# Estimation and Prediction for Stochastic Blockstructures Krzysztof Nowicki and Tom A. B. Snijders, 2001

Andrea Teruzzi, DSBA Bocconi '22

July 4, 2022

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- Introduction and Preview
- Discrete Relational Data
- 3 Stochastic Structures with Randomly Colored Vertices
- 4 Identifiability and Invariant Parameters
- **6** Gibbs Sampling for the Posterior Distribution

• The paper extends the approach of Nowicki and Snijders (1997) to a larger class of relational data.

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#### Set of vertices V

(1)

(2)

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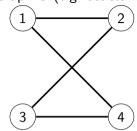
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Set of vertices V

(1)

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Graph G (e.g. assistance)



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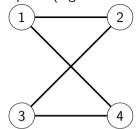
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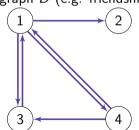
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(4)

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Digraph D (e.g. friendship)



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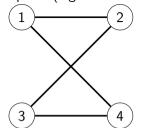
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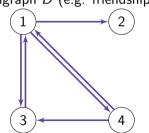
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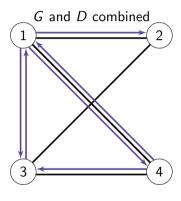
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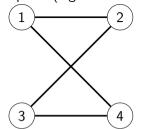
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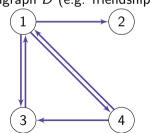
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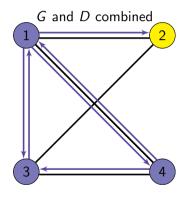
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• Given a set of n vertices labeled  $1, \ldots, n$ , we define the **set of pairs** for which the probability model applies:

$$\mathcal{N} \subset \mathcal{N}_0 = \{(i,j) \in \{1,\ldots,n\}^2 | i \neq j \}$$

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The aims of our probability model is take into account the mutual dependence of relation from i to j and from j to i. We define the **set of dyadic relations**:

$$\alpha^2 = \{\mathsf{a} = (\mathsf{a}_t, \mathsf{a}_v) | \mathsf{a}_t, \mathsf{a}_v \in \alpha\}$$

• We call  $A \subset \alpha^2$  the **alphabet** of pairwise relations. For every  $(i,j) \in \mathcal{N}$  exists  $a = (a_t, a_v) \in A$  describing the dyadic relation of between i and j.

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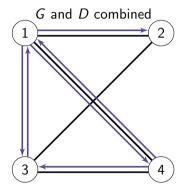
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- We denote  $r = |\mathcal{A}|, r_0 = |\mathcal{A}_0|, r_1 = \frac{1}{2}|\mathcal{A}_1| = |\mathcal{A}_{10}| = |\mathcal{A}_{11}|$

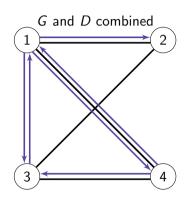
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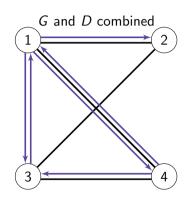


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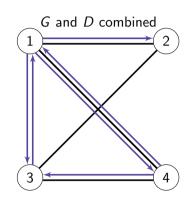
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#### Relational Data: Colored Relational Structure

The second aspect of the structure is a **discrete vertex characteristic**. The set of vertices  $\{1, \ldots, n\}$  is partitioned into c colors  $1, \ldots, c$  and we denote the set of colors  $C = \{1, \ldots, c\}$ .

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#### **Definition**

It is called **colored relational structure** a set  $\mathcal{N}$  of ordered pairs of vertices between which relations are given, with the vertices belonging to c categories stored in the vector  $\mathbf{x} = (x_i)_{i=1}^n$  with  $x_i \in \mathcal{C}$  and with a relational structure where the dyadic relations  $\mathbf{y} = (y_{ij})_{(i,j) \in \mathcal{N}}$  take values in  $\mathcal{A}$ .

We consider a stochastic setting and we denote the random adjacency matrix and the random vector of colors by  $(\mathbf{Y}, \mathbf{X})$ .

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In our particular framework, we will consider  $\mathbf{Y} = \mathbf{y}$  observed, but  $\mathbf{X}$  unknown (posteriori blockmodelling).

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# Stochastic blockmodel: P(X)

The ultimate goal of our analysis is specify a probability model for colored relational structures. In particular we are interested in:

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and the joint distribution of X to be:

$$P(X = x) = \theta_1^{m_1} \dots \theta_c^{m_c}$$
$$m_k = \sum_{i=1}^n I(x_i = k)$$

The vector  $(m_k)_{k\in\mathcal{C}}$  is **sufficient statistic** for the probability law of X.

Given the vector of colors  $\mathbf{X} = \mathbf{x}$ , the random vectors  $\mathbf{Y}_{ij}$  for  $(i,j) \in \mathcal{N}$  with i < j are **independent** with probabilities:

$$P(\mathbf{Y}_{ij} = a | \mathbf{X} = \mathbf{x}) = \eta_a(x_i, x_j)$$
 for  $a \in \mathcal{A}$  and  $x_i, x_j \in \mathcal{C}$ 

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which implies a **redundancy in parameters**  $\eta_a(k, h)$ .

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A non-redundant parameterization is obtained as follows:

$$\begin{cases} \eta_{\mathsf{a}}(k,h) & \text{for } \mathsf{a} \in \mathcal{A} \text{ and } k < h \\ \eta_{\mathsf{a}}(k,k) & \text{for } \mathsf{a} \in \mathcal{A}' \text{ and } k \in \mathcal{C} \end{cases}$$

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The **conditional joint distribution** P(y|x) is given by:

$$P(y|\mathbf{x},\boldsymbol{\theta},\boldsymbol{\eta}) = \left(\prod_{\mathsf{a}\in\mathcal{A}}\prod_{1\leq k< h\leq c}(\eta_{\mathsf{a}}(k,h))^{\mathsf{e}_{\mathsf{a}}(k,h)}\right) \times \left(\prod_{\mathsf{a}\in\mathcal{A}'}\prod_{k=1}^{c}(\eta_{\mathsf{a}}(k,k))^{\mathsf{e}_{\mathsf{a}}(k,k)}\right)$$

where  $e_a(k, h)$  counts the number of relations of type a from vertices of color k to vertices of color h and is a **sufficient statistic**.

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### Stochastic blockmodel

The stochastic blockmodel is then given by the joint distribution of (Y, X):

$$P(\mathbf{y}, \mathbf{x} | \boldsymbol{\theta}, \boldsymbol{\eta}) = P(\mathbf{x}) \times P(\mathbf{y} | \mathbf{x}, \boldsymbol{\theta}, \boldsymbol{\eta})$$

$$= \theta_1^{m_1} \times \dots \times \theta_c^{m_c}$$

$$\times \left( \prod_{\mathbf{a} \in \mathcal{A}} \prod_{1 \le k < h \le c} (\eta_{\mathbf{a}}(k, h)^{e_{\mathbf{a}}(k, h))} \right)$$

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$$\times \left( \prod_{\mathbf{a} \in \mathcal{A}'} \prod_{k=1}^{c} (\eta_{\mathbf{a}}(k, k))^{e_{\mathbf{a}}(k, k)} \right)$$

Because our model consider a stochastic structure (Y, X), with Y observed and X latent variable, the probability of observing edge pattern y is:

$$P(\mathbf{y}|\,oldsymbol{ heta},oldsymbol{\eta}) = \sum_{\mathbf{x} \in \mathcal{C}^n} P(\mathbf{y},\mathbf{x}|\,oldsymbol{ heta},oldsymbol{\eta})$$



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From the stochastic blockmodel:

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#### From the stochastic blockmodel:

• We assume a prior density  $f(\theta, \eta)$  for the parameters  $(\theta, \eta)$ , which we can update using y and inference about the parameters:

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$$P(x|y) = \int f(\boldsymbol{\theta}, \boldsymbol{\eta}, \mathbf{x}|\mathbf{y}) d\boldsymbol{\theta} d\boldsymbol{\eta}$$

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 $\implies$  **Gibbs sampling** is used to obtain the conditional distribution  $f(\theta, \eta, \mathbf{x} | \mathbf{y})$ , which we need to solve both problems.

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- Introduction and Preview
- Discrete Relational Data
- 3 Stochastic Structures with Randomly Colored Vertices
- 4 Identifiability and Invariant Parameters
- Gibbs Sampling for the Posterior Distribution

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### Identifiability

The parameters  $(\theta, \eta)$  in the joint distribution  $f(\theta, \eta, \mathbf{x}, \mathbf{y})$  are not identifiable. What matters is the partition defined by  $\mathbf{x}$ , not the colors labels  $1, \ldots, c$ .

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In particular, let S denote the group of permutation of  $\{1, \ldots, c\}$  and define  $h_s(\cdot)$  and  $s(\cdot)$  such that:

$$P(\mathbf{Y} = \mathbf{y} | \boldsymbol{\theta}, \boldsymbol{\eta}) = P(\mathbf{Y} = \mathbf{y} | h_s(\boldsymbol{\theta}, \boldsymbol{\eta}))$$
  
 $s(\mathbf{x}) = (s(x_1), \dots, s(x_n))$ 

for every permutation  $s \in \mathcal{S}$ .



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for every permutation  $s \in S$ . The transformation preserves the partition of the vertices and it implies:

$$P(\mathbf{x}|\mathbf{y}, \boldsymbol{\theta}, \boldsymbol{\eta}) = P(s(\mathbf{x})|\mathbf{y}, h_s(\boldsymbol{\theta}, \boldsymbol{\eta}))$$

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$$P(X_i = k | \mathbf{y}) = 1/c$$

independently from k.



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independently from k. We can deal with the invariance problem in some ways:

• Put restrictions on the parameters

e.g. 
$$\theta_1 < \theta_2 \cdots < \theta_c$$

However this approach is not always applicable and it may require some prior information (informative prior).



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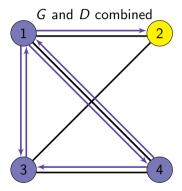
which are invariant w.r.t. the transformations  $h_s(\theta, \eta)$  and  $s(\mathbf{X})$ .

We can apply the expectation to these functions and find the following matrix and the three-way array:

$$\left(P(X_i = X_j | \mathbf{y})\right)_{1 \le i \ne j \le n}$$
 
$$\left(\mathbb{E}(\eta_{\mathsf{a}}(X_i, X_j) | \mathbf{y})_{1 \le i \ne j \le n, \, \mathsf{a} \in \mathcal{A}'}\right)$$



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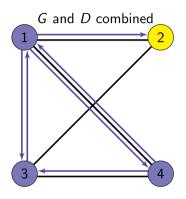




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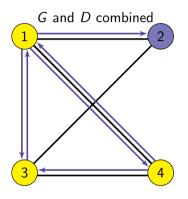
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$$I\{X_i=X_j\}$$

$X_i$	1	2	3	4
1	1	0	1	1
2	0	1	0	0
3	1	0	1	1
4	1	0	1	-



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#### Definition

**Gibbs Sampling** is a simulation method used to approximate a target posterior distribution. It is an iterative simulation scheme that, given a set of unknown random vectors, consists in drawing each random vector from its probability law conditioned on the values of all of the other random vectors.

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We apply this scheme to  $((\theta, \eta), X_1, X_2, \dots, X_n)$ . At each iteration, given the current values  $(\theta^{(p)}, \eta^{(p)}, \mathbf{X}^{(p)})$ :

**1** Draw  $(\theta^{(p+1)}, \eta^{(p+1)})$  from  $f(\theta, \eta | \mathbf{X}^{(p)}, \mathbf{y})$ 



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- ② For each  $i=1,\ldots,n$ : draw  $X_i^{(p+1)}$  from  $f(X_i|m{ heta}^{(p+1)},m{\eta}^{(p+1)},(X_j^{(p+1)})_{j< i},(X_k^{(p)})_{k>j})$

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We are left to specify the full conditional distribution for these two steps.

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  - For k < h,  $\eta(k,h) = (\eta_a(k,h))_{a \in \mathcal{A}}$  is an unconstrained probability vector of dimension  $r = |\mathcal{A}|$ .

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▶ For k = k,  $\eta(k, k)$  is constrained to  $\eta_{\mathsf{a}}(k, k) = \eta_{\pi(\mathsf{a})}(k, k)$ .



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transforming  $\eta(k, k)$  in a  $(r_0 + r_1)$ -dimensional (note  $r_0 + r_1 < r$ ) vectors without redundant elements for every  $k \in C$ .

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The posterior distribution of  $(\theta, \eta)$  given (y, x) is is largely tractable:

$$(m_k + T_k)_{k \in \mathcal{C}}$$
 for  $\boldsymbol{\theta}$   $(e_a(k,h) + E_a(k,h))_{a \in \mathcal{A}}$  for  $\boldsymbol{\eta}(k,h), \ 1 \leq k < h \leq c$   $(e_a(k,k) + E_a(k,k))_{a \in \mathcal{A}'}$  for  $\boldsymbol{\eta}^{(0)}(k,k), \ 1 \leq k \leq c$ 

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We can approximate  $\eta_a(X_i, X_j)$  using the average of  $\eta_a^{(p)}(X_i, X_j)$  drawn from the Gibbs sampler.

# Step 2: $f(X_i|\boldsymbol{\theta},\boldsymbol{\eta},\mathbf{x}_{-i})$

From the probability law of the stochastic block-model  $P(\mathbf{y}, \mathbf{x} | \boldsymbol{\theta}, \boldsymbol{\eta})$  we can derive:

$$P(X_i = k | \mathbf{y}, \boldsymbol{\theta}, \boldsymbol{\eta}, \{X_j\}_{j \neq i}) = Q\theta_k \prod_{\mathsf{a} \in \mathcal{A}} \prod_{h=1}^{\mathsf{c}} (\boldsymbol{\eta}_{\mathsf{a}}(k, h))^{d_{\mathsf{a}}(i, h)}$$

with  $d_a(i, k) = \sum_{j:(i,j) \in \mathcal{N}} I\{y_{ij} = a\}I\{x_j = k\}$  counting number of dyadic relations of type a from vertex i to vertices of color k and with Q a constant not depending on k.

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The relative frequency of  $X_i^{(p)} = X_j^{(p)}$  over the Gibbs sampler can be used to approximate the matrix of posterior predictive probabilities  $(P(X_i = X_j | \mathbf{y}))_{1 \le i \ne j \le n}$ 

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#### Adequacy of class structure

We can build some parameters for evaluating the adequacy of the obtained class structure:

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•  $I_y$  is the information of the observed relations with  $c \ge 2$ :

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This value is small when  $\eta$  and **X** determine to a large extent of the observed relations.

 H<sub>x</sub> measures the extent to which the distribution of X defines one clear-cut partition of vertices into classes.

$$H_{\times} = \frac{4}{n(n-1)} \sum_{i,j=1}^{n} \pi_{ij} (1 - \pi_{ij})$$

with  $\pi_{ij} = P(X_i = X_j | \mathbf{y})$ . If  $H_x$  is small it relatively clear if pair of vertices are in the same class or not.

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# Example – Adequacy parameters

С	ly	H <sub>x</sub>
2	.94	.24
3	.91	.21
4	.89	.26
5	.89	.24 .21 .26 .27

Figure 1: Parameter for the class structure for Kapferer's dataset

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To check to convergence of the Gibbs sampler:

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To check to convergence of the Gibbs sampler:

• Run multiple Gibbs sampler with different independent starting points and check that parameters  $H_x$  and  $I_y$  have similar values.

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#### Assign vertices to classes:

• For uniform prior, arbitrarily assign labels.

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To check to convergence of the Gibbs sampler:

- Run multiple Gibbs sampler with different independent starting points and check that parameters  $H_x$  and  $I_y$  have similar values.
- For invariant prior, check that the posterior predictive distribution of the sequence  $\mathbf{X}^{(p)}$  is uniform.

#### Assign vertices to classes:

- For uniform prior, arbitrarily assign labels.
- For nonuniform prior, labels are identified by the prior.

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#### Example – Estimated posterior probabilities I

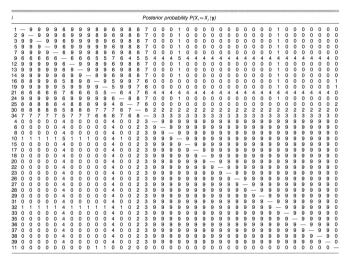


Figure 2: Estimated posterior probabilities  $P(X_i = X_i | \mathbf{y})$  for Kapferer's dataset

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### Example – Estimated posterior probabilities I

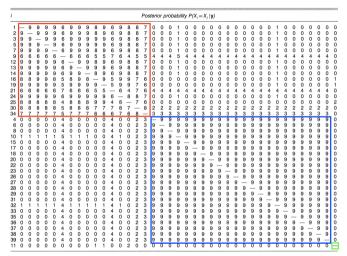


Figure 2: Estimated posterior probabilities  $P(X_i = X_i | \mathbf{y})$  for Kapferer's dataset

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# Example – Estimated posterior probabilities II

a     h $k=1$ $k=2$ $(0,0)$ 1     .27     .72 $(0,0)$ 2     .72     .78       3     .14     .31       1     .38     .19       .15     .15     .22       1     .03     .01 $(F,F)$ 2     .01     .01       3     .07     .04       1     .16     .03       .07     .04       (AF,AF)     2     .03     .05       3     .42     .07       (0,F)     2     .03     .00       3     .04     .03       1     .01     .00       3     .04     .03       1     .07     .01					
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	k = 3	k= 2	k= 1	h	а
(A, A)     2     .19     .15       3     .15     .22       1     .03     .01       (F,F)     2     .01     .01       3     .07     .04       1     .16     .03       (AF,AF)     2     .03     .05       3     .42     .07       1     .01     .00       (0,F)     2     .03     .00       3     .04     .03	.14 .31	.78	.72	1 2 3	(0,0)
$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	.15 .22	.15	.19	2	(A, A)
(AF, AF)     2     .03     .05       3     .42     .07       1     .01     .00       (0,F)     2     .03     .00       3     .04     .03	.07 .04	.01	.01	2	(F,F)
(0,F) 2 .03 .00 3 .04 .03	.42 .07	.05	.03		(AF, AF)
1 07 01	.05 .27	.00	.03	1 2 3	(0, <i>F</i> )
(A, AF) 2 .02 .00 3 .05 .03	.08 .04			1 2 3	(A, AF)

Figure 3: Estimated posterior probabilities  $\eta_a(X_i, X_i)$  for Kapferer's dataset

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