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“Statistical Independence” versus “Logical Indetermination”, two ways of generating clustering criteria through couplings : Application to graphs modularization

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Abstract This paper aims at comparing two coupling approaches as basic layers for building clustering criteria, suited for modularizing very large graphs. Although the scientific literature is not sparing with clustering criteria dedicated to graphs and networks decomposition, we shall nevertheless rework this subject, in this paper, by proposing a new symmetric and dual approach based on coupling functions, allowing to compare and calibrate them. To elaborate those coupling maps, we will briefly use “optimal transport theory” as a starting point, then we will derive two main families of criteria: those based upon “statistical independence” versus those based upon “logical indetermination”. Among others, we will use the so called “Monge’s properties”, applied to contingency matrices context, as specific tricks for putting forward some key features about those criteria. A further and deeper study is proposed, highlighting “logical indetermination”, because it is, by far, lesser known. Those dual and parallel criteria are perfectly suited for graphs clustering, this will be illustrated and shown on various types of graphs within this paper.

Keywords Correlation Clustering · Mathematical Relational Analysis · Logical Indetermination · Coupling Functions · Optimal Transport · Graph Theoretical Approaches

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1 Introduction

As mentioned in the abstract, this paper introduces two coupling approaches as basic layers for building clustering criteria, suited for modularizing very large graphs.

Graph clustering (or cliques partitioning of graphs) is a key topic, concerned with a very large dedicated literature. One of the reasons of this status is the recent and power use made by the GAFAM companies about very large graphs resulting of modern activities dealing with: *big social networks, cellphone communications networks, high speed financial trading, large IT networks, IOT networks etc.*, This is simultaneously associated with the IT capacity afforded today to store the really huge amounts of data, those activities force us to cope with. The sudden apparition of these big networks gave rise to a renewal of the so-called *graph theoretical domain*, used in that context for different purposes, such as: discovering the latent cliques, clustering the whole graph, isolating some key parts of interest within the network, etc. In other words, this massive and raw information contained inside the networks must be analyzed *per se*, and this leads obviously to mandatory techniques, among which graphs clustering plays a prominent role, with a lot of practical contextual applications.

At that stage two aspects must be differentiated : on the one hand (i) the existence of generic algorithms dealing with various *clustering criteria* as global objective functions, which can be changed according to the context, we want to address, or, on the other hand (ii), on the graph clustering criteria themselves, as soon as we must choose some of them as global objective functions, during the network analysis step. Both those points will be discussed throughout this article, although we shall theoretically insist essentially on the second point (ii).

Going back on the first point, (i) concerned with *generic algorithms*, it is well known that several methods were introduced to fit this purpose and notably the famous *Louvain's algorithm*, whose origin is quite recent [4], and which is recognized as a very *good tool* by the scientific community. It is based upon the optimization, (through some ad-hoc heuristics), of a global function called *modularity*, (we shall discuss this notion later on). In few words let us say that the global optimization is obtained iteratively by optimizing a local cost function: where two vertices are said to be *similar* if they are connected according to a weight which sufficiently differs from the mean weight of their neighborhood. The cost function, as we will see later, is built on the departure from the usual *independence coupling* function. The method has been naturally generalized in [6] where the authors proposed to choose a *candidate criterion* among a list of global criteria, different from the usual *modularity*. In her thesis [7], Patricia Conde-Cespedes, proposed some experiments on usual graphs, involving our criteria plus some others, showing that results may vary from one criterion to another, while being still consistent and interpretable. The process she has performed is exactly the fusion of (i)-(ii) in the same design. This, as already mentioned beforehand, is obtained by using the same

algorithmic process (in that case the generic Louvain’s one) applied with different *clustering criteria*. It is interesting to notice that the resulting numbers of classes (which is not fixed in advance by the method on the contrary of the k-means approach) were coherent and comparable from one criterion to another for most of the studied graphs.

To fulfill our (ii) objective, we will focus, in this paper, on two graph clustering criteria, the first one, quite classic and largely used, is called: *modularity* (\mathcal{M}^\times) (a kind of measure of the *deviation from statistical independence*), while the second (\mathcal{M}^+) is locally based on a deviation to another coupling function, already latent in a paper of Fréchet [9] and that we shall call *indetermination* or *logical indetermination* (notion introduced by J.F. Marcotorchino in his seminal papers [14] and [17]). Here we propose a theoretical approach to understand the behavior of both those criteria. The function (\mathcal{M}^+) has been already tested by Patricia Conde-Cespedes in her thesis [7] on peculiar graphs. We shall replicate, here, the experimental results she got, but we want both reanalyze more systematically the behavior of those criteria on the very simple model of Erdős-Renyi’s random graphs and bring much more solid bases to the theoretical interpretation of these chosen criteria (\mathcal{M}^\times) and (\mathcal{M}^+).

To express similarities between them, we will conduct a deep analysis of the two underlying coupling functions: the well-known *independence* (usually quoted with a \otimes) and the more recent *indetermination* (quoted with a \oplus) that we shall introduce later on.

The paper is structured as follows. In section 2 we propose a parallel discovery of two coupling functions (\otimes) and (\oplus) using discrete *optimal transport theory*. In section 3 is mentioned a list of dual properties related to Monge’s matrices. Section 4 deeply studies *indetermination* introducing properties that, to our knowledge, deserve to be put forward with regards to the too poor coverage which is devoted to them in the literature. Finally, Section 5 gathers a study about the behavior of the criteria based on those coupling functions on the general Erdős-Renyi’s random graph model, quoting similarities and differences through specific graphs.

2 Parallel discovery of two dual couplings

When we want to couple two marginal laws, the most common and straightforward way to proceed, consists in assuming *independence* and keep on computations. It is so well integrated in our mindset, that it appears naturally in real life applications, as soon as we want to build fast models up. In our scientific work, the approach is quite the same: when we use a very classical and usual criterion like the χ^2 index, we are measuring nothing but a deviation to *independence*.

Thinking about how we first introduced *independence*, we immediately suggest empiric experiences: let us say if we play a dice twice, how should we derive the resulting probabilities from a unique dice? Most of us will naturally apply *independence* coupling: it relies on empirical experiments.

Although being the most natural, it is not, by far, the only existing available coupling method; actually, as introduced by Sklar in [23], any copula function will lead to a coupling function behaving on two cumulative distribution functions. In this document, we link a coupling function to a given optimal transport problem. Hence, to follow a similar approach for *indetermination* coupling, we train ourselves first by extracting *independence* coupling from the optimization of a transport problem and we generalize the principle by applying the same approach to the *indetermination* case, but with a second and different transport problem.

We already introduced the term "coupling function" several times but let us define it formally, since it will be a key notion throughout the document.

Definition 1 (Coupling function)

Given $\mu = \mu_1 \dots \mu_p$ and $\nu = \nu_1 \dots \nu_q$ two discrete probabilities called marginal distributions (or simply margins), we want to define a probability function $\pi = \pi_{u,v} \{1 \leq u \leq p, 1 \leq v \leq q\}$ on the product space. A way for building it up, consists in making happen a coupling function C such that $\pi = C(\mu, \nu)$, satisfying the following constraints:

- (first margin) $C(\mu, \nu)_{u,\cdot} = \sum_{v=1}^q C(\mu, \nu)_{u,v} = \mu_u, \forall 1 \leq u \leq p$
- (second margin) $C(\mu, \nu)_{\cdot,v} = \sum_{u=1}^p C(\mu, \nu)_{u,v} = \nu_v, \forall 1 \leq v \leq q$
- (positivity) $C(\mu, \nu)_{u,v} \geq 0, \forall 1 \leq u \leq p, \forall 1 \leq v \leq q$

Remark 1

All coupling functions (or maps) we use will satisfy: $\pi_{u,v} = C(\mu, \nu)_{u,v} = C(\mu_u, \nu_v)$; this illustrates that π value on (u, v) only depends upon the value on the corresponding margins: μ_u and ν_v .

2.1 Some few words about Optimal Transport

Looking at Definition 1, we observe that a coupling function behaves as a copula in the discrete domain: acting on margins it derives a probability distribution on the product space.

We can imagine a lot of coupling functions, especially if we do not limit ourselves to Remark 1. The constraints that C has to respect, lead us to cope with some difficulties. This is the reason why we shall choose a systematic approach: minimizing a cost function and observe the link to *optimal transport* definition.

The ad-hoc discrete optimal transport problem we will be dealing with, typically looks like Problem 2, given hereafter (where MKP stands for Monge-Kantorovitch-Problem).

Before to introduce Problem 2 in detail, let us go back to the historical problem (here quoted Problem 1). It is, in fact, the merit of the French Mathematician Gaspard Monge to have been the first to address, in 1781, the problem, known as Problem of "*Remblais et déblais*". This problem can be simply turned as follows: what is the most efficient way (in terms of work

or minimization effort) to move a pile of sand to fill up an excavation of the same volume? This constraint of *volume incompressibility* makes the problem difficult.

Problem 1 (Original Monge Problem)

$$\min_{\mathcal{T}} \int_{\mathcal{X}} \mathbf{C}(x, \mathcal{T}(x)) dx$$

Using modern notations, a "sand pile" is represented by a probability measure $\mu \in \mathbb{P}(\mathcal{X})$ and a "hole to fill up" by a probability measure $\nu \in \mathbb{P}(\mathcal{Y})$. Those probability measures correspond to the margins of Definition 1. They are still in a continuous space, as we follow historical introduction, but we will come back later on to a discrete space. *A priori* holes have the same volumes as sand piles do, this implies:

$$0 < \mu(\mathcal{X}) = \nu(\mathcal{Y}) = 1$$

Let us also give a continuous transportation cost function $\mathbf{C} : \mathcal{X} \times \mathcal{Y} \rightarrow \mathbb{R}^+$.

A solution to this Problem 1 (if any) is called an optimal transport map or a Monge's solution. Let us remark that transport maps from μ to ν may not exist; for instance, this is the case if μ is a Dirac δ_a at point a whereas ν is not. But on a more general standpoint, one should also remark that the Monge's formulation is quite rigid in the sense that it requires that the whole mass of x in X should be assigned to the same target $\mathcal{T}(x)$ (no split is permitted). According to the difficulties of the Monge's problem, as commonly met in hard problem solving, the solution resides in the extension or relaxation of the research domain itself. It is exactly what happened to Monge's problem: in 1942, Leonid Kantorovich (Nobel Prize of Economy 1975) proposed a relaxed formulation of the Monge's problem that allows mass splitting; a discrete version of Problem 2 is presented below:

Problem 2 (Discrete Version of MKP)

$$\begin{aligned} & \min_{\pi} \sum_{u=1}^p \sum_{v=1}^q \mathbf{C}(\pi(u, v)) \pi(u, v) \\ & \text{subject to:} \\ & \sum_{v=1}^q \pi(u, v) = \mu_u; \forall u \in \{1, \dots, p\} \\ & \sum_{u=1}^p \pi(u, v) = \nu_v; \forall v \in \{1, \dots, q\} \\ & \pi(u, v) \geq 0; \forall (u, v) \in \{1, \dots, p\} \times \{1, \dots, q\} \end{aligned}$$

The choice of a cost function \mathbf{C} depends upon the applications we want to address. For instance, we can force the result π to concentrate as little information as possible, this means, we shall force it to be as close as possible

to the uniform law, referring to the product space (remember it has to verify the given margins). Other choice: we can, as well, minimize the entropy of π . Both those cases are usual approaches, introduced in some articles. They expect the global assignment to be as smooth as possible.

A MKP problem is essentially given by its cost function, while margins (μ, ν) may vary. This is the reason why we shall try to solve it with a model taking the fixed margins as parameters. Let us define now an optimal coupling function C associated to a given MKP problem with fixed margins given as parameters.

Definition 2 (MKP Problem Associated with Coupling function)

For a given MKP problem P , we can define a coupling function C^P by: $C^P(\mu, \nu) = \pi^*(P)$ provided that π^* exists as a unique solution of P with margins μ and ν .

Following Definition 2 we propose the solutions of two discrete optimal transport problems that we shall use in section 5: each implies a structured and well-defined criterion, suitable for graph clustering.

2.2 The Alan Wilson's Entropy Model: role of "independence"

First introduced by Sir Alan Wilson in 1969 for "Spatial Interaction Modeling" the "Flows Entropy Model" of Alan Wilson, can be found in his various publications: originated in [26], developed in [27], and refined in his book [28]. A fundamental justification of his approach corresponds to the following contextual situation: in a theoretical system, elements of which do not maintain affinities, it is advisable to determine the distribution of $\pi(u, v)$ (normalized frequency flows), supposing $\pi \geq 0$ which maximizes the entropy of the system under certain constraints. The objective function to be minimized is based upon the *Boltzmann's or Shannon's Entropies* so that the problem should be expressed as follows:

Problem 3 (Unbalanced PSIS)

$$\min_{\pi} - \sum_{u=1}^p \sum_{v=1}^q \pi(u, v) \ln(u, v)$$

In a situation where we have a total absence of information, the minimization of Problem 3 just amounts to satisfy the constraint that the cell values distribution is effectively a probability (i.e.: the sum of positive $\pi(u, v)$ is equal to 1 (summing up a joint probability distribution). The solution of this very simple "Program of Spatial Interaction System" (PSIS) can be expressed as follows.

$$\pi^*(u, v) = \frac{1}{pq} \tag{1}$$

In other words, when we ignore everything about the way the exchanges are built up, it is necessary to use Laplace's principle of "insufficient reason" and to consider that the world trade is uniformly distributed inside the system.

By using margins, let us say information about total exports (origins flows) and total imports (destination flows), degree of disorder of the system can be drastically reduced. Indeed, totals on rows and columns are no longer free, but must satisfy marginal values μ_u and ν_v , fixed by the application as expressed in Problem 4; solution of which is given by theorem 1.

Problem 4 (Balanced PSIS)

$$\min_{\pi} - \sum_{u=1}^p \sum_{v=1}^q \pi(u, v) \ln(\pi(u, v))$$

subject to:

$$\sum_{v=1}^q \pi(u, v) = \mu_u, \quad \forall 1 \leq u \leq p$$

$$\sum_{u=1}^p \pi(u, v) = \nu_v, \quad \forall 1 \leq v \leq q$$

$$0 \leq \pi_{u,v} \leq 1, \quad \forall 1 \leq u, v \leq q$$

Theorem 1

The solution of Problem 4 is $\pi^\times(u, v) = \mu_u \nu_v$.

Hence the coupling function associated to Problem 4 is nothing but "independence":

$$C^{Problem\ 4}(\mu, \nu)_{u,v} = C^\times(\mu, \nu)_{u,v} = (\mu \otimes \nu)_{u,v} = \mu_u \nu_v$$

We skip the proof of theorem 1 as it is similar to the one we will develop for theorem 2 which is less common.

As a conclusion, from the direct maximization of entropy, we get the solution expressed in terms of probability and remark that the associated coupling function is nothing but "independence" (expressed with a \otimes throughout the document). We also note that the degree of disorder is not total: flows possess an intensity which is proportional to the weights of the partners in the world trade exchanges matrix in case of an economic application.

2.3 The minimal trade model: role of "indetermination"

In the "Minimal Trade Model" (see [25], [14] and [17]), we still impose the objective function to respect the balanced marginal distributions and mass preserving constraints but we change its structure for getting a smoother breakdown of the origins-destinations n_{uv} values than in the Alan Wilson's entropy model (this explains the term "Minimal Trade"). We still suppose

$\pi(u, v) = \frac{n_{u,v}}{n_{..}}$, for any real application. In that case the criterion is a quadratic function measuring squared deviation of the cells values from the "no information" situation (the uniform joint distribution law related to Problem 3). As expected, in case of free margins, the solution remains the uniform law. Though, adding usual pre-conditioned constraints on margins, the least squared problem is Problem 5; solution of which is given by theorem 2.

Problem 5 (Minimal Trade Model)

$$\min_{\pi} \sum_{u,v} \left\{ \pi(u, v) - \frac{1}{pq} \right\}^2$$

subject to:

$$\begin{aligned} \sum_{v=1}^q \pi(u, v) &= \mu_u, \quad \forall 1 \leq u \leq p \\ \sum_{u=1}^p \pi(u, v) &= \nu_v, \quad \forall 1 \leq v \leq q \\ 0 &\leq \pi_{u,v} \leq 1, \quad \forall 1 \leq u, v \leq q \end{aligned}$$

Theorem 2

The solution of Problem 5 is $\pi^+(u, v) = \frac{\mu_u}{q} + \frac{\nu_v}{p} - \frac{1}{pq}$.

Hence the coupling function associated to Problem 5 is nothing but "indetermination":

$$C^{Problem\ 5}(\mu, \nu)_{u,v} = C^+(\mu, \nu)_{u,v} = (\mu \oplus \nu)_{u,v} = \frac{\mu_u}{q} + \frac{\nu_v}{p} - \frac{1}{pq}$$

A supplementary condition, which is exogenous with regard to the previous model, can be added on the margins (which are, by the way, constant values given *a priori*), this condition (see [14]) is a simple inequality which guarantees the positivity of the frequency Matrix $\pi^*(u, v)$ we are looking for:

$$p \min_u \mu_u + q \min_v \nu_v \geq 1 \quad (2)$$

From now on, we shall consider that Condition 2 applies whatever the breakdown of the μ_u and ν_v is. Furthermore since the Matrix $\pi(u, v)$ represents "frequencies", the last constraint of Problem 5 is playing a role of supplementary endogenous constraint, ensuring: $\pi(u, v) \leq 1$. Notice that in the "Adjustment to Fixed Margins for Contingency Table" case, the associated values n_{uv} must be integers, and therefore returns the problem much more complex to solve, relaxation of this integrity constraint leads formally to the Problem 5.

Remark 2 (Vanishing bias)

By developing the cost function, we obtain an interesting equality we will reuse

later on:

$$\sum_{u,v} \left(\pi(u,v) - \frac{1}{pq} \right)^2 = \sum_{u,v} \pi^2(u,v) - \frac{1}{pq} \quad (3)$$

so that the influence of the constant shift $\frac{1}{pq}$ in the squared model is disappearing.

Proof

The proof we propose directly comes from [25] and [17]. A generalization of the canonic additive form when we relax hypothesis 2 can be found in the thesis to come [3].

Using equality 3, the Lagrangian function associated to the previous minimization model can be turned into

$$\begin{aligned} \mathbf{L}(\pi, \lambda, \omega, \theta) &= \sum_{u=1}^p \sum_{v=1}^q \pi^2(u,v) \\ &\quad - \sum_{u=1}^p \lambda_u \left(\mu_u - \sum_{v=1}^q \pi(u,v) \right) \\ &\quad - \sum_{v=1}^q \omega_v \left(\nu_v - \sum_{u=1}^p \pi(u,v) \right) \\ &\quad - \theta \left(\sum_{u=1}^p \sum_{v=1}^q \pi(u,v) - 1 \right) \end{aligned}$$

Since the function to optimize is a convex one, the solution we are looking for is a minimum so that first order conditions apply and we have the following system of equations.

$$\frac{\partial \mathbf{L}(\pi, \lambda, \omega, \theta)}{\partial \pi(u,v)} = 2\pi(u,v) - \lambda_u - \omega_v - \theta = 0 \quad (4)$$

$$\frac{\partial \mathbf{L}(\pi, \lambda, \omega, \theta)}{\partial \lambda_u} = \mu_u - \sum_{v=1}^q \pi(u,v) = 0 \quad (5)$$

$$\frac{\partial \mathbf{L}(\pi, \lambda, \omega, \theta)}{\partial \omega_v} = \nu_v - \sum_{u=1}^p \pi(u,v) = 0 \quad (6)$$

When supposing $\sum_v \omega_v = 0$ as Lagrange multipliers are defined within a constant near we sum 4 on v to obtain $2\mu_u = 2 \sum_v \pi(u,v) = q\lambda_u + q\theta$ so that

$$\lambda_u + \theta = \frac{2\mu_u}{q}, \forall u \quad (7)$$

From 6 we get $2\nu_v = \sum_{u=1}^p 2\pi(u,v) = 4 \sum_{u=1}^p \lambda_u + \omega_v + \theta = 7 \sum_{u=1}^p \frac{2}{q}\mu_u + \omega_v = \frac{2}{q}\mu_u + p\omega_v$ so that

$$\omega_v = \frac{2\nu_v}{p} - \frac{2}{pq}, \forall v \quad (8)$$

Replacing into 4 $\lambda_u + \theta$ and ω_v by their value given respectively by 7 and 8 we obtain:

$$\pi^*(u, v) = \frac{\mu_u}{q} + \frac{\nu_v}{p} - \frac{1}{pq}, \forall (u, v)$$

Remark, since Condition 2 applies, the π^* expressed in the previous equation are nonnegative. We will go back to this expression, in the next sections and develop a deeper focus on it, explaining the true meaning of the term "indetermination" and some other consequences.

Remark 3 (Sum of uniform shift)

We notice that $\pi_{u,v} = \frac{\mu_u}{q} + \frac{\nu_v}{p} - \frac{1}{pq}$ can be expressed as $\pi_{u,v} - \frac{1}{pq} = \frac{1}{q} \left(\mu_u - \frac{1}{p} \right) + \frac{1}{p} \left(\nu_v - \frac{1}{q} \right)$ so that indetermination basically sums up the distances to uniformity for each margin.

2.4 Expected difference between coupling

Both coupling functions are extracted from an optimal transport problem concentrating values around the uniform. Hence differences between them should be small in a certain sense. We provide in this section a measure of their proximity. We evaluate the expected value of a norm between the two couplings under uniform laws. More precisely we suppose the two margins μ and ν follow the Dirichlet's law (basically the uniformity on probability distributions). We remind here the form of that law for our application.

Definition 3 (Dirichlet's Law)

The density of a Dirichlet law \mathcal{D}_p representing a uniform law among probability law on p elements is expressed as follows:

$$f(\mu_1, \dots, \mu_p) \prod_{k=1}^p d\mu_k = \frac{1}{B(p)} \prod_{k=1}^p \mu_k^0 \prod_{k=1}^p d\mu_k = \frac{1}{B(p)} \prod_{k=1}^p d\mu_k$$

where B is the multinomial Beta function.

Having expressed a density function for μ and ν (replace p by q), we apply them two coupling functions C^+ and C^\times . As a distance, we define:

$$\Delta_p = \mathbb{E}_{(\mu, \nu) \sim \mathcal{D}_p \otimes \mathcal{D}_q} \left[\sum_{u=1}^p \sum_{v=1}^q [(\mu \otimes \nu)_{u,v} - (\mu \oplus \nu)_{u,v}]^2 \right]$$

and compute its value through the sequence:

$$\begin{aligned} \Delta_p &= \mathbb{E}_{(\mu, \nu) \sim \mathcal{D}_p \otimes \mathcal{D}_q} \left[\sum_{u=1}^p \sum_{v=1}^q \left[\left(\mu_u - \frac{1}{p} \right) \left(\nu_v - \frac{1}{q} \right) \right]^2 \right] \\ &= \mathbb{E}_{\mu \sim \mathcal{D}_p} \left[\sum_{u=1}^p \left(\mu_u - \frac{1}{p} \right)^2 \right] \mathbb{E}_{\nu \sim \mathcal{D}_q} \left[\sum_{v=1}^q \left(\nu_v - \frac{1}{q} \right)^2 \right] \\ &= pq \mathbb{E}_{\mu \sim \mathcal{D}_p} \left[\left(\mu_1 - \frac{1}{p} \right)^2 \right] \mathbb{E}_{\nu \sim \mathcal{D}_q} \left[\left(\nu_1 - \frac{1}{q} \right)^2 \right] \end{aligned}$$

Now, we notice that we need to compute the variance of \mathcal{D}_p ; as it is a known law, we use the following property:

Proposition 1 (Variance of Dirichlet law)

$$\mathbb{V}_{X \sim \mathcal{D}_p}[X] = \frac{p-1}{p^2(p+1)}$$

Proposition 1 in particular, implies that margins will concentrate their values around $\frac{1}{p}$ and $\frac{1}{q}$ respectively as soon as p or q increases respectively. As we notice that couplings equal each other when any margin is uniform, this should imply that Δ_p converges to 0 if any of the two increases. This is exactly what happens, we have the expression:

$$\Delta_p = \frac{1}{pq} \left(\frac{p-1}{p+1} \cdot \frac{q-1}{q+1} \right) \leq \frac{1}{pq}$$

This last inequality confirms what was expected: as margins are concentrated around their means, the two couplings tend to be equal rapidly if p or q increases.

2.5 Structural Justification based upon an axiomatic result of Imre Csiszar

Although it seems arbitrary, our restriction to these two previous coupling functions, is all but a fortuitous decision: in [8], Csiszar actually shows that, provided we verify additional intuitive properties, we must restrict ourselves to use either least square or maximum entropy as canonic "distances" between probability distributions.

Let us rewrite our transport problems in terms of the notations he uses in [8]. We notice that problems 4 and 5 aims at reducing a distance from π to the uniform law (that term actually vanishes in both), where π must satisfy constraints on its margins leading to an eligible space $L_{\mu,\nu}$ inside the simplex S_n . In the first problem, the distance function is the entropy while in the second it is the norm \mathbb{L}_2 .

A general question is how to adapt a "prior guess" u_0 to verify a list of constraints. Let us say u_0 lives in S_n while the given constraints define a subspace $L \in \mathcal{L}$ (\mathcal{L} is the space of subspaces of S_n tuned by a finite list of affine constraints, see [8] for more details). To formalize it, Csiszar defines a *projection rule* Π as a function whose input is a set $L \in \mathcal{L}$ and which generates a method Π_L to project any prior guess u_0 to a vector in L :

$$\begin{aligned} \Pi : \mathcal{L} &\rightarrow (S_n \rightarrow S_n) \\ L &\rightarrow \Pi_L : (u_0 \rightarrow \Pi_L(u_0) \in L) \end{aligned}$$

The article then introduces a collection of "natural" properties that we gather hereafter.

- *consistency*: if $L' \subset L$ and $\Pi_L(S_n) \subset L'$ then $\Pi_{L'} = \Pi_L$; basically, if the result of a projection to a bigger space is always inside a smaller, then the projection on the two spaces are equivalent.

- *distinctness*: if L and L' are defined by a unique constraint and they are not equal, then $\Pi_L \neq \Pi_{L'}$ (unless they both contains the initial prior guess). Typically, in \mathbb{R}^2 , minimizing $\|\cdot\|$ on two lines returns a different result as soon as they do not both contain 0.
- *continuity*: Π is continuous with regards to $L \in \mathcal{L}$; it has a continuous relation with constraints.
- *scale invariant*: $\Pi_{\lambda L}(\lambda u) = \lambda u$ for any positive λ and any $u \in S_n$.
- *local*: for any subset $J \subset \{1, \dots, n\}$, $(\Pi_L)_J = (\Pi_{L'})_J$ as soon as $L_J = L'_J$ where L_J means we only keep constraints dealing with coordinates in J and $(\Pi_L)_J$ is the restriction of the resulting vector of Π_L to the J coordinates. This property indicates that the results of Π on a set of coordinates, only depends on constraints applied to those coordinates.
- *transitive*: for any $L' \subset L$, $\Pi_{L'} = \Pi'_L \circ \Pi_L$. We can first project on a bigger space without affecting the result.

All those properties appear as a must-have for defining a convenient projection rule. The main result of the paper [8] is that if Π is satisfying their combination then it is limited to two forms:

- $\Pi_L : u \rightarrow \operatorname{argmin}_{v \in L} \left[\sum_{i=1}^n \alpha_i (v_i - u_i)^2 \right]$ for a fixed vector α
- $\Pi_L : u \rightarrow \operatorname{argmin}_{v \in L} \left[\sum_{i=1}^n \alpha_i h_\beta(v_i | u_i) \right]$ for a fixed vector α with h_β being specific functions defined in the paper and which are equal to the entropy in the case $\beta = 1$

We already basically know that any convenient projection is coined out of \mathbb{L}_2 projections or entropy-like h_β functions. Adding a last property, similar to the Full Monge or Full Log Monge conditions that we introduce in section 3 restrict to $\alpha = \beta = 1$, hence to the two problems we treated in this document. This last property guarantees that the "no interaction" solution in case we omit constraints (as the one of problem 3) respects a proportional behavior. Namely, that if we update the total mass available (for instance in a monetary application), the resulting effect will be proportional on each component.

To come back to our transport problem, the "prior guess" is the uniform law while the subspace $L \subset S_n$ is defined using the margin constraints forced by μ and ν . Then, provided we verify quoted properties, the two cost functions we used cover an exhaustive view.

2.6 Conclusion deduced from the Optimal Transport overview

Using the generic formalism of "optimal transport", we found out two dual coupling functions. The first one "independence" is well-known while the second introduces the so-called "indetermination", which follows a dual sequence of properties induced by the use of sums rather than products; we shall give further details on that point. In section 4 we present some highlights on the specific properties of "indetermination" and study it *per se*. Now, let us keep on the parallel between those twins coupling functions in section 3 by introducing some properties on their corresponding contingency (or probability) matrices; leading to the \oplus notation.

3 Monge properties: a justification of the \oplus/\otimes notation

We introduce two classes of matrices, the first one is attributed to Gaspard Monge, from a basic idea appearing in his 1781 paper, (incidentally see [5], where a reference is given to Alan Hoffman¹ who first coined that point and consequently proposed the name: Monge's Matrices). For each of those Monge's matrices, we point out some remarkable equalities and, moreover, we link them to a corresponding coupling function. Doing so, we derive new properties on each of the two coupling functions we introduced in section 2.

3.1 Monge property – "Indetermination"

To introduce Monge's properties, we follow the exhaustive work of Rainer Burkard, Bettina Klinz and Rüdiger Rudolf exposed in the 66-pages-long article [5] and begin with definition 4.

Definition 4 (Monge and Anti-Monge matrix)

A $p \times q$ real matrix $c_{u,v}$ is said to be a Monge matrix if it satisfies:

$$c_{u,v} + c_{u',v'} \leq c_{u',v} + c_{u,v'} \quad \forall 1 \leq u \leq u' \leq p, 1 \leq v \leq v' \leq q$$

and an Anti-Monge matrix if:

$$c_{u,v} + c_{u',v'} \geq c_{u',v} + c_{u,v'} \quad \forall 1 \leq u \leq u' \leq p, 1 \leq v \leq v' \leq q$$

Remark 4 (Full-Monge matrix)

The important case for our purpose is the equality case when a matrix is both Monge and Anti-Monge, we will call this situation "Full-Monge" matrix.

$$c_{u,v} + c_{u',v'} = c_{u',v} + c_{u,v'} \quad \forall 1 \leq u \leq u' \leq p, 1 \leq v \leq v' \leq q$$

Although it is poorly studied, the last introduced equality fits perfectly our purpose. The inequalities on the contrary, are common and can be met in diverse situations such as cumulative distribution functions, or copula theory.

Remark 5 (Adjacent cells)

A straightforward but important derived property is the local adjacency cells equality: it is sufficient to satisfy the property of the remark 4 on adjacent cells, to ensure the obtainment of a "Full-Monge" matrix behavior for the global set of cells i.e.:

$$c_{u,v} + c_{u+1,v+1} = c_{u+1,v} + c_{u,v+1} \quad \forall 1 \leq u \leq p, 1 \leq v \leq q$$

¹ In 1961 Alan Hoffman (IBM Fellow and US Science Academy member) rediscovered Monge's observation see [13]. Hoffman showed that the Hitchcock–Kantorovich transportation problem can be solved by a very simple approach if its underlying cost matrix satisfies those Monge's properties

3	4	2	9		1/9	4/27	2/27	1/3
2	3	1	6		2/27	1/9	1/27	2/9
1	2	0	3		1/27	2/27	0	1/9
3	1	2	9		1/9	4/27	2/27	1/3
9	13	5	27		1/3	13/27	5/27	1

Fig. 1 Example of an indetermination coupling (Statistical counting vs Probability forms)

Remark 5 is a key property to study Monge matrices since it gives a direct $\mathcal{O}(pq)$ algorithm to verify if a matrix is Monge.

Besides, a question emerges: which density function verifies the full Monge property? The following Proposition 2 gives an interesting answer: all full Monge's matrices derive from the density of an "indetermination" structure.

Proposition 2 (Full-Monge matrix is equivalent to "Indetermination")

A "full Monge matrix" necessarily represents an "indetermination coupling".

Proof

Summing on u' and v' the equality of remark 4 we straightforwardly obtain:

$$\sum_{u'} \sum_{v'} c_{u,v} + c_{u',v'} - c_{u',v} - c_{u,v'} = pq c_{u,v} + c_{\cdot,\cdot} - qc_{\cdot,v} - pc_{u,\cdot} = 0 \rightarrow c_{u,v} = \frac{c_{u,\cdot}}{q} + \frac{c_{\cdot,v}}{p} - \frac{c_{\cdot,\cdot}}{pq}$$

By summarizing properties of Full-Monge Matrices we get the following Theorem 3.

Theorem 3 (Full-Monge matrices)

The $\pi_{u,v}$ cell values representing a probability matrix then the following properties are equivalent.

1. π is a Full-Monge matrix
2. $\pi_{u,v} = \pi_{u,v}^+ = \frac{\mu_u}{q} + \frac{\nu_v}{p} - \frac{1}{pq}$
3. π optimizes problem 5 for some given margins
4. All 2×2 sub-tables $\{u, v, u', v'\}$ extracted from π have the same sum on their diagonal and anti-diagonal

Last property of Theorem 3 is illustrated on Figure 1 and justifies the \oplus notation assigned to "indetermination". Indeed, if we take blue and red arrows we get the same resulting value: 0. Using the contingency form:

$$\text{blue arrows : } 3 + 2 - 1 - 4 = 0$$

$$\text{red arrows : } 3 + 2 - 4 - 1 = 0$$

Equality remains true for the probability form since we just have to divide the cell values by the total sum of the matrix (27 here).

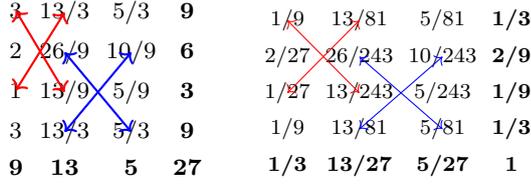


Fig. 2 Example of an "independence coupling" (Contingency vs Probability forms)

3.2 Log-Monge property – Independence

We present hereafter a similar class of Matrices related, now, to independence: called Log-Monge matrices. They are built on the same principle as before through definition 5.

Definition 5 (Full-Log-Monge Matrices)

A strictly positive $p \times q$ matrix $c_{u,v}$ is "Full-Log-Monge" when:

$$\ln(c_{u,v}) + \ln(c_{u',v'}) = \ln(c_{u',v}) + \ln(c_{u,v'}) \quad \forall 1 \leq u \leq u' \leq p, 1 \leq v \leq v' \leq q$$

To immediately get the correspondence, we propose a transposition from a property to another using logarithm in Remark 7. It supposes matrices to be strictly positive (for our probability application: whole discrete space must be reached).

Remark 6 (From Log-Monge to Monge)

We easily verify that c satisfies condition proposed in definition 5 if and only if $\ln(c)$ verifies the equivalent condition in definition 4 where logarithm is taken element-wise.

Using Remark 6, we can check that Full-Log-Monge property leads to interesting results and is linked to "independence coupling"; without detailing their obtainment, we gather those results within Theorem 4, dual of Theorem 3.

Theorem 4 (Full-Log-Monge Matrices)

Let $\pi_{u,v}$ be a strictly positive probability matrix then all the following statements are equivalent.

1. $\pi_{u,v}$ is Full-Log-Monge
2. $\pi_{u,v} = \pi_{u,v}^\times = \mu_u \nu_v$
3. π optimizes problem 3
4. All 2×2 sub-tables $\{u, v, u', v'\}$ extracted from π have the same product on their diagonal and anti-diagonal.

Figure 2 illustrates "Full Log-Monge" matrices and their properties related to "independence"; it justifies the usual \otimes notation.

In these matrices cell values are fractions; we want them to fulfil the same marginal values as those given in Figure 1. It is important to remark that both

those matrices (in Figure 1 and Figure 2) optimize a problem where the unique difference is the cost functions (since the margins are strictly identical). We immediately verify the last property of Theorem 4:

$$\text{blue arrows : } 3 * 13/9 - 1 * 13/3 = 0$$

$$\text{red arrows : } 26/9 * 5/3 - 13/3 * 10/9 = 0$$

3.3 Conclusion on the parallel coupling approaches

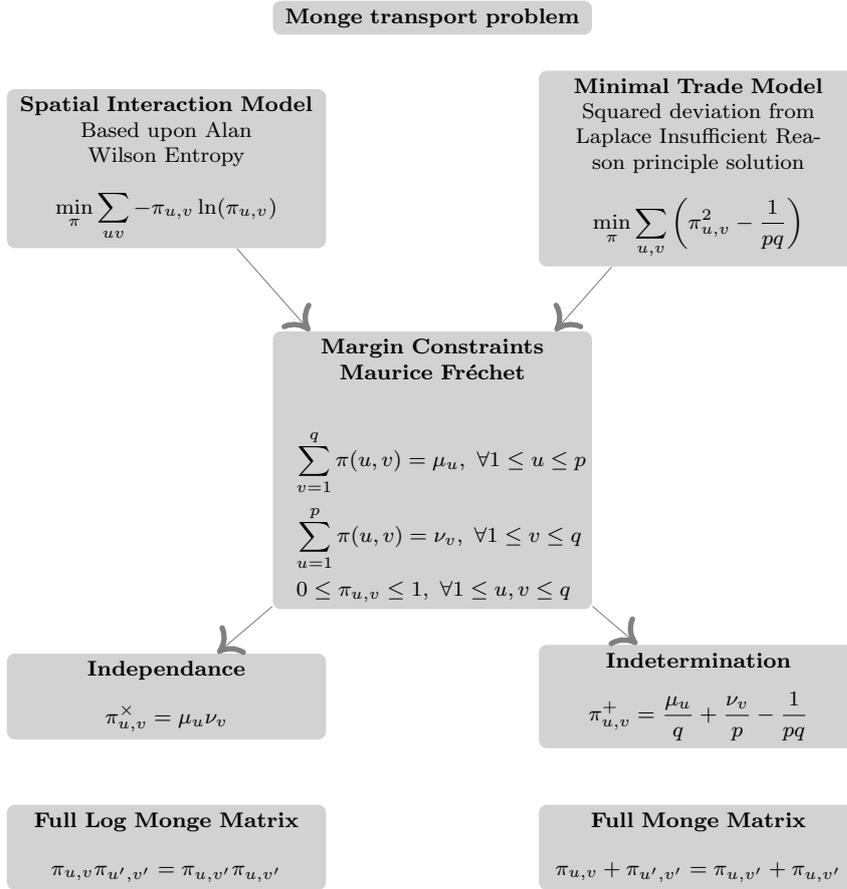


Fig. 3 View of the symmetry independence / indetermination

We propose here some concluding remarks about the parallel definitions and properties our coupling functions, "independence" and "indetermination", are fulfilling : this is illustrated by Figure 3.

Both appear as the result of a discrete optimization problem with fixed marginal constraints; only the choice of their cost function allows the user to discriminate among the two possible approaches. *A priori* one cannot really justify the reason of the choice of one cost function versus the other one. However in practice, there is no doubt for anybody, most of the statisticians will choose the "independence coupling" as a more classical and more comfortable, solution, but it should have been interesting, at least, on a fair intellectual standpoint, to answer the question of the interest of the other solution .

Along the same lines, introducing two "Full Monge Matrix" forms, we have shown that a property suitable for one situation generates by transposition a similar property for the other one: once again, this does not induce *a priori* any justification for the preponderance of "independence".

Choice of "independence" comes from its easy interpretative power as mentioned beforehand. Realizing an experience leading to "independence" is natural: we can explain and understand it. On the contrary, few articles propose to realize a coupling according to "indetermination" (whose formula is given by Theorem 2). In section 4, we shall essentially work on describing correctly this lesser known coupling, hoping this will help the reader to better understand its latent structure, before applying it within the graph clustering context.

4 Logical "indetermination" and "Condorcet's voting equilibrium"

In section 4, our latent goal is to better understand the "indetermination coupling", that we have until now essentially introduced on a theoretical point of view. Although obtained through a similar process, "independence coupling" is straightforwardly linked to classical empirical experiences. π^+ does not share this latent simplicity and interpreting it, *per se*, is clearly a domain which deserves to be investigated. We present an attempt for helping the reader to make an accurate picture about the "indetermination" concepts.

Interest for the coupling will be reinforced by its link with Condorcet's majority equilibrium and its presence in several statistical criteria as shown in section 5 devoted to graph clustering. Defining a "for" vs "against" notion will lead us to a formal equality interpreting "indetermination" in an other space. In fact we are faced with the famous "Condorcet's voting equilibrium", which amounts to exhibit the situation where the number of opinions "for" balances exactly the number of opinions "against".

In that case, we describe an equilibrium situation, verified on a probabilistic or statistical standpoint, characterizing any measure coupling two margins through "indetermination". The demonstration of this property requires the use of "Mathematical Relational Analysis" notations, which will be formally defined hereafter. We do not want in the context of this article to develop an exhaustive overview of this theory and its applications but pick up some results in connection with the goals we want to achieve; most of them being extracted from the following list of papers which gathers some of the most

important key features about the subject: [18], [14], [19], [22], [15], [16], [1], [2].

We also interpret the equilibrium between the "yes" (agreements) and the "no" (disagreements) (or "for" and "against" as well) as in an election as a voting "indetermination situation". This implies: since the number of votes "for" equals the number of votes "against" we are in a situation, where it is impossible to take a decision. The term: "indetermination" ("indeterminacy" or "uncertainty" should have been used as well) is a formal translation of this surprising situation (fortunately occurring rarely). First of all, let us introduce properly Relational Analysis notations that we shall use later on.

Definition 6 (Relational Analysis notations)

Let (u_1, \dots, u_n) and (v_1, \dots, v_n) be two n probabilistic draws of $U \sim \mu$ and $V \sim \nu$ respectively. We define two associated symmetric $n \times n$ matrices X and Y by

$$\begin{aligned} X_{i,j} &= \mathbb{1}_{u_i=u_j}, \quad \forall 1 \leq i, j \leq n \\ Y_{i,j} &= \mathbb{1}_{v_i=v_j}, \quad \forall 1 \leq i, j \leq n \end{aligned}$$

To understand the notation, let us begin with some remarks about definition 6. Basically, the two binary matrices X and Y (which correspond in fact to two binary equivalence relations based on the drawn modalities) represent agreements and disagreements of the two variables on a same draw of size n ; they are symmetric with 1 values on their diagonal. This relational coding has a lot of powerful properties, which will not be presented in this paper but which can be found in the articles we mentioned beforehand.

Definition 6 immediately provides us with an algorithm to transfer contingency representations to relational ones. The way back consists in noticing that:

$X_{i,j} = 1$ if and only if i and j share the same modality of $U \sim \mu$.

Hence we assign a modality to each class defined by the equivalence relation embedded in X : the only loss of information during this process resides in the names of modalities.

Now, we are ready to present the Theorem justifying the name "indetermination":

Theorem 5 (π^+ and Condorcet equilibrium)

π being a cross probability law on a set of $p \times q$ categorical variables, we shall say that π is an "indetermination coupling" on its margins, if and only if the expected number of "agreements" equals the number of "disagreements" on a 2 independent drawings of π .

Proof

Let π be a probability law on $p \times q$ categorical variables; it's defined through its values $\pi_{u,v}$, $1 \leq u \leq p$ and $1 \leq v \leq q$. U and V are random variables representing its margins. By n drawings through π , hence n samplings of (U, V) ,

U and V generates two partitions (equivalence relations) of the n individuals based on their modalities.

We will say that an agreement occurs when both partitions simultaneously gather or separate the individuals i and j . A disagreement occurs on the contrary when a classification regroupes i and j while the other one separates them. Formally, if X, Y encodes the n samplings as defined in Definition 6:

- $X_{i,j}Y_{i,j} = 1$, agreement of type 11, there are pq couples of classes possible for two individuals i and j to realize this type of agreement
- $\overline{X}_{i,j}\overline{Y}_{i,j} = 1$, agreement of type 00, there are $p(p-1)q(q-1)$ couples of classes of this type
- $X_{i,j}\overline{Y}_{i,j} = 1$, disagreement of type 10, there are $pq(q-1)$ couples of classes of this type
- $\overline{X}_{i,j}Y_{i,j} = 1$, disagreement of type 01, there are $p(p-1)q$ couples of classes of this type

As quantities vary according to their types of agreement or disagreement, we propose the following equality which establishes that the weighted number of agreements equals the weighted number of disagreements:

$$\frac{XY}{pq} + \frac{\overline{X}\overline{Y}}{p(p-1)q(q-1)} = \frac{X\overline{Y}}{pq(q-1)} + \frac{\overline{X}Y}{p(p-1)q} \quad (9)$$

Equality 9 is intrinsically important and appears notably in some articles among those we cited beforehand. It is defined on a draw of size n and linked to a contingency indetermination. We take two draws at random independently under π : (u_i, v_i) and (u_j, v_j) and introduce a probabilistic equality based on our 2 draws (u_i, v_i) and (u_j, v_j) :

$$\frac{\mathbb{E}_{\pi \otimes \pi}(X_{i,j}Y_{i,j})}{pq} + \frac{\mathbb{E}_{\pi \otimes \pi}(\overline{X}_{i,j}\overline{Y}_{i,j})}{p(p-1)q(q-1)} = \frac{\mathbb{E}_{\pi \otimes \pi}(X_{i,j}\overline{Y}_{i,j})}{pq(q-1)} + \frac{\mathbb{E}_{\pi \otimes \pi}(\overline{X}_{i,j}Y_{i,j})}{p(p-1)q} \quad (10)$$

We shall notice now that equality 10 precisely occurs when π equals the indetermination coupling of its margins with the formula introduced in Theorem 2. Let us compute the result of two-sized independent draws under π .

- $\mathbb{E}_{\pi \otimes \pi}(X_{i,j}Y_{i,j}) = \sum_{u_i, v_i} \sum_{u_j, v_j} \pi_{u_i, v_i} \pi_{u_j, v_j} \mathbb{1}_{u_i=u_j \& v_i=v_j} = \sum_{u, v} \pi_{u, v}^2$
- $\mathbb{E}_{\pi \otimes \pi}(\overline{X}_{i,j}\overline{Y}_{i,j}) = \sum_{u_i, v_i} \sum_{u_j, v_j} \pi_{u_i, v_i} \pi_{u_j, v_j} \mathbb{1}_{u_i \neq u_j \& v_i \neq v_j} = \sum_{u, v} \pi_{u, v} (1 - \pi_{u, \cdot} - \pi_{\cdot, v} + \pi_{u, v})$
- $\mathbb{E}_{\pi \otimes \pi}(X_{i,j}\overline{Y}_{i,j}) = \sum_{u_i, v_i} \sum_{u_j, v_j} \pi_{u_i, v_i} \pi_{u_j, v_j} \mathbb{1}_{u_i=u_j \& v_i \neq v_j} = \sum_{u, v} \pi_{u, v} (\pi_{u, \cdot} - \pi_{u, v})$

Inserting into equation 10, we get:

$$\begin{aligned} & \frac{\sum_{u,v} \pi_{u,v}^2}{pq} + \frac{\sum_{u,v} \pi_{u,v}(1 - \pi_{u,\cdot} - \pi_{\cdot,v} + \pi_{u,v})}{p(p-1)q(q-1)} \\ &= \frac{\sum_{u,v} \pi_{u,v}(\pi_{u,\cdot} - \pi_{u,v})}{pq(q-1)} + \frac{\sum_{u,v} \pi_{u,v}(\pi_{\cdot,v} - \pi_{u,v})}{p(p-1)q} \end{aligned}$$

Reducing to same denominator, we get:

$$\begin{aligned} & (p-1)(q-1) \sum_{u,v} \pi_{u,v}^2 + \sum_{u,v} \pi_{u,v}(1 - \pi_{u,\cdot} - \pi_{\cdot,v} + \pi_{u,v}) \\ &= (p-1) \sum_{u,v} \pi_{u,v}(\pi_{u,\cdot} - \pi_{u,v}) + (q-1) \sum_{u,v} \pi_{u,v}(\pi_{\cdot,v} - \pi_{u,v}) \end{aligned}$$

regrouping the similar terms yields:

$$pq \sum_{u,v} \pi_{u,v}^2 - p \sum_u \pi_{u,\cdot}^2 - q \sum_v \pi_{\cdot,v}^2 + 1 = 0$$

Making use of a classical equality similar to equation 3, we obtain:

$$pq \sum_{u,v} (\pi_{u,v} - \pi_{u,\cdot}/q - \pi_{\cdot,v}/p + 1/pq)^2 = 0$$

Finally it holds:

$$\pi_{u,v} = \frac{\pi_{u,\cdot}}{q} + \frac{\pi_{\cdot,v}}{p} - \frac{1}{pq}$$

We have proved that π equals π^+ if and only if the expected number of normalized agreements equals the expected number of disagreements on a 2-sized drawing.

In order to give a concrete example of the notion of "balanced voting" (also called Condorcet's Majority Voting Equilibrium), let us illustrate the concept of "indetermination" in a specific and interpretable case: criminal judgements in a judicial court.

Suppose we have two variables U, V . The first one U represents the result of the judgement (with 2 possible modalities: condemnation (modality 1) or release (modality 0)), while the second V represents the court case status (with 2 modalities as well: guilty (modality 1), innocent (modality 0)). Also, we have a distribution μ on the first variable and ν on the second. Associating a "moral index marker" on each case is pretty easy:

- 00: corresponds to release an innocent, counted as an agreement (good decision)
- 01: release a guilty, counted as a disagreement (bad decision)
- 10: condemnation of an innocent, counted as a disagreement (bad decision)
- 11: condemnation of a guilty case counted as an agreement (good decision)

Optimizing a type of against votes always occurs to the expense of the other type; a tolerance level between 01 and 10 is set depending on the society rules. Whatever the preferred "against type" (01 or 10), any society will try

to decrease as much as possible the total number of "controversial decisions". Hence the worst court situation would be to have exactly the same number of votes "against" and "for"; indeed, once that equality passed, reversing all judgements would improve efficiency. This particular criminal judgement "indetermination" situation occurs when agreements equal disagreements and corresponds to have the following equilibrium:

$$\text{cases } 00 + \text{cases } 11 = \text{cases } 10 + \text{cases } 01$$

i.e. expressed in probability:

$$\pi_{0,0} + \pi_{1,1} = \pi_{0,1} + \pi_{1,0}$$

Using the previously introduced equivalence of Theorem 3 (but here in a 2×2 context), we immediately recognize our "indetermination coupling situation".

5 Application to Graph clustering

5.1 Introduction

Conde Cespedes, in her thesis [7], gathered a large amount of graph clustering criteria, coming from the scientific literature; she took advantage of this task to give them a category label, depending upon their relationship with both "independence" or "indetermination". She compared them according to their ability to perform on various graphs, and collected and stored the obtained results. Although we are in the quite same line with Patricia Conde Cespedes, we restrict ourselves to investigate a focused study of both the canonic ones: "deviation to independence" and "deviation to indetermination" that we will reintroduce hereafter within the graph theoretical context.

First let us start with some usual definitions for a graph:

Definition 7 (Weighted graph)

A weighted graph G , is a graph which contains n vertices $1 \leq i \leq n$, which are connected each other through edges (i, j) linked with weights $a_{i,j}$ (representing a weighted incidence matrix). We also introduce the total weight $2M = \sum_{i,j} a_{i,j}$.

A basic way to randomly generate a graph is to use the Erdős-Rényi distribution:

Definition 8 (Erdős-Rényi)

Fixing a number n of vertices and $\epsilon \in [0, 1]$, we link any set of two vertices by independently drawing through a Bernoulli law with parameter ϵ leading to a 0 - 1 weight. The obtained graph is non directed and each weight is 0 or 1.

Remark 7

Adding a parameter p representing maximum weight, we can easily create a weighted graph by drawing a Binomial law with parameter (ϵ, p) while linking couples (instead of sets) generates oriented graphs.

As mentioned in section 1, our work will be devoted to the research of classes, groupings, clusters or cliques (whatever we call them) within a graph. They are defined through an equivalence relation as specified in definition 9:

Definition 9 (Graph clustering)

Let us call x , a matrix representation of a binary equivalence relation, the result of the clustering of a graph G . Then $x_{i,j}$ equals 0 or 1 and equals 1 if and only if the two vertices i and j are in the same class for x , and 0 if not.

Clustering algorithms aim at providing classes maximizing internal similarities as well as minimizing external ones. A first option is to take as input the number K of classes we are looking for, together with an associated distance (or dissimilarity index) and come up with a list of best representatives or "means" for each class. The output "means" tend to optimize the sum of distances from all vertices to their nearest mean. K-means algorithm whose idea goes back to the fifties (see² [24]) typically illustrates this option. Having fixed a distance and a number of classes, finding optimal means minimizing the sum of the distances remains a NP-hard problem. A second option, is to construct a local criterion c which assigns a weight $c_{i,j}$ to each (i, j) couple of vertices based on their similarity; the more similar they are, the higher the criterion is. We then build up a global criterion by summing up the local values $c_{i,j}$ if and only if i and j are in the same class as proposed in problem 6.

Problem 6 (Generic clustering problem)

$$\max_x M(c, x) = \sum_{i=1}^n \sum_{j=1}^n c_{i,j} x_{i,j}$$

subject to:

x is an equivalence relation

First let us remark that, as notably spotted in [15], [18], [22] an equivalence relation constraint can be written as :

- $x_{i,i} = 1, \forall 1 \leq i \leq n$ (reflexivity)
- $x_{i,j} = x_{j,i}, \forall 1 \leq i, j \leq n$ (symmetry)
- $x_{i,j} + x_{j,k} - x_{j,i} \leq 1, \forall 1 \leq i, j, k \leq n$ (transitivity)

Thanks to the linearity of these constraints, in addition to the linear expression of the criterion itself (in terms of the unknown $x_{i,j}$ values), the problem 6 although *a priori* NP-hard can be exactly solved (according to some conditions) through the integer relaxation of a good existing 0-1 linear programming code (see [18]), for problems sizes n lower than say 300. But in the context of networks and graphs clustering, the size n of the problem (here the number of vertices or nodes) can be really huge (millions for social networks) and the direct solving by linear programming, even specially tuned, is no longer possible; therefore, the use of robust heuristics becomes mandatory.

² factually this is the method of S. Lloyd(1957) rewritten by E.W. Forgy (1965) which corresponds to the oldest version of the K-means really used

”Louvain” Algorithm (see [10] or [21]) is adequately considered as one of these good and available heuristics, allowing to cope with this clustering task. This algorithm relies on two steps for globally maximizing the criterion $M(c, x)$ based on the local costs $c_{i,j}$ values.

0. Initially, each node in the network is assigned to its own community: there are as many as vertices.
1. In the first step, for each node i , the change from removing it from its community and adding it to all its neighbors’ is computed. If $M(c, x)$ increases for some, i is put in the locally optimal connected community. This process is applied repeatedly and sequentially to all nodes until no improvement of $M(c, x)$ occurs. Once this local maximum of modularity is reached, the first phase has ended.
2. In the second phase, the algorithm groups all the nodes in the same community and builds a new network where nodes are the communities from the previous phase. Links between nodes of the same community are now represented by self-loops on the new community node and links from multiple nodes in the same community or nodes in different communities are represented by weighted edges between communities.
3. Once the new network is created, the second phase is completed and the first phase can be re-applied to the new network.
4. It eventually ends when the improvement on $M(c, x)$ brought by the first step is less than a chosen threshold.

As mentioned beforehand, Louvain Algorithm is a good heuristic; it does not provide us with an exact optimal result systematically but just a quite good approximate one. Just for a rough comparison, K-means algorithm as well is getting an approximate solution but with a supplementary drawback: it imposes to fix *a priori* the number K of classes we want (which is completely out of context when dealing with social networks or huge graphs clustering; to guess the reasonable K clusters value is then impossible or extremely greedy in computer time). In addition to that, K-means as well as Louvain algorithm depends on vertices naming as they lexicographically and sequentially browses them.

Whatever the costs $c_{i,j}$ are, an optimal solution of the global criterion $M(c, x)$ exists, even if we are unable to find the optimum out, the generic Louvain algorithm gets approximate solutions which are quite satisfactory and often sufficient for practical purposes and for most of them, close to optimality. However, this aspect concerned with the optimality and the unicity of those solutions $x_{i,j}$ has been studied in a lot of articles and books and it is not our intention to discuss this point deeper in this paper. We will concentrate on some other characteristics: the choice between two canonic costs at the light of the previous sections.

5.1.1 Original Modularity – "Independence"

The original, famous, and well known Newman-Girvan's presentation of a global criterion for graphs clustering, see [10] or [21], has been introduced in the Louvain algorithm together with a global cost called "Modularity" defined by:

Definition 10 (Modularity)

Given a partition $x_{i,j}$ and a graph G with weighted function a on its edges, the global modularity returns to:

$$M^\times(G, x) = \frac{1}{2M} \sum_{i,j} \left[a_{i,j} - \frac{a_{i,\cdot} a_{\cdot,j}}{2M} \right] x_{i,j} \quad (11)$$

Let us first remark that the original modularity M^\times is nothing but our generic global cost function defined though Problem 6 with:

$$c_{i,j} = m^\times(G)_{i,j} = \frac{a_{i,j}}{2M} - \frac{a_{i,\cdot} a_{\cdot,j}}{(2M)^2}$$

and that the local gain $m^\times(G)_{i,j}$ to put two vertices in the same class is the local deviation to independence. Indeed, using definition 7, we know that $\pi_{i,j} = \frac{a_{i,j}}{2M}$ can be seen as a probability measure on $\{1 \dots n\}^2$ with margins $\mu_i = \frac{a_{i,\cdot}}{2M}$ so that m^\times rewrites:

$$m^\times(G)_{i,j} = 2M (\pi_{i,j} - \mu_i \mu_j)$$

and does express itself as a canonic *deviation to independence* criterion.

A second remark is that as $m^\times(G)_{i,j}$ expression does not contain absolute value or square elevation then non connected vertices will lead to negative weights preventing them from being allocated to the same class. If they are connected the importance of $m^\times(G)_{i,j}$ evolves positively as i and j have less connections ($a_{i,\cdot}$ and $a_{\cdot,j}$ small); here again this implies an appropriate behavior. More precisely, since independence ensures a coupling as uniform as possible with fixed margins (this is a solution of problem 3), m^\times appears as a fair construction. The criterion basically measures a distance between the observed linkage weight and an expected flat weight given by the average neighborhood.

5.1.2 Extended Modularity – "Indetermination"

Problem 6 basically represents an extension of the already introduced "Modularity criterion" towards a generic criterion based on a local input one.

We suggest an expression $m^+(G)_{i,j}$ which represents a deviation to indetermination. It will be used as a local cost function in 6 leading to a slightly different global formula $M^+(G, x)$ to optimize locally:

$$m^+(G)_{i,j} = a_{i,j} - \frac{a_{i,\cdot}}{n} - \frac{a_{\cdot,j}}{n} + \frac{2M}{n^2}$$

Symmetrically as m^\times , it ends up being a canonic *deviation to indetermination* criterion. Indeed, with $\pi_{i,j} = \frac{a_{i,j}}{2M}$, m^+ rewrites:

$$m^+(G)_{i,j} = 2M * \left(\pi_{i,j} - \frac{\mu_i}{n} - \frac{\mu_j}{n} + \frac{1}{n^2} \right)$$

The global criterion being:

$$M^+(G, x) = \sum_{i,j} \left[a_{i,j} - \frac{a_{i,\cdot}}{n} - \frac{a_{\cdot,j}}{n} + \frac{2M}{n^2} \right] x_{i,j} \quad (12)$$

We have seen in section 2.4, that the square difference between both couplings tends to be small. Moreover they share a lot of properties as shown in section 3 and section 4. In the same way, Patricia Conde noticed that a lot of statistical criteria (at least the most frequently used) measuring variables correlation are based either on a "distance to independence", or are straightforwardly related to a "distance to indetermination" (Patricia Conde gave an interesting list in [7]). According to these remarks, our canonic *deviation to indetermination* criterion M^+ deserves to have the same types of use as those dedicated to the Newman Girvan's M^\times .

5.2 Erdős-Renyi Experimental Tests

As already mentioned, solving problem 6 is NP-hard so that we cannot expect precise results, neither about the number of classes for a given criterion, nor about the prediction of the running time of Louvain algorithm on a given graph. Nevertheless, as it is based on optimizing a local criterion, we can compare directly their local values to extrapolate a common or a distinct global run.

We propose a comparative try based on Erdős-Renyi graphs to spot differences or similarity between $m^\times(G)_{i,j}$ and $m^+(G)_{i,j}$ values. The aim is to observe the distribution of both criteria on a typical graph. First, to simplify observations and as only the reference cost varies between m^+ and m^\times , we only keep it by subtracting $a_{i,j}$; it is formally defined in definition 11. Then, we generate graphs randomly, compute each criterion on random pairs of vertices and store the reference cost. The experiment is formally specified in algorithm 1 while the results are gathered within figure 4.

Definition 11 (Bias or reference cost)

The two bias derived from m^\times and m^+ are respectively:

$$\begin{aligned} - b_{i,j}^\times &= \frac{a_{i,\cdot} a_{\cdot,j}}{2M} \\ - b_{i,j}^+ &= \frac{a_{i,\cdot}}{n} + \frac{a_{\cdot,j}}{n} - \frac{2M}{n^2} \end{aligned}$$

On figure 4 we observe that both distributions are similar for any values of ϵ . Indeed, the curves are identical on their core values (those with a number of realizations upon 200). It is not really surprising because they both come from

Algorithm 1 Provides the distribution of two reference costs

Input n
Input ϵ

$L_+ \leftarrow []$
 $L_\times \leftarrow []$
for $R = 1 \dots 10000$ **do**
 $G \leftarrow \text{Erdős-Rényi}(n, \epsilon)$
 $(i, j) \leftarrow (\text{RandomUnif}(n), \text{RandomUnif}(n))$
 $L_+ \leftarrow L_+ + (b_{i,j}^+(G))$
 $L_\times \leftarrow L_\times + (b_{i,j}^\times(G))$
end for
return (L_+, L_\times)

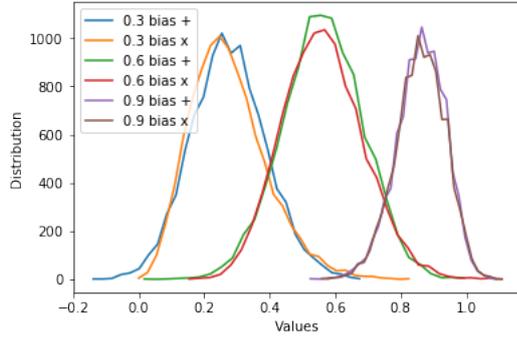


Fig. 4 Empirical distribution of the two reference costs $b_{i,j}^+$ and $b_{i,j}^\times$ for ϵ in $[0.3, 0.6, 0.9]$; X-axis gives the values of the bias, Y-axis gives the corresponding number of realizations

an optimization of a transport problem aiming at flattening the distribution (section 2) and they tend to be equal (section 2.4). We also notice on figure 4 that their common mean is equal to the value of ϵ , as it can be easily derived from the formulas.

A difference nevertheless remains: the bias b^+ has smaller extreme left-side values while the bias b^\times has higher extreme right-side values, which is particularly visible for $\epsilon = 0.3$ and $\epsilon = 0.6$ while not represented for $\epsilon = 0.9$.

Let us now compute theoretically both distributions under Erdős-Rényi graphs to confirm their symmetry. Value of $m^\times(G)_{i,j}$ as well as $m^+(G)_{i,j}$ only depends on the subsequent values of $a_{i,j}$, $a_{i,\cdot}$ and $a_{\cdot,j}$. Plus it's easy to get the corresponding probability of each event as expressed in proposition 3.

Proposition 3 (Probability values)

Let b be a binary value, $b \leq n_i \leq n$ and $b \leq n_j \leq n$; let us compute the following probability:

$$\begin{aligned} & \mathbb{P}(a_{i,j} = b, a_{i,\cdot} = n_i, a_{\cdot,j} = n_j) \\ &= \epsilon^b (1 - \epsilon)^{1-b} \binom{n-1}{n_i-b} \epsilon^{n_i-b} (1 - \epsilon)^{n-1-n_i+b} \binom{n-1}{n_j-b} \epsilon^{n_j-b} (1 - \epsilon)^{n-1-n_j+b} \end{aligned}$$

The corresponding value $m_{i,j}^+$ and $m_{i,j}^\times$ associated to a group (b, n_i, n_j) of the parameters being evident, we propose figure 5 which represents the difference between theoretical distributions of both criteria with $\epsilon = 0.3$.

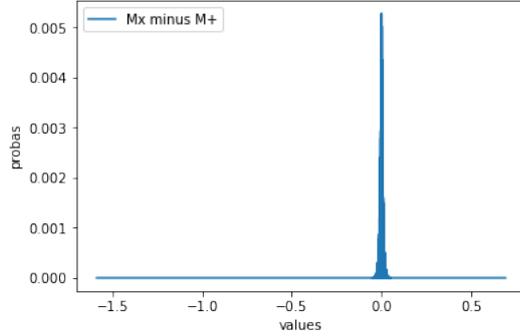


Fig. 5 Theoretical distribution of the difference $m^\times(G)_{i,j} - m^+(G)_{i,j}$ (same as $b_{i,j}^+ - b_{i,j}^\times$) on generated graphs

b^\times and b^+ have distinct forms but their proximity on highly probable values, given on Figure 5, illustrates section 2.4: if we couple two variables with n margins, expected difference is less than $\frac{1}{n^2}$.

Extreme values, on the contrary may differ drastically. Though it seems the opposite to Figure 4 as m^+ comes with higher values than m^\times , it's consistent because of the *minus* sign in the formula linking m with b .

Having noticed that b^+ and b^\times differ on their extreme values, we compute them on a general Erdős-Renyi graph (respecting the common value of $2M = n^2\epsilon$), and obtain the bounds:

$$\begin{aligned} -\epsilon &\leq b^+ \leq \frac{n}{n} + \frac{n}{n} - \epsilon = 2 - \epsilon \\ 0 &\leq b^\times \leq \frac{n \times n}{n^2\epsilon} = \frac{1}{\epsilon} \end{aligned}$$

As already expected with figure 5 the difference between extreme values is arbitrarily high.

5.3 Summary of an application to various graphs

The similar distributions found in section 5.2 must be confirmed through real life applications. We gather in table 1 the number of classes found by Patricia Conde-Cespedes, who applied both criteria on the same empirical graphs. She got similar results, as those we expected beforehand. We present here the list of graphs she used:

- Social network named "Zachary karate club" is frequently used in social network analysis and composed of 34 members from a Karate club of an American university (see [30]).
- Social network named "American College Football" gathers American football matches during year 2000. Each vertice is a team and connections represent a match (see [10]).
- "Jazz" social network represents collaborations between jazz musicians during years 1912 to 1940. Each vertice is a group and they are connected if they share a musician. Data were extracted from The Red Hot Jazz Archive (see [11]).
- "Internet" is a sub-graph of the Internet (see [12]).
- "Amazon" found on Amazon.com contains vertices representing products which are connected if they are frequently bought together (see [29]).
- "YouTube" where each vertice is a user. On YouTube, users can create groups, two users are connected in the graph if they joined the same group (see [20]).

Table 1 Number of classes found by each criteria on various graphs

	Karate	Football	Jazz	Internet	Amazon	YouTube
N (nb vertices)	34	115	198	69 949	334 863	1 134 890
M (sum of weights)	78	613	2 742	351 280	925 872	2 987 624
Number of classes for criteria M^\times	4	10	4	46	250	5 567
Number of classes for criteria M^+	4	10	6	39	246	13 985

Table 1 can be read as follows: for example, the "Internet" graph contains 69,949 vertices (nodes) with 351,280 edges (links); if we apply Louvain algorithm on, with the global criteria M^\times we usually find 46 communities, while M^+ leads to 39.

As anticipated in section 2.4 criteria are (in average) very close; consequently their resulting effect on various graphs is similar. Section 5.2 of the present paper provides the reader with an explanation of that assertion Patricia experimented in [7].

5.4 A general remark to differentiate the two criteria

While section 5.2 concludes on a global symmetric behavior of both criteria, reinforced by Patricia Condé's experimental results, summarized in section 5.3, it doesn't prevent them from being quite different on specific graphs.

Scanning up the local bias introduced in definition 11 we notice that the product form b^\times , will be small except if the mass $a_{i,\cdot} = a_{\cdot,i}$ of vertice i AND the mass of vertice j are high; the additive form of b^+ on the contrary will be small unless one of the two mass $a_{i,\cdot}$ OR $a_{\cdot,j}$ is big. Remembering m has to be high to lead to a merging:

- m^\times is penalized (by b^\times) if $a_{i,\cdot}$. AND $a_{\cdot,j}$ are big.
- m^+ is penalized (by b^+) as soon as $a_{i,\cdot}$. OR $a_{\cdot,j}$ is big.

To summary: to maximize additive form we cannot allow any of the two neighborhoods to wear large mass while the product form may accept one. Leveraging that remark we can build up specific graphs to differentiate the two criteria. Eventually, it enables us to exhibit very specific graphs kept as they are by a criterion while merged in one class by the other, we even propose unconnected vertices regrouped in the same class because of the overall weight distribution. The interested reader can refer to [3] for further details.

5.5 A common threshold on a particular form of graph

In this section 5.5, we present a curiosity: a form of graph on which criteria share a same merging threshold. Out of this curiosity, it presents several interests: first we are able to fix a threshold and secondly it is a training for a more general analyze.

We propose to work on a loop of n classes like the one in figure 6 (for which $n = 10$) and look for a threshold on $a_{i,i}^n$ (unique parameter) for the graph to be left intact by M^\times . As any vertice has the same environment, we may select any $b_{i,j}$: they are all equal. Counting edges, requiring $b_{i,j}^\times = b^\times \geq 1$ so that no merge can occur:

$$\begin{aligned} 2M &= n \times a_{i,\cdot} \\ a_{i,\cdot} &= 2 + a_{i,i}^n \\ \frac{a_{i,\cdot}^2}{2M} &\geq 2M \end{aligned}$$

and, solving a square equation ($u = a_{i,i}^n, u^2 + (4 - n)u + 2(2 - n) \geq 0$), we obtain $a_{i,i}^n \geq n - 2$. For instance, in our example, $n = 10$ so that 8 is the threshold explaining figure 6 is a convenient final graph for M^\times .

If we look at the behavior of M^+ on that very graph, we observe that our merging threshold equation is:

$$\begin{aligned} b_{i,j}^+ &\geq 1 \\ 2 * \frac{a_{i,\cdot}}{n} - \frac{2M}{n^2} &\geq 1 \\ 2 * \frac{a_{i,i}^n + 2}{n} - \frac{n(a_{i,i}^n + 2)}{n^2} &\geq 1 \\ a_{i,i}^n &\geq n - 2 \end{aligned}$$

Hence, while the graph form was coined for M^\times to have a threshold, we notice that not only M^+ also has one threshold but both are equal. The parallel properties of the two coupling functions appear here with a graph application.

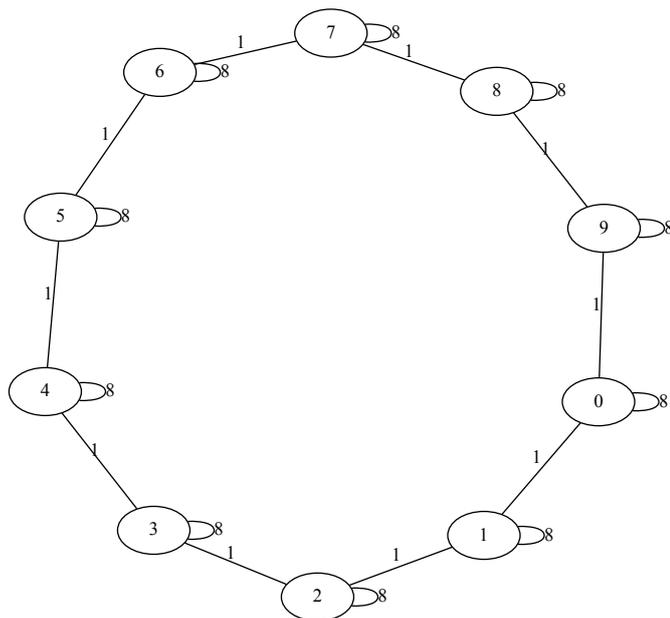


Fig. 6 Example of a convenient final graph clustering for M^\times

Remark 8 (Curiosity?) *As mentioned in remark 2.4, the two coupling functions are equal when one of the margin is uniform. Given the form of graph in figure 6, all vertices are symmetric one to another so that any distribution based on the neighborhood is uniform: it explains the result.*

6 Conclusions

First, we followed the historical line and introduced two basic notions extracted from Discrete Optimal Transport Theory: *independence* and *indetermination*. As recalled, the first one is the most intuitive and frequently used in mathematical articles as well as experimented in real life. The second notion appeared more surprising, poorly studied in the statistical literature but more commonly used by people working on Mathematical Relational Analysis Voting Theory and Analysis of Variance. Together, they cover the only two canonic projection costs as quoted in section 2.5.

To illustrate the usefulness of the parallel construction, we turned to applications and completed the track introduced by Patricia Conde in her thesis [7]. She gathered a list of graphs clustering criteria and classified them according to their deviation to one of the two previously mentioned coupling functions.

Section 5 reports a further analyze of the two canonical criteria. It gathers results about the general similarity of their application on various graphs as well as their extreme values to set one another apart. Subsection 2.4, notably, shows that they slightly differ and it explains the experimental results.

In each section, from optimal transport to graph theory, we insisted on the parallel between both notions together with their differences. As quoted beforehand, they appear as the two unique canonic structural solutions. A particularly curious situation is their duality when we pass from contingency to relational notations. It was first spotted in [17] and needs to be further understood. Generally, the differences between them needs to be scanned up, either to coin a macro criteria, or to chose wisely between one or another depending on the structure of the graph. In any case, the traditional use of *independence* at the expense of *indetermination* needs to be be further motivated and explained.

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