Analysing replicated point patterns in spatstat

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Abstract

This document describes spatstat's capabilities for fitting models to replicated point patterns. More generally it applies to data from a designed experiment in which the response from each unit is a spatial point pattern.

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1 Introduction

'Replicated point patterns' are datasets consisting of several point patterns which can be regarded as independent repetitions of the same experiment. For example, three point patterns taken from micrographs of three pipette samples of the same jug of milk, could be assumed to be replicated observations.

More generally we could have several experimental groups, with replicated point pattern data in each group. For example there may be two jugs of milk that were treated differently, and we take three pipette samples from each jug.

Even more generally our point patterns could be the result of a designed experiment involving control and treatment groups, covariates such as temperature, and even spatial covariates (such as image data).

This document describes some capabilities available in the spatstat package for analysing such data. For further detail, see Chapter 16 of the spatstat book [2].

2 Overview of software

The main components needed are:

- the model-fitting function mppm, an extension of the spatstat function ppm, that will fit Gibbs point process models to multiple point pattern datasets;
- support for the class "mppm" of point process models fitted by mppm (e.g. functions to print and plot the fitted model, analysis of deviance for Poisson models)
- some tools for exploratory data analysis;
- basic support for the data from such experiments by storing the data in a "hyperframe". A hyperframe is like a data frame, except that each entry in a column can be a point pattern or a pixel image, as well as a single number or categorical value.
- four example datasets.

3 Formulating the problem

We view the experiment as involving a series of 'units'. Each unit is subjected to a known set of experimental conditions (described by the values of the covariates), and each unit yields a response which is a spatial point pattern. The value of a particular covariate for each unit can be either a single value (numerical, logical or factor), or a pixel image.

Three important cases are:

independent replicates: We observe *n* different point patterns that can be regarded as independent replicates, i.e. independent realisations of the same point process. The 'responses' are the point patterns; there are no covariates.

replication in groups: there are K different experimental groups (e.g. control, aspirin, nurofen). In group k (k = 1, ..., K) we observe n_k point patterns which can be regarded as independent replicates within this group. We regard this as an experiment with $n = \sum_k n_k$ units. The responses are the point patterns; there is one covariate which is a factor (categorical variable) identifying which group each point pattern belongs to.

general case: there are covariates other than factors that influence the response. The point patterns are assumed to be independent, but no two patterns have the same distribution.

Examples of these three cases are given in the datasets waterstriders, pyramidal and demohyper respectively, which are installed in spatstat.

4 Installed datasets

The following datasets are currently installed in spatstat.

- waterstriders: Penttinen's [9] waterstriders data recording the locations of insect larvae on a pond in 3 independent experiments.
- pyramidal: data from Diggle, Lange and Benes [7] on the locations of pyramidal neurons in human brain, 31 human subjects grouped into 3 groups (controls, schizoaffective and schizophrenic).
- flu: data from Chen et al [5] giving the locations of two different virus proteins on the membranes of cells infected with influenza virus; 41 multitype point patterns divided into two virus types (wild and mutant) and two stain types.
- simba: simulated data from an experiment with two groups and 5 replicate point patterns per group.
- demohyper: simulated data from an experiment with two groups in which each experimental unit has a point pattern response and a pixel image covariate.

5 Lists of point patterns

First we need a convenient way to store the responses from all the units in an experiment.

An individual point pattern is stored as an object of class "ppp". The easiest way to store all the responses is to form a list of "ppp" objects.

5.1 Waterstriders data

The waterstriders data are an example of this type. The data consist of 3 independent point patterns representing the locations of insect larvae on a pond. See help(waterstriders).

```
> waterstriders
```

```
List of point patterns
```

```
Component 1:
```

Planar point pattern: 38 points

window: rectangle = $[0, 48.1] \times [0, 48.1] \text{ cm}$

Component 2:

Planar point pattern: 36 points

window: rectangle = [0, 48.8] x [0, 48.8] cm

Component 3:

Planar point pattern: 36 points

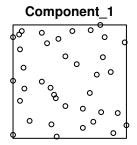
window: rectangle = $[0, 46.4] \times [0, 46.4] \text{ cm}$

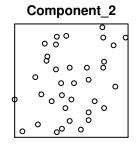
The waterstriders dataset is a list of point patterns. It is a list, each of whose entries is a point pattern (object of class "ppp"). Note that the observation windows of the three point patterns are not identical.

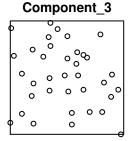
5.2 The class listof

For convenience, the waterstriders dataset also belongs to the class "listof". This is a simple mechanism to allow us to handle the list neatly — for example, we can provide special methods for printing, plotting and summarising the list.

> plot(waterstriders, main="")







Notice that the plot method displays each entry of the list in a separate panel. There's also the summary method:

> summary(waterstriders)

Summary of 3 point patterns

Component 1:

Planar point pattern: 38 points

Average intensity 0.01642455 points per square cm

Coordinates are given to 2 decimal places i.e. rounded to the nearest multiple of 0.01 cm

Window: rectangle = $[0, 48.1] \times [0, 48.1] \text{ cm}$

Window area = 2313.61 square cm

Unit of length: 1 cm

Component 2:

Planar point pattern: 36 points

Average intensity 0.0151169 points per square cm

Coordinates are given to 2 decimal places i.e. rounded to the nearest multiple of 0.01 $\ensuremath{\text{cm}}$

Window: rectangle = [0, 48.8] x [0, 48.8] cm Window area = 2381.44 square cm

Unit of length: 1 cm

Component 3:

Planar point pattern: 36 points

Average intensity 0.01672117 points per square cm

Coordinates are given to 2 decimal places i.e. rounded to the nearest multiple of 0.01 cm

Window: rectangle = $[0, 46.4] \times [0, 46.4] \text{ cm}$

Window area = 2152.96 square cm

Unit of length: 1 cm

5.3 Creating a list of object

For example, here is a simulated dataset containing three independent realisations of the Poisson process with intensity 100.

> X <- listof(rpoispp(100), rpoispp(100), rpoispp(100))</pre>

Then it can be printed and plotted.

> plot(X)

> X

Component 1:

Planar point pattern: 88 points

window: rectangle = [0, 1] x [0, 1] units

Component 2:

Planar point pattern: 97 points

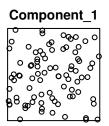
window: rectangle = $[0, 1] \times [0, 1]$ units

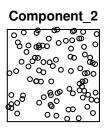
Component 3:

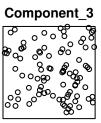
Planar point pattern: 97 points

window: rectangle = $[0, 1] \times [0, 1]$ units









To convert an existing list to the class listof, use as.listof.

6 Hyperframes

A hyperframe is like a data frame, except that its entries can be objects of any kind. A hyperframe is effectively a two-dimensional array in which each column consists of values of one type (as in a data frame) or consists of objects of one class.

The entries in a hyperframe can be point patterns, pixel images, windows, or any other objects.

To analyse an experiment, we will store **all** the data from the experiment in a single hyperframe. The rows of the hyperframe will correspond to different experimental units, while the columns represent different variables (response variables or covariates).

6.1 Creating hyperframes

The function hyperframe will create a hyperframe.

```
> hyperframe(...)
```

The arguments ... are any number of arguments of the form tag=value. Each value will become a column of the array. The tag determines the name of the column.

Each value can be either

- an atomic vector or factor (i.e. numeric vector, integer vector, character vector, logical vector, complex vector or factor)
- a list of objects which are all of the same class
- one atomic value, which will be replicated to make an atomic vector or factor
- one object, which will be replicated to make a list of identical objects.

All columns (vectors, factors and lists) must be of the same length, if their length is greater than 1.

For example, here is a hyperframe containing a column of numbers and a column of functions:

```
> H <- hyperframe(X=1:3, Y=list(sin,cos,tan))
> H

Hyperframe:
    X      Y
1 1 (function)
2 2 (function)
3 3 (function)
```

Note that a column of character strings will be converted to a factor, unless you set stringsAs-Factors=FALSE in the call to hyperframe. This is the same behaviour as for the function data.frame.

```
> G <- hyperframe(X=1:3, Y=letters[1:3], Z=factor(letters[1:3]),
+ W=list(rpoispp(100),rpoispp(100), rpoispp(100)),
+ U=42,
+ V=rpoispp(100), stringsAsFactors=FALSE)
> G
```

Hyperframe:

```
X Y Z W U V
1 1 a a (ppp) 42 (ppp)
2 2 b b (ppp) 42 (ppp)
3 3 c c (ppp) 42 (ppp)
```

This hyperframe has 3 rows. The columns named U and V are constant (all entries in a column are the same). The column named Y is a character vector.

6.2 Hyperframes of data

To analyse an experiment, we will store **all** the data from the experiment in a single hyperframe. The rows of the hyperframe will correspond to different experimental units, while the columns represent different variables (response variables or covariates).

Several examples of hyperframes are provided with the package, including demohyper, flu, simba and pyramidal, described above.

The simba dataset contains simulated data from an experiment with a 'control' group and a 'treatment' group, each group containing 5 experimental units. The responses in the control group are independent Poisson point patterns with intensity 80. The responses in the treatment group are independent realisations of a Strauss process (see help(simba) for details). The simba dataset is a hyperframe with 10 rows and 2 columns: Points (the point patterns) and group (a factor with levels control and treatment).

> simba

Hyperframe:

```
Points
               group
1
    (ppp)
             control
2
    (ppp)
             control
3
    (ppp)
             control
4
    (ppp)
             control
5
    (ppp)
             control
6
    (ppp) treatment
7
    (ppp) treatment
8
    (ppp) treatment
9
    (ppp) treatment
10
    (ppp) treatment
```

The pyramidal dataset contains data from Diggle, Lange and Benes [7] on the locations of pyramidal neurons in human brain. One point pattern was observed in each of 31 human subjects. The subjects were classified into 3 groups (controls, schizoaffective and schizophrenic). The pyramidal dataset is a hyperframe with 31 rows and 2 columns: Neurons (the point patterns) and group (a factor with levels control, schizoaffective and schizophrenic).

> pyramidal

Hyperframe:

	Neurons	group
1	(ppp)	control
2	(ppp)	control

```
3
                    control
     (ppp)
4
     (ppp)
                    control
5
     (ppp)
                    control
6
     (ppp)
                    control
7
     (ppp)
                    control
8
     (ppp)
                    control
9
     (ppp)
                    control
10
     (ppp)
                    control
11
     (ppp)
                    control
12
     (ppp)
                    control
13
     (ppp) schizoaffective
     (ppp) schizoaffective
14
     (ppp) schizoaffective
15
16
     (ppp) schizoaffective
17
     (ppp) schizoaffective
     (ppp) schizoaffective
18
19
     (ppp) schizoaffective
20
     (ppp) schizoaffective
21
     (ppp) schizoaffective
22
              schizophrenic
     (ppp)
              schizophrenic
23
     (ppp)
              schizophrenic
24
     (ppp)
              schizophrenic
25
     (ppp)
26
              schizophrenic
     (ppp)
27
              schizophrenic
     (ppp)
              schizophrenic
28
     (ppp)
29
              schizophrenic
     (ppp)
              schizophrenic
30
     (ppp)
              schizophrenic
31
     (ppp)
```

The waterstriders dataset is not a hyperframe; it's just a list of point patterns. It can easily be converted into a hyperframe:

```
> ws <- hyperframe(Striders=waterstriders)</pre>
```

6.3 Columns of a hyperframe

Individual columns of a hyperframe can be extracted using \$:

```
> H$X
[1] 1 2 3
> H$Y
1:
function (x) .Primitive("sin")
2:
function (x) .Primitive("cos")
```

```
3:
function (x)
               .Primitive("tan")
   The result of $ is a vector or factor if the column contains atomic values; otherwise it is a list of
objects (with class "listof" to make it easier to print and plot).
   Individual columns can also be assigned (overwritten or created) using $<-:
> H$U <- letters[1:3]
> H
Hyperframe:
  Х
              ΥU
1 1 (function) a
2 2 (function) b
3 3 (function) c
   This can be used to build up a hyperframe column-by-column:
> G <- hyperframe()
> G$X <- waterstriders
> G$Y <- 1:3
> G
Hyperframe:
      ΧY
1 (ppp) 1
2 (ppp) 2
3 (ppp) 3
     Subsets of a hyperframe
Other subsets of a hyperframe can be extracted with [:
> H[,1]
Hyperframe:
  Х
1 1
2 2
3 3
> H[2,]
Hyperframe:
              ΥU
2 2 (function) b
```

> H[2:3,]

```
Hyperframe:
   X       Y U
2 2 (function) b
3 3 (function) c
> H[1,1]
Hyperframe:
   X
1 1
```

The result of [is a hyperframe, unless you set drop=TRUE and the subset consists of only one element or one column:

```
> H[,1,drop=TRUE]
[1] 1 2 3
> H[1,1,drop=TRUE]
[1] 1
> H[1,2,drop=TRUE]
function (x) .Primitive("sin")
```

Currently there is no method for [<- that would allow you to assign values to a subset of a hyperframe.

7 Plotting

7.1 Plotting a list of object

The plot method for listof objects has formal arguments

```
> plot.listof(x, ..., main, arrange = TRUE, nrows = NULL, ncols = NULL)
```

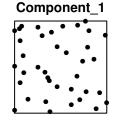
where main is a title for the entire page.

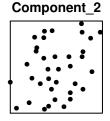
If arrange=TRUE then the entries of the list are displayed in separate panels on the same page (with nrows rows and ncols columns of panels), while if arrange=FALSE then the entries are just plotted as a series of plot frames.

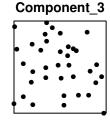
The extra arguments ... control the individual plot panels. These arguments will be passed to the plot method that displays each entry of the list. Suitable arguments depend on the type of entries.

> plot(waterstriders, pch=16, nrows=1)

waterstriders





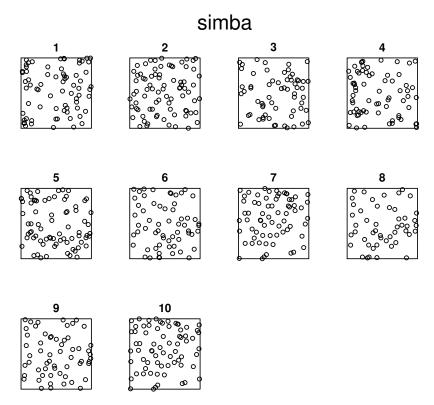


7.2 Plotting a hyperframe

7.2.1 Plotting one column

If h is a hyperframe, then the default action of plot(h) is to extract the first column of h and plot each of the entries in a separate panel on one page (actually using the plot method for class "listof").

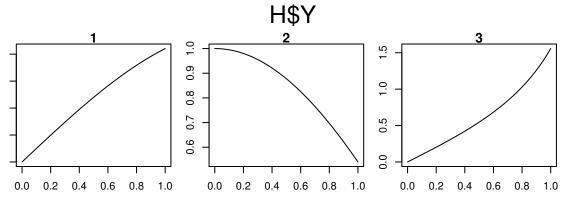
> plot(simba)



This only works if the entries in the first column are objects for which a plot method is defined (for example, point patterns, images, windows).

To select a different column, use \$ or [:

> H <- hyperframe(X=1:3, Y=list(sin,cos,tan))
> plot(H\$Y)



The plot can be controlled using the arguments for plot.listof (and, in this case, plot.function, since H\$Y consists of functions).

7.2.2 Complex plots

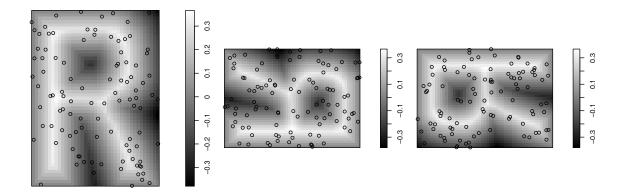
More generally, we can display any kind of higher-order plot involving one or more columns of a hyperframe:

> plot(h, e)

where h is a hyperframe and e is an R language call or expression that must be evaluated in each row to generate each plot panel.

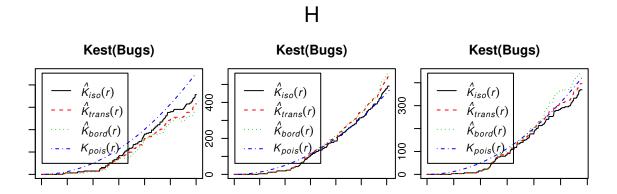
> plot(demohyper, quote({ plot(Image, main=""); plot(Points, add=TRUE) }))

demohyper



Note the use of quote, which prevents the code inside the braces from being evaluated immediately. To plot the K-functions of each of the patterns in the waterstriders dataset,

- > H <- hyperframe(Bugs=waterstriders)
- > plot(H, quote(plot(Kest(Bugs))), marsize=1)



8 Data analysis

8.1 Computing with hyperframes

Often we want to perform some computation on each row of a hyperframe.

In a data frame, this can be done using the command with:

```
> df <- data.frame(A=1:10, B=10:1)
> with(df, A-B)
[1] -9 -7 -5 -3 -1 1 3 5 7 9
```

In this example, the expression A-B is evaluated in each row of the data frame, and the result is a vector containing the computed values for each row. The function with is generic, and has a method for data frames, with.data.frame. The computation above was executed by with.data.frame.

The same syntax is available for hyperframes using the method with.hyperframe:

```
> with(h,e)
```

Here h is a hyperframe, and e is an R language construct involving the names of columns in h. For each row of h, the expression e will be evaluated in such a way that each entry in the row is identified by its column name.

```
> H <- hyperframe(Bugs=waterstriders)
> with(H, npoints(Bugs))
   2 3
 1
38 36 36
> with(H, distmap(Bugs))
List of pixel images
1:
real-valued pixel image
128 x 128 pixel array (ny, nx)
enclosing rectangle: [0, 48.1] x [0, 48.1] cm
2:
real-valued pixel image
128 x 128 pixel array (ny, nx)
enclosing rectangle: [0, 48.8] x [0, 48.8] cm
3:
real-valued pixel image
128 x 128 pixel array (ny, nx)
enclosing rectangle: [0, 46.4] x [0, 46.4] cm
```

The result of with.hyperframe is a list of objects (of class "listof"), or a vector or factor if appropriate.

Notice that (unlike the situation for data frames) the operations in the expression e do not have to be vectorised. For example, distmap expects a single point pattern, and is not vectorised to deal with a list of point patterns. Instead, the expression distmap(Bugs) is evaluated separately in each row of the hyperframe.

8.2 Summary statistics

One application of with.hyperframe is to calculate summary statistics for each row of a hyperframe. For example, the number of points in a point pattern X is returned by npoints(X). To calculate this for each of the responses in the simba dataset,

> with(simba, npoints(Points))

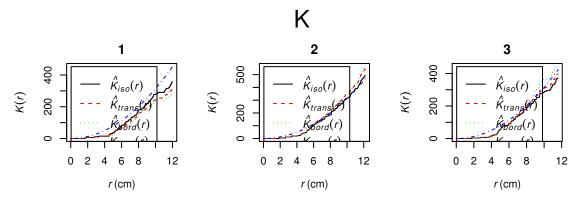
The summary statistic can be any kind of object. For example, to compute the empirical K-functions for each of the patterns in the waterstriders dataset,

> H <- hyperframe(Bugs=waterstriders)

> K <- with(H, Kest(Bugs))

To plot these K-functions you can then just type

> plot(K)



The summary statistic for each row could be a numeric vector:

- > H <- hyperframe(Bugs=waterstriders)
- > with(H, nndist(Bugs))

1:

- $[1] \ \ 9.190609 \ \ 5.850214 \ \ 2.817836 \ \ 1.850000 \ \ 5.500445 \ \ 5.966071 \ \ 1.850000 \ \ 7.107468$
- [9] 5.500445 9.190609 4.516426 4.964071 4.964071 3.309381 5.635672 1.654690
- [17] 1.654690 5.635672 5.258688 5.850214 6.792297 5.850214 5.140204 7.107468
- [25] 7.288155 5.140204 6.023164 5.258688 7.117092 5.500445 6.023164 6.472357
- [33] 6.365721 8.794800 4.636087 6.365721 5.153504 4.636087

2:

- [1] 7.288155 7.840159 7.288155 5.336216 4.824210 1.886637 1.886637
- [8] 5.140204 3.350493 5.500445 2.668108 3.350493 5.193197 4.470727
- [15] 2.668108 4.516426 4.086784 4.709331 5.966071 4.470727 5.550000
- [22] 5.258688 5.232590 5.232590 3.330000 3.330000 5.032544 2.616295
- [29] 2.616295 5.032544 4.455390 4.455390 5.550000 9.648420 6.158027
- [36] 11.682864

```
3:
 [1]
      5.990409 11.372357
                                     5.990409
                                                         5.171779
                                                                    5.258564
                          8.007128
                                               6.208679
 [8]
      5.171779
                6.215143
                          5.258564
                                     5.110000
                                               5.110000
                                                          3.724258
                                                                    3.724258
[15]
      3.869186
                3.869186
                                     4.251459
                                               4.968581
                                                          6.242828
                                                                    4.740000
                          5.470000
[22]
      4.740000
                4.251459
                          2.773193
                                     4.805767
                                               6.237123
                                                          1.828004
                                                                    1.828004
[29]
      5.110000 10.888329
                          5.110000
                                     4.638620
                                               4.136581
                                                          4.638620
                                                                    4.136581
[36] 11.917739
```

The result is a list, each entry being a vector of nearest neighbour distances. To find the minimum interpoint distance in each pattern:

8.3 Generating new columns

New columns of a hyperframe can be created by computation from the existing columns.

For example, I can add a new column to the simba dataset that contains pixel images of the distance maps for each of the point pattern responses.

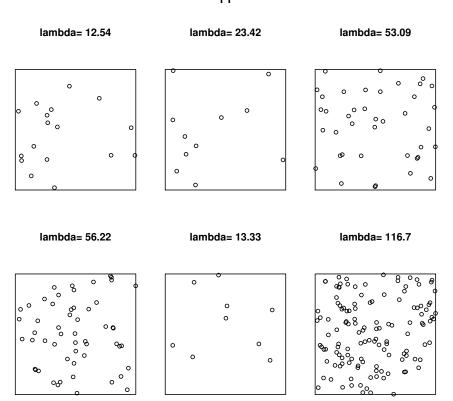
```
> simba$Dist <- with(simba, distmap(Points))</pre>
```

8.4 Simulation

This can be useful for simulation. For example, to generate Poisson point patterns with different intensities, where the intensities are given by a numeric vector lambda:

```
> lambda <- rexp(6, rate=1/50)
> H <- hyperframe(lambda=lambda)
> H$Points <- with(H, rpoispp(lambda))
> plot(H, quote(plot(Points, main=paste("lambda=", signif(lambda, 4)))))
```

Н



It's even simpler to generate 10 independent Poisson point patterns with the same intensity 50, say:

> H\$X <- with(H, rpoispp(50))

(the expression rpoispp(50) is evaluated once in each row, yielding a different point pattern in each row because of the randomness).

9 Exploratory data analysis

Before fitting models to the data, it is prudent to explore the data to detect unusual features and to suggest appropriate models.

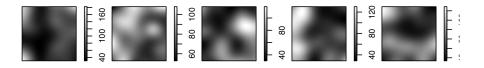
9.1 Exploring spatial trend and covariate effects

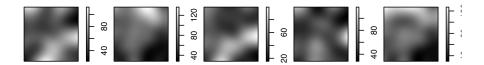
Points may be distributed non-uniformly either because they are intrinsically non-uniform ("spatial trend") or because their abundance depends on a spatial covariate ("covariate effects").

Non-uniformity of a point pattern can be investigated using the kernel smoothed intensity. This is the convolution of the point pattern with a smooth density called the kernel. Effectively each point in the pattern is replaced by a copy of the kernel, and the sum of all copies of the kernel is the kernel-smoothed intensity function. It is computed by density.ppp separately for each point pattern.

```
> plot(simba, quote(plot(density(Points), main="")), nrows=2)
```

simba





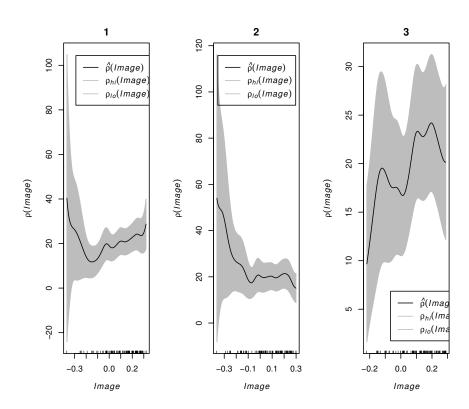
Covariate effects due to a real-valued spatial covariate (a real-valued pixel image) can be investigated using the command **rhohat**. This uses a kernel smoothing technique to fit a model of the form

$$\lambda(u) = \rho(Z(u))$$

where $\lambda(u)$ is the point process intensity at a location u, and Z(u) is the value of the spatial covariate at that location. Here ρ is an unknown, smooth function which is to be estimated. The function ρ expresses the effect of the spatial covariate on the point process intensity. If ρ turns out to be constant, then the covariate has no effect on point process intensity (and the constant value of ρ is the constant intensity of the point process).

- > rhos <- with(demohyper, rhohat(Points, Image))</pre>
- > plot(rhos)

rhos



9.2 Exploring interpoint interaction

Still to be written.

10 Fitting models of spatial trend

The command mppm fits models to multiple point patterns. Its syntax is very similar to that of lm and glm:

> mppm(formula, data, interaction, ...)

where formula is a formula describing the systematic trend part of the model, data is a hyper-frame containing all the data (responses and covariates), and interaction determines the stochastic interpoint interaction part of the model.

For example:

> mppm(Points ~ group, simba, Poisson())

Note that the formula has a left hand side, which identifies the response. This should be the name of a column of data.

10.1 Trend formula

The right side of formula is an expression for the linear predictor (effectively the **logarithm** of the spatial trend).

The variables appearing in the right hand side of formula should be either

- names of columns in data
- objects in the R global environment (such as pi and log)
- the reserved names x, y (representing Cartesian coordinates), marks (representing mark values attached to points) or id (a factor representing the row number in the hyperframe).

10.1.1 Design covariates

The variables in the trend could be 'design covariates'.

For example, to fit a model to the simba dataset in which all patterns are independent replicates of the same uniform Poisson process, with the same constant intensity:

```
> mppm(Points ~ 1, simba)
Point process model fitted to 10 point patterns
Call: mppm(Points ~ 1, simba)
Log trend formula: ~1
Fitted trend coefficients:
(Intercept)
    4.19419
```

Interaction for all patterns: Poisson process

To fit a model in which the two groups of patterns (control and treatment groups) each consist of independent replicates of a uniform Poisson process, but with possibly different intensity in each group:

```
> mppm(Points ~ group, simba)
Point process model fitted to 10 point patterns
Call: mppm(Points ~ group, simba)
Log trend formula: ~group
Fitted trend coefficients:
   (Intercept) grouptreatment
   4.2682979 -0.1541507
```

Interaction for all patterns: Poisson process

To fit a uniform Poisson process to each pattern, with different intensity for each pattern:

```
> mppm(Points ~ id, simba)
Point process model fitted to 10 point patterns
Call: mppm(Points ~ id, simba)
Log trend formula: ~id
```

Fitted trend coefficients:

(Intercept) id2 id3 id4 id5 id6 4.26267988 0.11934676 -0.11954515 -0.04317217 0.05480824 -0.15180601 id7 id8 id9 id10 -0.04317217 -0.37085958 -0.20223687 -0.01418463

Interaction for all patterns: Poisson process

10.1.2 Spatial covariates

The variables in the trend could be 'spatial covariates'.

For example, the demotyper dataset has a column Image containing pixel images.

> mppm(Points ~ Image, data=demohyper)

(Intercept) Image 2.9844838 0.3885543

Interaction for all patterns: Poisson process

This model postulates that each pattern is a Poisson process with intensity of the form

$$\lambda(u) = \exp(\beta_0 + \beta_1 Z(u))$$

at location u, where β_0, β_1 are coefficients to be estimated, and Z(u) is the value of the pixel image Image at location u.

It may or may not be appropriate to assume that the intensity of the points is an exponential function of the image pixel value Z. If instead we wanted the intensity $\lambda(u)$ to be proportional to Z(u), the appropriate model is

> mppm(Points ~ offset(log(Image)), data=demohyper)

which corresponds to an intensity proportional to Image,

$$\lambda(u) = \exp(\beta_0 + \log Z(u)) = e^{\beta_0} Z(u).$$

The offset indicates that there is no coefficient in front of $\log Z(u)$.

Alternatively we could allow a coefficient:

> mppm(Points ~ log(Image), data=demop)

which corresponds to a gamma transformation of Image,

$$\lambda(u) = \exp(\beta_0 + \beta_1 \log Z(u)) = e^{\beta_0} Z(u)^{\beta_1}.$$

11 Interpoint interaction

The stochastic interpoint interaction in a point process model is specified by the arguments interaction and (optionally) iformula in

> mppm(formula, data, interaction, ..., iformula=NULL)

11.1 Same interaction for all patterns

In the simplest case, the argument interaction is one of the familiar objects that describe the point process interaction structure. It is an object of class "interact" created by calling one of the functions

```
Poisson()
                           the Poisson point process
             Hardcore()
                           the hard core process
              Strauss()
                           the Strauss process
          StraussHard()
                           the Strauss/hard core point process
             Softcore()
                           pairwise interaction, soft core potential
                           pairwise interaction, piecewise constant
            PairPiece()
DiggleGatesStibbard()
                           Diggle-Gates-Stibbard pair potential
      DiggleGratton()
                           Diggle-Gratton pair potential
              Fiksel()
                           Fiksel pair potential
        LennardJones()
                           Lennard-Jones pair potential
             Pairwise()
                           pairwise interaction, user-supplied potential
            AreaInter()
                           area-interaction potential
                 Gever()
                           Geyer's saturation process
                BadGey()
                           multiscale Geyer saturation process
             Saturated()
                           Saturated pair model, user-supplied potential
            OrdThresh()
                           Ord process, threshold potential
                   Ord()
                           Ord model, user-supplied potential
         MultiStrauss()
                           multitype Strauss process
                           multitype Strauss/hard core process
    MultiStraussHard()
                Concom()
                           connected component interaction
                           hybrid of several interactions
                Hybrid()
```

In this 'simple' usage of mppm, the point process model assumes that all point patterns have exactly the same interpoint interaction, (with the same interaction parameters), and only differ in their spatial trend.

11.2 Hyperframe of interactions

> Rad <- hyperframe(R=radii)</pre>

More generally the argument interaction can be a hyperframe containing objects of class "interact".

For example, we might want to fit a Strauss process to each point pattern, but with a different Strauss interaction radius for each pattern.

Then radii is a vector of numbers which we could use as the values of the interaction radius for each case. First we need to make the interaction objects:

```
> Str <- with(Rad, Strauss(R))
    Then we put them into a hyperframe and fit the model:
> Int <- hyperframe(str=Str)
> mppm(Points ~ 1, simba, interaction=Int)

Point process model fitted to 10 point patterns
Call: mppm(Points ~ 1, simba, interaction = Int)
Log trend formula: ~1
```

```
Fitted trend coefficients: (Intercept)
4.372376
```

```
Interaction for each pattern:
                                      Strauss process
Interaction 1:
                      Strauss(r = 0.06525, gamma = 0.8158)
                      Strauss(r = 0.06588, gamma = 0.8158)
Interaction 2:
Interaction 3:
                      Strauss(r = 0.06567, gamma = 0.8158)
                      Strauss(r = 0.06511, gamma = 0.8158)
Interaction 4:
Interaction 5:
                      Strauss(r = 0.05764, gamma = 0.8158)
Interaction 6:
                      Strauss(r = 0.07948, gamma = 0.8158)
Interaction 7:
                      Strauss(r = 0.07608, gamma = 0.8158)
                      Strauss(r = 0.09014, gamma = 0.8158)
Interaction 8:
```

An important constraint is that all of the interaction objects in one column must be *instances of the same process* (e.g. Strauss) albeit possibly having different parameter values. For example, you cannot put Poisson and Strauss processes in the same column.

Strauss(r = 0.07943, gamma = 0.8158)

Strauss(r = 0.07684, gamma = 0.8158)

11.3 Interaction formula

Interaction 9:

Interaction 10:

If interaction is a hyperframe, then the additional argument iformula may be used to fully specify the interaction.

(An iformula is also required if interaction has more than one column.)

The iformula should be a formula without a left hand side. Variables on the right hand side are typically the names of columns in interaction.

11.3.1 Selecting one column

If the right hand side of iformula is a single name, then this identifies the column in interaction to be used as the interpoint interaction structure.

```
> h <- hyperframe(Y=waterstriders)
> g <- hyperframe(po=Poisson(), str4 = Strauss(4), str7= Strauss(7))
> mppm(Y ~ 1, data=h, interaction=g, iformula=~str4)

Point process model fitted to 3 point patterns
Call: mppm(Y ~ 1, data = h, interaction = g, iformula = ~str4)
Log trend formula: ~1
```

```
Fitted trend coefficients: (Intercept)
-3.522586
```

Interaction formula: "str4

Interactions defined for each pattern:

Interaction 'str4': Strauss(r = 4, gamma = 0.2556)

11.3.2 Interaction depending on design

The iformula can also involve columns of data, but only those columns that are vectors or factors. This allows us to specify an interaction that depends on the experimental design. [This feature is experimental.] For example

```
> fit <- mppm(Points ~ 1, simba, Strauss(0.07), iformula = ~Interaction*group)
```

Since Strauss(0.1) is not a hyperframe, it is first converted to a hyperframe with a single column named Interaction.

The iformula = Interaction*group specifies (since group is a factor) that the interpoint interaction shall have a different coefficient in each experimental group. That is, we fit a model which has two different values for the Strauss interaction parameter γ , one for the control group and one for the treatment group.

When you print the result of such a fit, the package tries to do 'automatic interpretation' of the fitted model (translating the fitted interaction coefficients into meaningful numbers like γ). This will be successful in *most* cases:

> fit

```
Point process model fitted to 10 point patterns
Call: mppm(Points ~ 1, simba, Strauss(0.07), iformula = ~Interaction *
Log trend formula: ~1
Fitted trend coefficients:
               (Intercept)
                                        grouptreatment
                 4.1979786
                                             0.4389735
Interaction: grouptreatment
                -0.9545881
                      Strauss(r = 0.07, gamma = 1.071)
Interaction 1:
                      Strauss(r = 0.07, gamma = 1.071)
Interaction 2:
                      Strauss(r = 0.07, gamma = 1.071)
Interaction 3:
Interaction 4:
                      Strauss(r = 0.07, gamma = 1.071)
Interaction 5:
                      Strauss(r = 0.07, gamma = 1.071)
Interaction 6:
                      Strauss(r = 0.07, gamma = 0.4122)
```

```
Interaction 7: Strauss(r = 0.07, gamma = 0.4122)
```

Interaction 8: Strauss(r = 0.07, gamma = 0.4122)

Interaction 9: Strauss(r = 0.07, gamma = 0.4122)

Interaction 10: Strauss(r = 0.07, gamma = 0.4122)

Thus we see that the estimate of the Strauss parameter γ for the control group is 1.071, and for the treatment group 0.4122 (the correct values in this simulated dataset were 1 and 0.5).

The fitted model can also be interpreted directly from the fitted canonical coefficients:

> coef(fit)

```
(Intercept) Interaction
4.19797857 0.06839639
grouptreatment Interaction:grouptreatment
0.43897349 -0.95458813
```

The last output shows all the coefficients β_j in the linear predictor for the (log) conditional intensity. The interpretation of the model coefficients, for any fitted model in R, depends on the *contrasts* which were applicable when the model was fitted. This is part of the core R system: see help(contrasts) or options(contrasts). If you did not specify otherwise, the default is to use treatment contrasts. This means that, for an explanatory variable which is a factor with N levels, the first level of the factor is used as a baseline, and the fitted model coefficients represent the factor levels $2, 3, \ldots, N$ relative to this baseline.

In the output above, there is a coefficient for (Intercept) and one for grouptreatment. These are coefficients related to the group factor. According to the "treatment contrasts" rule, the (Intercept) coefficient is the estimated effect for the control group, and the grouptreatment coefficient is the estimated difference between the treatment and control groups. Thus the fitted first order trend is $\exp(4.198) = 66.55$ for the control group and $\exp(4.198 + 0.439) = 103.2$ for the treatment group. The correct values in this simulated dataset were 80 and 100.

The remaining coefficients in the output are Interaction and Interaction:grouptreatment. Recall that the Strauss process interaction term is $\gamma^{t(u,x)} = \exp(t(u,x)\log\gamma)$ at a spatial location u, for a point pattern x. Since we're using treatment contrasts, the coefficient Interaction is the estimate of $\log \gamma$ for the control group. The coefficient Interaction:grouptreatment is the estimate of the difference in $\log \gamma$ between the treatment and control groups. Thus the estimated Strauss interaction parameter γ is $\exp(0.0684) = 1.071$ for the control group and $\exp(0.0684 + (-0.9546)) = 0.4122$ for the treatment group. The correct values were 1 and 0.5.

11.3.3 Completely different interactions for different cases

In the previous example, when we fitted a Strauss model to all point patterns in the simba dataset, the fitted model for the patterns in the control group was close to Poisson ($\gamma \approx 1$). Suppose we now want to fit a model which is Poisson in the control group, and Strauss in the treatment group. The Poisson and Strauss interactions must be given as separate columns in a hyperframe of interactions:

```
> interaction=hyperframe(po=Poisson(), str=Strauss(0.07))
```

What do we write for the iformula? The following will not work:

```
> iformula=~ifelse(group=="control", po, str)
```

This does not work because the Poisson and Strauss models are 'incompatible' inside such expressions. The canonical sufficient statistics for the Poisson and Strauss processes do not have the same dimension. Internally in mppm we translate the symbols po and str into matrices; the dimensions of these matrices are different, so the ifelse expression cannot be evaluated.

Instead we need something like the following:

```
> iformula=~I((group=="control")*po) + I((group=="treatment") * str)
```

The letter I here is a standard R function that prevents its argument from being interpreted as a formula (thus the * is interpreted as multiplication instead of a model interaction). The expression (group=="control") is logical, and when multiplied by the matrix po, yields a matrix.

So the following does work:

```
> g <- hyperframe(po=Poisson(), str=Strauss(0.07))</pre>
> fit2 <- mppm(Points ~ 1, simba, g,</pre>
                iformula=~I((group=="control")*po)
                        + I((group=="treatment") * str))
> fit2
Point process model fitted to 10 point patterns
Call: mppm(Points ~ 1, simba, g, iformula = ~I((group == "control") *
Log trend formula: ~1
Fitted trend coefficients:
                                    I((group == "control") * po)
                     (Intercept)
                       4.3914128
                                                               NA
I((group == "treatment") * str)
                      -0.6994845
Active interactions:
                             (10 x 2 matrix)
Interaction 1:
                       Poisson process
Interaction 2:
                       Poisson process
Interaction 3:
                       Poisson process
                       Poisson process
Interaction 4:
Interaction 5:
                       Poisson process
Interaction 6:
                       Strauss(r = 0.07, gamma = 0.4968)
Interaction 7:
                       Strauss(r = 0.07, gamma = 0.4968)
```

Interaction 8: Strauss(r = 0.07, gamma = 0.4968)

Interaction 9: Strauss(r = 0.07, gamma = 0.4968)

Interaction 10: Strauss(r = 0.07, gamma = 0.4968)

12 Random effects

12.1 Mixed effects models

It is also possible to fit models that include 'random effects'. Effectively, some of the coefficients in the model are assumed to be Normally-distributed random variables instead of constants.

12.1.1 Mixed Poisson model

Consider the simplest model of a uniform Poisson process which we fitted to the 3 point patterns of waterstriders. It might be sensible to assume that each pattern is a realisation of a Poisson process, but with random intensity. In each realisation the intensity λ is constant across different locations, but it is a different, random value in different realisations. This example is called a 'mixed Poisson process' and belongs to the class of 'Cox processes' (Poisson processes with random intensity functions). Let's assume further that the log-intensity is a Normal random variable. Then the model is a (very degenerate) special case of a 'log-Gaussian Cox process'.

To fit such a model we use the standard techniques of mixed effects models [8, 6, 10]. The mixed Poisson process which we discussed above would be written in standard form

$$\lambda_i(u) = \exp(\mu + Z_i) \tag{1}$$

for the *i*th point pattern, where μ is a parameter to be estimated (the 'fixed effect') and $Z_i \sim N(0, \sigma^2)$ is a zero-mean Normal random variable (the 'random effect' for point pattern *i*). In the simplest case we would assume that Z_1, \ldots, Z_n are independent. The variance σ^2 of the random effects would be estimated. One can also estimate the individual realised values z_i of the random effects for each point pattern, although these are usually not of such great interest. Since the model includes both fixed and random effects, it is called a "mixed-effects" model.

12.1.2 Dependence structure

When we formulate a random-effects or mixed-effects model, we must specify the dependence structure of the random effects. In the model above we assumed that the Z_i are independent for all point patterns i. If the experiment consists of two groups, we could alternatively assume that $Z_i = Z_j$ whenever i and j belong to the same group. In other words all the patterns in one group have the same value of the random effect. So the random effect is associated with the group rather than with individual patterns. This could be appropriate if, for example, the groups represent different batches of a chemical. Each batch is prepared under slightly different conditions so we believe that there are random variations between batches, but within a batch we believe that the chemical is well-mixed.

12.1.3 Random effects are coefficients

In the mixed Poisson model (1), the random effect is an additive constant (with a random value) in the log-intensity. In general, a random effect is a *coefficient* of one of the covariates. For example if v

is a real-valued design covariate (e.g. 'temperature'), with value v_i for the *i*th point pattern, then we could assume

$$\lambda_i(u) = \exp(\mu + Z_i v_i) \tag{2}$$

where $Z_i \sim N(0, \sigma^2)$ are independent for different i. This model has a random effect in the dependence on v.

We could also have a random effect for a spatial covariate V. Suppose V_i is a real-valued image for the *i*th pattern (so that $V_i(u)$ is the value of some covariate at the location u for the *i*th case). Then we could assume

$$\lambda_i(u) = \exp(\mu + Z_i V_i(u)) \tag{3}$$

where $Z_i \sim N(0, \sigma^2)$ are independent for different *i*. This kind of random effect would be appropriate if, for example, the images V_i are not 'normalised' or 'standardised' relative to each other (e.g. they are images taken under different illumination). Then the coefficients Z_i effectively include the rescaling necessary to standardise the images.

12.2 Fitting a mixed-effects model

The call to mppm can also include the argument random. This should be a formula (with no left-hand side) describing the structure of random effects.

The formula for random effects must be recognisable to lme. It is typically of the form

$$x_1 + ... + x_n \mid g$$

or

$$x_1 + ... + x_n \mid g_1/.../g_m$$

where $x1 + \ldots + xn$ specifies the covariates for the random effects and g or $g1/\ldots/gm$ determines the grouping (dependence) structure. Here g or $g1, \ldots, gm$ should be factors.

To fit the mixed Poisson model (1) to the waterstriders, we want to have a random intercept coefficient (so x is 1) that varies for different point patterns (so g is id). The reserved name id is a factor referring to the individual point pattern. Thus

```
> H <- hyperframe(P=waterstriders)
> mppm(P ~ 1, H, random=~1/id)

iteration 1
Point process model fitted to 3 point patterns
Call: mppm(P ~ 1, H, random = ~1 | id)
Log trend formula: ~1
Fixed effects:
(Intercept)
   -4.131233
Random effects:
    (Intercept)
1 6.779163e-10
2 -1.826395e-09
3 1.148479e-09
```

Random effects summary:

Random effects:

Formula: ~1 | id

(Intercept) Residual StdDev: 2.84701e-05 1

Variance function:

Structure: fixed weights

Formula: ~invwt

Interaction for all patterns: Poisson process

To fit the mixed effects model (2) to the coculture data with the AstroIm covariate, with a random effect associated with each well,

> mppm(Neurons ~ AstroIm, random=~AstroIm|WellNumber)

13 Studying the fitted model

Fitted models produced by mppm can be examined and validated in many ways.

13.1 Fits for each pattern

13.1.1 Subfits

The command subfits takes an mppm object and extracts, for each individual point pattern, the fitted point process model for that pattern that is implied by the overall fit. It returns a list of objects of class ppm.

```
> H <- hyperframe(W=waterstriders)
> fit <- mppm(W ~ 1, H)
> subfits(fit)
1:
Stationary Poisson process
Intensity: 0.01606306
             Estimate
                           S.E.
                                  CI95.lo
                                            CI95.hi Ztest
                                                                Zval
(Intercept) -4.131233 0.1640366 -4.452739 -3.809727
                                                       *** -25.18482
2:
Stationary Poisson process
Intensity: 0.01606306
             Estimate
                           S.E.
                                  CI95.lo
                                            CI95.hi Ztest
                                                                Zval
(Intercept) -4.131233 0.1616836 -4.448127 -3.814339
                                                       *** -25.55134
Stationary Poisson process
Intensity: 0.01606306
             Estimate
                           S.E.
                                  CI95.lo
                                            CI95.hi Ztest
                                                                Zval
(Intercept) -4.131233 0.1700466 -4.464518 -3.797948
                                                       *** -24.29472
```

In this example the result is a list of three ppm objects representing the implied fits for each of the three point patterns in the waterstriders dataset. Notice that the fitted coefficients are the same in all three models.

Note that there are some unresolved difficulties with the implementation of subfits. Two completely different implementations are supplied in the package; they are called subfits.old and subfits.new. The old version would occasionally crash. Unfortunately the newer version subfits.new is quite memory-hungry and sometimes causes R to hang. We're still working on this problem. So for the time being, subfits is the same as subfits.old. You can change this simply by reassigning, e.g.

```
> subfits <- subfits.new
```

13.1.2 Fitting separately to each pattern

For comparison, we could fit a point process model separately to each point pattern dataset using ppm. The easy way to do this is with with.hyperframe.

To fit a separate uniform Poisson point process to each of the three waterstriders patterns,

```
> H <- hyperframe(W=waterstriders)
> with(H, ppm(W))
1:
Stationary Poisson process
Intensity: 0.01642455
             Estimate
                           S.E.
                                  CI95.lo CI95.hi Ztest
log(lambda) -4.108978 0.1622214 -4.426926 -3.79103
                                                     *** -25.32944
2:
Stationary Poisson process
Intensity: 0.0151169
                           S.E.
                                  CI95.lo CI95.hi Ztest
             Estimate
                                                                Zval
log(lambda) -4.191942 0.1666667 -4.518602 -3.865281
                                                      *** -25.15165
3:
Stationary Poisson process
Intensity: 0.01672117
                                 CI95.lo CI95.hi Ztest
            Estimate
                          S.E.
                                                              7.val
log(lambda) -4.09108 0.1666667 -4.417741 -3.764419
                                                     *** -24.54648
```

The result is again a list of three fitted point process models (objects of class ppm), but now the fitted coefficients are different.

13.2 Residuals

One standard way to check a fitted model is to examine the residuals.

13.2.1 Point process residuals

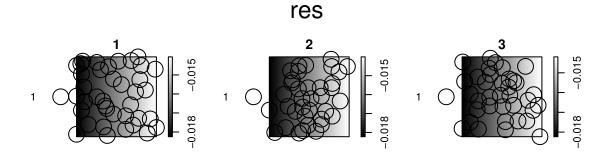
Some recent papers [4, 1] have defined residuals for a fitted point process model (fitted to a *single* point pattern). These residuals are implemented in **spatstat** as **residuals.ppm** and apply to an object of class **ppm**, that is, a model fitted to a *single* point pattern.

The command residuals.mppm computes the point process residuals for an mppm object.

```
> fit <- mppm(P ~ x, hyperframe(P=waterstriders))
> res <- residuals(fit)</pre>
```

The result is a list, with one entry for each of the point pattern datasets. Each list entry contains the point process residuals for the corresponding point pattern dataset. Each entry in the list is a signed measure (object of class "msr") as explained in the help for residuals.ppm). It can be plotted:

> plot(res)

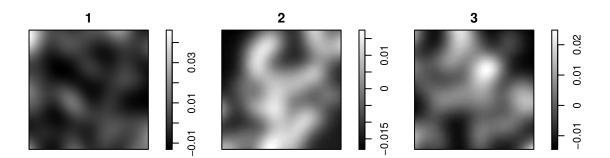


You probably want the smoothed residual field:

```
> smor <- with(hyperframe(res=res), Smooth(res, sigma=4))</pre>
```

> plot(smor)

smor



13.2.2 Sums of residuals

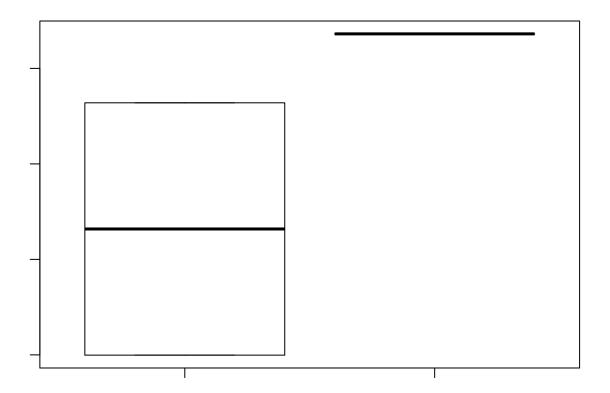
It would be useful to have a residual that is a single value for each point pattern (representing how much that point pattern departs from the model fitted to all the point patterns).

That can be computed by *integrating* the residual measures using the function integral.msr:

```
> fit <- mppm(P ~ x, hyperframe(P=waterstriders))
> res <- residuals(fit)
> totres <- sapply(res, integral.msr)</pre>
```

In designed experiments we can plot these total residuals against the design covariates:

```
> fit <- mppm(Points~Image, data=demohyper)
> resids <- residuals(fit, type="Pearson")
> totres <- sapply(resids, integral.msr)
> areas <- with(demohyper, area.owin(as.owin(Points)))
> df <- as.data.frame(demohyper[, "Group"])
> df$resids <- totres/areas
> plot(resids~Group, df)
```



13.2.3 Four-panel diagnostic plots

Sometimes a more useful tool is the function diagnose.ppm which produces a four-panel diagnostic plot based on the point process residuals. However, it is only available for ppm objects.

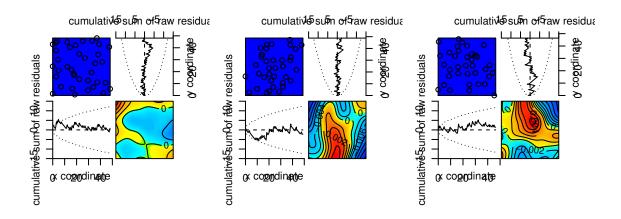
To obtain a four-panel diagnostic plot for each of the point patterns, do the following:

- 1. fit a model to multiple point patterns using mppm.
- 2. extract the individual fits using subfits.
- 3. plot the residuals of the individual fits.

For example:

```
> fit <- mppm(P ~ 1, hyperframe(P=waterstriders))
> sub <- hyperframe(Model=subfits(fit))
> plot(sub, quote(diagnose.ppm(Model)))
```

sub



(One could also do this for models fitted separately to the individual point patterns.)

13.2.4 Residuals of the parameter estimates

We can also compare the parameter estimates obtained by fitting the model simultaneously to all patterns (using mppm) with those obtained by fitting the model separately to each pattern (using ppm).

One could also try deletion residuals, etc.

13.3 Goodness-of-fit tests

13.3.1 Quadrat count test

The χ^2 goodness-of-fit test based on quadrat counts is implemented for objects of class ppm (in quadrat.test.ppm) and also for objects of class mppm (in quadrat.test.mppm).

This is a goodness-of-fit test for a fitted **Poisson** point process model only. The model could be uniform or non-uniform and the intensity might depend on covariates.

```
> H <- hyperframe(X=waterstriders)
> # Poisson with constant intensity for all patterns
> fit1 <- mppm(X~1, H)
> quadrat.test(fit1, nx=2)
        Chi-squared test of fitted Poisson model 'fit1' using quadrat counts
        Pearson X2 statistic
data: fit1
X2 = 2.0691, df = 11, p-value = 0.003524
alternative hypothesis: two.sided
Pooled test
Quadrats of component tests:
List of spatial objects
1:
2 by 2 grid of tiles
2 by 2 grid of tiles
3:
2 by 2 grid of tiles
> # uniform Poisson with different intensity for each pattern
> fit2 <- mppm(X ~ id, H)
> quadrat.test(fit2, nx=2)
        Chi-squared test of fitted Poisson model 'fit2' using quadrat counts
        Pearson X2 statistic
data: fit2
X2 = 1.8596, df = 9, p-value = 0.01301
alternative hypothesis: two.sided
Pooled test
Quadrats of component tests:
List of spatial objects
1:
2 by 2 grid of tiles
2:
2 by 2 grid of tiles
```

3:

2 by 2 grid of tiles

See the help for quadrat.test.ppm and quadrat.test.mppm for further details.

13.3.2 Kolmogorov-Smirnov test

The Kolmogorov-Smirnov test of goodness-of-fit of a Poisson point process model compares the observed and predicted distributions of the values of a spatial covariate.

We want to test the null hypothesis H_0 that the observed point pattern \mathbf{x} is a realisation from the Poisson process with intensity function $\lambda(u)$ (for locations u in the window W). Let Z(u) be a given, real-valued covariate defined at each spatial location u. Under H_0 , the observed values of Z at the data points, $Z(x_i)$ for each $x_i \in \mathbf{x}$, are independent random variables with common probability distribution function

$$F_0(z) = \frac{\int_W \lambda(u) \mathbf{1} \{ Z(u) \le z \} du}{\int_W \lambda(u) du}.$$

We can therefore apply the Kolmogorov-Smirnov test of goodness-of-fit. This compares the empirical cumulative distribution of the observed values $Z(x_i)$ to the predicted c.d.f. F_0 .

The test is implemented as kstest.ppm. The syntax is

> kstest.mppm(model, covariate)

where model is a fitted model (of class "mppm") and covariate is either

- a function(x,y) making it possible to compute the value of the covariate at any location (x,y)
- a pixel image containing the covariate values
- a list of functions, one for each row of the hyperframe of original data
- a list of pixel images, one for each row of the hyperframe of original data
- a hyperframe with one column containing either functions or pixel images.

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