

# Nonparametric likelihood based estimation of linear filters for point processes

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**Abstract** We consider models for multivariate point processes where the intensity is given nonparametrically in terms of functions in a reproducing kernel Hilbert space. The likelihood function involves a time integral and is consequently not given in terms of a finite number of kernel evaluations. The main result is a representation of the gradient of the log-likelihood, which we use to derive computable approximations of the log-likelihood and the gradient by time discretization. These approximations are then used to minimize the approximate penalized log-likelihood. For time and memory efficiency the implementation relies crucially on the use of sparse matrices. As an illustration we consider neuron network modeling, and we use this example to investigate how the computational costs of the approximations depend on the resolution of the time discretization. The implementation is available in the R package `ppstat`.

**Keywords** Multivariate point processes · Penalization · Reproducing kernel Hilbert spaces · `ppstat`

## 1 Introduction

Reproducing kernel Hilbert spaces have become widely used in statistics and machine learning, [Bishop \(2006\)](#), [Hastie et al. \(2009\)](#), [Scholkopf and Smola \(2001\)](#), where they provide a means for nonparametric estimation of nonlinear functional relations. They have a long history in the statistical literature, with noteworthy relations to splines and other basis expansion techniques, as well as Gaussian process theory,

(see [Berlinet and Thomas-Agnan 2004](#), [Wahba 1990](#)). A typical application is to estimation of a mean value that depends on one or more predictor variables. As a function of the predictor variables the mean is assumed to be in a Hilbert space, and the estimator is obtained by penalized estimation in the linear Hilbert space—using the Hilbert space norm for penalization. If we use the squared error loss, the so-called representer theorem states that for a reproducing kernel Hilbert space the estimation problem is, in fact, a finite dimensional optimization problem. The optimization problem is given in terms of a finite number of kernel evaluations, see ([Hofmann et al. 2008](#)) for a recent review. The representer theorem holds for any loss function, which is a function of a finite number of continuous linear functionals.

In this paper we show how to use reproducing kernel Hilbert space techniques for nonparametric point process modeling of e.g. neuron network activity. A network of neurons is a prime example of an interacting dynamical system, and the characterization and modeling of the network activity is a central scientific challenge, see e.g. [Pillow et al. \(2008\)](#). Data consist of a collection of spike times, which can be measured simultaneously for multiple neurons. The spike times are discrete event times and the appropriate modeling framework is that of multivariate point processes. From a prediction viewpoint the objective is to predict the next spike time of a given neuron as a function of the history of the spike times for all neurons.

A natural modeling approach is via the conditional intensity, which specifies how the history affects the immediate intensity—or rate—of the occurrence of another spike. The negative log-likelihood for a point process model is given directly in terms of the intensity, but the representer theorem, Theorem 9 in [Hofmann et al. \(2008\)](#), does not hold in general, (see [Hansen 2013](#)). The reason is that the log-likelihood involves a time-integral, see (4) below, and the log-likelihood

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is consequently not a function of a *finite* number of continuous linear functionals in general. This is the main problem that we address in this paper.

To motivate our general nonparametric model class we briefly review the classical linear Hawkes process introduced in Hawkes (1971). We consider in the following  $p$  different counting processes of discrete events, e.g. spike times. We let  $(N_t^j)$  denote the  $j$ 'th of the counting processes, for  $j = 1, \dots, p$ , and we assume first that the intensity of a new event for the  $i$ 'th process is  $Y_t^i = \sum_{j=1}^p Y_t^{ij}$  where

$$Y_t^{ij} = \int_0^{t-} e^{\alpha_{ij}(t-s)+\beta_{ij}} dN_s^j. \tag{1}$$

The intensity process  $Y^i$  jumps by  $e^{\beta_{ij}}$  whenever an event occurs in the  $j$ 'th process, and the  $\alpha_{ij}$ -parameters control the smooth exponential behavior in between jumps. The intensity specifies the conditional probability of observing an event immediately after time  $t$  in the sense that

$$P(N_{t+\delta}^i - N_t^i = 1 \mid \mathcal{F}_t) \simeq \delta Y_t^i,$$

where  $\mathcal{F}_t$  denotes the history of all events preceding time  $t$ , (see e.g. Jacobsen 2006 or Andersen et al. 1993). Note the upper integration limit,  $t-$ , which means that the integral w.r.t.  $N_s^j$  only involves events strictly before  $t$ . This is an essential requirement for correct likelihood computations, see (4) below.

It follows from (1) that if  $\sigma_j < t$  denotes the last of the  $j$ 'th events before  $t$ ,

$$Y_t^{ij} = e^{\alpha_{ij}(t-\sigma_j)} Y_{\sigma_j+}^{ij}.$$

This provides an efficient way of computing the intensity process. In fact, it follows that  $(Y_t^{ij})_{i,j=1,\dots,p}$  is a  $p^2$ -dimensional Markov process, and that there is a one-to-one correspondence between this process and the multivariate counting process  $(N_t^1, \dots, N_t^p)$ .

Our interest is to generalize the model given in terms of (1) to non-exponential integrands, and, in particular, to allow those integrands to be estimated nonparametrically. A consequence is that the Markov property will be lost, and that the intensity computation will be more demanding.

The integral (1) can be understood as a linear filter of the multivariate counting process  $(N_t^1, \dots, N_t^p)$ , and we will consider the generalization of such linear filters to processes of the form

$$X_t^i = \sum_{j=1}^p \int_0^{t-} g_{ij}(t-s) dN_s^j \tag{2}$$

with  $g_{ij}$  general functions in a suitable function space. The positive  $Y^i$  process is a special case with  $g_{ij}(s) = e^{\alpha_{ij}s+\beta_{ij}}$ . If we allow for negative integrands in (2) the linear filter can take negative values, in which case it cannot be an intensity.

We therefore consider transformations of  $X_t^i$ , such that the intensity is given by  $\varphi(X_t^i)$  for a general but fixed function  $\varphi : \mathbb{R} \rightarrow [0, \infty)$ .

In this paper we are particularly concerned with efficient computation and minimization of the penalized negative log-likelihood as a function of the nonparametric components  $g_{ij}$ , with  $g_{ij}$  in a reproducing kernel Hilbert space  $\mathcal{H}$ . We consider algorithms for standard quadratic penalization  $\sum_{ij} \|g_{ij}\|^2$ , with  $\|\cdot\|$  the Hilbert space norm on  $\mathcal{H}$ . We will throughout assume that the  $g_{ij}$ -functions are variation independent, which imply that the computation and minimization of the joint penalized negative log-likelihood can be split into  $p$  separate minimization problems. To ease notation we will thus subsequently consider the modeling of one counting process  $N_t$  in terms of  $N_t^1, \dots, N_t^p$ , where  $N_t$  can be any of the  $p$  counting processes. All computations presented were carried out in R using the `ppstat` package. It implements the models of multivariate point processes through linear filters that are treated in this paper.

## 2 Likelihood computations for point processes specified by linear filters

We assume that we observe a simple counting process  $(N_s)_{0 \leq s \leq t}$  of discrete events on the time interval  $[0, t]$ . The jump times of  $N_s$  are denoted  $\tau_1 < \dots < \tau_{N_t}$ . We let  $\mathcal{H}$  denote a reproducing kernel Hilbert space of functions on  $[0, t]$  with reproducing kernel  $R : [0, t] \times [0, t] \rightarrow \mathbb{R}$ , and we let  $g = (g_1, \dots, g_p) \in \mathcal{H}^p$ . We assume that  $R$  is continuous in which case the functions in  $\mathcal{H}$  are also continuous, see Theorem 17 in Berlinet and Thomas-Agnan (2004). With  $N^1, \dots, N^p$  counting processes with corresponding event times  $\sigma_j^i$  we introduce

$$\begin{aligned} X_s(g) &= \sum_{i=1}^p \int_0^{s-} g_i(s-u) dN_u^i \\ &= \sum_{i=1}^p \sum_{j:\sigma_j^i < s} g_i(s - \sigma_j^i). \end{aligned}$$

As a function of  $g$  we note that  $X_s : \mathcal{H}^p \rightarrow \mathbb{R}$  being a sum of function evaluations is a continuous linear functional. Indeed, we can express  $X_s$  in terms of inner products with the kernel as

$$X_s(g) = \sum_{i=1}^p \sum_{j:\sigma_j^i < s} \langle R(s - \sigma_j^i, \cdot), g_i \rangle. \tag{3}$$

The process  $X_s(g)$  is called the *linear predictor* process. We consider the model of  $(N_s)_{0 \leq s \leq t}$  where the intensity is given as  $\lambda_s(g) = \varphi(X_s(g))$  with  $\varphi : \mathbb{R} \rightarrow [0, \infty)$  a known

function. The objective is to estimate the  $g_i$ -functions in  $\mathcal{H}$ . In most applications we will include a baseline parameter as well, in which case the linear predictor becomes  $\beta_0 + X_s(g)$ . In order not to complicate the notation unnecessarily we take  $\beta_0 = 0$  in the theoretical presentation.

From Corollary II.7.3 in Andersen et al. (1993) it follows that the negative log-likelihood w.r.t. the homogeneous Poisson process is given as

$$\ell(g) = \int_0^t \varphi(X_s(g)) \, ds - \sum_{k=1}^{N_t} \log \varphi(X_{\tau_k}(g)). \tag{4}$$

If  $\varphi$  is the identity the time integral has a closed form representation in terms of the antiderivatives of  $g_i$ , but in general it has to be computed numerically. We should note that  $\ell$  is convex as a function of  $g$  if  $\varphi$  is convex and log-concave.

The following proposition gives the gradient of  $\ell$  in the reproducing kernel Hilbert space. This result is central for our development and understanding of a practically implementable minimization algorithm of the penalized negative log-likelihood.

**Proposition 1** *If  $\varphi$  is continuously differentiable the gradient in  $\mathcal{H}$  w.r.t.  $g_i$  is*

$$\begin{aligned} \nabla_i \ell(g) &= \sum_j \int_{\sigma_j^i}^t \varphi'(X_s(g)) R(s - \sigma_j^i, \cdot) \, ds \\ &\quad - \sum_j \sum_{k: \sigma_j^i < \tau_k} \frac{\varphi'(X_{\tau_k}(g))}{\varphi(X_{\tau_k}(g))} R(\tau_k - \sigma_j^i, \cdot). \end{aligned} \tag{5}$$

The proof of Proposition 1 is given in Sect. 7. It is a special case of Proposition 3.6 in Hansen (2013) if  $\mathcal{H}$  is a Sobolev space. However, since we restrict attention to counting process integrators in this paper, in contrast to Hansen (2013) where more general integrator processes are allowed, we can give a relatively elementary proof for  $\mathcal{H}$  being any reproducing kernel Hilbert space with a continuous kernel.

Computations of  $\ell$  as well as the gradient involve the computation of  $X_s(g)$ . Without further assumptions a direct computation of  $X_s(g)$  on a grid of  $n$  time points involves in the order of  $n \sum_{i=1}^p N_t^i$  evaluations of the  $g_i$ -functions. In comparison, (1) can be computed recursively with the order of  $np$  evaluations of the exponential function.

In this paper we consider three techniques for reducing the general costs of computing  $X_s(g)$ .

- **Bounded memory.** The filter functions  $g_i$  are restricted to have support in  $[0, A]$  for a fixed  $A$ .
- **Preevaluations.** The filter functions are preevaluated on a grid in  $[0, A]$ .

- **Basis expansions.** The filter functions are of the form  $g = \sum_k \beta_k B_k$  for fixed basis functions  $B_k$ , and

$$X_s(g) = \sum_k \beta_k X_s(B_k).$$

The linear filters  $X_s(B_k)$  are precomputed.

### 3 Time discretization

In this section we discuss the time discretizations necessary for the practical implementation of an optimization algorithm in  $\mathcal{H}$ . We assume that all filter functions  $g_i$  have a prespecified support restricted to  $[0, A]$ , and that  $\mathcal{H}$  is restricted to be a space of functions with support in  $[0, A]$ . We approximate time integrals by right Riemann sums with functions evaluated in the grid

$$0 = t_0 < t_1 < \dots < t_n = t$$

and corresponding interdistances  $\Delta_l = t_l - t_{l-1}$  for  $l = 1, \dots, n$ . We will assume that the collection of event times is a subset of this grid and denote the corresponding subset of indices by  $I_{\text{jump}} \subseteq \{0, \dots, n\}$ .

We need an implementable representation of the linear predictor as well as the functional gradient given by (5). A possible representation of  $g_i$  itself is via the  $N$ -dimensional vector  $\mathbf{g}_i$  of its evaluations in a grid

$$0 = \delta_0 < \delta_1 < \dots < \delta_N = A,$$

that is,  $\mathbf{g}_{ik} = g_i(\delta_k)$  for  $k = 0, \dots, N - 1$ . We let  $\mathbf{g}$  denote the  $N \times p$  matrix with columns  $\mathbf{g}_i$  for  $i = 1, \dots, p$ . Define

$$h_{lik} = \#\{j \mid \delta_k \leq t_l - \sigma_j^i < \delta_{k+1}\} \mathbf{1}(\sigma_j^i < t_l)$$

as the number of events for  $N^i$  in  $(t_l - \delta_{k+1}, t_l - \delta_k]$ . The indicator  $\mathbf{1}(\sigma_j^i < t_l)$  ensures that if  $\sigma_j^i = t_l$  then  $h_{li0} = 0$ , which, in turn, ensures that the approximation of the linear predictor below does not anticipate events. It is the intention that the grid is chosen such that the  $h_{lik}$ 's take the values 0 and 1 only. The linear predictor for given  $g_i$ 's evaluated in the grid points is approximated as

$$\xi_l := \sum_{i,k} h_{lik} \mathbf{g}_{ik} \tag{6}$$

$$\simeq \sum_{i=1}^p \sum_{j: t_l - A \leq \sigma_j^i < t_l} g_i(t_l - \sigma_j^i) \tag{7}$$

$$= \sum_{i=1}^p \int_{t_l - A}^{t_l^-} g_i(t_l - u) dN_u^i.$$

To formally handle the lower limit in the integral correctly,  $h_{li(N-1)}$  should be redefined to be 1 if  $\sigma_j^i = t_l - A$ . Such a

redefinition will typically have no detectable consequences, whereas handling the case  $\sigma_j^i = t_l$  correctly is crucial to avoid making the approximation anticipating. An approximation of the negative log-likelihood in  $g$  is then obtained as

$$\ell^{\text{approx}}(\mathbf{g}) = \sum_l \varphi(\xi_l) \Delta_l - \sum_{l \in I_{\text{jump}}} \log \varphi(\xi_l). \tag{8}$$

If we use the same  $\delta$ -grid for evaluating the kernel  $R$ , we get the gradient approximation from Proposition 1

$$\begin{aligned} \nabla_i \ell^{\text{approx}}(\mathbf{g}) &= \sum_k \left( \sum_l \varphi'(\xi_l) \Delta_l h_{lik} \right) R(\delta_k, \cdot) \\ &\quad - \sum_k \left( \sum_{l \in I_{\text{jump}}} \frac{\varphi'(\xi_l)}{\varphi(\xi_l)} h_{lik} \right) R(\delta_k, \cdot). \end{aligned} \tag{9}$$

We observe that

$$\nabla_i \ell^{\text{approx}}(\mathbf{g}) \in \text{span} \{R(\delta_0, \cdot), \dots, R(\delta_{N-1}, \cdot)\}.$$

The consequence is that any descent algorithm based on  $\nabla_i \ell^{\text{approx}}(\mathbf{g})$  stays in the finite dimensional subspace spanned by  $R(\delta_0, \cdot), \dots, R(\delta_{N-1}, \cdot)$  – if it starts in this subspace. As we show below, there is a unique element in this subspace with evaluations  $\mathbf{g}_i$ , and the discretization effectively restricts  $g_i$  to be a function in this subspace.

### 3.1 The direct approximation

The  $N \times N$  Gram matrix  $\mathbb{G}$  is given as  $\mathbb{G}_{kl} = R(\delta_k, \delta_l)$ . The vector  $\mathbf{g}_i$  can be identified with the unique function  $g_i = \sum_k \beta_{ik}^0 R(\delta_k, \cdot)$  obtained by solving

$$\mathbf{g}_i = \mathbb{G} \beta_i^0.$$

This is the minimal norm element whose evaluations coincide with  $\mathbf{g}_i$ . Since  $\mathbb{G}$  is positive definite there are several possible ways to factorize  $\mathbb{G}$  such that  $\mathbb{G} = U U^T$ . For the Cholesky factorization  $U$  is lower triangular, and for the spectral decomposition the columns of  $U$  are orthogonal. For any such factorization

$$\mathbf{g}_i = U \underbrace{U^T \beta_i^0}_{\beta_i} = U \beta_i.$$

Note how the  $\beta_i^0$ - and thus the  $\beta_i$ -parameter representation of the evaluations  $\nabla_i \ell^{\text{approx}}(\mathbf{g})(\delta_k)$  can be read directly from (9). We observe that the squared norm of  $g_i$  equals

$$\|g_i\|^2 = (\beta_i^0)^T \mathbb{G} \beta_i^0 = \|\beta_i\|_2^2$$

with  $\|\cdot\|_2$  denoting the ordinary Euclidean norm on  $\mathbb{R}^N$ . The parametrization in terms of  $\beta_i$  is thus an isometry from  $\mathbb{R}^N$  into  $\mathcal{H}$ . The objective function—the penalized negative log-likelihood approximation—can be computed as

$$\ell^{\text{approx}}(U\beta) + \lambda \sum_i \|\beta_i\|_2^2 \tag{10}$$

using (8), and the  $\beta_i$ -gradient can be computed as

$$U^T \nabla_i^\beta \ell^{\text{approx}}(U\beta) + 2\lambda \beta_i,$$

where

$$\begin{aligned} \nabla_i^\beta \ell^{\text{approx}}(\mathbf{g})_k &= \sum_l \varphi'(\xi_l) \Delta_l h_{lik} \\ &\quad - \sum_{l \in I_{\text{jump}}} \frac{\varphi'(\xi_l)}{\varphi(\xi_l)} h_{lik}. \end{aligned} \tag{11}$$

The use of (8) and (11)—and (6)—requires the computation of  $h_{lik}$ . This can either be done on-the-fly (a matrix free method) or by precomputing the  $n \times (pr)$ -dimensional sparse matrix  $\mathbf{H} = (h_{lik})$ . In practice, an incomplete factorization of  $\mathbb{G}$  with  $U$  an  $N \times q$  matrix is used. This reduces the number of computations a little, and the transition between the  $\mathbf{g}_i$  vectors of evaluations and the  $\beta_i$ -parameters becomes numerically more stable. The implementation in `ppstat` uses the spectral decomposition, and  $q$  is determined by a threshold on the size of the eigenvalues for  $\mathbb{G}$  relative to the largest eigenvalue. The default choice on the threshold in `ppstat` is  $10^{-8}$ .

### 3.2 The basis approximation

Choose a set of basis functions  $B_1, \dots, B_q$  such that

$$\text{span}\{B_1, \dots, B_q\} \subseteq \text{span}\{R(\delta_0, \cdot), \dots, R(\delta_{N-1}, \cdot)\}.$$

Precompute the  $n \times q$  model matrices  $\mathbf{Z}^i$  of basis filters

$$\mathbf{Z}_{lj}^i = \sum_k h_{lik} B_j(\delta_k).$$

With  $g_i = \sum_j \beta_{ij}^0 B_j$ , the  $n$ -dimensional linear predictor is given as  $\xi = \sum_i \mathbf{Z}^i \beta_i^0$ , and  $\ell^{\text{approx}}(\beta^0)$  can be computed using (8). The Gram matrix,  $\mathbb{G}$ , is given by  $\mathbb{G}_{kl} = \langle B_k, B_l \rangle$ , and we let  $\mathbb{G} = V V^T$ . In terms of the parametrization  $\beta_i = V^T \beta_i^0$  we find that

$$\|g_i\|^2 = (\beta_i^0)^T \mathbb{G} \beta_i^0 = \|\beta_i\|_2^2,$$

thus  $\beta_i$  provides an isometric parametrization from  $\mathbb{R}^q$  into  $\mathcal{H}$ . The objective function becomes

$$\ell^{\text{approx}}(V^{-1}\beta) + \lambda \sum_i \|\beta_i\|_2^2, \tag{12}$$

and the gradient is

$$\begin{aligned} & \sum_l \varphi'(\xi_l) \Delta_l (\mathbf{z}_l^i V^{-1})^T - \sum_{l \in I_{\text{jump}}} \frac{\varphi'(\xi_l)}{\varphi(\xi_l)} (\mathbf{z}_l^i V^{-1})^T + 2\lambda \beta_i \\ &= (V^{-1})^T \left( \sum_l \varphi'(\xi_l) \Delta_l (\mathbf{z}_l^i)^T - \sum_{l \in I_{\text{jump}}} \frac{\varphi'(\xi_l)}{\varphi(\xi_l)} (\mathbf{z}_l^i)^T \right) + 2\lambda \beta_i \\ &= (V^{-1})^T \nabla_{\mathbf{z}_l^i}^{0, \text{approx}} (V^{-1} \beta) + 2\lambda \beta_i, \end{aligned}$$

where

$$\nabla_{\mathbf{z}_l^i}^{0, \text{approx}} (\beta^0) = \sum_l \varphi'(\xi_l) \Delta_l (\mathbf{z}_l^i)^T - \sum_{l \in I_{\text{jump}}} \frac{\varphi'(\xi_l)}{\varphi(\xi_l)} (\mathbf{z}_l^i)^T$$

is the gradient in the  $\beta_i^0$  parametrization.

### 4 Statistical theory

In the preceding sections we reduced the infinite dimensional optimization problem to an approximate finite dimensional one, and we introduced isometric parametrizations in terms of a finite dimensional parameter  $\beta$ . In this section we discuss the statistical theory for the case where  $X_s(g) = X_s^T \beta$  for a vector process  $X_s$ , and the estimator of  $\beta$  is obtained by penalized maximum-likelihood estimation using the penalty  $\lambda \|\beta\|_2^2$ . If  $\varphi(X_s^T \beta)$  is the intensity of the counting process, the process  $M_s = N_s - \int_0^s \varphi(X_u^T \beta) du$  is a local martingale. The derivative of the negative log-likelihood can be expressed as a stochastic integral w.r.t.  $M$ ,

$$\begin{aligned} D_\beta \ell(\beta) &= \int_0^t \varphi'(X_s^T \beta) X_s^T ds - \int_0^t \frac{\varphi'(X_s^T \beta)}{\varphi(X_s^T \beta)} X_s^T dN_s \\ &= - \int_0^t \frac{\varphi'(X_s^T \beta)}{\varphi(X_s^T \beta)} X_s^T dM_s. \end{aligned} \tag{13}$$

Since the angle bracket of the local martingale  $M$  is  $\langle M \rangle_t = \int_0^t \varphi(X_s^T \beta) ds$ , cf. (2.4.2) in Andersen et al. (1993), it follows from (2.3.7) in Andersen et al. (1993) that the angle bracket of the vector process (13) is

$$\int_0^t X_s X_s^T \frac{\varphi'(X_s^T \beta)^2}{\varphi(X_s^T \beta)^2} d\langle M \rangle_s = \int_0^t X_s X_s^T \frac{\varphi'(X_s^T \beta)^2}{\varphi(X_s^T \beta)} ds.$$

Under sufficient integrability conditions, see e.g. Proposition 4.6.2 in Jacobsen (2006), the mean of the angle bracket equals the covariance matrix  $K$  of (13), which is the Fisher information matrix. This suggests the estimator

$$\hat{K} = \int_0^t X_s X_s^T \frac{\varphi'(X_s^T \hat{\beta})^2}{\varphi(X_s^T \hat{\beta})} ds$$

of the Fisher information, which can be computed using the same time discretization as otherwise used for likelihood and gradient computations.

From (13) we find the penalized likelihood estimating equation in the  $\beta$ -parametrization

$$\Psi(\beta) := - \int_0^t \frac{\varphi'(X_s^T \beta)}{\varphi(X_s^T \beta)} X_s^T dM_s + 2\lambda \beta^T = 0. \tag{14}$$

The covariance matrix of  $\Psi(\beta)$  defined above coincides with the Fisher information matrix  $K$ , and the mean of its derivative is

$$J := E D_\beta \Psi(\beta) = K + 2\lambda I.$$

A corresponding estimator of  $J$  is  $\hat{J} = \hat{K} + 2\lambda I$ . If  $\hat{\beta}_\lambda$  solves (14), a Taylor expansion of  $\Psi(\hat{\beta}_\lambda)$  around  $\beta$  yields

$$0 = \Psi(\hat{\beta}_\lambda) \simeq \Psi(\beta) + D_\beta \Psi(\beta)(\hat{\beta}_\lambda - \beta),$$

which implies the approximation

$$\hat{\beta}_\lambda - \beta \simeq -D_\beta \Psi(\beta)^{-1} \Psi(\beta) \simeq -J^{-1} D_\beta \ell(\beta) - 2\lambda J^{-1} \beta.$$

If, moreover, the distributional approximation

$$D_\beta \ell(\beta) \overset{\text{approx}}{\sim} \mathcal{N}(0, K)$$

can be justified, these heuristic derivations suggest that

$$\hat{\beta}_\lambda \overset{\text{approx}}{\sim} \mathcal{N}(\beta - 2\lambda J^{-1} \beta, J^{-1} K J^{-1}).$$

We will not attempt to establish sufficient technical conditions in an asymptotic framework to rigorously justify this approximation of the distribution of  $\hat{\beta}_\lambda$ , but see Vaart (1998) for a treatment of standard asymptotic theory, and Chapter VI in Andersen et al. (1993) for a treatment in a counting process framework. We use the distributional approximation to compute pointwise confidence intervals based on the sandwich estimator

$$\hat{J}^{-1} \hat{K} \hat{J}^{-1}$$

of the approximate covariance matrix of  $\hat{\beta}_\lambda$ .

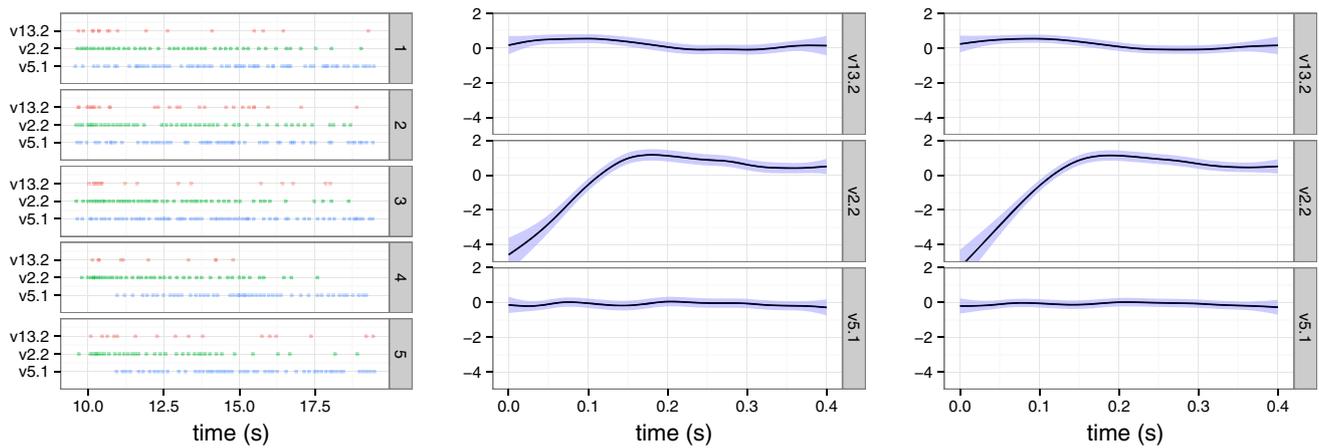
With  $\ell(\hat{\beta}_\lambda)$  the negative log-likelihood in the penalized estimator we also introduce Takeuchi’s information criterion

$$\text{TIC} = \ell(\hat{\beta}_\lambda) + \text{tr}(\hat{J}^{-1} \hat{K}),$$

see Chapter 2 in Claeskens and Hjort (2008). The penalization parameter  $\lambda$  can be chosen by minimizing TIC.

### 5 Results

We investigated the use of both the direct approximation and the basis expansion using cubic B-spline basis functions on a test data set of neuron spike times. The data set consisted of multichannel measurements of spinal neurons from a turtle.



**Fig. 1** *Left* Data example consisting of three spike tracks from five independent multichannel measurements of turtle spinal neurons during a stimulation period. *Middle* Estimates of the  $h_i$ 's in the model of  $v2.2$  using the direct approximation to minimize (10) with  $n = 20,609$ ,  $N = 200$  and  $q = 33$ . The value of  $\lambda = 0.125$  was chosen by minimizing TIC. The baseline estimate is  $\hat{\beta}_0 = 1.04$ . *Right* Similar

estimates of the  $h_i$ 's using a B-spline basis expansion to minimize (12) with  $q = 33$ , and with  $\lambda = 2$  chosen by minimizing TIC. The baseline estimate is  $\hat{\beta}_0 = 1.05$ . The point-wise approximate 95% confidence intervals were obtained using a sandwich estimator of the asymptotic variance

The measurements were replicated 5 times and each time the spike activity was recorded over a period of 40 seconds. A 10 seconds stimulation was given within the observation window. We used the spike times for 3 neurons labeled  $v2.2$ ,  $v13.2$  and  $v5.1$  during the stimulation period, see Fig. 1

The likelihood and gradient algorithms are implemented in the R package `ppstat`, which supports optimization of the objective function via the R function `optim` using the BFGS-algorithm. The `ppstat` package offers a formula based model specification with an interface familiar from `glm`. The direct approximation is implemented via the `ppKernel` function, and the basis expansion is implemented via the `ppSmooth` function. A typical call has the form

```
ppKernel(v2.2 ~ k(v13.2)+k(v2.2)+k(v5.1),
  data = spikeData,
  family = Hawkes('log'),
  support = 0.4,
  lambda = 0.125
)
```

which will include a baseline parameter in addition to the three nonparametric filter functions. The data set contained in the object `spikeData` must be of class `MarkedPointProcess` from the supporting R package `processdata`. The grid of  $n$  time points is determined when the `MarkedPointProcess` object is constructed. The choice of  $\varphi$  is specified as an “inverse link function”—being ‘log’ in the call above. That is, in the call above,  $\varphi(x) = e^x$ .

Figure 1 shows the estimated  $h_i$ 's obtained with  $\varphi(x) = e^x$ ,  $A = 0.4$ ,  $n = 20,609$ ,  $N = 200$  and  $q = 33$  and using either the direct approximation with the Sobolev kernel

or the basis expansion with a B-spline basis. The estimates were computed by minimizing (10) and (12), respectively. The Sobolev kernel is the reproducing kernel for the Sobolev Hilbert space consisting of twice weakly differentiable functions with the second derivative being square integrable. Its precise form depends on which inner product is chosen, but for common choices  $R(\delta_k, \cdot)$  is a cubic spline. The resulting model shows that a  $v2.2$  spike results in a depression of the  $v2.2$ -intensity in the first 0.1 s after the spike followed by an elevation of the  $v2.2$ -intensity. A  $v13.2$  spike appears to result in a small but significant elevation of the  $v2.2$ -intensity, whereas a  $v5.1$  spike appears to have no significant effect on the  $v2.2$ -intensity.

The `ppstat` package supports a number of different choices of  $\varphi$ . In addition to some familiar link functions it supports two parametrized classes of functions. The `root` class is given as

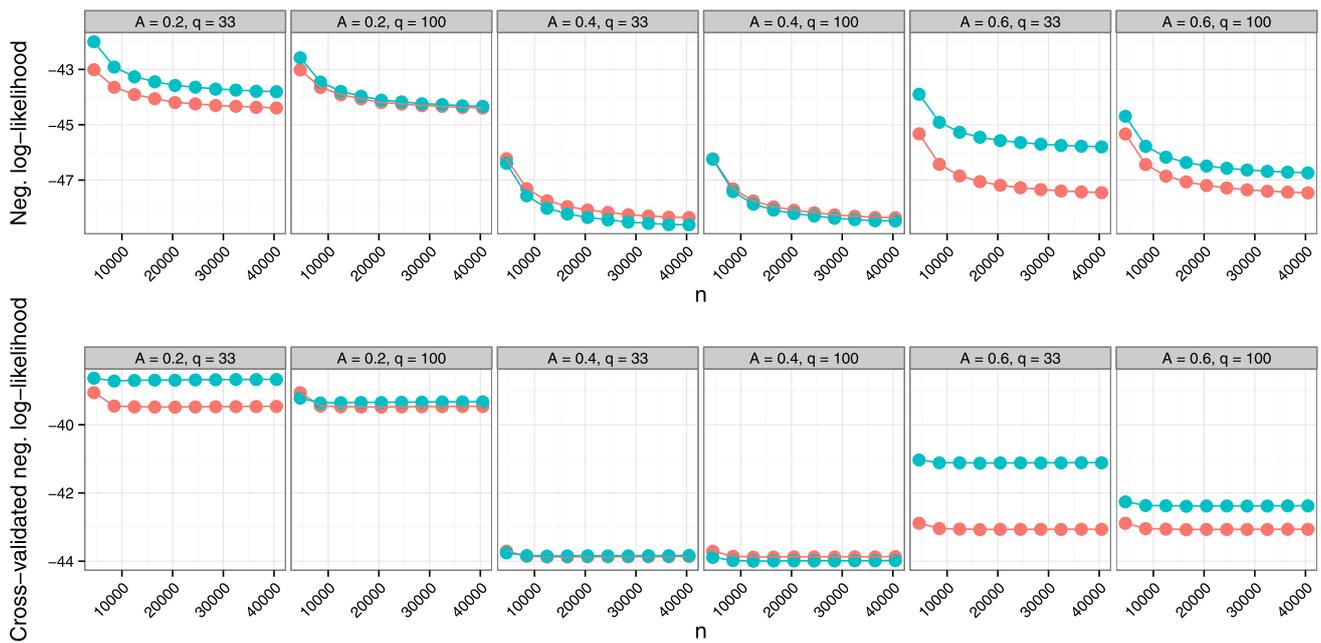
$$\varphi(x) = \begin{cases} x^{c+1} & \text{for } x \leq 0 \\ 0 & \text{for } x > 0, \end{cases}$$

which for  $c = 0$  (the default value) amounts to  $\varphi(x) = \max\{x, 0\}$ . The `logaffine` class is given as

$$\varphi(x) = \begin{cases} e^x & \text{for } x \leq c \\ e^c(x - c + 1) & \text{for } x > c. \end{cases}$$

They all map  $\mathbb{R}$  continuously into  $[0, \infty)$ . Moreover, for the `logaffine` class the  $\varphi$  function is continuously differentiable, whereas for the `root` class this is only true for  $c > 1$ .

The appropriate choice of  $\varphi$  is not straightforward, and there are several considerations that need to be taken into account. One possibility, that we have used, is to optimize the model fit to data. However, one must pay attention to the



**Fig. 2** Top Average negative log-likelihood on the training data for the direct approximation red (dark) filled circle and for the basis expansion cyan (light) filled circle for  $N = 400$ ,  $A = 0.2, 0.4, 0.6$  and  $q = 33, 100$ . Bottom Cross-validated negative log-likelihood

fact that not all combinations of  $\varphi$  and linear filters will result in non-exploding point processes, (see Gjessing et al. 2010). This will be particularly problematic if we were to simulate data from the model. It is difficult to give theoretical results on the non-explosion or stability of a point process if  $\varphi$  grows super linearly, (see e.g. Brémaud and Massoulié 1996) where  $\varphi$  is assumed to be Lipschitz to establish results on stability of point processes.

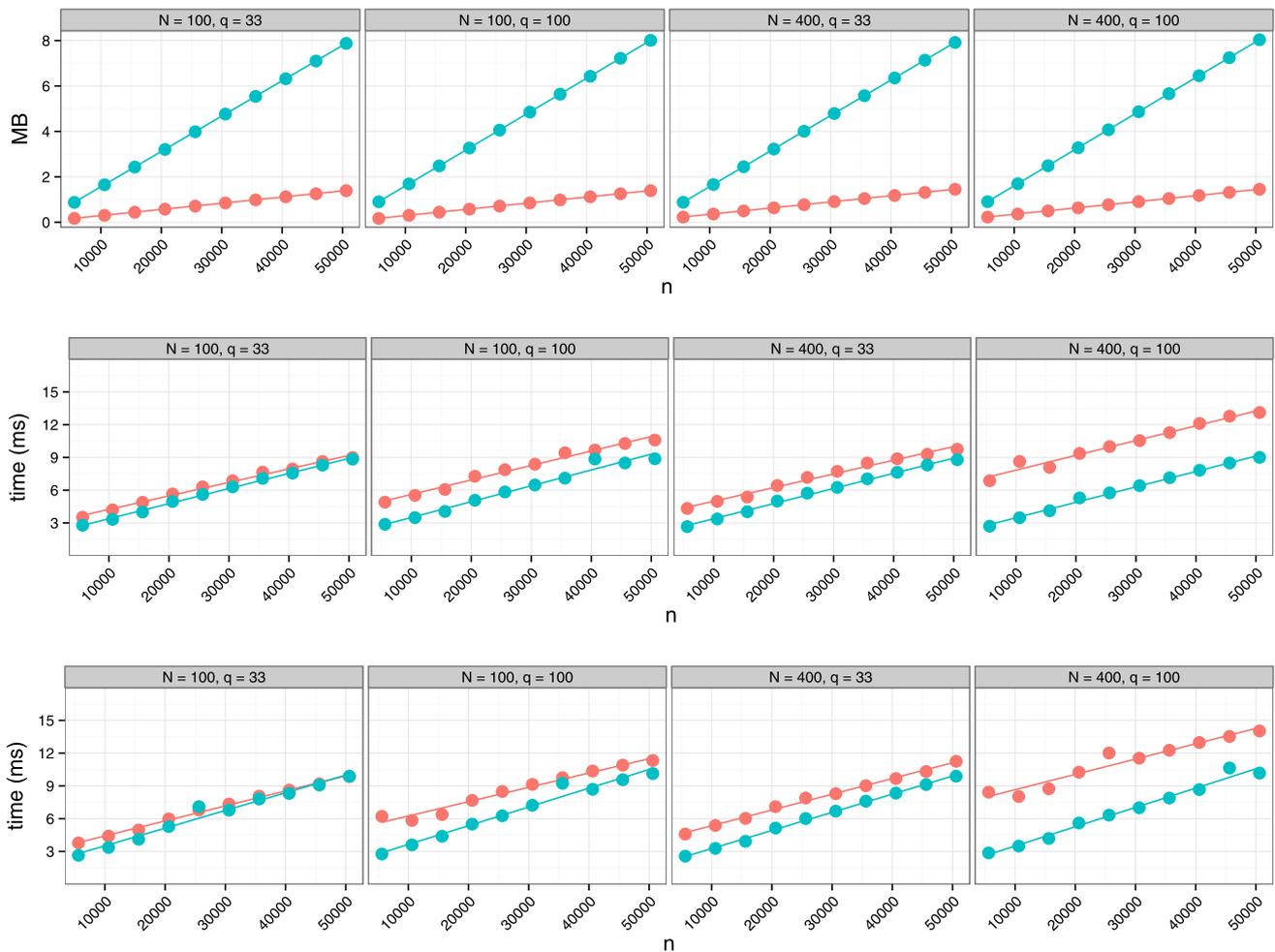
We chose to consider the `logaffine` class and to optimize over  $c$  to achieve the best model fit. Since the optimal choice of the penalization parameter  $\lambda$  may be affected by the choice of  $c$ , we minimized TIC over a grid of  $c$  and  $\lambda$  values. When the memory bound on the linear filters was chosen as  $A = 0.4$ , the optimal choice of  $c$  was effectively  $+\infty$ , meaning that  $\varphi(x) = e^x$  was optimal.

We then investigated how several of the other model and approximation choices affected the model fit. The data set consists of five replications, and we used cross-validation to iteratively fit the model on four of the five replications (the training data) and validate it on the last. We did this for different combinations of  $A$ ,  $n$  and  $q$  that determine the memory bound, the resolution of the time discretization and the dimension of the actual parameter space. We fixed  $N = 400$  for these computations. For the basis expansion the number of B-spline basis functions was chosen explicitly to be either  $q = 33$  or  $q = 100$ . For the direct approximation the choice of threshold on the spectrum was tuned to result in  $q = 33$  or  $q = 100$ . The negative log-likelihood per replication was used as a measure of model fit, and it was in all cases computed using the finest time discretization (largest  $n$ ). Figure

2 shows that the fit generally improved on the training data as  $n$  increased, but above  $n = 20,000$  the improvement was small. The cross-validated negative log-likelihood was, however, almost unaffected by the choice of  $n$  used for fitting the model. Only the coarsest discretization resulted in a slightly worse fit. Figure 2 also shows that among the three choices of  $A$ ,  $A = 0.4$  was best both in terms of model fit on the training data and in the cross-validation. Finally, the choice of  $q$  did not play a role for the direct approximation in terms of model fit, whereas for the basis expansion the use of more basis functions resulted in a slightly better model fit, in particular for  $A = 0.6$ .

We then investigated the memory usage and the computation times of the direct approximation and the basis expansion. The memory usage was obtained using the R function `object.size` and the computation times were computed as the average of 80 replicated likelihood or gradient evaluations. The interest was on how they scale with the numbers  $n$ ,  $N$  and  $q$ . The implementation relies on precomputation of the  $\mathbf{H}$  or  $\mathbf{Z}$  matrices, which are stored as sparse matrices as implemented in the R package `Matrix`. Note that for the basis approximation the choice of  $N$  only affects the pre-computation of the model matrix and not the likelihood and gradient computations.

Figure 3 shows that the basis expansion used more memory for storing  $\mathbf{Z}$ , and that the memory usage as a function of  $n$  had a somewhat larger slope than for the direct approximation. We should note that the memory usage for neither of the methods showed a noticeable dependence upon  $N$  or  $q$ . Storing the matrices as non-sparse matrices the



**Fig. 3** Top Memory usage for storing the  $\mathbf{H}$ -matrix for the direct approximation *red (dark) filled circle* and the  $\mathbf{Z}$ -matrix for basis expansion *cyan (light) filled circle* for  $N = 100, 400$  and  $q = 33, 100$ . Middle Log-likelihood computation time. Bottom Gradient computation time

$\mathbf{Z}$ -matrix required 119 MB and the  $\mathbf{H}$ -matrix required 465 MB for  $n = 50,000$ ,  $N = 400$  and  $q = 100$ . In comparison, the sparse versions required 8 MB and 1.5 MB, respectively.

Figure 3 shows, furthermore, that likelihood and gradient computations were generally faster when the basis expansion was used. More importantly, Fig. 3 shows that computation time for the direct approximation depended upon  $N$  as well as  $q$ , and that the computation times for the basis expansion, using the B-spline basis, were remarkably independent of  $q$ . Note also that the slope on the computation times, as a function of  $n$ , is slightly smaller for the direct approximation than for the basis expansion. The dominating contribution to the computations are the matrix-vector products  $\mathbf{H}(U\beta)$  and  $\mathbf{Z}(V^{-1}\beta)$ . The former scales approximately like  $aNpn + p^2Nq$  and the latter like  $bqpn + p^2q^2$ , where  $a$  and  $b$  are the fraction of non-zero entries in the matrices. Our results reflect that  $aN < bq$ .

## 6 Discussion

The two approximations considered in this paper differ in terms of what is precomputed. Computing the matrix  $\mathbf{H}$  upfront as in the direct approximation should require only a fraction of the memory required for storing the  $\mathbf{Z}$ -matrices. This was confirmed by our implementation. We also showed that the storage requirements for the direct approximation did not depend noticeably on the number  $N$  of  $\delta$ -grid points when  $\mathbf{H}$  is stored as a sparse matrix. The tradeoff is an increased computation time, which depends on the resolution determined by  $N$  and  $q$ .

The storage requirements for  $\mathbf{Z}$  can easily become prohibitively large. A choice of basis functions with local support, such as B-splines used here, can compensate partly for this. It is unlikely that it is useful to precompute  $\mathbf{Z}^i V^{-1}$ , as this will destroy the computational benefits of the basis with local support.

For the basis expansion it is possible to precompute the model matrix in a slightly different and more direct way. Instead of precomputing the  $q \times N$  basis function evaluations  $B_j(\delta_k)$  we can compute  $\mathbf{Z}_{ij}^i$  directly as

$$\mathbf{Z}_{ij}^i = \sum_{k:t_l - A < \sigma_k^i < t_i} B_j(t_l - \sigma_k^i).$$

This may be more accurate but since  $n \gg N$  in typical applications this comes at the cost of many more basis function evaluations. Whether this is critical in terms of the time to compute  $\mathbf{Z}^i$  depends upon how costly a single basis function evaluation is relative to the computation of the  $h_{lik}$ 's. We have not presented data on the computational costs of the precomputations, but they were observed to be small compared to the costs of the actual optimization.

We observed that the fitted models obtained by either the direct approximation using the Sobolev kernel or the B-spline basis expansion were almost identical. This is not surprising given the fact that  $R(\delta_k, \cdot)$  is a cubic spline. In the actual implementation there are minor differences—for the B-spline expansion the linear part is, for instance, not penalized whereas all parts of the kernel fit is penalized. In conclusion, the B-spline basis expansion is currently to be preferred if the storage requirements can be met. The implementation of the direct approximation does, however, offer an easy way to use alternative kernels and thus alternative reproducing kernel Hilbert spaces.

We illustrated the general methods and the implementation using neuron network data. In practice, there are many model choices to be made besides the choice of appropriate discretizations. We have shown how some of these choices, e.g. the choice of  $\varphi$  and the choice of  $\lambda$ , can be made by minimizing TIC. The choice of  $A$  can be made on a data driven basis in a similar way. Neuron network activity is just one example of a multivariate interacting dynamical system that is driven by discrete events. Other examples include high-frequency trading of multiple financial assets, (see Hautsch 2004), and chemical reaction networks as discussed in Anderson and Kurtz (2011) and Bowsher (2010). The Markovian linear Hawkes model (1) was also considered in Chapter 7 in Hautsch (2004), and the typical models of chemical reactions are Markovian multitype birth-death processes. Markovian models are often computationally advantageous, as they offer more efficient intensity and thus likelihood computations. With the implementation in the R package `ppstat` we have made more flexible yet computationally tractable nonparametric and non-Markovian models available.

### 7 Proof of Proposition 1

Function evaluations are represented in terms of the kernel by inner products as given by (3). This gives that

$$X_s(g) = \sum_{i=1}^p \left\langle \sum_{j:\sigma_j^i < s} R(s - \sigma_j^i, \cdot), g_i \right\rangle. \tag{15}$$

If  $\psi$  is a continuously differentiable function we find that

$$\begin{aligned} & \frac{\psi(X_s(g + \varepsilon h)) - \psi(X_s(g))}{\varepsilon} \\ &= \frac{\psi(X_s(g) + \varepsilon X_s(h)) - \psi(X_s(g))}{\varepsilon} \rightarrow \psi'(X_s(g))X_s(h) \end{aligned}$$

for  $\varepsilon \rightarrow 0$ . This is clearly a continuous linear functional. Using (15) and differentiating only w.r.t. the  $i$ 'th coordinate of  $g$  we find that the corresponding gradient in  $\mathcal{H}$  is

$$\nabla_i \psi(X_s(g)) = \psi'(X_s(g)) \sum_{j:\sigma_j^i < s} R(s - \sigma_j^i, \cdot).$$

Taking  $\psi = \log \varphi$  this yields the gradient of the second term in the negative log-likelihood,  $\sum_{k=1}^{N_t} \log \varphi(X_{\tau_k}(g))$ , directly. For the first term we take  $\psi = \varphi$ , but we need to ensure that we can interchange the order of integration and differentiation. To this end the following norm bound on  $\nabla_i \varphi(X_s(g))$  is useful

$$\begin{aligned} \|\nabla_i \varphi(X_s(g))\| &\leq |\varphi'(X_s(g))| \sum_{j:\sigma_j^i < s} \|R(s - \sigma_j^i, \cdot)\| \\ &\leq C_t N_t^i \sup_{s \in [0, t]} \sqrt{R(s, s)} < \infty. \end{aligned}$$

Here  $C_t = \sup_{s \in [0, t]} |\varphi'(X_s(g))|$  is finite because  $X_s(g)$  is continuous in  $s$  and  $\varphi'$  is assumed continuous. We have also used that  $\|R(s - \sigma_j^i, \cdot)\|^2 = R(s - \sigma_j^i, s - \sigma_j^i)$  and the fact that  $R$  is continuous to conclude that the bound is finite. The bound shows that

$$\sum_j \int_{\sigma_j^i}^t \varphi'(X_s(g)) R(s - \sigma_j^i, \cdot) ds$$

is an element in  $\mathcal{H}$ , and the required interchange of integration and differentiation is justified by the bound. This completes the proof.  $\square$

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