Model-Based Multiple Instance Learning

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Abstract—While Multiple Instance (MI) data are point patterns—sets or multi-sets of unordered points—appropriate statistical point pattern models have not been used in MI learning. This article proposes a framework for model-based MI learning using point process theory. Likelihood functions for point pattern data derived from point process theory enable principled yet conceptually transparent extensions of learning tasks, such as classification, novelty detection and clustering, to point pattern data. Furthermore, tractable point pattern models as well as solutions for learning and decision making from point pattern data are developed.

Index Terms—Multiple instance learning, point pattern, point process, random finite set, classification, novelty detection, clustering.

1 INTRODUCTION

Multiple instance (MI) learning is the sub-area of machine learning dedicated to point pattern data, i.e., data in which an observation is a set or multi-set of unordered points [1], [2]. Stemming from research on handwritten digit recognition in 1990 [3], MI learning has emerged as an important topic in pattern recognition with a host of techniques and applications, see e.g., the surveys [1], [2]. Nonetheless, to the best of our knowledge, MI learning based on statistical point pattern models have not yet been investigated, despite the fundamental role of statistical models in machine learning.

A statistical data model is specified by the likelihood function which can be interpreted as how likely an observation is, given the parameters of the underlying model. The likelihood can be used to determine the “best” labels for input observations in classification (supervised learning), the “best” cluster parameters in clustering (unsupervised learning), and outliers in novelty detection (semi-supervised learning) [4], [5], [6]. The data likelihood function thus plays a fundamental role in model-based data analysis.

Given a set of observations, $\mathbf{x} = (x_1, x_2, \ldots, x_m)$, the likelihood of observing these data is given by the joint (probability) density:

$$p(x_1, ..., x_m) = \prod_{i=1}^{m} p_f(x_i) \tag{1}$$

Suppose on day 1 we observe one apple landing at $x_1$, and on day 2 we observe two apples landing at $x_2$ and $x_3$ (see Fig. 1), which of these daily landing patterns is more likely to be a novelty? Since there is no ‘novel’ training data in novelty detection, the common practice (see e.g., [4]) is to examine the ‘normal’ likelihoods of the landing patterns

$$p(x_1) = p_f(x_1) = 0.2,$n$$p(x_2, x_3) = p_f(x_2) p_f(x_3) = 0.36.$n$$

Figure 1. Distribution of landing positions. Position $x_1 = 0.8$ m is 3 times less likely than $x_2 = 0.4$ m and $x_3 = -0.4$ m which are equally likely. Credit: clipartbest.com (apple tree clipart)

To identify outliers. Intuitively, the pattern observed on day 1 is more likely to be a novelty since $p(x_1) < p(x_2, x_3)$. However, had we measured distance in centimeters, then $p(x_1) = 0.002 > p(x_2, x_3) = 0.000036$, thereby, contradicting the previous conclusion! This phenomenon arises from the incompatibility in the measurement units of the likelihoods because $p(x_1)$ is measured in “m$^{-1}$” whereas $p(x_2, x_3)$ is measured in “m$^{-2}$” or “cm$^{-2}$”, i.e., we are not “comparing apples with apples.”

Figure 2. Distribution of discrete landing positions.

The joint density of the landing positions also suffers from another problem. To eliminate the effect of unit incompatibility, we assume that there are only 201 positions

To motivate the development of suitable likelihood functions for point patterns, let us consider an example in novelty detection. Suppose that apples fallen from an apple tree land on the ground independently from each other, and that the daily point patterns of landing positions are inde-
numbered from $-100$ to $100$, evenly spaced on the interval $[-1 m, 1 m]$. Thus, instead of a probability density on $[-1 m, 1 m]$ we now have a (unit-less) probability mass function on the discrete set $\{-100, \ldots, 100\}$, as shown in Fig. 2. Four point patterns from the ‘normal’ training data set are shown in Fig. 3a while Fig. 3b shows 2 new observations $X^{(1)}$ and $X^{(2)}$. Since $X^{(2)}$ has only 1 feature, whereas $X^{(1)}$ and the ‘normal’ observations each have around 10 features, it is intuitive that $X^{(2)}$ is novel. However, its likelihood is much higher than that of $X^{(1)}$ ($0.009$ versus $2 \times 10^{-23}$). This counter intuitive phenomenon arises from the lack of appropriate cardinality information in the likelihood.

Figure 3. (a) ‘Normal’ observations. (b) New observations: $p(X^{(1)}) \approx 2 \times 10^{-23}$ and $p(X^{(2)}) = 0.009$.

The simple example above demonstrates that the joint probability density of the constituent points is not the likelihood of a point pattern. In particular, it suffers from incompatibility in the unit of measurement and does not appropriately account for the number of elements in each point pattern. Worse, such inconsistency in a likelihood function could lead to erroneous results in more complex MI learning tasks. Hence, a proper notion of probability density for random point pattern is needed.

This paper proposes a model-based approach to MI learning using point process theory—the study of random counting measures [12], [13], [14]. Likelihood functions derived from point process theory are probability densities of random point patterns, which incorporate both cardinality and feature information, and avoid the unit of measurement inconsistency. Moreover, they enable the extension of model-based formulations for learning tasks such as classification, novelty detection, and clustering to point pattern data in a conceptually transparent yet principled manner. Such a framework, facilitates the development of tractable point pattern models as well as solutions for learning and decision making. Specifically:

- In MI classification, we propose solutions based on learning point process models from fully observed training data, and develop an inexpensive classifier using a tractable class of models;
- In MI novelty detection, where observations are ranked according to their likelihoods, we show that the standard point process probability densities are not suitable for point patterns and develop suitable ranking functions;
- In MI clustering we propose solutions by introducing point process mixture models, and develop inexpensive algorithms for known and unknown number of clusters using a tractable class of models.

These developments have been partially reported in [15], [16], [17], respectively. This article provides a more complete study, under a unified exposition. In Section 2 we discuss the importance of point pattern data and MI learning as well as reviewing basic concepts from point process theory. Subsequent sections present the proposed framework for model-based MI learning, in progression from: supervised, namely classification, in Section 3; semi-supervised, namely novelty detection, in Section 4; to unsupervised, namely clustering, in Section 5.

2 Background

2.1 Point pattern

A point pattern is a set or multi-set of unordered points. While a multi-set is different from a set in that it may contain repeated elements, a multi-set can also be equivalently expressed as a set. Specifically, a multi-set with elements $x_1$ of multiplicity $N_1$, $x_2$ of multiplicity $N_2$, can be represented as the set $\{(x_1, N_1), \ldots, (x_m, N_m)\}$.

Point patterns are ubiquitous in nature, for example the locations of trees or bird nests (‘statistical ecology’); the positions of stars and galaxies (‘astrostatistics’); the locations of point-like defects in a silicon crystal wafer (materials science); the locations of neurons in brain tissue; or the home addresses of individuals diagnosed with a disease (‘spatial epidemiology’), and many more, see e.g., [18]. Point patterns also arise in numerous machine learning tasks.

In natural language processing and information retrieval, the ‘bag-of-words’ representation treats each document as a multi-set of words [7], [8], [9]. Specifically, the Naïve Bayes (NB) model was used for document classification (or text categorization), where each document is represented by a set of words and their frequencies.

In image and scene categorization, the ‘bag-of-visual-words’ representation treats each image as a set of its key points [10] or local patches [9]. The ‘bag-of-visual-words’ is an efficient representation that captures sufficient information from the original images to enable good image classification results to be achieved. The data likelihood is assumed to be the joint density of the visual-words, and were approximated using NB in [10] and Variational Message Passing in [19].

In transaction data, each datum is a set of items belonging to a transaction, such as market basket data [20], [21] and web log data [10]. Bayesian clustering of transaction data were investigated in [20], [21], [10] using the joint density of items as the data likelihood, which was then approximated by the NB model.

In general, sparse data can be efficiently represented by point patterns. Each sparse observation is an array with most elements taking the same value(s) [22], and can be represented as a ‘bag-of-features’ when the constituent features are not ordered, or as a linked-list when the constituent features are ordered. Document and image data mentioned earlier are examples of sparse data that can be represented as point patterns. High-dimensional data in modern applications, e.g., gene data [23], recommendation data [25], are often sparse.
The emerging area of machine learning dedicated to point pattern data is commonly known as Multiple Instance (MI) learning [11, 12]. Approaches to MI learning are classified into three paradigms: Instance-Space, Embedded-Space, or Bag-Space. The Instance-Space paradigm operates on individual observations within each point pattern. The Embedded-Space paradigm transforms the point patterns into vectors of a common dimension to be processed by vector classifiers, whereas the Bag-Space paradigm operates directly on the point patterns themselves. The Bag-Space paradigm addresses the problem at the most fundamental level and preserves the information content of the data, which could otherwise be compromised in the data transformation process (as in the Embedded-Space approach). However, there are no model-based algorithms in the Bag-Space paradigm.

Given the abundance as well as importance of point pattern data, it is surprising that their mathematical models have not received much attention in machine learning. Specifically, mathematically principled likelihood functions have not received much attention in machine learning. Pattern data, it is surprising that their mathematical mod-

2.2 Point Process

This section outlines the elements of point process theory and presents some basic models for point pattern data. For further detail on point processes, we refer the reader to textbooks such as [13, 12, 14].

A point pattern can be characterized as a counting measure on the space of features \( \mathcal{X} \). Given a point pattern \( X \), a counting measure \( N \) is defined, for each (compact) set \( A \subseteq \mathcal{X} \), by

\[
N(A) = \text{number of points of } X \text{ occurring in } A. \quad (2)
\]

The values of the counting variables \( N(A) \) for all subsets \( A \) provide sufficient information to reconstruct the point pattern \( X \) [13, 12]. The points of \( X \) are the set of \( x \) such that \( N(\{ x \}) > 0 \). A point pattern is said to be: finite if it has a finite number of points, i.e., \( N(\mathcal{X}) < \infty \); and simple if it contains no repeated points, i.e., \( N(\{ x \}) \leq 1 \) for all \( x \in \mathcal{X} \).

Formally a point process is defined as a random counting measure. A random counting measure \( N \) may be viewed as a collection of random variables \( N(A) \) indexed by \( A \subseteq \mathcal{X} \). A point process is finite if its realizations are finite almost surely, and simple if its realizations are simple almost surely.

In this work we are interested in likelihood functions for finite point patterns. For a countable feature space \( \mathcal{X} \), the likelihood function \( f \) is simply the probability of the point pattern. More concisely,

\[
f(\{x_1, ..., x_i\}) = p_c(i) \sum_{\pi} p(x_{\pi(1)}, ..., x_{\pi(i)} | i),
\]

where: \( \pi \) denotes a permutation of \( \{1, 2, ..., i\} \); \( p(x_1, ..., x_i | i) \) is the joint probability of the features \( x_1, ..., x_i \) given that there are \( i \) features; and \( p_c(i) \) is the probability that there are \( i \) features. Conceptually, likelihoods for point patterns in a countable space is straightforward and requires no further discussion. Hereon, we consider point processes on a compact subset \( \mathcal{X} \) of \( \mathbb{R}^d \).

2.2.1 Probability Density

The probability density of a point process is the Radon-Nikodym derivative of its probability distribution with respect to a dominating measure \( \mu \), usually an unnormalised probability distribution of a Poisson point process.

Let \( \nu \) be a (non-atomic \( \sigma \)-finite) measure on \( \mathcal{X} \). A Poisson point process on \( \mathcal{X} \) with intensity measure \( \nu \) is a point process such that

- for every (compact) set \( A \subset \mathcal{X} \), the random variable \( N(A) \) is Poisson distributed with mean \( \nu(A) \),
- if \( A_1, ..., A_m \subset \mathcal{X} \) are disjoint (compact) sets, then the random variables \( N(A_1), ..., N(A_m) \) are independent.

In general the probability density of a point process may not exist [28, 29]. To ensure that probability densities are available, we restrict ourselves to finite point processes [29]. Further, in many applications involving uncountable feature spaces, the observed point patterns do not have repeated elements, and hence can be modeled as a simple point process. A simple finite point process is equivalent to a random finite set [29], i.e., a random variable taking values in \( F(\mathcal{X}) \), the space of finite subsets of \( \mathcal{X} \).

The probability density \( f: F(\mathcal{X}) \to [0, \infty) \) of a random finite set is usually taken with respect to the dominating measure \( \mu \), defined for each (measurable) \( T \subseteq F(\mathcal{X}) \), by (see e.g., [30, 14, 31]):

\[
\mu(T) = \sum_{i=0}^{\infty} \frac{1}{i!U^i} \int 1_T(\{x_1, ..., x_i\}) d(x_1, ..., x_i),
\]

where \( U \) is the unit of hyper-volume in \( \mathcal{X} \), \( 1_T(\cdot) \) is the indicator function for \( T \), and by convention the integral for \( i = 0 \) is the integrand evaluated at \( \emptyset \). The measure \( \mu \) is the unnormalized distribution of a Poisson point process with unit intensity \( 1/U \) when \( \mathcal{X} \) is bounded. For this choice of reference measure, it was shown in [31] that the integral of \( f \) is given by

\[
\int f(X) \mu(dX) = \sum_{i=0}^{\infty} \frac{1}{i!U^i} \int f(\{x_1, ..., x_i\}) d(x_1, ..., x_i),
\]

which is equivalent to Mahler’s set integral [32, 33] and that densities relative to \( \mu \) can be computed using Mahler’s set derivative [32, 33]. Note that the reference measure \( \mu \) and the integrand \( f \) are all dimensionless.

The probability density of a random finite set, with respect to \( \mu \), evaluated at \( \{x_1, ..., x_i\} \) can be written as [28, p. 27] (Eqs. (1.5), (1.6), and (1.7)):

\[
f(\{x_1, ..., x_i\}) = p_c(i) i! U^i f_i(x_1, ..., x_i),
\]

where \( p_c(i) \) is the cardinality distribution, and \( f_i(x_1, ..., x_i) \) is a symmetric function[denoting the joint probability density of \( x_1, ..., x_i \) given cardinality \( i \). Note that by convention \( f_0 = 1 \) and hence \( f(\emptyset) = p_c(0) \). It can be seen from

1. Since \( f_m \) is symmetric, the notations \( f_m(\{x_1, ..., x_m\}) \) and \( f_m(\{x_1, ..., x_m\}) \) can be used interchangeably.
that the probability density \( f \) captures the cardinality information as well as the dependence between the features. Also, \( U^i \) cancels out the unit of the probability density \( f_i(x_1, ..., x_i) \) making \( f \) unit-less, thereby avoids the unit mismatch.

2.2.2 Intensity and Conditional Intensity

The intensity function \( \lambda \) of a point process is a function on \( X \) such that for any (compact) \( A \subset X \)

\[
\mathbb{E} \left[ N(A) \right] = \int_A \lambda(x) dx.
\]

(7)

The intensity value \( \lambda(x) \) is interpreted as the instantaneous expected number of points per unit hyper-volume at \( x \).

For a hereditary probability density \( f \), i.e., \( f(X) > 0 \) implies \( f(Y) > 0 \) for all \( Y \subset X \), the conditional intensity at a point \( u \) is given by [29]

\[
\lambda(u, X) = \frac{f(X \cup \{u\})}{f(X)}.
\]

(8)

Loosely speaking, \( \lambda(u, X) \) \( du \) can be interpreted as the conditional probability that the point process has a point in an infinitesimal neighbourhood \( du \) of \( u \) given all points of \( X \) outside this neighbourhood. The intensity function is related to the conditional intensity by

\[
\lambda(u) = \mathbb{E} \left[ \lambda(u, X) \right].
\]

(9)

For a Poisson point process the conditional intensity equals the intensity.

The probability density of a finite point process is completely determined by its conditional intensity [12], [14]. Certain point process models are convenient to formulate in terms of the conditional intensity rather than probability density. Using the conditional intensity also eliminates the normalizing constant needed for the probability density. However, the functional form of the conditional intensity must satisfy certain consistency conditions.

2.2.3 IID cluster model

Imposing the independence assumption among the features, the model in [6] reduces to the IID-cluster model [13], [12]:

\[
f(X) = p_c(|X|) |X|! \left[ \prod_{j \in X} f_j \right]^X,
\]

(10)

where \( |X| \) denotes the cardinality (number of elements) of \( X \), \( p_c \) is a probability density on \( X \), referred to as the feature density, and \( h^X = \prod_{x \in X} h(x) \), with \( h^0 = 1 \) by convention. Sampling from an IID-cluster can be accomplished by first sampling the number of points from the cardinality distribution \( p_c \), and then sampling the corresponding number points independently from the feature distribution \( p_f \).

When the cardinality distribution \( p_c \) is Poisson with rate \( \rho \) we have the celebrated Poisson point process [13], [12]:

\[
f(X) = \rho^{|X|} e^{-\rho} \left[ \prod_{j \in X} p_f \right]^X.
\]

(11)

The Poisson point process model is completely determined by the intensity function \( \lambda = \rho p_f \). Note that the Poisson cardinality distribution is described by a single non-negative number \( \rho \), hence there is only one degree of freedom in the choice of cardinality distribution for the Poisson point process model.

2.2.4 Finite Gibbs model

A well-known general model that accommodates dependence between its elements is a finite Gibbs process, which has probability density of the form [12], [14]:

\[
f(X) = \exp \left( V_0 + \sum_{i=1}^{|X|} \sum_{\{x_1,...,x_i\} \subset X} V_i(x_1, ..., x_i) \right),
\]

(12)

where \( V_i \) is called the \( i \)th potential, given explicitly by

\[
V_i(x_1, ..., x_i) = \sum_{Y \subseteq \{x_1,...,x_i\}} (-1)^{|\{x_1,...,x_i\}| - |Y|} \log f(Y).
\]

Gibbs models arise in statistical physics, where \( \log f(X) \) may be interpreted as the potential energy of the point pattern. The term \(-V_1(x)\) can be interpreted as the energy required to create a single point at a location \( x \), and the term \(-V_2(x_1, x_2)\) can be interpreted as the energy required to overcome the force between the points \( x_1 \) and \( x_2 \).

Note that any hereditary probability density of a finite point process can be expressed in the Gibbs form [29]. The Poisson point process is indeed a first order Gibbs model. Another example is the hardcore model, where every pair of distinct points is at least \( r \) units apart. In this case, \( V_1(x) \) is a constant and

\[
V_2(x_1, x_2) = \begin{cases} 0, & \|x_1 - x_2\| > r \\ -\infty, & \|x_1 - x_2\| \leq r \end{cases}.
\]

The next three sections show how point process models are used in model-based point pattern classification, novelty detection and clustering.

3 Model-based MI Classification

Classification is the supervised learning task that uses fully-observed training input-output pairs \( D_{\text{train}} = \{(X_n, y_n)\}_{n=1}^N \) to determine the output class label \( y \in \{1, ..., K\} \) of each input observation [5], [6]. This fundamental machine learning task is the most widely used form of supervised machine learning, with applications spanning many fields of study.

In MI learning, model-based classifiers for point patterns have not been investigated. Existing classifiers in the Bag-Space paradigm are based on distances between point patterns, such as Hausdorff [34], [35], Chamfer [36], Earth Mover’s [37], [38]. Such classifiers do not require any underlying data models and are simple to use. However, they may perform poorly with high dimensional inputs due to the curse of dimensionality, and are often computationally intractable for large datasets [6], not to mention that the decision procedure is unclear. On the other hand, knowledge of the underlying data model can be used to exploit statistical patterns in the training data, and to devise optimal decision procedures.

Using the notion of probability density for point process from subsection 2.2.1 the standard model-based classification formulation directly extends to MI classification:

- In the training phase, we seek likelihoods that “best” fit the training data. Specifically, for each \( k \in \{1, ..., K\} \), we seek a likelihood function \( f(\cdot | y = k) \) that best fit the training input point patterns in
\( \mathcal{D}_{train}^{(k)} = \{ X : (X, k) \in \mathcal{D}_{train} \} \), according to criteria such as maximum likelihood (ML) or Bayes optimal if suitable priors on the likelihoods are available.

- In the classifying phase, the likelihoods (learned from training data) are used to classify input observations. When a point pattern \( X \) is passed to query its label, the Bayes classifier returns the mode of the class label posterior \( p(y = k \mid X) \) computed from the likelihood and the class prior \( p \) via Bayes’ rule:

\[
p(y = k \mid X) \propto p(y = k)f(X \mid y = k). \tag{13}
\]

The simplest choices for the class priors are the uniform distribution, and the categorical distribution, usually estimated from the training data via

\[
p(y = k) = \frac{1}{N_{\text{train}}} \sum_{n=1}^{N_{\text{train}}} \delta_{i[n]}[k],
\]

where \( \delta_{i[j]} \) is the Kronecker delta, which takes on the value 1 when \( i = j \), and zero otherwise. Hence, the main computational effort in model-based classification lies in the training phase.

### 3.1 Learning Point Process Models

Learning the likelihood function for class \( k \) boils down to finding the value(s) of the parameter \( \theta_k \) such that the (parameterized) probability density function \( f(\cdot \mid y = k, \theta_k) \) best explains the observations \( X_1, \ldots, X_N \) in \( \mathcal{D}_{train}^{(k)} \). In this subsection, we consider a fixed class label and its corresponding observations \( X_1, \ldots, X_N \), and omit the dependence on \( k \).

Methods for learning point process models have been available since the 1970’s, see e.g., [14], [29]. We briefly summarize some recognized techniques and presents ML for IID cluster models as a tractable MI classification solution.

#### 3.1.1 Model fitting via summary statistics

The method of moments seeks the parameter \( \theta \) such that the expectation of a given statistic of the model point process parameterized by \( \theta \) is equal to the statistic of the observed point patterns [29]. However, this approach is only tractable when the solution is unique and the expectation is a closed form function of \( \theta \), which is usually not the case in practice, not to mention that moments are difficult to calculate.

The method of minimum contrast seeks the parameter \( \theta \) that minimizes some dissimilarity between the expectation of a given summary statistic (e.g., the K-function) of the model point process and that of the observed point patterns [29]. Provided that the dissimilarity functional is convex in the parameter \( \theta \), this approach can avoid some of the problems in the method of moments. However, in general the statistical properties of the solution are not well understood, not to mention the numerical behaviour of the algorithm used to determine the minimum.

#### 3.1.2 Maximum likelihood (ML)

In the ML approach, we seek the ML estimate (MLE) of \( \theta \):

\[
\hat{\theta}(f; X_{1:N}) = \arg \max_{\theta} \left( \prod_{n=1}^{N} f(X_n \mid \theta) \right). \tag{14}
\]

The MLE has some desirable statistical properties such as asymptotic normality and optimality [29]. However, in general, there are problems with non-unique maxima. Moreover, analytic MLEs are not available because the likelihood of many Gibbs models contains an intractable normalizing constant (which is a function of \( \theta \)) [14].

To the best of our knowledge, currently there is no general ML technique for learning generic models such as Gibbs from real data. Numerical approximation method proposed in [59] and Markov Chain Monte Carlo (MCMC) method proposed in [40] are highly specific to the chosen model, computationally intensive, and require careful tuning to ensure good performance. Nonetheless, simple models such as the IID-cluster model [10] admits an analytic MLE (see subsection 3.1.4).

Remark: The method of estimating equation replaces the ML estimation equation

\[
\frac{d}{d\theta} \left( \sum_{n=1}^{N} \log(f(X_n \mid \theta)) \right) = 0 \tag{15}
\]

by an unbiased sample approximation of the general equation

\[
E_\theta [\Psi(\theta, X)] = 0, \text{ i.e.,}
\sum_{n=1}^{N} \Psi(\theta, X_n) = 0. \tag{16}
\]

For example, \( \Psi(\theta, X_n) = \frac{d}{d\theta} \log(f(X_n \mid \theta)) \) results in ML since it is well-known that [15] is an unbiased estimating equation. Setting \( \Psi(\theta, X_n) \) to the difference between the empirical value and the expectation of the summary statistic results in the method of moments. Takacs-Fiksel is another well-known family of estimating equations [31], [42].

#### 3.1.3 Maximum Pseudo-likelihood

Maximum pseudo-likelihood (MPL) estimation is a powerful approach that avoids the intractable normalizing constant present in the likelihood while retaining desirable properties such as consistency and asymptotic normality in a large-sample limit [43], [44]. The key idea is to replace the likelihood of a point process (with parameterized conditional intensity \( \lambda_0(u; X) \)) by the pseudo-likelihood:

\[
PL(\theta; X_{1:N}) = \prod_{n=1}^{N} e^{-f \lambda_0(u; X_n)} \left[ \lambda_0(\cdot; X_n) \right]^{X_n}. \tag{17}
\]

The rationale behind this strategy is discussed in [43]. Up to a constant factor, the pseudo-likelihood is indeed the likelihood if the model is Poisson, and approximately equal to the likelihood if the model is close to Poisson. The pseudo-likelihood may be regarded as an approximation to the likelihood which neglects the inter-point dependence.

An MPL algorithm has been developed by Baddeley and Turner in [45] for point processes with sufficient generality such as Gibbs whose conditional intensity has the form

\[
\lambda(u, X) = \exp \left( \sum_{i=1}^{k} \sum_{\{x_{i-1}, \ldots, x_1\} \subseteq X} V_i(u, x_1, \ldots, x_{i-1}) \right).
\]

By turning the pseudo-likelihood of a general point process into a classical Poisson point process likelihood, MPL can be implemented with standard generalized linear regression
software [15]. Due to its versatility, the Baddeley-Turner algorithm is the preferred model fitting tool for point processes.

The main hurdle in the application of the Baddeley-Turner algorithm to MI classification is the computational requirement. While this may not be an issue in spatial statistics applications, the computational cost is still prohibitive with large data sets often encountered in MI learning. On the other hand, disadvantages of MPL (relative to ML) such as small-sample bias and inefficiency [44], [46] become less significant with large data. Efficient algorithms for learning general point process models is an ongoing area of research. Nonetheless, the Baddeley-Turner algorithm is a promising tool for complex MI classification problems.

3.1.4 ML Learning for IID-Clusters

Computationally efficient algorithms for learning point process models are important because MI learning usually involves large data sets (compared to applications in spatial statistics). Since learning a general point process is computationally prohibitive, the IID-cluster model [10] provides a good trade-off between tractability and versatility by neglecting interactions between the points.

Since an IID-cluster model is uniquely determined by its cardinality and feature distributions, we consider a parameterization of the form:

\[ f(X | \xi, \varphi) = p_\xi(|X|) |X|! U^{|X|} p_\varphi^X, \]  

where \( p_\xi \) and \( p_\varphi \) are the parameterized cardinality and feature distributions respectively. Learning the underlying parameters of an IID-cluster model amounts to estimating the parameter \( \theta = (\xi, \varphi) \) from training input data.

The form of the IID-cluster likelihood function allows the MLE to separate into the MLE of the cardinality parameter \( \xi \) and MLE of the feature parameter \( \varphi \). This is stated more concisely in Proposition 1 (the proof is straightforward, but included for completeness).

**Proposition 1.** Let \( X_1, ..., X_N \) be \( N \) i.i.d. realizations of an IID-cluster with parameterized cardinality distribution \( p_\xi \) and feature density \( p_\varphi \). Then the MLE of \( (\xi, \varphi) \), is given by

\[ \begin{align*}
\hat{\xi} &= \hat{\theta}(p_\xi; |X_1|, ..., |X_N|), \\
\hat{\varphi} &= \hat{\theta}(p_\varphi; \psi^N_{n=1} X_n),
\end{align*} \]  

where \( \psi \) denotes disjoint union.

**Proof:** Using (18), we have

\[ \prod_{n=1}^{N} f(X_n | \xi, \varphi) = \prod_{n=1}^{N} p_\xi(|X_n|) |X_n|! U^{|X_n|} p_\varphi^X_n \]

\[ = \prod_{n=1}^{N} |X_n|! U^{|X_n|} \prod_{n=1}^{N} p_\xi(|X_n|) \prod_{n=1}^{N} p_\varphi^X_n \]

Hence, to maximize the likelihood we simply maximize the second and last products in the above separately. This is achieved with (19) and (20). \( \square \)

Observe from Proposition 1 that the MLE of the feature density parameter is identical to that used in NB, e.g., if the feature density is a Gaussian, then the MLEs of the mean and covariance are:

\[ \begin{align*}
\hat{\mu} &= \frac{1}{N} \sum_{n=1}^{N} X_n, \\
\hat{\Sigma} &= \frac{1}{N} \sum_{n=1}^{N} (x - \hat{\mu})(x - \hat{\mu})^T.
\end{align*} \]  

Consequently, learning the IID-cluster model requires only one additional task of computing the MLE of the cardinality parameters, which is relatively inexpensive.

For a categorical cardinality distribution, i.e., \( \xi = (\xi_1, ..., \xi_M) \) where \( \xi_k = Pr(|X| = k) \) and \( \sum_{M}^{1} \xi_k = 1 \), the MLE of the cardinality parameter is given by

\[ \hat{\xi}_k = \frac{1}{N} \sum_{n=1}^{N} \delta_k(|X_n|). \]  

Note that to avoid over-fitting, the standard practice of placing a Laplace prior on the cardinality distribution can be applied, i.e. replacing the above equation by \( \xi_k \propto \epsilon + \sum_{n=1}^{N} \delta_k(|X_n|) \), where \( \epsilon \) is a small number.

For a Poisson cardinality distribution parameterized by the rate \( \xi = \rho \), the MLE is given by

\[ \hat{\rho} = \frac{1}{N} \sum_{n=1}^{N} |X_n|. \]

It is also possible to derive MLEs for other families of cardinality distributions such as Panjer, multi-Bernoulli, etc.

Remark: Proposition 1 also extends to Bayesian learning for IID-clusters if the prior on \( (\xi, \varphi) \) separates into priors on \( \xi \) and \( \varphi \). Following the arguments in the proof of Proposition 1 the maximum posteriori (MAP) estimate of \( (\xi, \varphi) \) separates into MAP estimates of \( \xi \) and \( \varphi \). Typically a (symmetric) Dirichlet distribution \( Dir(\eta/K, ..., \eta/K) \), with dispersion \( \eta \) on the unit \((M - 1)\)-simplex, can be used as a prior on the categorical cardinality distribution. The prior for \( \varphi \) depends on the form of the feature density \( p_\varphi \) (see also subsection 5.2 for conjugate priors of the Poisson model).

Indeed, Bayesian learning for point process models can also be considered as a variation of the Bayesian point pattern clustering problem in subsection 5.2.

4 MODEL-BASED MI NOVELTY DETECTION

Novelty detection is the semi-supervised task of identifying observations that are significantly different from the rest of the data [4], [47]. In novelty detection, there is no novel training data, only ‘normal’ training data is available. Hence it is not a special case of classification nor clustering [48], [49], and is a fundamental problem in its own right.

Similar to classification, novelty detection involves a training phase and a detection phase. Since novel training data is not available in novelty detection, input observations are ranked according to how well they fit the ‘normal’ training data and those not well-fitted are deemed novel or anomalous [48], [49]. The preferred measure of goodness of fit is the ‘normal’ likelihoods of the input data. To the best of our knowledge, there are no MI novelty detection solutions in the literature.

In this section we present a model-based solution to MI novelty detection. The training phase in novelty detection is the same as that for classification. However, in the detection phase the ranking of likelihoods is not applicable to point
pattern data, even though point process probability density functions are unit-less and incorporates both feature and cardinality information. In subsection 4.1, we discuss why such probability densities are not suitable for ranking input data, while in subsection 4.2, we propose a suitable ranking function for MI novelty detection.

4.1 Probability density and likelihood

This subsection presents an example to illustrate that the probability density of a point pattern does not necessarily indicate how likely it is. For this example, we reserve the term likelihood for the measure of how likely or probable a realization is.

![Probability density and likelihood](image)

Consider two IID-cluster models with a common cardinality distribution but different uniform feature densities as shown in Fig. 4. Since the feature density is uniform, point patterns with the same cardinality are equally likely, and consequently their likelihoods should be proportional to the cardinality distribution.

![Cardinality and feature distributions of 2 IID-clusters](image)

If the probability density were an indication of how likely a point pattern is, then the plot of probability density against cardinality should resemble the cardinality distribution. However, this is not the case. Fig. 4 indicates that for the IID-cluster with ‘short’ feature density, the probability density tends to decrease with increasing cardinality (Fig. 5a). This phenomenon arises because the feature density given cardinality $n$ is $0.05^n$, which vanishes faster than the $n!$ growth (for $n \leq 20$). The converse is true for the IID-cluster with ‘tall’ feature density (Fig. 5b). Thus, point patterns with highest/least probability density are not necessarily the most/least probable.

Such problem arises from the non-uniformity of the reference measure. A measure $\mu$ is said to be uniform if for any measurable region $A$ with $\mu(A) < \infty$, all points of $A$ (except on set of measure zero) are equi-probable under the probability distribution $\mu/\mu(A)$. One example is the Lebesgue measure $\text{vol}$ on $\mathbb{R}^n$: given any bounded measurable region $A$, the probability distribution $\text{vol}(\cdot)/\text{vol}(A)$ is uniform on $A$, i.e., all realizations in $A$ are equally likely. The probability density (as a Radon-Nikodym derivative) at a point $X$ is the ratio of probability measure to reference measure at an infinitesimal neighbourhood of $X$, i.e.

$$f(X) = \frac{P(dX)}{\mu(dX)}.$$  

Hence, unless the reference measure is uniform, $f(X)$ is not a measure of how likely $X$ is. This is also true even for probability densities on the real line. For example, the probability density of a zero-mean Gaussian distribution with standard variance 1 relative to the (uniform) Lebesgue measure is the usual Gaussian curve shown in Fig. 6a, while its density relative to a zero-mean Gaussian distribution with variance 0.8 is shown in Fig. 6b, where the most probable point has the least probability density value.

![Density of a zero-mean unit-variance Gaussian w.r.t. Lebesgue measure](image)

The reference measure $\mu$ defined by (4) is not uniform because for a bounded region $T \subseteq \mathcal{F}(\mathcal{X})$, the probability distribution $\mu/\mu(T)$ is not necessarily uniform (unless all points of $T$ have the same cardinality). Hence, probability densities of input point patterns relative to $\mu$ are not indicative of how well they fit the ‘normal’ data model.

Remark: In novelty detection we are interested in the likelihood of the input point pattern whereas in Bayesian
classification we are interested in its likelihood ratio. The posterior class probability
\[ p(y \mid X) = \frac{p(y)f(X \mid y)}{\int p(y)f(X \mid y)dy} = \frac{p(y)p(DX \mid y)/\mu(dx)}{\int p(y)p(DX \mid y)/\mu(dx)dy} = \frac{p(y)P(DX \mid y)}{\int p(y)P(DX \mid y)dy} \]
is the ratio, at an infinitesimal neighbourhood \(dx\), between the joint probability \(P(dx \mid y)\), and the probability \(P(dx)\), which is invariant to the choice of reference measure. In essence, the normalizing constant cancels out the influence of the reference measure, and hence, problems with the non-uniformity of the reference measure do not arise.

### 4.2 Ranking functions

To the best of our knowledge, it is not known whether there exists a uniform reference measure on \(\mathcal{F}(X)\) that dominates the probability distributions of interest (so that they admit uniformity of the reference measure, and hence, problems with the non-uniformity of the reference measure do not arise.

The probability density \(f(X)\) is the product of the cardinality distribution \(p_c(|X|)\), the cardinality-conditioned feature (probability) density \(f_{X|X}(X)\), and a trans-dimensional weight \(|X|\|f\|^{X^|X|}\). Note that the cardinality distribution and the conditional feature density completely describes the point process. The conditional density \(f_{X|X}(X)\) enables the ranking of point patterns of the same cardinality, but cannot be used to rank across different cardinalities because it takes on different units of measurement. The weights \(|X|\|f\|^{X^|X|}\) reconcile for the differences in dimensionality and unit of measurement between \(f_{X|X}(X)\) of different cardinalities. However, the example in subsection 4.1 demonstrates that weighting by \(|X|\|f\|^{X^|X|}\) leads to probability densities that are inconsistent with likelihoods.

In the generalization of the maximum a posteriori (MAP) estimator to point patterns [33], the consistency requirement: for a given cardinality \(n\), the expected ranking value is proportional to the probability of cardinality \(n\), i.e.,
\[ \mathbb{E}_{X \mid |X| = n}[r(X)] \propto p_c(n). \] (26)

**Proposition 2.** For a point process with probability density \(f(X)\), a ranking function consistent with the cardinality distribution, i.e., satisfies (26), is given by
\[ r(X) \propto \frac{p_c(|X|)}{||f_{X|X}(X)||^2} f_{X|X}(X) \] (27)
where \(| \cdot |\|_2\) denotes the \(L_2\)-norm.

**Proof:** Noting from (6) that \(f(X \mid |X| = n) = n!U^n f_n(X)\delta_n \|X\|\), and using the integral (5) we have
\[ \mathbb{E}_{X \mid |X| = n}[f_n(X)] = \int f_n(X) f(X \mid |X| = n) \mu(dx) = \frac{n!U^n}{n!U^n} \int (f_n(\{x_1, \ldots, x_n\}))^2 d(x_1, \ldots, x_n) = ||f_n||^2_2. \]
Hence
\[ \mathbb{E}_{X \mid |X| = n}[r(X)] \propto \mathbb{E}_{X \mid |X| = n}[\frac{p_c(|X|)}{||f_{X|X}(X)||^2} f_{X|X}(X)] \]
\[ = \frac{p_c(n)}{||f_n||^2_2} \mathbb{E}_{X \mid |X| = n}[f_n(X)] = p_c(n). \]

Note that \(||f_{X|X}(X)||^2_2\) has units of \(U^{-|X|}\), which is the same as the unit of \(f(X)\), rendering the ranking function \(r\) unitless, thereby avoids the unit of measurement inconsistency described in section 4.1.

For an IID-cluster with feature density \(p_f\) the ranking function reduces to
\[ r(X) \propto p_c(|X|) \left( \frac{p_f}{||p_f||^2_2} \right)^X. \] (28)
The feature density \(p_f\), in the example of subsection 4.1, is uniform and so \(||p_f||^2_2 = 1\) on its support. Hence the ranking is equal to the cardinality distribution, as expected. Fig. 7 illustrates the effect of dividing a non-uniform feature density \(p_f\), by its energy \(||p_f||^2_2\), ‘tall’ densities become shorter and ‘short’ densities become taller, providing the right adjustment for multiplying together many large/small numbers.

![Probability density divided by energy](image-url)

**Figure 7.** Probability density divided by energy: (a) ‘short’ Gaussian (mean = 0, variance = 1); (b) ‘tall’ Gaussian (mean = 0, variance = 0.05).
5 Model-Based MI Clustering

The aim of clustering is to partition the dataset into groups so that members in a group are similar to each other whilst dissimilar to observations from other groups [6]. A partitioning of a given set of observations \( \{X_1, \ldots, X_N\} \) is often represented by the (latent) cluster assignment \( y_1:N \), where \( y_n \) denotes the cluster label for the \( n\text{th} \) observation. Clustering is an unsupervised learning problem since the labels are not included in the observations [55]. Indeed it can be regarded as classification without training and is a fundamental problem in data analysis. Comprehensive surveys on clustering can be found in [50], [52], [53].

In MI learning, model-based pattern clustering have not been investigated. To the best of our knowledge, there are two clustering algorithms for point patterns: the Bag-level MI Clustering (BAMIC) algorithm [54], and the Maximum Margin MI Clustering (M3IC) algorithm [55]. BAMIC adapts the \( k \)-medoids algorithm with the Hausdorff distance as a measure of dissimilarity between point patterns [54]. On the other hand, in M3IC, the clustering was posed as a non-convex optimization problem which is then relaxed and solved via a combination of the Constrained Concave-Convex Procedure and Cutting Plane methods [55]. While these algorithms are simple to use, they lack the ability to exploit statistical trends in the data, not to mention computational problems with high dimensional inputs and large datasets [6].

In this section, we propose a model-based approach to the clustering problem for point pattern data. Mixture modeling is the most common probabilistic approach to clustering, where the aim is to estimate the cluster assignment \( y_1:N \) via likelihood or posterior inference [6]. The point process formalism enables direct extension of mixture models to point pattern data. In particular, the finite mixture point process model for problems with known number of clusters is presented in subsection 5.1, while the infinite mixture point process model for problems with unknown number of clusters is presented in subsection 5.2.

5.1 Finite Mixture Model

A finite mixture model assumes \( K \) underlying clusters labeled 1 to \( K \), with prior probabilities \( \pi_1, \ldots, \pi_K \), and characterized by the parameters \( \theta_1, \ldots, \theta_K \) in some space \( \Theta \). Let \( f(X_n | \theta_k) \triangleq f(X_n | y_n = k, \theta_k) \) denote the likelihood of \( X_n \) given that cluster \( k \) generates an observation. Then

\[
f(X_{1:N}, y_{1:N} | \pi_{1:K}, \theta_{1:K}) = \prod_{n=1}^{N} \pi_{y_n} f(X_n | \theta_{z_n}),
\]

Marginalizing the joint distribution [29] over the cluster assignment \( y_1:N \) gives the data likelihood function

\[
f(X_{1:N} | \pi_{1:K}, \theta_{1:K}) = \prod_{n=1}^{N} \sum_{k=1}^{K} \pi_k f(X_n | \theta_k).
\]

Thus, in a finite mixture model, the likelihood of an observation is a mixture of \( K \) probability densities. Hence the application of the finite mixture model requires the number of clusters to be known apriori. The posterior probability of cluster label \( y_n = k \) (i.e., the probability that, given \( \pi_{1:K}, \theta_{1:K} \) and \( X_n \), cluster \( k \) generates \( X_n \)) is

\[
p(y_n = k | X_n, \pi_{1:K}, \theta_{1:K}) = \frac{\pi_k f(X_n | \theta_k)}{\sum_{k=1}^{K} \pi_k f(X_n | \theta_k)}.
\]

Next we detail an ML solution to point pattern clustering using EM with an IID-cluster mixture model. Instead of presenting a Bayesian solution for the finite mixture model, in subsection 5.2 we extend it to address an unknown number of clusters, and develop a solution using Gibbs sampling, which can be simplified to the finite mixture case.

5.1.1 EM clustering via IID-cluster mixture model

The EM algorithm maximizes the data likelihood [30] by generating a sequence of iterates \( \{\psi(i)\}_{i=0}^{\infty} \) using the following two steps [56], [57]:

- **E-step:** Compute \( Q(\psi | \psi(i-1)) \), defined as

\[
\mathbb{E}_{y_{1:N} | X_{1:N}, \psi(i-1)} \log(f(X_{1:N} | y_{1:N} | \psi))
= \sum_{k=1}^{K} \sum_{n=1}^{N} \log(\pi_k f(X_n | \theta_k)) p(y_n = k | X_n, \psi(i-1)).
\]

- **M-step:** Find \( \psi(i) = \arg\max_{\psi} Q(\psi | \psi(i-1)) \).

The expectation \( Q(\psi(i) | \psi(i-1)) \) increases after each EM iteration, and consequently converges to a (local) maximum [56], [57]. In practice, the iteration is terminated at a user defined number \( N_{\text{iter}} \) or when increments in \( Q(\psi(i) | \psi(i-1)) \) falls below a given threshold. The optimal cluster label estimate is the mode of the cluster label posterior [31].

Following the arguments from [60], the M-step can be accomplished by separately maximizing \( Q(\pi_{1:K}, \theta_{1:K} | \psi(i-1)) \) over \( \theta_1, \ldots, \theta_K \) and \( \pi_{1:K} \). Using Lagrange multiplier with constraint \( \sum_{k=1}^{K} \pi_k = 1 \), yields the optimal weights:

\[
\pi_k(i) = \frac{1}{N} \sum_{n=1}^{N} p(y_n = k | X_n, \psi(i-1)).
\]

The \( k\text{th} \) optimal component parameter depends on the specific form of \( f(X_n | \theta_k) \), and is intractable in general.

Fortunately, close form solutions can be derived for special cases of the IID-cluster mixture model, i.e., a finite mixture point process model with

\[
f(X | \theta_k) = p_{\psi_k}(|X|) |X|! p_{\psi_k}^X,
\]
where $\theta_k = (\xi_k, \varphi_k)$ with $\xi_k$ and $\varphi_k$ denoting the parameters of the cardinality and feature distributions, respectively. Similar to Proposition 1, the IID-cluster form allows separate maximization over $\xi_k$ and $\varphi_k$.

- For a categorical cardinality distribution with maximum cardinality $M$: $\xi_k = (\xi_{k,0}, \ldots, \xi_{k,M})$ belongs to the unit $(M + 1)$-simplex, the iteration is

$$
\xi_{k,m}^{(i)} = \frac{\sum_{n=1}^{N} \delta_{m,n} |X_n| p(y_n = k | X_n, \psi^{(i-1)})}{\sum_{m=0}^{M} \sum_{n=1}^{N} \delta_{m,n} |X_n| p(y_n = k | X_n, \psi^{(i-1)})}.
$$

Like MLE, a Laplace prior can be used to address over-fitting (see subsection 3.1.4).

- For a Poisson cardinality distribution: $\xi_k > 0$ is the mean cardinality, the iteration is

$$
\xi_k^{(i)} = \frac{\sum_{n=1}^{N} |X_n| p(y_n = k | X_n, \psi^{(i-1)})}{\sum_{n=1}^{N} p(y_n = k | X_n, \psi^{(i-1)})}.
$$

Iterates for other families such as Panjer, or multi-Bernoulli can also be derived.

- For a Gaussian feature distribution: $\varphi_k = (\mu_k, \Sigma_k)$ is the mean and covariance pair, the iteration is

$$
\mu_k^{(i)} = \frac{\sum_{n=1}^{N} p(y_n = k | X_n, \psi^{(i-1)}) \sum_{x \in X_n} x}{\sum_{n=1}^{N} |X_n| p(y_n = k | X_n, \psi^{(i-1)})},
$$

$$
\Sigma_k^{(i)} = \frac{\sum_{n=1}^{N} p(y_n = k | X_n, \psi^{(i-1)}) \sum_{x \in X_n} (x - \mu_k^{(i)}) (x - \mu_k^{(i)})^{T}}{\sum_{n=1}^{N} |X_n| p(y_n = k | X_n, \psi^{(i-1)})},
$$

where $K_k^{(i)}(x) = (x - \mu_k^{(i)}) (x - \mu_k^{(i)})^{T}$.

### 5.2 Infinite Mixture Model

For an unknown number of cluster, finite mixture models are no longer directly applicable. Bayesian non-parametric modeling (see e.g., [61], [62]) addresses the unknown number of clusters by modeling the set of mixture parameters as a point process. Thus, the observations and the clusters are all modeled as point processes.

In a finite mixture model, the number of components (and clusters) is fixed at $K$. The mixture parameter $\psi = (\pi_{1:K}, \theta_{1:K})$ is a point in $(\mathbb{R}_+ \times \Theta)^K$, such that $\sum_{i=1}^{K} \pi_i = 1$. Under the Bayesian framework, it is further assumed that $\theta_{1:K}$ follows a given distribution on $\Theta^K$, and that $\pi_{1:K}$ follows a distribution on the unit $(K - 1)$-simplex, e.g. a Dirichlet distribution.

An infinite mixture model addresses the unknown number of components by considering the mixture parameter $\Psi$ as a point pattern in $(\mathbb{R}_+ \times \Theta)$ such that $\sum_{(\omega, \theta) \in \Psi} \pi = 1$. Further, under the Bayesian non-parametric framework, we furnish $\Psi$ with a prior distribution, thereby modeling the mixture parameter as a point process on $(\mathbb{R}_+ \times \Theta)$. The simplest model would be the Poisson point process, but the resulting component weights do not necessarily sum to one. Nonetheless, these weights can be normalized to yield a tractable point process model for the mixture parameter [63], [64]. More concisely, let $\Xi$ be a Poisson point process on $(\mathbb{R}_+ \times \Theta)$ with intensity measure $\nu_{\Xi}^{-1} e^{-\nu_{\Xi}} d\omega dG_0(d\theta)$, i.e., the product of an improper gamma distribution and the base distribution $G_0$. Then the prior model for the mixture parameter is given by

$$
\Psi = \left\{ (\nu_{\Xi}^{-1} \omega, \theta) : (\omega, \theta) \in \Xi \right\},
$$

where $\nu_{\Xi} = \sum_{(\omega, \theta) \in \Xi} \omega$. Note that (34) is no longer a Poisson point process because each component element involves the sum $\nu_{\Xi}$, thereby violating the independence condition.

To specify an explicit form for the prior distribution of the mixture parameter, note that each point $(\nu_{\Xi}^{-1} \omega, \theta)$ can be equivalently represented by atom at $\theta$ with weight $\nu_{\Xi}^{-1} \omega$, and hence the point process (34) can be represented by the random atomic distribution $G$ on $\Theta$, defined by

$$
G(A) = \nu_{\Xi}^{-1} \sum_{(\omega, \theta) \in \Xi} \omega 1_A(\theta).
$$

It was shown in [63] that $G$ follows a Dirichlet process $DP(\eta, G_0)$, with parameter $\eta$ and base distribution $G_0$. Noting that the cluster parameter $\theta_n$ for $X_n$ can be regarded as a sample from $G$, the data generation process for this model can be summarized as follows

$$
G \sim DP(\eta, G_0)
$$

$$
\theta_n \sim G
$$

$$
X_n \sim f(\cdot|\theta_n).
$$

The cluster assignment and the mixture parameters, including the number of clusters, can be automatically learned from the data via posterior inference. Analogous to finite mixture models, computing the posteriors are intractable in general and often require MCMC methods. Next we detail a (collapsed) Gibbs sampler to simulate the cluster label posterior $p(y_{1:N} | X_{1:N})$ for point pattern clustering.

#### 5.2.1 Gibbs Sampling for Poisson mixture model

A Gibbs sampler simulates the posterior $p(y_{1:N} | X_{1:N})$ via a Markov Chain $\{y_{1:n}^{(i)}\}_{i=0}^{\infty}$ in which $y_{1:n}^{(i)}$ is generated from $y_{1:n}^{(i-1)}$ by iterating:

$$
y_{1:n}^{(i)} \sim p_n(\cdot | y_{1:n-1}^{(i)}, y_{1:n+1:N}^{(i)}, X_{1:N}),
$$

for $n = 1, \ldots, N$, where

$$
p_n(y_n | y_{1:n-1}, y_{n+1:N}, X_{1:N}) \propto p(y_n | X_{1:N})
$$

is the $n^{th}$ conditional probability. After the so-called pre-convergence period, samples from the Markov chain are effectively distributed from the cluster label posterior. However, the actual distribution of the samples depends on the starting value. In practice, the pre-convergence samples, known as burn-ins, are discarded, and the post-convergence samples are used for inference.

While Gibbs sampling is efficient, it requires the conditionals to be easily computed and sampled. Using the notation $-n = \{1, \ldots, N\} - \{n\}$, the $n^{th}$ conditional for the cluster labels of the infinite point process mixture can be written as

$$
p(k | y_{-n}, X_{1:N}) = p(y_n = k | z_{-n}, X_n, X_{-n})
$$

$$
\propto f(X_n | y_n = k, y_{-n}, X_{-n}) p(y_n = k | y_{-n}, X_{-n})
$$

$$
= f(X_n | y_n = k, y_{-n}, X_{-n}) p(y_n = k | y_{-n})
$$

where the last line follows from the fact that given $X_{-n}$ and $y_{-n}$, $y_n$ is independent of $X_{-n}$. Using the Polya urn characterization [63] of the Dirichlet process, we have

$$
p(y_n = k | y_{-n}) = \frac{(1 - 1_{y_n \neq k}(k)) \eta + \sum_{j \neq k} \delta_{y_n}(k)}{N - 1 + \eta}
$$

(37)
where the sum over \( -n \) is called the popularity of \( k \). Further, note in the first term of (35) that, given \( y_n = k, y_{-n} \) and \( X_{-n}, X_n \) only depends on \( X(k) = \{ X_j \in X_n : y_j = k \} \), the set of observations in \( X_n \) that belongs to cluster \( k \) (in fact its cardinality is the popularity of \( k \)). Hence

\[
f(X_n|y_n = k, y_{-n}, X_{-n}) = \int \frac{f(X_n|\theta_k)G(d\theta_k|X(k))}{f(X_n|\theta_k)} \, d\theta_k = \int f(X_n|\theta_k)G(d\theta_k|X(k)), \tag{38}
\]

which is the predictive likelihood for cluster \( k \) of the point pattern \( X_n \). In general the predictive likelihood, and consequently the conditionals, are intractable.

Fortunately, an analytic predictive likelihood can be derived for a Poisson point process mixture, i.e., a point process mixture with

\[
f(X|\theta_k) = \xi_k^{|X|} e^{-\xi_k(U^{X} \phi)} p^X_{\phi_k}
\]

where \( \theta_k = (\xi_k, \varphi_k) \) with \( \xi_k \) and \( \varphi_k \) denoting the mean cardinality and parameter of the feature distribution. In the following, we propose a family of conjugate priors for Poisson point processes and exploit conjugacy to derive the predictive likelihood for the Poisson mixture model.

**Proposition 3.** Let \( H(d\varphi|\gamma) \) be a conjugate prior distribution with respect to the feature density \( p_\varphi \) of a Poisson point process likelihood \( f(X|\xi, \varphi) \). Then the distribution given by

\[
G_0(\xi, \varphi|\alpha, \beta, \gamma) = \int \frac{\beta^\alpha}{\Gamma(\alpha)} e^{\beta \xi} d\xi H(d\varphi|\gamma)
\]

is conjugate with respect to \( f(X|\xi, \varphi) \). Moreover, the predictive likelihood of \( X \) given a finite collection \( Z \) of point patterns is

\[
f(X|Z) = \frac{\Gamma(\alpha + |Z|) \beta^{\alpha |Z|}}{\Gamma(\alpha)(\beta + 1)^{\alpha + |Z|}} \int p^X_{\varphi} H(d\varphi|\gamma). \tag{41}
\]

where \( \alpha = \alpha + \sum_{Z \in Z} |Z|, \beta = \beta + |Z| \) and \( H(d\varphi|\gamma) \propto \prod_{Z \in Z} p^Z_{\varphi} H(d\varphi|\gamma) \) also has the same form, which we denote by \( \tilde{H}(d\varphi|\gamma) \).

Proof: Since \( H(d\varphi|\gamma) \) and \( p_\varphi \) are conjugate, i.e., \( H(d\varphi|\gamma) \) and \( p_\varphi(z) H(d\varphi|\gamma) / \int p_\varphi(z) H(d\varphi|\gamma) \) have the same form, it follows by induction that \( p^X_{\varphi} H(d\varphi|\gamma) / \int p^X_{\varphi} H(d\varphi|\gamma) \) also has the same form, which we denote by \( \tilde{H}(d\varphi|\gamma) \).

Using Bayes’ rule

\[
G(\xi, \varphi|Z, \alpha, \beta, \gamma) \propto f(Z|\xi, \varphi) G_0(\xi, \varphi|\alpha, \beta, \gamma) \\
\propto \xi^{|Z|} e^{\xi(U^{Z} \phi)} p^Z_{\varphi} e^{-\beta \xi} \xi^{\alpha} \xi^{\beta} \tilde{H}(d\varphi|\gamma)
\]

which takes on the same form as (40). Hence (40) is conjugate with respect to \( f(Z|\xi, \varphi) \). Further, iterating the above argument through the elements of \( Z \) yields

\[
G(\xi, \varphi|Z, \alpha, \beta, \gamma) \propto \xi^{|Z|} e^{-\beta \xi} d\xi \tilde{H}(d\varphi|\gamma)
\]

Substituting this into the predictive likelihood

\[
f(X|Z) = \int \frac{f(X|\xi, \varphi)G(\xi, \varphi|Z, \alpha, \beta, \gamma)}{f(X|\xi, \varphi)} \, d\xi d\varphi
\]

together with some algebraic manipulations yields (41).

For an infinite Poisson mixture model with base measure \( G_0 \) given by (40), where \( H(d\varphi|\gamma) \) is conjugate with respect to the feature density \( p_\varphi \) of the constituent Poisson point process components, the predictive likelihood (38) is given by \( f(X_n|X(k)) \).

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