

## Score tests for pairwise interaction parameters of Gibbs point processes

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**Abstract:** Pairwise interaction Gibbs processes with density belonging to a  $m$ -parameter exponential family are frequently used as models for point processes exhibiting inhibition or repulsion between the events. The normalizing constant of the probability density is untractable analytically and many procedures to make inference in these Gibbs processes have been proposed in the literature such as pseudo-likelihood methods, analytical approximations, Markov chain Monte Carlo or perfect sampling methods. In this paper, we propose a score test for the interaction parameters of the Gibbsian exponential family processes that does not requires the calculation of the normalizing constant and whose distribution under the null hypothesis can be simulated providing then an exact Monte Carlo test.

**Key words:** Gibbs point processes; point process; Poisson process; spatial pattern; Strauss process.

## 1 Introduction

Gibbs processes have been frequently used in spatial statistics as models for random point patterns, particularly those showing inhibition between events, or more regularly spread than Poisson processes with the same intensity of events. One of the main attractive aspects of these models is that their probability distribution is characterized by a small number of parameters which have physical interpretation. However, inference about these parameters are complicated due to the presence of a normalizing constant which can not be obtained explicitly even in very simple cases.

Several inference approaches for the parameters of these models have been suggested in the literature such as the Takacs-Fiksel estimating equation method (Takacs, 1986; Fiksel, 1988), the pseudo-likelihood method (Besag, 1977), analytical approximations for the normalizing constant (Ogata and Tanemura, 1981, 1984), maximum likelihood estimation through Markov chain Monte Carlo methods for evaluation of the normalizing constant (Geyer and Møller, 1994).

In this paper, we present a score test for the interaction parameter of pairwise interaction Gibbs processes, a widely used class of models. We show that an exact Monte Carlo test can be obtained without resource to analytical approximation

or MCMC methods. The test is easily implemented in a high-level environment such as R.

## 2 Preliminaries

Let  $W$  be a known, bounded subset of  $d$ -dimensional space  $R^d$ , where  $d \geq 1$ . The data consist of a spatial point pattern  $\varphi = \{\mathbf{x}_1, \dots, \mathbf{x}_n\}$  observed in  $W$ , where  $n \geq 0$  is not fixed and  $\mathbf{x}_i \in W \subset R^d$ . We consider inference conditional on the total number  $n$  of observed events since  $n$  typically will not provide substantial information on the interaction between events.

A particular and widely used class of Gibbs processes are the homogeneous pairwise interaction processes for which the density with respect to the Poisson process with intensity measure 1 is given by

$$f(\varphi; \boldsymbol{\theta}) = C(\boldsymbol{\theta}) \exp \left\{ - \sum_{i < j} \phi(\mathbf{x}_i, \mathbf{x}_j; \boldsymbol{\theta}) \right\}, \quad (2.1)$$

where  $C(\boldsymbol{\theta})$  is the normalizing constant and  $\phi(\cdot)$  a potential function depending on  $\boldsymbol{\theta}$ . It is common to work with an isotropic point process where the potential function depends only on the relative distance between  $\mathbf{x}_i$  and  $\mathbf{x}_j$ :

$$f(\varphi; \boldsymbol{\theta}) = C(\boldsymbol{\theta}) \exp \left\{ - \sum_{i < j} \phi(|\mathbf{x}_i - \mathbf{x}_j|; \boldsymbol{\theta}) \right\}. \quad (2.2)$$

In this paper, we focus on isotropic pairwise interaction Gibbs point process models for which the density belongs to a  $m$ -parameter exponential family:

$$f(\varphi; \boldsymbol{\theta}) = C(\boldsymbol{\theta}) \exp\{-\boldsymbol{\theta}^t \mathbf{T}\} = C(\boldsymbol{\theta}) \exp \left\{ - \sum_{k=1}^m \theta_k T_k(\varphi) \right\}, \quad (2.3)$$

where  $\boldsymbol{\theta}^t = (\theta_1, \dots, \theta_m)$  and  $\mathbf{T}^t = (T_1, \dots, T_m)$  with  $T_k(\varphi) = \sum_{i < j} \phi_k(|\mathbf{x}_i - \mathbf{x}_j|)$  and not involving unknown parameters. We allow  $\theta_k$  to be equal to  $\infty$ , as we explain below.

Several famous models appear as special cases of model (2.3). For example, the Strauss process (Strauss, 1975) with fixed number  $n$  of events can be written as

$$f(\varphi; \theta) = C(\theta) \exp\left\{-\theta \sum_{i < j} I[|\mathbf{x}_i - \mathbf{x}_j| < r]\right\} = C(\theta) \exp\{-\theta T(\varphi)\}, \quad (2.4)$$

where  $I[\cdot]$  is the indicator function,  $r$  is a known constant and  $T(\varphi)$  is the number of unordered pairs of events which lie closer than  $r$  units. In order to have integrable density, we need to impose the additional constraint  $\theta > 0$ . This implies that only patterns showing inhibition or repulsion between events can be

generated by this model. We allow  $\theta = \infty$  implying that the measurable set of configurations with any two events lying closer than  $r$  units has null probability.

The step function pair potential model is a generalization of Strauss process with

$$f(\varphi; \boldsymbol{\theta}) = C(\boldsymbol{\theta}) \exp \left\{ - \sum_{k=1}^m \theta_k \sum_{i < j} I[r_k < |\mathbf{x}_i - \mathbf{x}_j| \leq r_{k+1}] \right\}, \quad (2.5)$$

where the cutpoints  $r_k$  are known with  $r_1 = 0$  and, occasionally,  $r_{m+1} = \infty$ . Hence,  $T_k(\varphi)$  is the number of unordered pairs of events with distance between  $r_k$  and  $r_{k+1}$ .

Another famous model belonging to the exponential family is the soft core model discussed by Ogata and Tanemura (1984). Loosely speaking, their model weights configurations with events close to each other with values increasing smoothly with distance between them rather than having hard thresholds as in (2.4) or (2.5). More specifically, the density is defined as:

$$f(\varphi; \boldsymbol{\theta}) = C(\boldsymbol{\theta}) \exp \left\{ - \sum_{i < j} \left( \frac{\sigma}{|\mathbf{x}_i - \mathbf{x}_j|} \right)^{2/\nu} \right\}, \quad (2.6)$$

where  $0 < \nu < 1$  is known.

Under the null hypothesis  $H_0 : \boldsymbol{\theta} = \mathbf{0}$  the Gibbs process (2.3) is simply a homogeneous Poisson process. Therefore, before undertaking complicated inference procedures to fit Gibbs processes, there is interest in testing if either the observed process is compatible with the simpler homogeneous Poisson process or if there is evidence of interaction between the events.

### 3 A score test for the interaction parameter

These inferential problems with the  $K$  function motivates our proposal described next, a score test for the hypothesis  $H_0 : \boldsymbol{\theta} = \mathbf{0}$ . This score test has two main advantages: since it is based in the likelihood function, it provides a less ad-hoc approach to the problem in hand; it inherits the optimality property of the score test of being the locally most powerful test of  $H_0$ .

A score test can be derived for the Gibbs model (2.3) to test the null hypothesis  $H_0 : \boldsymbol{\theta} = \mathbf{0}$  versus the alternative hypothesis  $H_1 : \boldsymbol{\theta} \neq \mathbf{0}$ , meaning that at least one entry of  $\boldsymbol{\theta}$  is different from zero. It will be useful to denote by  $H_{\boldsymbol{\theta}}$  the simple hypothesis that  $\boldsymbol{\theta}$  is the true parameter vector.

Since we are conditioning in the total number events observed in  $W$ , the log-likelihood function of configuration  $\varphi$  is

$$l(\boldsymbol{\theta}) = \log C(\boldsymbol{\theta}) - \sum_k \theta_k T_k(\varphi).$$

It is clear that

$$\mathbf{T}(\varphi) = (T_1(\varphi), \dots, T_m(\varphi))^t,$$

with  $T_k(\varphi) = \sum_{i < j} \phi_k(|\mathbf{x}_i - \mathbf{x}_j|)$ , is a natural sufficient statistic for the parameter  $\boldsymbol{\theta}$ .

The score statistic is given by

$$\frac{\partial l}{\partial \boldsymbol{\theta}} = \frac{1}{C(\boldsymbol{\theta})} \frac{\partial C(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} - \mathbf{T}(\varphi).$$

We know that  $\mathbf{0} = E_{\boldsymbol{\theta}}(\partial l / \partial \boldsymbol{\theta})$ , which implies that

$$\frac{\partial C(\boldsymbol{\theta})}{\partial \boldsymbol{\theta}} = C(\boldsymbol{\theta}) E_{\boldsymbol{\theta}}(\mathbf{T}(\varphi))$$

and therefore

$$\frac{\partial l}{\partial \boldsymbol{\theta}} \Big|_{\boldsymbol{\theta}=\mathbf{0}} = E_{\mathbf{0}}(\mathbf{T}(\varphi)) - \mathbf{T}(\varphi), \quad (3.1)$$

a contrast between expected under the null hypothesis and the observed value of the sufficient statistic. In the one-dimensional case, large values of (3.1) or, equivalently, small values of  $T(\varphi)$  lead to rejection of  $H_0$ .

Under  $H_0$ , the value  $E_{\mathbf{0}}(\mathbf{T}(\varphi))$  can be easily evaluated by simple Monte Carlo by generating many independent configurations of  $n$  i.i.d. uniform points in the sampling window  $W$  and taking the average of the values of the test statistic. Note that it is trivial to generate uniform variables and we can make the empirical evaluation as accurate as we wish by increasing the number of replications.

Alternatively, explicit analytical functions can be calculated if  $\mathbf{T}(\varphi)$  and the sampling window  $W$  are simple enough. For example, consider the Strauss process (2.4) where

$$T(\varphi) = \sum_{i < j} I[|\mathbf{x}_i - \mathbf{x}_j| < r].$$

Then

$$E_0(T(\varphi)) = \sum_{i < j} P(|\mathbf{x}_i - \mathbf{x}_j| < r) = \frac{n(n-1)}{2} P(B),$$

where  $B$  is the event that two independently and uniformly distributed random points  $\mathbf{x}$  and  $\mathbf{y}$  in the sampling window  $W$  are less than  $r$  units apart. Hence,

$$P(B) = E_{\mathbf{x}}[P(B|\mathbf{x})] = E_{\mathbf{x}}[A(\mathbf{x})],$$

where  $A(\mathbf{x})$  is the proportion of the intersection area between a circle centered at  $\mathbf{x}$  and with radius  $r$  and the sampling window  $W$ . If  $W$  has a simple geometry, this probability can be calculated explicitly. For example, if  $W$  is a square with side  $s$  larger than  $r$ , then

$$P(B) = \frac{r^4}{2} - \frac{8r^3}{3} + r^2\pi,$$

as shown in Taylor *et al.*(2001).

The covariance matrix of the test statistic is associated with the second derivative of the log-likelihood function and the Fisher information  $I(\mathbf{0})$ :

$$\frac{\partial^2 l}{\partial \boldsymbol{\theta} \partial \boldsymbol{\theta}^t} \Big|_{\mathbf{0}} = I(\mathbf{0}) = \mathbf{Var}_{\mathbf{0}} \mathbf{T}(\varphi) .$$

As before, under  $H_0$ , the value  $\mathbf{Var}_{\mathbf{0}} \mathbf{T}(\varphi)$  can be easily evaluated by simple Monte Carlo with any desired precision. Alternatively, analytical calculations can be performed if  $T(\varphi)$  is not too complicated and the sampling window  $W$  has a simple geometry.

Hence, for the local alternative  $H_{\boldsymbol{\theta}}$ , we can use the score test with test statistic  $U$  given by the quadratic form

$$U = (\mathbf{E}_{\mathbf{0}}(\mathbf{T}(\varphi)) - \mathbf{T}(\varphi))^t I^{-1}(\mathbf{0}) (\mathbf{E}_{\mathbf{0}}(\mathbf{T}(\varphi)) - \mathbf{T}(\varphi)), \quad (3.2)$$

which is the locally most powerful test in the sense that it maximizes the power function derivative vector module at  $\boldsymbol{\theta} = \mathbf{0}$  (Cox and Hinkley, 1974, page 113).

To complete the test definition, we need to find the critical region. One alternative is to use a normal approximation to the  $U$  statistic. Another alternative less dependent on asymptotic arguments is an *exact* Monte Carlo test, implemented as follows. Generate a large number  $B$  of independent patterns with  $n$  events under  $H_0$  and indexed by  $b = 2, \dots, B+1$ . Each pattern  $\varphi_b$  is obtained simply by sampling  $n$  points in  $W$  independently and with uniform distribution. For each pattern  $\varphi_b$ , including the observed one indexed as  $b = 1$ , evaluate the sufficient statistics  $T_b = T(\varphi_b)$ .

Assuming that  $\mathbf{E}_{\mathbf{0}}(T(\varphi))$  and  $\mathbf{Var}_{\mathbf{0}} \mathbf{T}(\varphi)$  can be calculated analytically, evaluate the test statistic values  $u_2, \dots, u_{B+1}$  with the simulated patterns as well as the  $u_1$  observed value of the test statistic. Under the null hypothesis, the values  $u_1, \dots, u_{B+1}$  are independently and identically distributed. The value of  $u_1$  based on the observed pattern is ranked amongst the values  $u_2, \dots, u_{B+1}$ . Then, if  $u_1$  ranks  $k$ -th largest or higher, the one-sided *exact*  $p$ -value is  $k/(B+1)$ . In fact, we obtain, under the null hypothesis, a random sample of  $B+1$  observations from the appropriate null distribution of  $U$ , and the rank of the observed statistic must provide an exact significance level for the test.

Monte Carlo tests were introduced by Barnard (1963). A critical region based on the null distribution of  $U$  is different from that based on the exact Monte Carlo test, both with the same significance level. This implies that it is possible to have a value of  $u_1$  declared significant in an exact analytical test but declared non significant in an exact Monte Carlo test, and vice versa. Hope (1968) showed that there is a slight power loss resulting from Monte Carlo tests rather than analytically deriving the critical region with the power differences decreasing to zero as  $B$  goes to infinity. Marriott (1979) investigated this power loss and concludes that, to make the power differences small for a test at the 5% level,  $B = 99$  is adequate while  $B = 499$  should be used if a test at level 1% is desired.

If  $\mathbf{E}_{\mathbf{0}}(T(\varphi))$  and  $\mathbf{Var}_{\mathbf{0}} \mathbf{T}(\varphi)$  can not be calculated analytically, we can use an *additional* set of simulated patterns to calculate both moments with any desired precision under the null hypothesis and plug in these estimates to evaluate

$u_1, \dots, u_{B+1}$ . The fact that we use an additional set of simulations guarantees that  $u_1, \dots, u_{B+1}$  are independent and identically distributed under the null hypothesis. This implies that, if  $u_1$  ranks  $k$ -th largest or higher, the one-sided  $p$ -value  $k/(B+1)$  is still exact.

When  $\mathbf{T}$  is one-dimensional, the test can be based simply on the ranks of the statistic  $T = T(\varphi)$  because, in this case, the test statistic could be defined as

$$U = \frac{E_0(T(\varphi)) - T(\varphi)}{\sqrt{\text{Var}_0(T(\varphi))}} \quad (3.3)$$

and therefore the ranks of  $T$  and  $U$  are in reverse order. Hence, critical regions can be equivalently based on the null hypothesis distribution of  $T$ , obtained by Monte Carlo, rather than that of  $U$ . Therefore, there is no need to calculate the moments of  $T$  under the null hypothesis. This simplification is not possible when the sufficient statistic  $\boldsymbol{\theta}$  has dimension larger than one. In this case, we need to work with the test statistic  $U$  based on the quadratic form (3.2) and there is a need to estimate or calculate analytically the moments  $E_{\mathbf{0}}(T(\varphi))$  and  $\text{Var}_{\mathbf{0}}T(\varphi)$ .

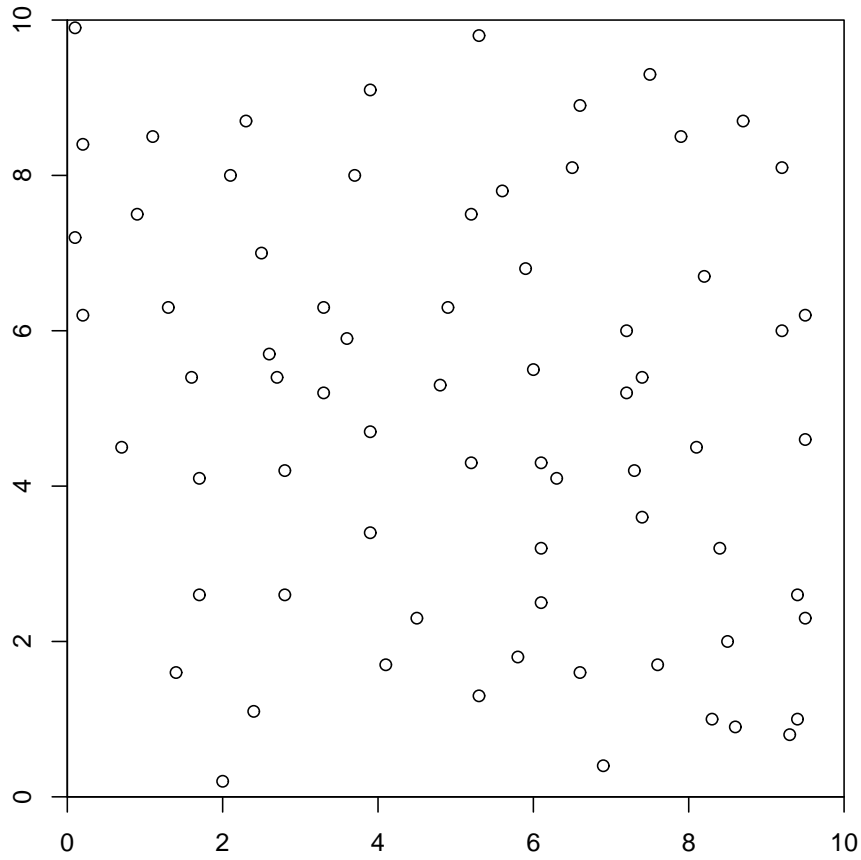
Both, the test statistic and its sampling distribution based on the null hypothesis, are calculated with no edge correction (Ripley, 1988). Thus, the Monte Carlo distribution is the true distribution of  $U$  under the null hypothesis, conditionally on the observed number of events. Therefore, no correction for edge effects is necessary to apply our test.

## 4 Application of the method

Figure 1 shows a dataset with the spatial locations of 71 Swedish pine saplings in a  $10m \times 10m$  square. Ripley (1981) fitted by trial and error a Strauss process with density (2.4) to this dataset, obtaining  $r = 0.7$  and  $\gamma = 0.20$ . Ripley (1998) used the pseudo-likelihood method to estimate  $\theta$  for fixed  $r$ , obtaining  $\theta = 0.15$ . Letting  $r$  fixed at the same value as Ripley's analysis, we tested the hypothesis that the process is a homogeneous Poisson process versus the hypothesis that it is a Strauss process with unknown parameter  $\theta$ .

In this case, we obtained  $t_1 = T(\varphi) = 12$  for the observed number of pairs of events within distance  $r = 0.7$  from each other. Since there is only one parameter, we can find the critical region simply considering the null hypothesis of  $T$  obtained by Monte Carlo simulation. In this case, 999 simulations of 72 independent and identically uniformly distributed events in the square produced values  $t_2, \dots, t_{999}$  with  $t_1$  smaller than all of the simulated values. Hence, the  $p$ -value is  $1/1000$ , a strong evidence to reject the null hypothesis.

Inference on the parameter  $r$  is not simple and the solution has been the adoption of a step function model such as (2.5) where we make the dependence of the model on the definition of a distance threshold less demanding. For the example considered here, we used 5 intervals determined by  $r_1 = 0, r_2 = 0.25, r_3 = 0.5, r_4 = 0.75, r_5 = 1.0$ , and  $r_6 = 1.5$ . Then,  $\boldsymbol{\theta}$  is a vector whose  $k$ -th element is  $\sum_{i < j} I[r_k < |\mathbf{x}_i - \mathbf{x}_j| \leq r_{k+1}]$ , with  $k = 1, \dots, 5$ .



**Figure 1** *Spatial locations of 71 Swedish pine saplings in a 10m × 10m square.*

The observed vector  $\mathbf{T}$  had the counts (1, 8, 8, 24, 111) whereas its null hypothesis expected value, evaluated through 999 Monte Carlo simulations, is (4.87, 14.07, 22.41, 30.52, 82.40) and the standard deviation is (2.16, 3.88, 5.02, 5.79, 10.63). The evaluation of the quadratic form (3.2) in the 999 simulations gave an exact p-value of 0.002 for testing the hypothesis that  $\boldsymbol{\theta} = (\theta_1, \dots, \theta_5) = \mathbf{0}$ .

## 5 A relationship between the $K$ -function and the score test

The most common way to test if an observed point process could have been generated by a homogeneous Poisson point process is to use the  $K$ -function introduced by Ripley (1977) to analyze point patterns. For a stationary point process, it is defined using the conditional expectation given an event at a specified location:

$$K(r) = \lambda^{-1} E(N(B_r) - 1 | N(\mathbf{0}) = 1),$$

where  $\lambda$  is the first-order intensity, and  $N(B_r)$  is the number of events within a circle centered at the origin  $\mathbf{0}$  and with radius  $r$ . Ignoring edge correction, an estimate of  $K(r)$  is

$$\widehat{K}(r) = \frac{2|W|}{n(n-1)} \sum_{i < j} I[|\mathbf{x}_i - \mathbf{x}_j| < r] = \frac{2|W|}{n(n-1)} T_r(\varphi),$$

where  $T_r(\varphi)$  is the sufficient statistic for the parameter  $\theta$  in the Strauss model (2.4) with known  $r$ . Hence, the  $K$ -function is proportional  $T_r(\varphi)$  and tests of  $H_0$  based on  $T_r(\varphi)$  can be seen as equivalent to a test based on the  $K$ -function for a fixed distance  $r$ .

In fact, tests based on the  $K$ -function scan its values in a range of distances  $r$  searching for departures from  $H_0$ . Agreement with  $H_0$  is characterized by the  $K$ -function staying within pointwise 95% confidence intervals. Hence, the scale  $r$  where one finds the most extreme departure of the  $K$ -function can be interpreted then as value of  $r$  where the most extreme standardized score statistic  $T_r(\varphi)$  is observed.

Note that the  $K$ -function test uses a simultaneous procedure. Confidence intervals of confidence level  $1 - \alpha$  are obtained at each distance  $r$  generating a confidence *envelope* of nominal level  $1 - \alpha$  to the  $K$ -function. The upper envelope limit is drawn by connecting the upper intervals' endpoints for a set of  $r$  values. Likewise, the lower envelope limit is obtained by connecting the lower intervals' endpoints. Hence, the  $K$ -function envelope confidence level refers to the pointwise intervals and not the envelope itself. As a consequence, although the nominal error type I probability of the  $K$ -function test is equal to  $\alpha$ , its real error type I is larger and unknown. Usual solutions such as Bonferroni corrections are not feasible because too many correlated tests are involved in the  $K$ -function test. This is unfortunate but this problem has not been solved yet.



## 6 Discussion and conclusion

The score test requires fitting only the simpler model under the null hypothesis  $H_0$  and this is its main advantage of the score test in comparison with the likelihood ratio test. We showed that for the exponential family model (2.3), the evaluation of the score statistic is very simple, irrespective of the normalizing constant complexity in the Gibbs model density. For some regions with simple geometry, we can have an analytical expression for this score test statistic.

In the independent random variables sample context, the score test approaches its asymptotic distribution more slowly than the likelihood ratio statistic and this is its main disadvantage in comparison with the likelihood ratio test. Therefore, significance levels derived from the score statistic and based on its asymptotic distribution can be misleading, particularly in small samples. A necessary further research step is a thorough analysis of the asymptotic behavior of the score test, based on extensive simulations, for the case of a heavily dependent sample represented by densities such as (2.3).

Because of this difficulty with the asymptotic distribution of the score test, we suggest the use of the Monte Carlo approach to obtain the null hypothesis distribution of the test statistic  $U$ . There are several advantages in adopting this approach. First, although the null hypothesis distribution of  $U$  is not known, it can be simulated with no approximation whatsoever. Hence, we can easily generate a very large number  $B$  of independent realizations of  $U$  to obtain its null approximation with any desired level of accuracy. Second, the Monte Carlo test  $p$ -value is exact, whatever the number  $B$  of simulations generated. Finally, simulation under the null hypothesis is so simple for present day computer resources that there is no compelling reason to resort to unnecessarily complicated analytical approximations.

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