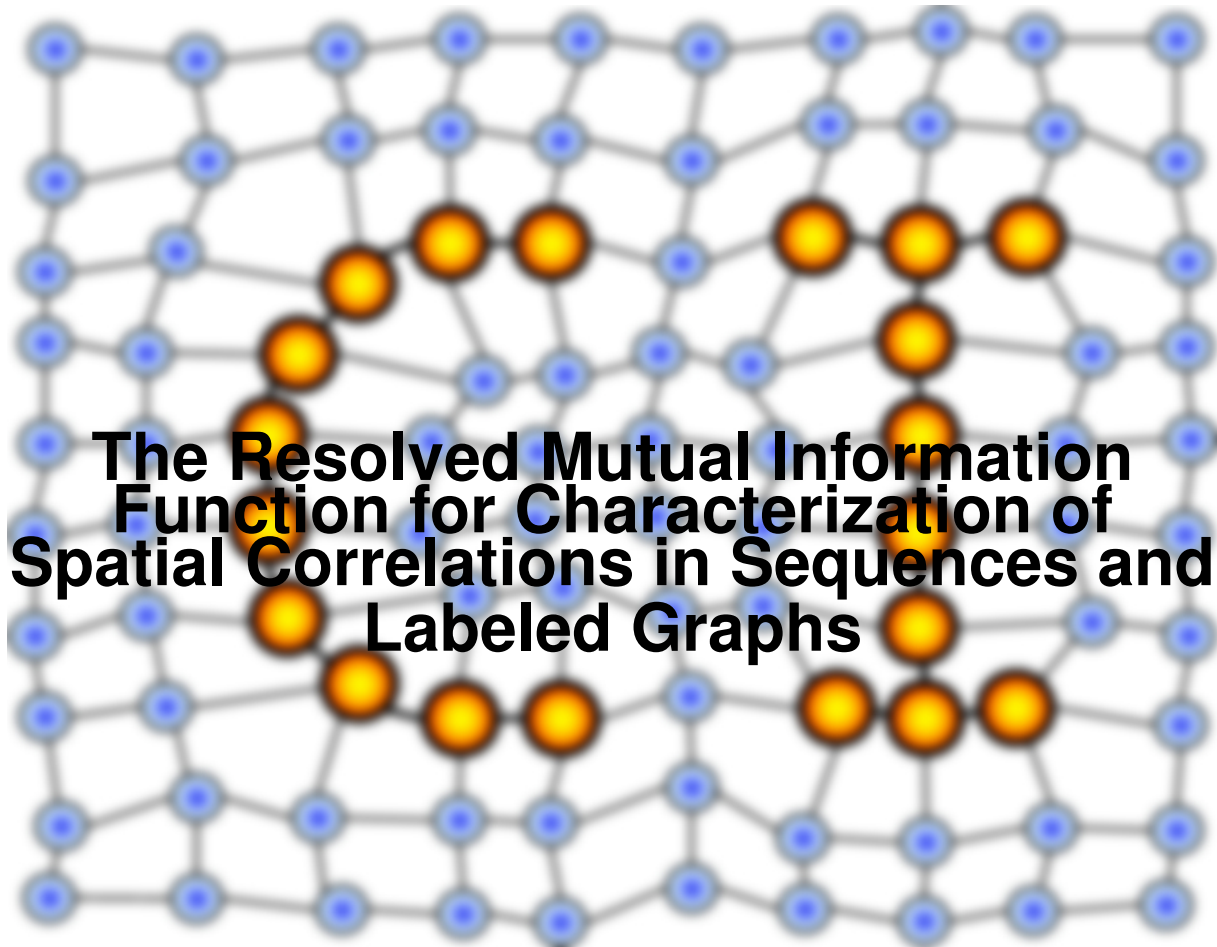


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The Resolved Mutual Information Function for Characterization of Spatial Correlations in Sequences and Labeled Graphs

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Abstract

In this technical report we collect and propose some useful quantities, notations, and approaches regarding information theoretic concepts, which might be helpful in machine learning when analyzing sequences and labeled graphs. In particular, we introduce resolved mutual information functions, which can be seen as a determining feature (profile) to characterize the spatial correlations in those data objects.

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1 Introduction

Information theoretic measures become more and more popular in applications far away from signal processing, information science and physics [33]. Among them, molecular-biological topics are one of the most promising areas as well as natural language processing [1, 45]. For example, sequence processing in biology and text analysis in linguistics are treated with very similar mathematical methods of information theory [29]. Those approaches comprise also methods which generate characteristic features of sequences or texts allowing a further processing by machine learning methods for clustering, classification and novelty detection, to name just a few application areas.

In this report, we consider some information theoretic quantities, which gained interest and generalize respective concepts to motivate further applications and the transfer to other application areas [6]. We will use these quantities to characterize spatial correlations and dependencies in sequences as well as in labeled graphs. Particularly, we will focus on quantities derived from the mutual information and related divergence measures [44]. Thereby, we will not restrict the approaches to the Shannon paradigm for the quantities but give also attention to computationally and theoretically interesting alternatives like Rényi divergences [35, 37]. Yet, we will start with the most prominent Shannon concepts.

2 Information Theoretic Quantities Related to the Shannon Concept of Information

2.1 Concepts, Basic Definitions and Mutual Information Functions

The Shannon entropy $H(X)$ of a random quantity $X \subseteq \mathcal{X}$ with the density measure $p(x)$ is the expectation value

$$\mathbb{E} \left[\log \left(\frac{1}{p(x)} \right) \right] = \int_{\mathcal{X}} p(x) \cdot \log \left(\frac{1}{p(x)} \right) dx \quad (1)$$

of the information $\log \left(\frac{1}{p(x)} \right)$, such that we have

$$H(X) = \mathbb{E} \left[\log \left(\frac{1}{p(x)} \right) \right] \quad (2)$$

for this entropy. The maximum value of $H(X)$ is obtained for an uniform density $p(x)$ and, hence, $H(X)$ serves as a measure of uncertainty [29]. The non-symmetric Kullback-Leibler divergence of $p(x)$ to a random quantity $Y \subseteq \mathcal{Y} = \mathcal{X}$ with density $p(y)$ is given as

$$D_{KL}(X \parallel Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x) \cdot \log \left(\frac{p(x)}{p(y)} \right) dy dx \quad (3)$$

yielding a zero value for $p(x) \equiv p(y)$ [23]. Thus, the Kullback-Leibler divergence $D_{KL}(X \parallel Y)$ can be taken as a dissimilarity measure between $p(x)$ and $p(y)$ [31]. The mutual information

$$I(X, Y) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(x) \cdot p(y)} \right) dy dx \quad (4)$$

quantifies the joint information of $p(x)$ and $p(y)$ with $p(x, y)$ being the joint density [23, 37]. Hence, the mutual information is the Kullback-Leibler divergence $D_{KL}(p(x, y) \parallel p(x) \cdot p(y))$ between the joint probability and the product of the marginal probabilities. Equivalently, we can write the mutual information as

$$I(X, Y) = \int_{\mathcal{X}} F(x, Y) dx$$

with

$$F(x, Y) = \int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(x) \cdot p(y)} \right) dy \quad (5)$$

describing a *mutual information relation* of a particular object (value) x of the random quantity X with respect to the random quantity Y . We denote $F(x, Y)$ as the (feature) *resolved mutual information* (rMI).

The mutual information $I(X, Y)$ can be written in terms of the Shannon entropies as

$$\begin{aligned} I(X, Y) &= H(X) + H(Y) - H(X, Y) \\ &= H(X) - H(X|Y) \end{aligned} \quad (6)$$

with the conditional entropy

$$\begin{aligned} H(X|Y) &= H(X, Y) - H(Y) \\ &= - \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(y)} \right) dy dx. \end{aligned} \quad (7)$$

Combining (6) and (7), the mutual information $I(X, Y)$ is obtained to be

$$\begin{aligned} I(X, Y) &= - \int_{\mathcal{X}} p(x) \cdot \log(p(x)) dx + \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(y)} \right) dy dx \\ &= - \int_{\mathcal{X}} \left(\int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(y)} \right) dy - p(x) \cdot \log(p(x)) \right) dx \end{aligned}$$

as an alternative formulation. From this we can conclude that for the rMI in eq. (5) the relation

$$F(x, Y) = -p(x) \cdot \log(p(x)) + \int_{\mathcal{Y}} p(x, y) \cdot \log \left(\frac{p(x, y)}{p(y)} \right) dy$$

holds.

The *cross mutual information* for sequences $X(t)$ and $Y(t + \tau)$ at time t with shift $\tau \geq 0$ is defined as

$$I(X(t), Y(t + \tau)) = \int_{\mathcal{X}} \int_{\mathcal{Y}} p(x(t), y(t + \tau)) \cdot \log \left(\frac{p(x(t), y(t + \tau))}{p(x(t)) \cdot p(y(t + \tau))} \right) dy dx \quad (8)$$

which yields by setting $Y(t + \tau) = X(t + \tau)$

$$I(X(t), X(t + \tau)) = \int_{\mathcal{X}} \int_{\mathcal{X}} p(x(t), x(t + \tau)) \cdot \log \left(\frac{p(x(t), x(t + \tau))}{p(x(t)) \cdot p(x(t + \tau))} \right) dx(t + \tau) dx$$

as the *auto mutual information* at time t with shift (delay) τ [22, 12]. If $p(x(t))$ is independent from t , only the joint probability $p(x(t), x(t + \tau))$ remains t -dependent or, more precisely, it becomes dependent only on the shift τ such that we simply write $p(x, x(\tau))$ for this. Thus, the auto mutual information in dependence on the shift τ is obtained as

$$I(X, \tau) = \int_{\mathcal{X}} \int_{\mathcal{X}} p(x, x(\tau)) \cdot \log \left(\frac{p(x, x(\tau))}{p(x) \cdot p(x(\tau))} \right) dx(\tau) dx \quad (9)$$

as an information theoretic analagon to the auto-correlation function. In [25, 26] this shift-dependent auto mutual information is denoted as the *mutual information function* (MIF). Adapting the rMI

from eq. (5) to the auto mutual information $I(X, \tau)$ we result the function

$$\begin{aligned} F(x, \tau) &= \int_{\mathcal{X}} p(x, x(\tau)) \cdot \log \left(\frac{p(x, x(\tau))}{p(x) \cdot p(x(\tau))} \right) dx(\tau) \\ &= \int_{\mathcal{X}} p(x, x(\tau)) \cdot \log \left(\frac{p(x, x(\tau))}{p(x(\tau))} \right) dx(\tau) - p(x) \cdot \log(p(x)) \end{aligned} \quad (10)$$

which can be seen as a quantity characterizing the inherent correlations of the sequence values $x(t)$. We denote $F(x, \tau)$ as the (feature) *resolved mutual information function* (rMIF), which trivially fulfills

$$I(X, \tau) = \int_{\mathcal{X}} F(x, \tau) dx \quad (11)$$

according to its definition. For (finite) discrete distributions it becomes simply a matrix \mathbf{F} . Hence, we can compare those matrices by an arbitrary matrix norm, e.g. by the Frobenius norm (metric) [14, 18].

2.2 Applications of Mutual Information Functions for Sequence Analysis in Bioinformatics

The consideration of organization processes, structuring and self-organization as well as information transfer belong to the key aspects of living systems [36, 9, 15, 16]. Thus information theoretic concepts play an important role in sequence analysis for understanding and analyzing RNA- and DNA- as well as protein sequences to explain biological systems [1].

Long-range correlations in sequences are well-known and intensively studied also in alignment free sequence comparison [28, 27, 32, 46]. The use of MIF as alternative to correlations was firstly investigated in [26] and this idea was renewed in [3] and [40]. It is followed by several studies using MIF for different topics like *in silico* comparison of bacterial strains using mutual information [41]. In [2], the MIF was renamed to be the *average mutual information profile* (AMI-profile) and proposed to serve as a genomic signature. This notation was taken over in the review [45] about information theoretic methods for sequence analysis. Following this notation, we denote the feature resolved mutual information function (rMIF) $F(x, \tau)$ from eq. (10) in this context also as the (feature) *resolved average mutual information profile* (rAMI-profile).

3 Rényi Information Concepts and α -scaled Mutual Information Functions

The Rényi-entropy

$$H_{\alpha}(X) = \frac{1}{1-\alpha} \log \left(\int_{\mathcal{X}} (p(x))^{\alpha} dx \right)$$

is a generalization of the Shannon-entropy, where $\alpha > 0$ and $\alpha \neq 1$ is a parameter [34]. Depending on the context it is also denoted as α -entropy. In the limit $\alpha \rightarrow 1$, the Shannon entropy is obtained. The Rényi-mutual-information (RMI) or α -mutual information (α -MI) is defined as

$$I_{\alpha}(X, Y) = \frac{1}{\alpha-1} \log \left(\int_{\mathcal{X}} \int_{\mathcal{Y}} \frac{(p(x, y))^{\alpha}}{(p(x))^{\alpha-1} \cdot (p(y))^{\alpha-1}} dy dx \right) \quad (12)$$

as outlined in [35]. This mutual information is widely applied in data analysis and pattern recognition as well as in information theoretic machine learning [10, 17, 21, 24, 33, 38, 44, 30, 4]. In analogy to the resolved mutual information rMI $F(x, Y)$ from eq. (10), we denote

$$F_\alpha(x, Y) = \int_{\mathcal{Y}} \frac{(p(x, y))^\alpha}{(p(x))^{\alpha-1} \cdot (p(y))^{\alpha-1}} dy \quad (13)$$

as the α -scaled resolved mutual information (α -rMI) or as α -scaled object dependent average mutual information profile (α -AMI-profile) in bioinformatics context.

The Rényi variant of the *cross mutual information* for sequences $X(t)$ and $Y(t + \tau)$ at time t with shift $\tau \geq 0$ is defined as

$$I_\alpha(X(t), Y(t + \tau)) = \frac{1}{\alpha - 1} \log \left(\int_{\mathcal{X}} \int_{\mathcal{Y}} \frac{(p(x(t), y(t + \tau)))^\alpha}{(p(x(t)))^{\alpha-1} \cdot (p(y(t + \tau)))^{\alpha-1}} dy(t + \tau) dx(t) \right) \quad (14)$$

which gives by setting $Y(t + \tau) = X(t + \tau)$

$$I_\alpha(X(t), X(t + \tau)) = \frac{1}{\alpha - 1} \log \left(\int_{\mathcal{X}} \int_{\mathcal{X}} \frac{(p(x(t), x(t + \tau)))^\alpha}{(p(x(t)))^{\alpha-1} \cdot (p(x(t + \tau)))^{\alpha-1}} dx(t + \tau) dx(t) \right)$$

as the Rényi variant of the *auto mutual information* at time t with shift (delay) τ . Again, if $p(x(t))$ is independent from t , only the joint probability $p(x(t), x(t + \tau))$ remains t -dependent such that it becomes dependent only on the shift τ and we simply write $p(x, x(\tau))$ for this. Hence, the Rényi auto mutual information in dependence on the shift τ is obtained as

$$I_\alpha(X, \tau) = \frac{1}{\alpha - 1} \log \left(\int_{\mathcal{X}} \int_{\mathcal{X}} \frac{(p(x, x(\tau)))^\alpha}{(p(x))^{\alpha-1} \cdot (p(x(\tau)))^{\alpha-1}} dx(\tau) dx \right)$$

and denoted as Rényi variant of, or α -scaled mutual information function (α -MIF). Accordingly, the α -scaled resolved version of α -MIF $I_\alpha(X, \tau)$ is

$$F_\alpha(x, \tau, X) = \int_{\mathcal{X}} \frac{(p(x, x(\tau)))^\alpha}{(p(x))^{\alpha-1} \cdot (p(x(\tau)))^{\alpha-1}} dx(\tau) \quad (15)$$

describing again the inherent correlations of the sequence and, hence, can serve as a characterizing quantity. We denote this function as the α -scaled resolved mutual information function (α -rMIF). In bioinformatics context it is denoted as α -scaled object dependent average mutual information profile (α -rAMI-profile). We immediately have

$$I_\alpha(X, \tau) = \frac{1}{\alpha - 1} \log \left(\int_{\mathcal{X}} F_\alpha(x, \tau) dx \right)$$

in complete analogy to eq. (11).

In contrast to eq. (6) being valid for the (Shannon) mutual information, now the inequality

$$I_\alpha(X, Y) \neq H_\alpha(X) + H_\alpha(Y) - H_\alpha(X, Y) \quad (16)$$

holds for RMI. Thus, the RMI is not based on the Rényi-entropy in a straightforward way as the Shannon mutual information is based on the Shannon entropy [17]. This problem arises from the difficulty to define a conditional Rényi entropy to be consistent with the setting in the Shannon case [8, 11, 42]. According to [20, 19] we can distinguish at least: [5, 43]

- Jizba-Arimitsu conditional Rényi-entropy

$$H_\alpha^{\text{JA}}(X|Y) = H_\alpha(X, Y) - H_\alpha(Y) \quad (17)$$

- Arimoto conditional Rényi-entropy

$$H_\alpha^{\text{A}}(X|Y) = \frac{\alpha}{1-\alpha} \log \left(\int_{\mathcal{X}} p(x) \left(\int_{\mathcal{Y}} (p(x|y))^\alpha dy \right)^{1/\alpha} dx \right) \quad (18)$$

- Hayashi conditional Rényi-entropy

$$H_\alpha^{\text{H}}(X|Y) = \frac{1}{1-\alpha} \log \left(\int_{\mathcal{X}} p(x) \left(\int_{\mathcal{Y}} (p(x|y))^\alpha dy \right) dx \right) \quad (19)$$

It can be shown that $H_\alpha^{\text{H}}(X|Y) \leq H_\alpha^{\text{A}}(X|Y)$ is valid using the Jensen's inequality [20]. Obviously, $H_\alpha^{\text{JA}}(X|Y)$ can be interpreted as an extension of the conditional Shannon entropy $H(X|Y)$ because the definition (17) precisely coincides with Shannon chain rule (7).

The non-negative Rényi- α -divergence is defined as

$$D_\alpha(X \parallel Y) = \frac{1}{\alpha-1} \log \left(\int_{\mathcal{X}} \int_{\mathcal{Y}} \frac{(p(x))^\alpha}{(p(y))^{\alpha-1}} dy dx \right) \quad (20)$$

with the limit $\lim_{\alpha \rightarrow 1} D_\alpha(X \parallel Y) = D_{KL}(X \parallel Y)$ being valid.

4 Resolved Mutual Information Functions for Characterization of Spatial Correlations between Nodes in Labeled Graphs

The above concepts for the (resolved) mutual information function for sequences can be easily transferred to labeled graphs. We assume a set \mathcal{G} of graphs G_k , each of which consists of N_k nodes n_j with node labels $l_j \in \mathcal{L}$ determining the class/type of the node regarding some given classification scheme \mathcal{L} . Further, let $\mathbf{D}^{(k)} \in \mathbb{R}^{N_k \times N_k}$ be the matrix of the, possibly directed and weighted, minimum graph distances (shortest path) between the node pairs of the graph G_k and $d_{\max} = \max_{i,j,k} (D_{i,j}^{(k)})$ the maximum node distance for all graphs to be considered. For undirected graphs, $\mathbf{D}^{(k)}$ is symmetric.

Let, $\mathcal{I}_{T,R} = [0, T]$ be an interval with a partition $P_T = \{\tau_0 = 0, \tau_1, \dots, \tau_R = T\}$ such that $\tau_i < \tau_j$ holds for $i < j$. The *dominating distance* $\tau_i(z)$ for a given value z is defined by the inequalities $\tau_{i-1} < z \leq \tau_i$ to be valid. Let $p(l)$ be the probability of the label $l \in \mathcal{L}$ in a graph G and $p(l, l')$ the respective joint probabilities.

Using these definitions we can determine in analogy to (9) the Shannon mutual information function (MIF) for graph as

$$I(G_k, \tau_r) = \sum_{i=1}^{N_k} \sum_{j=1}^{N_k} \delta(\tau_r, \tau_i(D_{i,j}^{(k)})) \cdot p(l_i, l_j) \cdot \log \left(\frac{p(l_i, l_j)}{p(l_i) \cdot p(l_j)} \right) \quad (21)$$

where

$$\delta(z, z') = \begin{cases} 1 & \text{for } z = z' \\ 0 & \text{for } z \neq z' \end{cases}$$

is the Kronecker-symbol and $\tau_r \in P_T$. Accordingly, the resolved MIF (rMIF) for graphs reads as

$$F(l_i, \tau, G_k) = \sum_{j=1}^{N_k} \delta(\tau_r, \tau_i(D_{i,j}^{(k)})) \cdot p(l_i, l_j) \cdot \log\left(\frac{p(l_i, l_j)}{p(l_i) \cdot p(l_j)}\right) \quad (22)$$

with $l_i \in \mathcal{L}$.

Applying the Rényi-variants α -MIF and α -rMIF to graphs, we obtain

$$I_\alpha(G_k, \tau) = \frac{1}{\alpha - 1} \log\left(\sum_{i=1}^{N_k} \sum_{j=1}^{N_k} \delta(\tau_r, \tau_i(D_{i,j}^{(k)})) \cdot p(l_i, l_j) \cdot \frac{(p(l_i, l_j))^\alpha}{p(l_i)^{\alpha-1} \cdot p(l_j)^{\alpha-1}}\right)$$

and

$$F_\alpha(l_i, \tau, G_k) = \sum_{j=1}^{N_k} \delta(\tau_r, \tau_i(D_{i,j}^{(k)})) \cdot p(l_i, l_j) \cdot \frac{(p(l_i, l_j))^\alpha}{p(l_i)^{\alpha-1} \cdot p(l_j)^{\alpha-1}}$$

respectively.

5 Conclusion

In this technical report we provide information theoretic concepts and quantities to characterize spatial correlations in sequences and labeled graphs. In particular, we introduced several types of mutual information functions for both, Shannon and Rényi information theoretic approaches. These functions/quantities can be used to compare those objects (sequences/graphs) in machine learning approaches regarding their inherent spatial correlations. Respective applications we see for sequence analysis in bioinformatics and text analysis as well as for social relation analysis by means of graphs as well as for other relational graphs, e.g. chemical structural formulae.

In the future work we will extend these approaches to further mutual information concept related to other widely considered entropy measures and information theoretic quantities, e.g. Tsallis-entropies and divergences or more general α -, β - and γ -divergences with related mutual informatin concepts .

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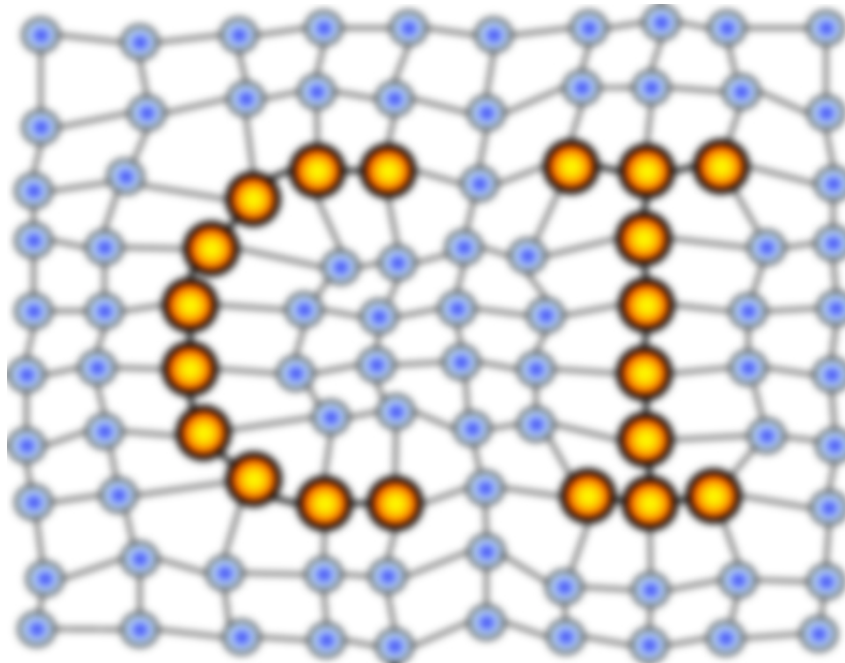
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