -\sum_{n=1}^{M} \int_{t_{i-1}}^{t} \lambda^*_n(t') dt' \right], \quad t_{i-1} < t \leq t_i.$$  \hspace{1cm} (2)

We also use the notation $\Lambda^*_m(t)$ to describe the cumulative conditional intensity:

$$\Lambda^*_m(t) = \lambda_m(t|\mathcal{H}_t) = \int_{t_{i-1}}^{t} \lambda^*_m(t') dt', \quad t_{i-1} < t \leq t_i.$$  \hspace{1cm} (3)

which allows Equation (2) to be written as $p^*_m(t) = \lambda^*_m(t) \exp \left[ -\sum_{n=1}^{M} \Lambda^*_n(t) \right]$.

In a multi-class setting, where exactly one label (displayed as the indicator function $\mathbb{1}$) is present in any event, the log-likelihood of a sequence $\mathcal{H}$ is a form of categorical cross-entropy:

$$\log p_{\text{multi-class}}(\mathcal{H}) = \sum_{m=1}^{M} \sum_{i=1}^{N} \mathbb{1}_{i,m} \log p^*_m(t_i) - \sum_{m=1}^{M} \int_{w_{-}}^{w_{+}} \lambda^*_m(t') dt', \hspace{1cm} (4)$$

where $\mathcal{H}_{t_0} = \mathcal{H}_{t_N} = \{\}$, and $t_0 = w_-$ but does not correspond to an event.

For clarity, an event $e_i$ may be written $e_i = \{t^m_i | m \in \mathcal{M}_i\}$ where $\mathcal{M}_i$ is the set of labels at time $t_i$. 

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In a multi-label setting, where at least one label is present in any event, the log-likelihood of a sequence $\mathcal{H}$ is a form of binary cross-entropy:

$$\log p_{\text{multi-label}}(\mathcal{H}) = \log p_{\text{multi-class}}(\mathcal{H}) + \sum_{m=1}^{M} \sum_{i=1}^{N} (1 - \mathbb{1}_{i,m}) \log \left[ 1 - p_m^*(t_i) \right]. \quad (5)$$

This setting should be especially useful to model EHRs, as a single medical consultation usually includes various events, such as diagnoses or prescriptions, all happening at the same time.

### 2.2 Neural temporal point processes

![Encoder/decoder architecture of Neural TPPs.](image)

Given a query time $t$, the sequence $\mathcal{H}$ is filtered to the events $\mathcal{H}_t$ in the past of $t$. The encoder maps $\mathcal{H}_t$ to continuous representations $Z_t = \{ z_i \}_{i \in H_t} = \text{Enc}(\mathcal{H}_t; \theta_{\text{Enc}})$. Each $z_i$ can be considered as a contextualised representation for the event at $t_i$. Given $Z_t$ and $t$, the decoder outputs $\text{Dec}(t, Z_t; \theta_{\text{Dec}}) \in \mathbb{R}^M$ that the conditional intensity and conditional cumulative intensity are derived from without any learnable parameters.

Encoder-decoder architectures have proven effective for Natural Language Processing (NLP) (Cho et al., 2014; Kiros et al., 2015; Hill et al., 2016; Vaswani et al., 2017). Existing Neural TPPs also exhibit this structure: the encoder creates event representations based only on information about other events; the decoder takes these representations and the decoding time to produce a new representation. The output of the decoder produces the conditional intensity and conditional cumulative intensity at that decoding time. For more detail, see Figure 1.

### 3 Previous work

While a Neural TPP encoder can be readily chosen from existing sequence models such as Recurrent Neural Networks (RNNs), choosing a decoder is much less straightforward due to the integral in Equation (2). Existing work can be categorised based on the relationship between the conditional intensity $\lambda^*(t)$ and conditional cumulative intensity $\Lambda^*(t)$. We focus on three approaches:

- Closed form likelihood: the conditional density $p^*(t)$ is closed form,
- Analytic conditional intensity: only $\lambda^*(t)$ is closed form, $\Lambda^*(t)$ is estimated numerically,
- Analytic cumulative conditional intensity: only $\Lambda^*(t)$ is closed form, $\lambda^*(t)$ is computed through differentiation.

#### 3.1 Closed form likelihood

The closed form likelihood approach implies that the contribution from each event toward the likelihood, i.e. the conditional density $p_m^*(t) = \lambda_m^*(t) \exp[-\sum_{n=1}^{M} \Lambda_n^*(t)]$ is closed form.

A well-known example is the Hawkes process (Hawkes, 1971; Nickel and Le, 2020), which models the conditional intensity as $\lambda_m^*(t; \{ \mu, \alpha, \beta \}) = \mu_m + \sum_{n=1}^{M} \alpha_{m,n} \sum_{\tau_i > t} \exp[-\beta_{m,n}(t - \tau_i)]$ with learnable parameters $\mu \in \mathbb{R}_0^M$, $\alpha \in \mathbb{R}_0^{M \times M}$, and $\beta \in \mathbb{R}^{M \times M}$. The closed form of $\Lambda_m^*(t; \theta)$ comes from the simple exponential linear $t$-dependence of $\lambda_m^*(t; \theta)$, which limits the model flexibility. Du (2016) leveraged the same closed form, conditioning an exponential linear decoder on the output of a RNN encoder (RMTPP). As with the Hawkes process, the model can only model exponential dependence in time. Additionally, it assumes labels are conditionally independent of time given a history, which we will show is a limiting assumption in domains like modelling EHRs.
An alternative to taking $\lambda^*(t)$ and $\Lambda^*(t)$ closed form is to take $p^*(t)$ closed form. Shchur et al. (2020) directly approximate the conditional density using a log-normal mixture (LNM). With a sufficiently large mixture, $p^*(t)$ can approximate any conditional density, and is a more flexible model than the RMTTP. However, as in Du (2016), labels are modelled conditionally independent of decoding time.

While none of the Neural TPP methods have been applied to modelling EHRs, Islam et al. (2017) uses a non-neural TPP model by combining a conditional Poisson process with a Gaussian distribution to predict in hospital mortality using EHR data.

## 3.2 Analytic conditional intensity

The analytic conditional intensity approach approximates the conditional intensity with a NN whose output is positive $\lambda^*_m(t; \theta) = \text{Dec}(t, \mathcal{Z}_t; \theta_{\text{Dec}})_m \in \mathbb{R}_{\geq 0}$, and whose integral with respect to $t$ must be approximated numerically.

The positivity constraint is satisfied by requiring the final activation function to be positive. Early Neural TPPs employed exponential activation (Du 2016). Recently, the scaled softplus activation $\sigma_+(x_m) = s_m \log(1 + \exp(x_m/s_m)) \in \mathbb{R}_{\geq 0}$ with learnable $s \in \mathbb{R}^M$ has gained popularity (Mei and Eisner 2017). Ultimately, writing a neural approximator for $\lambda^*_m(t)$ is relatively simple as there is no constraint on the NN architecture itself. Of course, this does not mean it is easy to train.

To approximate the integral, Monte Carlo (MC) estimation can be employed $\Lambda^*_m(t; \theta) \approx \text{MC}[\text{Dec}(t', \mathcal{Z}_t; \theta_{\text{Dec}}), t', 0, t]$ given a sampling strategy (Mei and Eisner 2017). Zhu et al. (2020) also applies this strategy for spatio-temporal point process, which jointly models times and labels, but only uses an embedding layer as an encoder.

## 3.3 Analytic conditional cumulative intensity

The analytic conditional cumulative intensity approach approximates the conditional cumulative intensity with a NN whose output is positive $\Lambda^*_m(t; \theta) = \text{Dec}(t, \mathcal{Z}_t; \theta_{\text{Dec}})_m \in \mathbb{R}_{\geq 0}$, and whose derivative is positive and approximates the conditional intensity $\lambda^*_m(t; \theta) = d\text{Dec}(t, \mathcal{Z}_t; \theta_{\text{Dec}})_m/dt \in \mathbb{R}_{\geq 0}$. This derivative can be computed using backpropagation. The benefit of the cumulative intensity approach consists in removing the variance induced by MC estimation. However, as the cumulative intensity is monotonic, it entails specific constraints on the NN.

Omi et al. (2019) uses a Multi-Layer Perceptron (MLP) with positive weights in order to model a monotonic decoder. It also uses tanh activation functions, and a softplus final activation function to ensure a positive output. However, this model does not handle labels, and has been criticised by Shchur et al. (2020) for lacking the property $\lim_{t \to +\infty} \Lambda^*_m(t; \theta) = +\infty$, due to its tanh activation.

## 4 Proposed models

Our main goal is to model the joint distribution of EHRs over time and labels, which inherently includes long-term dependencies in time. However, the recency bias of RNNs makes it difficult for them to model non-sequential dependencies (Bahdanau et al. 2016; Ravfogel et al. 2019). Additionally, RNNs do not meet the explainability standard required for real-world application.

To overcome these hurdles, in this section we develop the necessary building blocks to define self-attention and attention-based Neural TPPs that directly model either the conditional intensity $\lambda^*_m(t)$ or the conditional cumulative intensity $\Lambda^*_m(t)$.

### 4.1 Positive approximators

In order to model a positive intensity $\lambda^*_m(t)$, we chose to model directly $\log \lambda^*_m(t)$ with a NN, without adding a positive activation function on the last layer. We also use MC estimation with a uniform sampling strategy and only one sample per time interval, following the insight of Mei and Eisner (2017) that this yields satisfactory results while keeping the training of the NN efficient.

Using this strategy, we designed a decoder based on a MLP (MLP Monte Carlo, or MLP-MC), and one using the attention mechanism (Attn-MC). For more details, see Appendix B.
Table 1: Properties of datasets used for evaluation.

| Dataset          | # classes | Task type | # events | Avg. length | Train | Valid | Test |
|------------------|-----------|-----------|----------|-------------|-------|-------|------|
| Hawkes (ind.)    | 2         | Multi-class | 457,788  | 19          | 16,384| 4,096 | 4,096|
| Hawkes (dep.)    | 2         | Multi-class | 607,512  | 25          | 16,384| 4,096 | 4,096|
| MIMIC-II         | 75        | Multi-class | 2,419    | 4           | 585   | NA    | 65   |
| Stack Overflow   | 22        | Multi-class | 480,413  | 72          | 5,307 | NA    | 1,326|
| Retweets         | 3         | Multi-label | 2,087,866 | 104         | 16,000| 2,000 | 2,000|
| Ear infection    | 39        | Multi-label | 14,810   | 2           | 8,179 | 1,022 | 1,023|
| Synthea          | 357       | Multi-label | 496,625  | 43          | 10,524| 585   | 585  |

4.2 Positive monotonic approximators

Modelling $\Lambda^*_m(t)$ with a decoder is more difficult from a design perspective. First, the Decoder$(t, Z_t; \theta)$ must be positive, which as discussed above is not too difficult. In practice we model $\Lambda^*_m(t_i)$, which has the properties $\Lambda^*_m(t_i) = 0$ and $\lim_{t \to \infty} \Lambda^*_m(t) = \infty$. The first of these is satisfied by parameterising the decoder as $\text{Decoder}(t, Z_t; \theta) = f(t, Z_t; \theta) - f(t_i, Z_t; \theta)$. The second can be satisfied in two ways. The simplest is to add a Poisson term $\lambda \to \lambda + \mu$ to the conditional intensity. An alternative is to use a non-saturating activation function, however, Rectified Linear Unit (ReLU) cannot be used, as $\frac{d^2 \text{ReLU}(x)}{dx^2} = 0$, for $x \neq 0$, which means that the resulting conditional intensity produced by such a decoder would be equivalent to a Poisson process. We investigate one possibility in Appendix A. For our purposes, adding a Poisson term is sufficient.

Now we need a $f(t, Z_t; \theta)$ such that $df(t, Z_t; \theta)/dt > 0$. If we assume that $f$ is given by a $L$-layer NN, where the output of each layer $f_i$ is fed into the next $f_{i+1}$, then we can write $f(t) = (f_L \circ \cdots \circ f_2 \circ f_1)(t)$. Then, providing each step of processing produces an output that is a monotonic function of its input, i.e. $df_i/df_{i-1} \geq 0$ and $df_1/dt \geq 0$, then $f(t)$ is a monotonic function of $t$.

In order to make each of these NN blocks monotonic, we performed modifications on several of them. In addition, due to the importance of the derivative for this modelling approach, we use the adaptive Gumbel activation (Farhadi et al., 2019), which allows the network to adapt its first derivative more flexibly than a tanh activation. For more details see Appendix A.

We designed two decoders modelling the cumulative intensity: one based on a MLP (MLP Cumulative, or MLP-CM) and one using the attention mechanism (Attn-CM). For more details, see Appendix B.

5 Evaluation

5.1 Datasets

The statistics of all datasets used are summarised in Table 1.

Hawkes Processes This synthetic data allows us to have access to a theoretically infinite amount of data. Moreover, as we know the intensity function, we were able to compare each of our modelled intensity against the true one. We designed two different Hawkes datasets: one consisting of two independent processes, **Hawkes (independent)**, and a second one allowing interactions between two processes, **Hawkes (dependent)**.

Baselines We also compared our models on datasets commonly used to evaluate TPPs. We use: MIMIC-II, a medical dataset of clinical visits to Intensive Care Units, Stack Overflow, which classifies users on this question answering website, and Retweets, which consists in streams of retweet events by different types of Twitter users. Further details about the datasets and their preprocessing can be found in Du (2016); Mei and Eisner (2017).

Synthetic EHRs We used the Synthea simulator (Walonoski et al., 2018) which generates patient-level EHRs using human expert curated Markov processes.
Table 2: Evaluation on multi-class tasks. In both tables, (†) indicates a model newly presented in this work. Best performance and performances whose confidence intervals overlap the best are boldened.

| Encoder | GRU | MIMIC-II | Stack Overflow | Hawkes (ind.) | Hawkes (dep.) |
|---------|-----|----------|----------------|--------------|--------------|
| Decoder | F1 score | NLL/time | F1 score | NLL/time | NLL/time | NLL/time |
| CP      | .691 (0.83) | 6.78 (1.99) | .325 (0.004) | .553 (0.003) | .623 (0.002) | .774 (0.004) |
| RMTPP   | .215 (1.12) | 11.4 (3.57) | .284 (0.005) | .592 (0.006) | .610 (0.004) | .731 (0.004) |
| LNM     | .705 (1.17) | 6.33 (1.37) | .314 (0.003) | .548 (0.004) | .605 (0.001) | .727 (0.001) |
| MLP-CM† | .166 (0.83) | 12.2 (3.57) | .305 (0.016) | .573 (0.004) | .609 (0.005) | .728 (0.003) |
| MLP-MC† | .657 (0.85) | 9.33 (3.17) | .339 (0.006) | .538 (0.005) | .607 (0.005) | .727 (0.000) |
| Attn-CM† | .189 (1.10) | 10.4 (2.34) | .286 (0.017) | .589 (0.012) | .613 (0.003) | .732 (0.002) |
| Attn-MC† | .638 (1.12) | 8.19 (2.94) | .294 (0.020) | .587 (0.020) | .610 (0.002) | .734 (0.006) |

Encoder SA

| Decoder | F1 score | NLL/time | F1 score | NLL/time | NLL/time | NLL/time |
|---------|----------|----------|----------|----------|----------|----------|
| CP      | .686 (0.67) | 7.25 (1.44) | .326 (0.003) | .555 (0.003) | .622 (0.001) | .774 (0.002) |
| RMTPP   | .709 (0.76) | 4.24 (2.66) | .288 (0.002) | .592 (0.002) | .609 (0.005) | .734 (0.002) |
| LNM     | .632 (0.20) | 7.76 (2.42) | .305 (0.003) | .561 (0.006) | .607 (0.005) | .730 (0.004) |
| MLP-CM† | .159 (0.88) | 12.7 (3.45) | .292 (0.003) | .634 (0.042) | .611 (0.005) | .733 (0.002) |
| MLP-MC† | .567 (0.94) | 9.14 (3.04) | .312 (0.014) | .568 (0.006) | .607 (0.006) | .729 (0.002) |
| Attn-CM† | .186 (0.82) | 11.4 (3.90) | .269 (0.011) | .665 (0.047) | .614 (0.001) | .733 (0.001) |
| Attn-MC† | .700 (0.70) | 6.01 (2.61) | .310 (0.009) | .567 (0.009) | .609 (0.007) | .728 (0.001) |

We created a dataset utilising all of Synthea’s modules, Synthea (Full), as well as a dataset generated solely from the ear infection module Synthea (Ear Infection). Ear infection was selected for a simpler benchmark as the generation process demonstrated temporal dependence. For each task, we generated approximately 10,000 patients, and we kept 10% of the data for validation and testing, using 5 different folds randomly chosen. Moreover, we only kept the first 400 events of each sequence to optimise GPU utilisation.

We filtered out all events except conditions and medications. For each patient, we transformed event times by subtracting their birth date, then multiplying by $10^{-5}$. When provided, their death date is used as the end of the observation window $w+$, otherwise we use the latest event in their history.

5.2 Models

We chose two different encoders: a Gated Recurrent Unit (GRU), and a Self-Attention module (SA). We combined these with different decoders: a conditional Poisson process (CP), a RMTPP (Du [2016]), a log-normal mixture (LNM) (Shchur et al. [2020]), and our decoders, a MLP and an attention-based NN, both modelling the intensity (MLP-CM, Attn-CM) or its cumulative (MLP-MC, Attn-MC). For more details, see Appendix B.

We modified the transformer (Vaswani et al. [2017]) following Xiong et al. [2020]. Specifically, we set the LayerNorm before the multi-head attention module and the fully forward network.

To every model, we add a Poisson process, giving a learnable base intensity. Specifically, $\lambda_{\text{total}}(t) = \alpha_1 \mu + \alpha_2 \lambda^c(t)$ where $\alpha = \text{softmax}(\alpha)$ and $\alpha$ are learnable. We found that initialising $\alpha$ such that $\alpha_1 \sim e^{3}\alpha_2$, i.e. starting the combined TPP as mostly Poisson, was beneficial for convergence.

We chose to set these models with only one layer, both for the encoder and the decoder. We also chose the size of each layer to be 8 for the small datasets (Hawkes and MIMIC-II), 32 for the medium ones (Ear infection, Stack Overflow and Retweets), and 64 for Synthea. Our batch size was set between 32 and 512, depending on our GPU memory availability. In order to quickly fit the Poisson process, we used the Noam learning rate scheduler (Vaswani et al. [2017]), with a maximum learning rate value of $5e^{-6}$.
Table 3: Evaluation on multi-label tasks. (*) indicates that these models were trained using a different time scale for stability, therefore, their NLLs cannot be compared with the other models.

| Encoder | GRU | Retweets | Synthea (Ear infection) | Synthea (Full) |
|---------|-----|----------|-------------------------|---------------|
|         | ROC-AUC | NLL/time | ROC-AUC | NLL/time | ROC-AUC | NLL/time |
| CP      | .611 (.001) | 5.71 (1.02) | .786 (.015) | 37.6 (7.76) | .850 (.014) | 89.6 (3.15) |
| RMTPP   | .532 (.003) | -9.05 (1.40) | .672 (.013) | 36.7 (4.25) | .616 (.043) | 62.2 (6.63) |
| LNM     | .521 (.010) | -10.9 (2.11) | .765 (.008) | 26.7 (5.35) | .770 (.010) | 9.49 (6.37) |
| MLP-CM† | .533 (.001) | -10.4 (.301) | .742 (.050) | 30.4 (7.03) | .692 (.051) | 34.2 (14.5) |
| MLP-MC† | .536 (.001) | -183 (1.70)* | .842 (.014) | 25.3 (4.76) | .616 (.043) | 62.2 (6.63) |
| Attn-CM† | .526 (.001) | -10.0 (.535) | .799 (.028) | 27.1 (4.95) | .508 (.000) | 50.9 (2.51) |
| Attn-MC† | .534 (.001) | -9.66 (.231) | .858 (.010) | 25.0 (4.51) | .818 (.012) | 25.4 (3.82) |

Encoder SA

| CP      | .608 (.001) | 4.85 (.021) | .792 (.009) | 38.6 (8.96) | .825 (.020) | 91.2 (4.24) |
| RMTPP   | .535 (.001) | -8.70 (.087) | .675 (.068) | 42.9 (9.01) | .593 (.029) | 67.8 (6.13) |
| LNM     | .528 (.007) | -10.9 (1.29) | .767 (.007) | 26.2 (5.51) | .760 (.014) | 27.5 (27.2) |
| MLP-CM† | .512 (.001) | -8.93 (.180) | .684 (.094) | 33.8 (15.3) | .589 (.123) | 62.8 (30.8) |
| MLP-MC† | .535 (.000) | -9.65 (.153) | .853 (.008) | 26.0 (5.13) | .785 (.011) | 10789 (914)* |
| Attn-CM† | .517 (.001) | -8.54 (.168) | .697 (.059) | 31.4 (6.90) | .503 (.004) | 85.0 (3.01) |
| Attn-MC† | .521 (.007) | -8.69 (1.08) | .809 (.040) | 27.7 (5.47) | .769 (.056) | 38.4 (11.1) |

0.01 and 10 epochs of warming-up. We also used the Adam optimizer (Kingma and Ba, 2017) for all experiments, and set the number of epochs to 1000, with a patience of 100.

All our models are trained using Maximum Likelihood Estimation (MLE) of the data, and evaluated using a F1 metric for multi-class datasets, and a ROC-AUC metric for the multi-label ones. We also report Negative Log Likelihood (NLL) normalised by time, to make this metric meaningful across sequences defined on different time intervals (NLL/time).

6 Results

We want to first stress that none of the metrics we are reporting is a perfect measure of performance. Indeed, on one hand, the F1 (Table 2) and ROC-AUC (Table 3) metrics only measure the ability to correctly predict the label of the next event when it happens. These metrics do not penalise a model for inaccurate predictions in the inter-event interval, as it is shown on Figure 2.

On the other hand, the NLL is prone to overfit: if a Neural TPP accurately guesses when an event will happen, it has the incentive to endlessly increase the intensity at that time, reducing the overall NLL without improving the resulting model in a meaningful way. Ideally, a model should perform well on both metrics.

We also decided to run a simple conditional Poisson (CP) decoder, which we believe to be a good test of suitability of datasets. We expect this model to perform well in terms of F1/ROC-AUC, and poorly in terms of NLL, as it is unable to reduce its intensity in regions where no events happen. However,
we found that on the MIMIC-II and StackOverflow datasets, GRU-CP has both a competitive NLL and F1 score. This indicates that these datasets may not be well suited to benchmarking TPPs and we suggest caution for future work using these datasets. All other datasets seem to be suitable for TPPs. We focus here on EHRs, and discuss the Hawkes and Retweets results in Appendix C.

Although the cumulative-based models have theoretical benefits compared with their Monte Carlo counterparts, they are in practice harder to train. This may explain their relatively poor performance on datasets such as on MIMIC-II and Synthea (Full), and the high variance between F1/ROC-AUC scores on these datasets. Moreover, using a GRU encoder achieves marginally better results than using SA, whereas, the latter produces information on its internal modelling mechanism (see Figure 3).

7 Conclusion

In this work we gathered and proposed several neural network parameterisations of TPPs, evaluating them on synthetic EHRs, as well as common benchmarks. Given the significant out-performance of our models on synthetic EHRs, labels should be modelled jointly with time, rather than be treated as conditionally independent; a common simplification in the TPP literature. We also note that common TPP metrics are not good performance indicators
on their own. For a fair comparison we recommend using multiple metrics, each capturing distinct performance characteristics.

By employing a simple test that checks a dataset’s validity for benchmarking TPPs, we demonstrated potential issues within several widely-used benchmark datasets. We recommend caution when using those datasets, and that our test be run as a sanity check of any new evaluation task.

Finally, we have demonstrated that attention-based TPPs appear to transmit pertinent EHR information and perform favourably compared to existing models. This is an exciting line for further enquiry in EHR modelling, where human interpretability is essential. Future work should apply these models to real EHR data to investigate medical relevance.

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Broader impact statement

Overview

In this paper, we demonstrate that Temporal Point Processes perform favourably in modelling Electronic Health Records. We embarked on this project aware that as high impact systems, Clinical Decision Support tools must ultimately provide explanations (Holzinger et al., 2017) to ensure clinician adoption (Miller, 2019) and provide accountability (Mittelstadt et al., 2016) whilst being mindful of the call for researchers to build interpretable ML models (Rudin, 2019). Our results demonstrate that our attention based model performs favourably against less interpretable models. As attention could carry medically interpretable information our innovation contributes towards the development of medically useful AI tools.

Aware of both the need for transparency in the research community (Pineau et al., 2020) and for sensitive handling of health data (Kalkman et al., 2019), we opted to use open source synthetic EHRs. We provide all trained models, benchmarked datasets and a high quality deterministic codebase to allow others to easily implement and benchmark their own models. We also make the important contribution of highlighting existing benchmark datasets as inappropriate; continuing to develop temporal models using these datasets may slow development of useful technologies or cause poor outputs if applied to EHR data.

Turning to the potential impact of our technology, we begin by briefly discussing the benefits temporal EHR models could bring to healthcare before, with no less objectivity, analysing harms which could occur, raising questions for further reflection.

The potential benefits of EHR modelling

Healthcare systems today are under intense pressure. Chronic disease prevalence is rising (Raghupathi and Raghupathi, 2018), costs of care are increasing, resources are constrained and outcomes are worsening (Topol, 2019). 23% of UK deaths in 2017 were classed as avoidable (Office for National Statistics, 2017); clinician diagnostic error is estimated at 10-15% (Graber, 2013) and EHR data suffers from poor coding and incompleteness which affects downstream tasks (Jetley and Zhang, 2019). Our research contributes techniques which could be used to:

- More accurately impute missing EHR data.
- Identify likely misdiagnoses.
- Predict future health outcomes.
- Identify higher risk patients for successful health interventions.
- Design optimal care pathways.
- Optimise resource management.
• Identify previously undiscovered links between health conditions.

Clearly, implemented well, temporal EHR modelling could provide immense benefit to our society. These benefits outweigh possible harms on the provision that they are well mitigated. Hence we devote the rest of the discussion to evaluating potential harms.

**Potential Harms of EHR Modelling**

There are a number of ways in which the temporal modelling of EHRs could create societal harm. To examine these risks we evaluate them by topic, framed as a series of case studies.

**Poor Health Outcomes Through Data Bias**

Bias can mean many things when discussing the application of AI to healthcare. As such, we would encourage researchers to use Suresh and Guttag (2020)'s framework to better identify and address the specific challenges that arise when modelling health data. All are relevant to our technology but we will specifically focus on issues arising from historical, representation and aggregation biases. Importantly, we anticipate these biases would be more easily identified due to the interpretability of our attention-based technique.

Scenario: Temporal EHR modelling is deployed to predict future health having been trained on historical health records.

**Societal harm**

Societal groups who have historically been discriminated against continue to receive below standard healthcare.

**Examples of historical biases**

Historically, the majority of medical trials have been conducted on white males (Morley et al., 2019) providing greater health information on this population group. We also know that clinicians are fallible to human biases. For example: women are less likely than men to receive optimal care despite being more likely to present with hypertension and heart failure (Li Shanshan et al., 2016); They are often not diagnosed with diseases due to human bias (Suresh and Guttag, 2020) and are less likely than men to be given painkillers when they report they are in pain (Calderone, 1990); African Americans more likely to be misdiagnosed with schizophrenia than white patients (Gara et al., 2018).

Scenario: Temporal EHR modelling is deployed to predict future health and develop care plans. One model is used for a diverse population group.

**Societal harm**

Demographics’ varying symptom patterns and care plan needs are not accounted for, resulting in below optimal health outcomes for the majority.

**Examples of aggregation biases**

It has been shown that the risk factors for carotid artery disease differ by ethnicity (Gijsberts et al., 2015) yet prevention plans are developed on data from almost exclusively a white population. A common measurement for diabetes widely used for diagnosis and monitoring differs in value across ethnicities and genders (Herman and Cohen, 2012).

Scenario: Researchers select proxies to represent metrics within their model without considering broader socioeconomic factors.

**Societal harm**

Societal groups are subject to allocation biases where they do not receive the same standard of healthcare compared to advantaged groups.

**Example of poor proxy selection**

Obermeyer et al. (2019) analysed a model in current commercial use which identifies high risk patients for care interventions used medical costs as a proxy for illness. It was found that black people were much sicker than white people with the same risk score as historical and socioeconomic factors mean that black people do not receive parity in health care and treatments.
Scenario: Biased models are deployed as clinician-in-the-loop with the intention of using a human to protect against model biases.

Societal harm

The clinician cannot redress model biases, causing the above mentioned harms to persist.

Example of human-in-the-loop failure

Humans are subject to confirmation bias (Green and Chen, 2019) and Obermeyer et al. (2019) found that whilst clinicians can redress some disparity in care allocation, they do not adjust the balance to that of a fair algorithm.

Recommendations:

- Researchers must employ caution when using proxies such as “diagnosed with condition X” equals “has condition X”.
- Models must be evaluated against the intended recipient populations.
- We call on all institutions deploying temporal EHR models to assess fair performance in the target population, and, on policy makers to provide benchmarked patient datasets on which fair and safe performance of models must be demonstrated before deployment.

Questions for reflection:

- How do we best formulate the problems temporal EHR modelling is trying to solve to prevent discriminatory harms?
- If temporal EHR modelling was deployed, what techniques would be used to protect society from the reinforcement of structural inequalities and structural injustices (Jugov and Ypi, 2019)?
- How do you construct adequate benchmarking datasets to test the suitability of a temporal EHR model for a given population?
- What evidence is needed to demonstrate the clinical effectiveness of a temporal model (Greaves et al., 2018)?

Poor care provision through lack of contextual awareness

Scenario: A temporal model is trained in a perfectly unbiased way and is deployed for use.

Societal harm

As the model is not aware of emergent health outcomes, information provided is out of sync with modern medical knowledge. Potentially resulting in sub-optimal care plan recommendations and predictions.

Example of lack of contextual awareness

Consider training on a cohort of 100 year old patients. They lived through the second world war, ate rations, never took a contraceptive pill and were retiring as computers became commonplace. Individuals approaching old age in the future will likely have very different health trajectories. By their nature, modelling of EHR data will be context blind (Caruana et al., 2015). For example, if a new drug is found to prevent the development of Type 2 diabetes, model predictions will be out of sync with patient outcomes, it would view the prescription of this better drug as an error.

Questions for reflection:

- How would we develop temporal EHR models to correct dynamically for non-stationary processes (changing medical knowledge)?
- How do we introduce contextual awareness to temporal EHR models?
Restrictions in health access

Scenario: A perfect model is deployed to be used by health insurers to identify high cost patients. Those who can be assisted by interventions are helped. The model identifies a set of individuals who are unavoidably costly, due to health issues beyond their control.

Societal harm

This may cause a shift in the economic model of the society in which the EHR model is deployed (Balasubramanian et al., 2018).

Examples of economic impact

Temporal models will make increasingly accurate predictions about how much each individual’s healthcare will cost over a lifetime. In countries where healthcare is not universal insurers and providers will adjust their actuarial models, moving away from pooled risk healthcare costs. Health insurers increase premiums to an unfeasibly high amount for costly individuals, preventing their access to healthcare and pricing models change for those who are able to access care. Governments are forced to determine whether to use social security to provide universal healthcare. If it is not the divide between those who can access healthcare and those who can’t potentially widens with ripple effects across the broader economy.

Questions for reflection:

- How do we as a society determine how to carry the cost of healthcare provision?
- What level of risk granularity should health insurance companies be privy to?

Changes to the Doctor / Patient relationship and agency

Scenario: Temporal EHR modelling causes a paradigm shift towards solely data-centred medicine. Reducing a patient solely to their datapoints. Theoretically, the model can predict a patient’s death.

Societal harm

Agency is removed from both the patient and the doctor. Knowledge of death raises existential questions and changes individuals’ behaviours.

Example of solely data-centred medicine

The doctor is left to evaluate symptoms solely on datapoints (Kleinpeter, 2017). A patient’s ability to fully express what it means to inhabit their body and feel illness (or not) is removed. They may feel unable to decline or deviate from recommended treatment plans, impacting the patient’s perception of bodily autonomy.

Scenario: Temporal EHR models are deployed in consumer health and wellness applications with the current narrative of empowering an individual to take control of their health (Morley and Floridi, 2019a).

Societal harm

The burden of disease prevention is shifted to the individual who has proportionally little control over macro health issues, tantamount to victim blaming (Morley and Floridi, 2019a).

Example of empowerment ineffectiveness

Many factors of health are not solvable with applications. For example, those on low incomes can’t afford healthy foods and other socioeconomic factors prevent individuals from accessing healthcare (de Freitas and Martin, 2015).

Recommendations:

- Policy makers should contemplate how far into the future various institutions should be permitted to predict peoples’ health.
- We encourage future researchers to view consumer applications that use temporal EHR modelling as digital companions (Morley and Floridi, 2019b).
Questions for reflection:

- How many years in advance should predictive health technologies be able to predict?
- How much clinical decision-making should we be delegating to AI-Health solutions [di Nucci, 2019]?
- How can we develop temporal EHR models to account for the socioeconomic and historical factors which contribute to poor health outcomes?
- How do we incorporate into temporal EHR modelling an ethical focus on the end user, and their expectations, demands, needs, and rights [Morley and Floridi, 2020]?

Wider reaching applications

The temporal modelling of irregular data could be applied to many domains. For example, education and personalised learning, crime and predictive policing, social media interactions and more. Each of these applications raises questions around the societal impact of improved temporal modelling. We hope that the above analysis provides stimulation when developing its beneficial usage.

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A Positive monotonic building blocks

As discussed in Section 4.2, if \( f(t) \) is given by a \( L \)-layer NN, where the output of each layer \( f_i \) is fed into the next \( f_{i+1} \), then we can write \( f(t) = (f_{L} \circ \cdots \circ f_{2} \circ f_{1})(t) \). Application of the chain rule

\[
\frac{df(t)}{dt} = \frac{df_{L}}{df_{L-1}} \cdot \frac{df_{L-1}}{df_{L-2}} \cdots \frac{df_{2}}{df_{1}}
\]

shows that a sufficient solution to achieving \( \frac{df(t)}{dt} \geq 0 \) is to enforce each step of processing to be a monotonic function of its input, i.e. \( \frac{df_{i}}{df_{i-1}} \geq 0 \) and \( \frac{df_{1}}{dt} \geq 0 \) implies \( f(t) \) is a monotonic function of \( t \).

As well as the monotonicity constraint, as we are interested in intensities that can decay as well as increase, it needs to be possible that the second derivative of \( f(t) \) can be negative

\[
\frac{d\lambda(t|\mathcal{H}_t)}{dt} \sim \frac{d^2\lambda(t|\mathcal{H}_t)}{dt^2} \sim \frac{d^2 f(t|\mathcal{H}_t)}{dt^2} < 0
\]

for some history \( \mathcal{H}_t \).

Here we collect all of the modifications we employ to ensure our architectures comply with this restriction.

A.1 Linear projections

A linear projections are a core component of dense layers, and can be made monotonic by requiring every element of the projection matrix is at least 0

\[
f(x) = Wx, \quad df(x)_{i}/dx_{j} = W_{i,j} \geq 0 \quad \forall \ i, j.
\]

One solution to this problem is to parameterise the \( W \) as a positive \( g \) transformation of some auxiliary parameters \( V \) such that \( W = g(V) \geq 0 \). Taking \( g \) as ReLU leads to issue during training: any weight which reaches zero will become frozen no longer be updated by the network, harming convergence properties. We also experimented using softplus and sigmoid activations. These have the issue where the auxiliary weights \( V \) can be pushed arbitrarily negative and, when the network needs them again, training needs to pull them very far back for little change in \( W \), again harming convergence. This approach is also burdened with additional computational cost.

The most effective approach, which we employ in our models, involves modifying the forward pass such that any weights below some small \( \epsilon > 0 \) are set to \( \epsilon \). This \( \epsilon \) can be thought of as a lower bound on the derivative, has no computational overheads, and none of the issues discussed in the approaches above. In our experiments we take \( \epsilon = 10^{-30} \).
A.2 Dense activation functions

ReLU
The widely used ReLU activation clearly satisfies the monotonicity constraint, however

\[
\frac{d \text{ReLU}(x)}{dx} = \begin{cases} 
0 & \text{if } x \leq 0 \\
1 & \text{if } x > 0,
\end{cases}
\]

\[
\frac{d^2 \text{ReLU}(x)}{dx^2} = 0.
\]

As the second derivative is 0 then

\[
\frac{d \lambda^*_m(t)}{dt} = 0
\]

which means that any cumulative model using the ReLU activation is equivalent to the conditional Poisson process \( \lambda(\tau|H_t) = \mu(H_t) \) introduced in Section 4.2. We cannot use ReLU in a cumulative model.

Tanh
Omi et al. (2019) proposed to use the \( \tanh \) activation function which doesn’t have the constraints of ReLU:

\[
\frac{d \tanh(x)}{dx} = \text{sech}^2(x) \in (0, 1),
\]

\[
\frac{d^2 \tanh(x)}{dx^2} = 2 \tanh(x) \text{sech}^2(x) \in (c_-, c_+),
\]

where \( c_\pm = \log(2 \pm \sqrt{2})/2 \). \( \tanh \) meets our requirements of a positive first derivative and a non-zero second derivative.

Gumbel
An alternative to \( \tanh \) is the adaptive Gumbel activation introduced in Farhadi et al. (2019):

\[
\sigma(x_m) = 1 - [1 + s_m \exp(x_m)]^{-\frac{1}{s_m}}
\]

where \( \forall m : s_m \in \mathbb{R}_{>0} \), and \( m \) is a dimension/activation index. For brevity, we will refer to this activation function as the Gumbel activation, and while its analytic properties we will drop the dimension index \( m \), however, since the activation is applied element-wise, the analytic properties discussed directly transfer to the vector application case.

Its first and second derivatives match our positivity and negative requirements

\[
\frac{d\sigma(x)}{dx} = \exp(x) [1 + s \exp(x)]^{-\frac{c_+}{s}} \in (0, 1/e),
\]

\[
\frac{d^2\sigma(x)}{dx^2} = \exp(x) [1 - \exp(x)] [1 + s \exp(x)]^{-\frac{c_+}{s}} \in (c_-, c_+),
\]

where \( c_\pm = (\pm \sqrt{5} - 2) \exp[\pm (\sqrt{5} - 3)/2] \). The Gumbel activation shares many of the limiting properties of the tanh activation.

\[
\lim_{x \to -\infty} \sigma(x) = 0, \quad \lim_{x \to \infty} \sigma(x) = 1, \quad \lim_{x \to \pm \infty} \frac{d\sigma(x)}{dx} = \lim_{x \to \pm \infty} \frac{d^2\sigma(x)}{dx^2} = 0.
\]

For our purposes, the key advantage of the Gumbel over tanh are the learnable parameters \( s_m \). These parameters control the magnitude of the gradient through equation Equation (13) and the magnitude of the second derivative through Equation (14). The maximum value of the first derivative is obtained at \( x = 0 \), which corresponds to the mode of the Gumbel distribution, and for any value of \( s \)

\[
\max_x \frac{d\sigma(x)}{dx} = (1 + s)^{-\frac{c_+}{s}}.
\]

By sending \( s \to 0 \) we get the largest maximum gradient of \( 1/e \) which occurs in a short window in \( x \), and by sending \( s \to \infty \) we get the smallest maximum gradient of \( 0 \), which occurs for all \( x \). This allows the activation function to control its sensitivity changes in the input, and allows the NN to be selective in where it wants fine-grained control over its first and second derivatives gradient (i.e. produce therefore have an output that changes slowly over a large range in the input values), and where it needs the gradient to be very large in a small region of the input.

These properties are extremely beneficial for cumulative modelling, and we employ the Gumbel activation in all of these models.
Gumbel-Softplus Although \textit{tanh} and adaptive Gumbel meet our positivity and negativity requirements, they share a further issue raised by Shchur et al. (2020) in that their saturation ($\lim_{x \to \infty} \sigma(x) = 1$) does not allow the property $\lim_{t \to \infty} \Lambda^m_\ast(t) = \infty$, leading to an ill-defined joint probability density $p^\ast_m(t)$. To solve this, we introduce the Gumbel-Softplus activation:

$$\sigma(x_m) = \text{gumbel}(x_m) [1 + \text{softplus}(x_m)],$$

where gumbel is defined in Equation (12), and softplus is the parametric softplus function:

$$\text{softplus}(x_m) = \log (1 + s_m \exp(x_m))$$

This activation function has the property $\lim_{t \to \infty} \sigma(t) = \infty$, in addition to satisfying the positivity and negativity constraints.

A.3 Attention activation functions

In addition to the activation functions used in the dense layers of NNs, the attention block requires another type of activation. This is indicated in Equation (52), as the attention logits $E_{i,j}$ are passed through a function $g$ to produce the attention coefficients $\alpha_{i,j}$. Generally, this activation function is the Softmax function (see Equation (53)), however, this function is not monotonic:

$$\frac{\partial \text{softmax}(x_i)}{\partial x_j} = \text{softmax}(x_i) [\delta_{ij} - \text{softmax}(x_j)] < 0 \; \forall \; i \neq j,$$

where $\delta_{ij}$ is the Kronecker delta function.

Consequently, we chose to use the sigmoid activation function instead of the softmax when the modelled function required to be monotonic. Indeed, the sigmoid function is monotonic:

$$\frac{\partial \sigma(x)}{\partial x} = \sigma(x) [1 - \sigma(x)] > 0.$$

The softmax activation function has the nice property of making the attention coefficient sum to one, therefore forcing the network to attend to a limited number of points. This can make the interpretation of the attention coefficient easier. However, using a softmax could potentially lead to a decrease of performance if the points shouldn’t strictly compete for contribution to the intensity under the generating process. As a result, we believe that choosing a sigmoid or a softmax is not straightforward. We use sigmoid for cumulative approximators, and softmax everywhere else.

A.4 Layer normalisation

The final layer of the Transformer requiring modification issue is layer normalisation, a layer which dramatically improves the convergence speed of these models.

Modifying this layer requires realising that any layer requiring the division by the sum of activations (for example, even $L_2$ normalisation) will result in a negative derivative occurring somewhere. Indeed, this is the underlying reason for the negative elements of the softmax Jacobian in Equation (19).

It follows that any kind of normalisation cannot explicitly depend on the current set of activations. Taking inspiration from batch normalisation, we construct an exponential moving average form of Layer normalisation during training. When performing a forward pass, the means and standard deviations are taken from these moving averages and are treated as constants. After the forward pass, the means and standard deviations are then updated in a similar fashion to batch normalisation.

Finally, taking the gain parameter positive as discussed in Appendix A.1 results in a monotonic form of layer normalisation.

We employ this form of layer normalisation in the cumulative self-attention decoder (SA-CM), otherwise we use the standard form.

---

8This modification could equally be applied to the \textit{tanh} activation.
A.5 Encoding

**Temporal Encoding for monotonic approximators** The temporal embedding of Equation (54) is not monotonic in \( t \) and therefore cannot be used in any conditional cumulative approximator. (Vaswani et al., 2017) noted that a learnable temporal encoding had similar performance to the one presented in Equation (55). In order to model the conditional cumulative intensity \( \Lambda^*_m(t) \), we will instead use a MLP

\[
\text{ParametricTemporal}(t) = \text{MLP}(t; \theta \geq \epsilon) \in \mathbb{R}^{d_{\text{Model}}},
\]

where \( \theta \geq \epsilon \) indicates that all projection matrices have positive values in all entries. Biases may be negative. If we choose monotonic activation functions for the MLP, then it is a monotonic function approximator (Sill, 1998).

The temporal encoding of an event at \( t_i \) with labels \( M_i \) is then

\[
x_i = \text{TemporalEncode}(t_i, M_i) = v_i(M_i) \sqrt{d_{\text{Model}}} + \text{ParametricTemporal}(t_i) \in \mathbb{R}^{d_{\text{Model}}},
\]

A.6 Double backward trick

When using a marked neural network based on the cumulative intensity, one issue comes from the fact that neural networks accumulate gradients. Specifically, the way that autograd is implemented in commonly used deep learning frameworks means that it is not possible to compute \( \frac{\partial}{\partial t} \Lambda^*_m(t) \) for a single \( m \). The value of the derivative will always be accompanied by the derivatives of all \( m \) due to gradient accumulation, i.e. one can only compute the sum \( \sum_{m=1}^{M} \frac{\partial}{\partial t} \Lambda^*_m(t) \) but not an individual \( \frac{\partial}{\partial t} \Lambda^*_m(t) \).

A way of solving this issue is to split \( \Lambda^*_m(t) \) into individual \( M \) components, and to compute the gradient for each of them. However, this method is not applicable to high values of \( M \) due to computational overhead. Another way to solve this issue is to use the double backward trick which allows to compute this gradient without having to split the cumulative intensity.

This trick is based on the following: we define a \( B \times L \times M \) (Batch size \( \times \) Sequence length \( \times \# \) classes) tensor \( a \) filled with zeros, and compute the Jacobian vector product

\[
\text{jvp} = \left( \frac{\partial}{\partial t} \Lambda^*_m(t) \right)^T a \in \mathbb{R}^{B \times L}.
\]

We then define second tensor \( b \) of shape \( B \times L \times M \), filled with ones, and we compute the following Jacobian vector product:

\[
\left( \frac{\partial}{\partial a} \text{jvp} \right)^T b = \left\{ \frac{\partial}{\partial a} \left[ \left( \frac{\partial}{\partial t} \Lambda^*_m(t) \right)^T a \right] \right\}^T b
\]

\[
= \left( \frac{\partial}{\partial t} \Lambda^*_m(t) \right)^T b
\]

\[
= \frac{\partial}{\partial t} \Lambda^*_m(t) \in \mathbb{R}^{B \times L \times M}
\]

This recovers the element-wise derivative of the cumulative intensity function as desired, with the number of derivative operations performed being independent of the number of labels \( M \).

A.7 Modelling the log cumulative intensity

We also investigated an alternative which is to let the decoder directly approximate \( \log \Lambda^*_m(t) \). We have then:

\[
\frac{\partial}{\partial t} \log \Lambda^*_m(t) = \frac{\Lambda^*_m(t)}{\Lambda^*_m(t)} \frac{\partial}{\partial t} \Lambda^*_m(t),
\]

\[
\log \Lambda^*_m(t) = \log \Lambda^*_m(t) + \log \left( \frac{\partial}{\partial t} \Lambda^*_m(t) \right).
\]
While we didn’t use this method to produce our results, we implemented it in our code-base. The advantage of this method is that the log intensity is directly modelled by the network, and its disadvantage is that the subtraction of the exponential terms to compute \( \Lambda_m^*(t) - \Lambda_n^*(t) \) can lead to numerical instability.

## B Taxonomy

We ran our experiments using 2 encoders: SA and GRU, and 7 decoders: CP, RMTTP, LNM, MLP-CM, MLP-MC, Attn-CM, Attn-MM. We combined these encoders and decoders to form models, which are defined by linking an encoder with a decoder: for instance, GRU-MLP-CM denotes a GRU encoder with a MLP-CM (for cumulative) decoder. We present here these different components.

For the implementations of these models, as well as instances trained on the tasks in our setup, please refer to code base supplied in the supplementary material.

### Label embeddings

Although Neural TPP encoders differ in how they encode temporal information, they share a label embedding step. Given labels \( m \in M_t \), localised at time \( t \), the \( D_{\text{emb}} \) dimensional embedding \( v_i \) is

\[
v_i = f_{\text{pool}} \left( W_i = \{ w^{(m)} | m \in M_t \} \right) \in \mathbb{R}^{D_{\text{emb}}},
\]

where \( w^{(m)} \) is the learnable embedding for class \( m \), and \( f_{\text{pool}}(W) \) is a pooling function, e.g. mean pooling: \( f_{\text{pool}}(W) = \sum_{w \in W} w/|W| \), or max pooling: \( f_{\text{pool}}(W) = \oplus_{i=1}^{D_{\text{emb}}} \max(\{ w_{\alpha} | w \in W \}) \).

### B.1 Encoders

**GRU**

We follow the default equations of the GRU NN:

\[
\begin{align*}
    r_i &= \sigma (W^{(1)} x_t + b^{(1)} + W^{(2)} h_{(i-1)} + b^{(2)}) \\
    z_i &= \sigma (W^{(3)} x_t + b^{(3)} + W^{(4)} h_{(i-1)} + b^{(4)}) \\
    n_i &= \tanh (W^{(5)} x_t + b^{(5)} + r_i \circ (W^{(6)} h_{(i-1)} + b^{(6)})) \\
    h_i &= (1 - z_i) \circ n_i + z_i \circ h_{(i-1)},
\end{align*}
\]

where \( h_i, r_i, z_i \) and \( n_i \) are the hidden state, and the reset, update and new gates, respectively, at time \( t \). \( x_t \) is the input at time \( t \), defined by Equation (54). \( \sigma \) designs the sigmoid function and \( \circ \) is the Hadamard product.

**Self-attention (SA)**

We follow Equation (52) and Equation (55) to form our attention block. The keys, queries and values are linear projections of the input: \( q = W_k x, k = W_k x, v = W_v x \), with the input \( X = \{ x_1, x_2, \ldots, x \} \), with each \( x_i \) defined by Equation (55). We also apply a Layer Normalisation layer before each attention and feedforward block:

\[
\begin{align*}
    Q' &= \text{LayerNorm}(Q), \\
    Q' &= \text{MultiHeadAttn}(Q', V) \\
    Q' &= Q' + Q \\
    Z &= \text{LayerNorm}(Q') \\
    Z &= \{ W^{(2)} \text{ReLU}(W^{(1)} z_i + b^{(1)}) + b^{(2)} \} \\
    Z &= Z + Q',
\end{align*}
\]

where MultiHeadAttn is defined by Equation (56). We summarise these equations by:

\[
Z = \text{Attn}(Q = \mathcal{X}, \mathcal{V} = \mathcal{X}) \equiv \text{SA} (\mathcal{X}).
\]

\(^9\) In the multi-class setting, only one label appears at each time \( t_i \), and so \( v_i \) is directly the embedding for that label, and pooling has no effect.
B.2 Decoders

For every decoder, we use when appropriate the same MLP, composed of two layers: one from \( D_{\text{hid}} \) to \( D_{\text{hid}} \), and another from \( D_{\text{hid}} \) to \( M \), where \( D_{\text{hid}} \) is either 8, 32 and 64 depending on the dataset, and \( M \) is the number of marks.

We also define the following terms for every decoder: \( t \), a query time, \( z_t \equiv z_{t,\mathcal{H}_t} \), the representation for the latest event in \( \mathcal{H}_t \), i.e. the past event closest in time to \( t \), and \( t_i \), the time of the previous event. In addition, we define \( q_t \), the representation of the query time \( t \). For the cumulative models, \( q_t = \text{ParametricTemporal}(t) \), and for the Monte-Carlo models, \( q_t = \text{Temporal}(t) \), following Equation (21) and Equation (54), respectively.

### Conditional Poisson (CP)

The conditional Poisson decoder returns:

\[
\lambda_m^*(t) = \log(\text{MLP}(z_t)), \quad \Lambda_m^*(t) = \text{MLP}(z_t)(t - t_i),
\]

where the MLP is the same in both equations.

### RMTPP

Given the same elements as for the conditional Poisson, the RMTPP returns:

\[
\begin{align*}
\lambda_m^*(t) &= \left[ W^{(1)} z_t + w^{(2)} (t - t_i) + b^{(1)} \right], \\
\Lambda_m^*(t) &= \frac{1}{w^{(2)}} \left[ \exp(W^{(1)} z_t + b^{(1)}) - \exp(W^{(1)} z_t + w^{(2)} (t - t_i) + b^{(1)}) \right],
\end{align*}
\]

where \( W^{(1)} \in \mathbb{R}^{D_{\text{hid}} \times M}, w^{(2)} \in \mathbb{R}, \) and \( b^{(1)} \in \mathbb{R}^M \), are learnable parameters.

### Log-normal mixture (LNM)

Following [Shchur et al. (2020)](Shchur2020), the log-normal mixture model returns:

\[
\bar{p}^* = \sum^K_{k=1} \frac{1}{w_k} \frac{1}{(t - t_i) \sigma_k \sqrt{2\pi}} \exp \left[ \frac{-\log(t - t_i) - \mu_k)^2}{2\sigma_k^2} \right], \quad \bar{p}_m^* = \bar{p}^* \rho_m(\mathcal{H}_t)
\]

where \( w, \sigma, \mu \in \mathbb{R}^K \) are mixture weights, distribution means and standard deviations, and are outputs of the encoder. These parameters are defined by:

\[
\begin{align*}
&\mathbf{w} = \text{softmax}(W^{(1)} z_{t_i} + b^{(1)}), \\
&\mathbf{\sigma} = \exp(W^{(2)} z_{t_i} + b^{(2)}), \quad \mathbf{\mu} = W^{(3)} z_{t_i} + b^{(3)}.
\end{align*}
\]

### MLP Cumulative (MLP-CM)

The MLP-CM returns:

\[
\log \lambda_m^*(t) = \log \frac{\partial \Lambda_m^*(t)}{\partial t}, \quad \Lambda_m^*(t) = \text{MLP}([q_t, z_t]; \theta_{\geq t}),
\]

where the square brackets indicate a concatenation.

### MLP Monte Carlo (MLP-MC)

The MLP-MC returns:

\[
\log \lambda_m^*(t) = \text{MLP}([q_t, z_t]), \quad \Lambda_m^*(t) = \text{MC} [\lambda_m^*(t'), t', t_i, t],
\]

where MC represents the estimation of the integral \( \int_{t_i}^t \lambda_m^*(t') dt' \) using a Monte-Carlo sampling method.

### Attention Cumulative (Attn-CM)

For the Attn-CM and Attn-MC, the attention block differs from the SA encoder: the queries \( W_q q \) are defined from the query representations, and the keys \( W_k z \) and values \( W_v z \) are defined from the encoder representations.

The Attn-CM returns:

\[
\log \lambda_m^*(t) = \log \frac{\partial \Lambda_m^*(t)}{\partial t}, \quad \Lambda_m^*(t) = \text{Attn} (\mathcal{Q} = \{ q_t \}, \mathcal{V} = z),
\]

where Transformer refers to Equation (40), with \( x = q \) as input. Moreover, the components of this Attention are modified following Appendix [A]. In particular the ReLU activation is replaced by a Gumbel.
Attention Monte Carlo (Attn-MC) The Attn-MC returns:
\[
\log \lambda^*_m(t) = \text{Attn}(Q = \{q_i\}, V = Z), \quad \Lambda^*_m(t) = \text{MC} [\lambda^*_m(t'), t', t_i, t],
\]
where MC represents the estimation of the integral \( \int_{t_i}^t \lambda^*_m(t') dt' \) using a Monte-Carlo sampling method.

C Additional results

C.1 Hawkes datasets

The parameters of our Hawkes datasets are:

Independent:
\[
\mu = \begin{bmatrix} 0.1 \\ 0.05 \end{bmatrix}, \quad \alpha = \begin{bmatrix} 0.2 & 0.0 \\ 0.0 & 0.4 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \end{bmatrix},
\]

Dependent:
\[
\mu = \begin{bmatrix} 0.1 \\ 0.05 \end{bmatrix}, \quad \alpha = \begin{bmatrix} 0.2 & 0.1 \\ 0.2 & 0.3 \end{bmatrix}, \quad \beta = \begin{bmatrix} 1.0 & 1.0 \\ 1.0 & 2.0 \end{bmatrix}.
\]

C.2 Hawkes results

A useful property of these datasets is that we can visually compare the modelled intensities with the intensity of the underlying generating process. On each dataset, Hawkes (independent) and Hawkes (dependent), all models perform similarly, with the exception of the conditional Poisson. We present results for the SA-MLP-MC on Figure 4.

C.3 Retweets results

On the Retweets dataset, while the conditional Poisson model significantly outperforms TPP models in terms of ROC-AUC, the opposite is true in terms of NLL/time. This is probably due to the fact that TPPs can model the intensity decay that occurs when a tweet is not retweeted over a certain period of time. We compare on Figure 5 the intensity functions of a SA-CP and a SA-MLP-MC.

D Transformer architecture

Attention block The key component of the Transformer is attention. This computes contextualised representations \( q'_i = \text{Attention}(q_i, \{k_j\}, \{v_j\}) \in \mathbb{R}^{d_{\text{model}}} \) of queries \( q_i \in \mathbb{R}^{d_{\text{model}}} \) from linear combinations of values \( v_j \in \mathbb{R}^{d_{\text{model}}} \) whose magnitude of contribution is governed by keys \( k_j \in \mathbb{R}^{d_{\text{model}}}
\]

\[
\text{Attention}(q_i, \{k_j\}, \{v_j\}) = \sum_j \alpha_{i,j} v_j, \quad \alpha_{i,j} = g(E_{i,j}), \quad E_{i,j} = \frac{q_i^T k_j}{\sqrt{d_k}}
\]

where \( \alpha_{i,j} \) are the attention coefficients, \( E_{i,j} \) are the attention logits, and \( g \) is an activation function that is usually taken to be the softmax

\[
\text{softmax}(E_{i,j}) = \frac{\exp(E_{i,j})}{\sum_k \exp(E_{i,k})}.
\]
We experimented with having where \( \nu \) is a learnable parameter of the model, however, this made the model extremely difficult to optimise. Note that \( \tilde{\beta} = 1 \) for a language model. In addition, \( \beta \) does not change the relative frequency of the rotational subspaces in the temporal embedding from the form in [Vaswani et al., 2017]. The encoding with temporal information of an event at \( t_i \) with labels \( M_i \) is then

\[
x_i = \text{TemporalEncode}(t_i, M_i) = v_i(M_i) \sqrt{d_{\text{model}}} + \text{Temporal}(t_i) \in \mathbb{R}^{d_{\text{model}}}.
\]

**Multi-head attention** Multi-head attention produces \( q_h \) in order to jointly attend to information from different subspaces at different positions

\[
\text{MultiHead}(q_i, \{k_j\}, \{v_j\}) = W^{(o)} \left[ \bigoplus_{h=1}^{H} \text{Attention} \left( W_h^{(q)} q_i, W_h^{(k)} k_j, W_h^{(v)} v_j \right) \right],
\]

where \( W_h^{(q)}, W_h^{(k)}, W_h^{(v)} \in \mathbb{R}^{d_q \times d_{\text{model}}}, W_h^{(v)} \in \mathbb{R}^{d_v \times d_{\text{model}}}, \) and \( W^{(o)} \in \mathbb{R}^{d_{\text{model}} \times h d_v} \) are learnable projections.