Learning Scale Free Network by Node Specific Degree Prior

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Abstract

Learning the network structure underlying data is an important problem in machine learning. This paper introduces a novel prior to study the infernece of scale-free networks, which are widely used to model social and biological networks. The prior not only favors a desirable global node degree distribution, but also takes into consideration the relative strength of all the possible edges adjacent to the same node and the estimated degree of each individual node. To fulfill this, ranking is incorporated into the prior, which makes the problem challenging to solve. We employ an ADMM (alternating direction method of multipliers) framework to solve the Gaussian Graphical model regularized by this prior.

1. Introduction

Graphical models are widely used to describe the relationship between variables (or features). Estimating the structure of an undirected graphical model from a dataset has been extensively studied (Meinshausen & Bühlmann, 2006; Yuan & Lin, 2007; Friedman et al., 2008; Banerjee et al., 2008; Wainwright et al., 2006). Among those methods, $l_1$ penalty is usually used to regulate the log-likelihood function in order to generate a sparse graph structure. In Gaussian Graphical Models (GGMs) for example, we assume that the observed data follows a multivariate Gaussian distribution with a covariance matrix $\Sigma$. It is known that the network dependency structure is encoded in the zero pattern of precision matrix $\Omega = \Sigma^{-1}$. Then the $l_1$ penalized problem can be formulated as minimizing the negative log-likelihood function with an $l_1$ penalty on $\Omega$. However, the mostly-used $l_1$ penalty assumes that any pair of variables is equally likely to form an edge. This is inconsistent with many real-world networks such as gene networks and social networks, which are better described as scale-free networks.

A scale-free network (BARABÁSI & Bonabeau, 2003) consists of nodes with degree following the power-law distribution. In particular, a scale-free network may contain a few hub nodes, whose degrees are usually much larger than non-hub nodes. That is, the hub nodes are more likely to form an edge than the non-hub nodes. In a gene network, a hub usually represents a gene playing functions in many biological processes (Zhang & Horvath, 2005; Goh et al., 2007). There are examples papers studying inference of scale-free networks by improving the reweighted $l_1$ norm on the model parameters, say $\Omega$ in GGMs. For example, (Peng et al., 2009) proposed a joint regression sparse method to learn scale free networks by setting the penalty proportional to the estimated degrees. (Candes et al., 2008) proposed a method that iteratively reweighs the penalty in the $l_1$ norm based on the inverse of the previous estimation of $\Omega$. This method can suppress the large bias in the $l_1$ norm when the magnitude of the non-zero entries vary a lot and is also closer to the $l_0$ norm. Some recent papers follow the idea of node-based learning using group lasso...
(Friedman et al., 2010b; Meier et al., 2008; Tan et al., 2014; Friedman et al., 2010a; Mohan et al., 2014). Since group lasso penalty favors similar edge patterns for the variables in the same group, the nodes from different groups that interact weakly may be totally disconnected in the inferred networks. As such, group lasso may only produce edges adjacent to nodes with a large degree (i.e., hubs).

The methods above indeed improve their performance over the $l_1$ norm, but none of them can fit well the scale-free property of the target network. (Liu & Ihler, 2011) minimizes the negative log likelihood with a scale-free prior, where the degree is approximated by the $l_1$ norm. However, the objective function is non-convex, and is hence hard to optimize. (Defazio & Caetano, 2012) introduces another way to approximate the global node degree distribution by the submodular convex envelope of the node degree function. The convex envelope, also named as the Lovasz extension, tackles the above problem by introducing a convex penalty. These methods consider only the global degree distribution, but not the degree of each individual node.

To improve the inference of scale-free networks, this paper introduces a new prior, which not only favors a desirable global node degree distribution, but also takes into consideration the relative strengths of all the possible edges adjacent to the same node and the expected degree of each individual node. To fulfill this, we use node and edge ranking to dynamically determine the relative strength of one potential edge and to estimate the degree of an individual node. As dynamic ranking is used in the prior, the objective function is very challenging to optimize. This paper describes a novel ADMM (alternating direction method of multipliers) (Boyd et al., 2011) method to optimize our objective function.

2. Model

2.1. Notation & Preliminaries

Let $G = (V,E)$ denote a graph, where $V$ is vertex set $(p = |V|)$ and $E$ is edge set. Let $A$ denote the adjacency matrix of $G$, i.e., $A_{ij} = 1$ if and only if $(i,j) \in E$. The graph structure is encoded in the zero pattern of the estimated $X$, i.e. the edge formed by $X$ is $E(X) = \{(u,v) \mid [X_{uv}] \neq 0\}$. Let $F(X)$ denote the objective function describing the graph structure, which usually is negative log-likelihood (NLL). For example, in GGMs, $F(X) = tr(XS) - \log \det X$, where $S$ is the empirical covariance matrix of data $Z$. To induce sparsity of the parameter $X$, a $l_1$ penalty of $X$ is applied. The objective can then be formulated as

$$\hat{X} = \arg \min_X F(X) + \lambda \|X\|_1. \quad (1)$$

Given a $p \times p$ matrix $X$, we define two permutation functions. Let $(X_i)\_1$ be a permutation of a row vector $X_i$ (excluding the element $X_{i,i}$), satisfying $|X_{i,i}| \geq |X_{i,j}| \geq ... \geq |X_{i,p-1}|$. Let $(j,X_i)$ denote the index of the $j^{th}$-ranked element. When the context is clear, we use $X_{i,(j)}$ to indicate this element. Let $A$ and $B$ be two positive vectors with $p - 1$ and $p$ elements, respectively. Denote $X_{i} \circ A = \sum_{u=1}^{|X_{i,(u)}|} [X_{i,(u)}]A_u$. Let $[X,A,B]$ be a permutation of $X$ based upon $A$ and $B$ satisfying $X_{[1,X,A,B]} \circ A + B_2 \geq X_{[2,X,A,B]} \circ A + B_2 \geq \geq X_{[p,X,A,B]} \circ A + B_p$, where $[j,X,A,B]$ denote the $j^{th}$-ranked row. When $B$ is zero, we also write $[X,A,B]$ as $[X,A]$ and $[j,X,A,B]$ as $[j,X,A]$, respectively.

A natural way to learn a sparse graph is to add a $l_1$ penalty to regulate $F(X)$. However, $l_1$ norms doest not fit well for a scale free network. The main reason is that the node degree in scale free networks follows the power-law distribution, i.e., $P(d) \propto d^{-\alpha}$ where $d$ is the degree and $\alpha$ is a constant usually ranging from 2 to 3, rather than uniform distribution. A simple prior to favor scale free networks is the sum of the logarithm of node degree as follows:

$$\lambda \sum_{v=1}^p \alpha \log(d_v + 1), \quad (2)$$

where $d_v = ||X_v||_0 = \sum_{u=1}^p I[X_{uv} \neq 0]$ and $I$ is the indicator function. The constant $I$ is added to $d_v$ to handle the situation when $d_v = 0$. The $l_0$ norm in (2) is non-differentiable and thus, hard to optimize. Although it can be approximated by the $l_1$ norm(Liu & Ihler, 2011), a better approximation based on submodular function and Lovasz extension is introduced recently (Defazio & Caetano, 2012). The definition of submodular function and Lovasz extension are as follows.

Definition 1. Given a set $V = \{1,2,\ldots,p\}$, a set function $S : 2^V \rightarrow R$ is a submodular if and only if $S(\phi) = 0$ and for any $A \subseteq V$ and $B \subseteq V$ we have $S(A) + S(B) \leq S(A \cap B) + S(A \cup B)$.

Definition 2. Given weight $W = \{w_1,w_2,\ldots,w_p\}$ for nodes in $V$ where $w_i \geq 0$. Assume $w_{j_1} \geq w_{j_2} \geq \cdots \geq w_{j_u}$, then the Lovasz extension of the above-defined submodular function $S$ is $f_S(W) = \sum_{u=1}^p w_{j_u} (S(\{j_1,j_2,\ldots,j_u\}) - S(\{j_1,j_2,\ldots,j_{u-1}\})$. The relationship between the submodular function and Lovasz extension is described by the following proposition.

Proposition 1. The minimal value of the submodular function is equal to the minimal value of Lovasz extension if $W \in [0,1]^p$, i.e.

$$\min_{A \subseteq V} S(A) = \min_{W \in [0,1]^p} f_s(W) \quad (3)$$

By using Lovasz extension, instead of directly optimizing the set function, which usually involves an exponential number of combinations, we can optimize with respect
to real-valued variable $W$. We can further assume that $W \in R^p$, which is still a reasonable relaxation of the submodular function (Defazio & Caetano, 2012).

Let $X_{uv}$ denote the estimated interaction strength between two nodes $u$ and $v$. Denote the set function $d_E(\{(u,v), i = 1, \ldots, m\}) = \sum_{i=1}^{m} I[X_{uv} \neq 0]$. Let $d_E(v)$ denote $d_E(\{(u,v), u \in V\})$ which simply is the definition of degree for node $v$ in the set function language. Let $h_E(\{(u,v), i = 1, \ldots, m\}) = \log(\sum_{i=1}^{m} I[X_{uv} \neq 0] + 1)$. To favor the power-law distribution, the log-likelihood for the edge set $E$ can be written as $S(E) = \sum_{v \in V} h_E(v) = \sum_{v \in V} \log(d_E(v) + 1)$. It is easy to prove that both $S(E)$ and $h_E(v)$ are submodular. Note that even though we use $h_E(v)$ and $d_E(v)$ to represent the set functions, they are actually defined on a set of edges between nodes $v$ and the others.

This set function is hard to optimize. To make the optimization problem easier to tackle, (Defazio & Caetano, 2012) introduced the Lovasz extension of $h_E(v)$.

**Proposition 2.** The Lovasz extension of $h_E(v)$ is

$$
\sum_{u=1}^{p-1} |X_{v,(u)}| \left(h_E(\{(v, (1, X_v))\}, \ldots, (v, (u, X_v))) - h_E(\{(v, (1, X_v))\}, \ldots, (v, (u-1, X_v)))\right),
$$

Further, it is easy to show that eq.(4) is equivalent to the following equation.

$$
\sum_{u=1}^{p-1} |X_{v,(u)}| \left(\log(u+1) - \log(u)\right).
$$

Let $h'(u) = (\log(u+1) - \log(u))$. The Lovasz extension of a single node $v$ is

$$
\sum_{u=1}^{p-1} h'(u) |X_{v,(u)}|
$$

Therefore, instead of optimizing Eq.(1), which is usually difficult to achieve, we can optimize the following objective function.

$$
F(X) + \lambda \sum_{v=1}^{p} \sum_{u=1}^{p-1} h'(u) |X_{v,(u)}|
$$

Meanwhile, Lovasz extension can be interpreted as a reweighted $l_1$ norm. However, in order to use this norm, all the potential edges adjacent to node $v$ have to be sorted in a descending fashion according to their estimated strengths, i.e. their absolute values.

### 2.2. Dynamic Node Specific Prior

In this section we present our new prior by exploiting more detailed information in the estimated matrix $X$. Intuitively, given a node $u$, if we rank all the potential edges adjacent to $u$ in descending order by $|X_{u,v}|$ where $v \in V - u$, then $(u,v)$ with a higher rank is more likely to be a true edge than those with a lower rank. In addition, if both nodes $u$ and $v$ have large degrees, then $(u,v)$ is more likely to be a true edge. We introduce a new prior called “dynamic node specific penalty” to model these two intuitions.

To model the first one, we introduce a non-decreasing positive sequence $H$ and the following prior.

$$
\sum_{u=1}^{p-1} H(v) |X_{u,(v)}|
$$

Where $(v)$ represents the node ranked in the $v^{th}$ position. When $H$ is a constant, the prior above simply is $l_1$ norm. In the experiment, we set $H(v) = \log(v+1)^{0.15}$ for $v = 1, 2, ..., p - 1$. The intuition is to use a slowly increasing penalty such that a pair $(u,v)$ with a larger estimated $|X_{u,v}|$ has a smaller penalty. On the other hand, $(u',v')$ with a relatively smaller estimated $|X_{u',v'}|$ should not be punished too much.

To model the second intuition, we use a prior function for each individual node based upon its estimated degree. Ideally, we would like to rank all the nodes by their degrees, but this information is not available in most cases, so we rank them in descendingly by Lovasz extension. Here we use the Lovasz extension instead of the $l_1$ norm for approximate ranking because the former favors non-equal signals rather than equal but weak signals (Defazio & Caetano, 2012). Let $E(k)$ denote the expected number of nodes with degree $k$. We can estimate $E(k)$ from the prior degree distribution $p_d(k) \propto d^{-\alpha}$ when $\alpha$ is given. Let all the nodes are ranked in descending order by their degree, we use $\tau$ to denote the rounded expected degree of the $i^{th}$ ranked node based on power-law prior, such that $\tau_1 \geq \tau_2 \geq \cdots \geq \tau_p$.

Then for the $i^{th}$-ranked node we define

$$
g(i) = \frac{1}{H(\tau_i)}
$$

and our dynamic node specific prior function as follows.

$$
\Omega(X) = \sum_{v=1}^{p} g(v) X_{v,X,h'} \circ H
$$

Our prior function is dynamic and non-uniform since it depends on the ranking of nodes according to its estimated degree. This prior has the following properties.

- Given the $v^{th}$-ranked node with approximate degree $\tau_v$, the penalty for the $X_{[v,X,h'],(u)}$ such that $u \leq \tau_v$
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is less than or equal to 1, and the penalty for those $u > \tau_u$ is larger than 1. This implies that Eq.(10) is consistent with the expected degree for each node. And dynamically modeling the expected degree of each node allows the degree distribution to follow the power law.

- If node $i$ 's degree is higher than node $j$'s, then variable $X_{i,(u)}$ has a smaller penalty than $X_{j,(u)}$.
- The penalty for $X_{u,v}$ depends on the expected degree of nodes $u$, $v$ and the ranking of $(u,v)$ among all the possible edges adjacent to node $u$ or $v$.

3. Optimization

With prior defined in (10), we have the final form of the objective function:

$$F(x) + \beta \sum_{v=1}^{p} g(v) X_{[v,x,h']} \circ H$$ (11)

Here $\beta$ is used to control sparsity level. The challenge for minimizing Eq.(11) lies in the fact that both edge and node ranking are involved in the optimization procedure. We use an ADMM algorithm to solve it by introducing dual variables $Y$ and $U$. The detailed procedure of ADMM is described as follows:

$$X^{t+1} = \arg \min_X F(X) + \frac{\beta}{2} \|X^t - Y^t + U^t\|_F^2$$ (12)

$$Y^{t+1} = \arg \min_Y \beta \Omega(Y) + \frac{\beta}{2} \|X^{t+1} - Y + U^t\|_F^2$$ (13)

$$U^{t+1} = U^t + X^{t+1} - Y^{t+1}$$ (14)

For the first sub-problem, we can use any first-order method such as gradient descent to optimize it since we assume that $F(X)$ is convex. Here we describe a novel procedure for (13).

Let $A = X^{t+1} + U^t$, and $\lambda = \frac{\beta}{\rho}$. Minimizing (13) is equivalent to

$$\min_Y \frac{1}{2} \|Y - A\|_F^2 + \lambda \Omega(Y),$$ (15)

which can be relaxed as

$$\min_Y \frac{1}{2} \|Y - A\|_F^2 + \lambda \sum_{v=1}^{p} g(v) Y_{[v]} \circ H$$

s.t. $g([v]) = g([v,Y,h'])$ 1 \leq v \leq p. (16)

Here, we simply use $[\cdot]$ to denote a permutation of \{1, 2, ..., p-1\}, and use $[v]$ to denote the $v^{th}$ element of this permutation. (16) can be relaxed by solving the following problem until $g([v,Y,H,\delta]) = g([v,Y,h'])$ 1 \leq v \leq n.

$$\min_{Y,\delta} \frac{1}{2} \|Y - A\|_F^2 + \lambda \sum_{v=1}^{p} g(v) \{Y_{[v,Y,H,\delta]} \circ H\}$$ (17)

Here $\delta(v)$ is the dual variables we introduced and would typically be updated as $\delta(v) = \mu \cdot (g([v,Y,H,\delta]) - g([v,Y,h'])$, where $\mu$ is the step size. To solve (17), we use algorithm 1, an algorithm similar to dual decomposition.

Algorithm 1 Node rank updating

1: Randomly generate $Y^0$. Set $t = 0, \delta^0 = 0$ and compute $[Y^0, H, \delta^0]$
2: while TRUE do
3: $Y^{t+1} = \arg \min_Y \frac{1}{2} \|Y - A\|_F^2 + \lambda \sum_{v=1}^{p} g(v) Y_{[v,Y',H,\delta']} \circ H$
4: $\delta^{t+1} = \delta^t + \mu (g([Y^{t+1}, H, \delta^t]) - \delta^t)$
5: if $[Y^{t+1}, H, \delta^t] = [Y^t, H, \delta^t] = [Y^{t+1}, h^t]$ then
6: break
7: else
8: $\delta^{t+1} = \delta^t + \mu (g([Y^{t+1}, H, \delta^t]) - \delta^t)$
9: end if
10: $t = t + 1$
11: end while

Theorem 1. The output of algorithm 1 satisfies

$$Y' = \arg \min_Y \{\frac{1}{2} \|Y - A\|_F^2 + \lambda \sum_{v=1}^{p} g(v) Y_{[v,Y',H,\delta]} \circ H\}$$ (18)

Please refer to supplementary for proof of Theorem 1.

Solving line 3-4 in Algorithm 1 is not so trivial. The problem can be reformulated as

$$\min_{v=1}^{p} \{\frac{1}{2} \|Y_v - A_v\|_F^2 + Y_v \circ H'(v)\}.$$ (19)

where $H'(v) = \lambda g(v) H(u)$. Since $Y$ is symmetric, problem (19) can be re-formulated as follows,

$$\min_{v=1}^{p} \{\frac{1}{2} \|Y_v - A_v\|_F^2 + Y_v \circ H'\}$$ s.t. $Y = Y^T$. (20)

Problem (20) can be solved iteratively by introducing the Lagrangian term $< \sigma, Y - Y^T >$, where $\sigma$ is updated by $\sigma + = Y - Y^T$. Then (20) can be decomposed into $n$ independent sub-problems each iteration:

$$\frac{1}{2} \|Y_v - A_v - \sigma^T + \sigma\|_F^2 + Y_v \circ H'$$ (21)
Theorem 2. Let $y$ of elements in $T$ into $\{C\}$ denote this method as “Hub”. When testing this method, we use $\alpha$ to control the sparsity, i.e. the number of edges in predicted graph.

Recently (Defazio & Caetano, 2012) proposed a Lovasz extension approach to approximate degree by a convex function. However, the resultant penalty is counter-intuitive since it assigns a larger penalty to the node with a larger expected degree.

(Tan et al., 2014) proposes a method specifically for a graph with a few hubs and applied a group lasso penalty. In particular, they decomposed $X$ as $Z + V + V^T$, where $Z$ is a sparse symmetric matrix, and $V$ is a matrix whose column are almost entirely zero or entirely non-zero. Intuitively $Z$ describes the relationship between non-hubs, and $V$ describes the relationship between hubs. They formulated the problem as follows.

$$\min_{V,Z} F(X) + \lambda_1 \|Z\|_1 + \lambda_2 \|V\| + \lambda_3 \sum_{j=1}^p \|V_j\|_2$$

subject to $X = Z + V + V^T$.

An ADMM algorithm is used to solve this problem. We denote this method as “Hub”. When testing this method, we use $\lambda_3 = 0.01$ to yield the best performance in our simulations. Besides, we set $\lambda = \lambda_1 = \lambda_2$ to obtain the graph with a desired level of sparsity.

Our method involves 2 hyper-parameters: $\gamma$ and $\beta$. Meanwhile, $\gamma$ is the hyper parameter for the power-law distribu-
5. Results

We tested our method on a real gene expression dataset and two types of simulated networks: (1) a scale-free network generated by Barabasi-Albert (BA) model and (2) a network with a few hubs. We generated the data for the simulated scale-free network by its corresponding Multivariate Gaussian distribution. We compared our method (denoted as "DLovasz") with graphical lasso ("Glasso") (Friedman et al., 2008), neighborhood selection ("NS") (Meinshausen & Bühlmann, 2006), reweighted $l_1$ regularization ("RW") (Liu & Ihler, 2011) and a recent hub detection method ("Hub") (Tan et al., 2014).

5.1. Performance on Scale-Free Networks

We generated a network of 500 nodes ($p = 500$) by the BA model. Each entry $\Omega_{uv}$ of the precision matrix is set to 0.3 if $(u, v)$ forms an edge, and 0 otherwise. To make the precision matrix positive definite, we set the diagonal of $\Omega$ to be the minimum eigenvalue of $\Omega$ plus 0.2. In total we generate 250 data samples from the corresponding multivariate Gaussian distribution ($n = 250$). The hyper-parameters of all the methods are set as described in the last section.

![Figure 2. Simulation results on a scale free network. Gaussian Graphical Model is used and $n = 250$ and $p = 500$. X-axis is the number of predicted edges and Y-axis is the number of correctly predicted edges.](image2.png)

Our method is not sensitive to the hyper-parameter $\gamma$. In Figure 2, the predictions with different $\gamma$ ($\gamma = 2.1, 2.5, 2.9$) yield almost the same result. Hence we use $\gamma = 2.5$ in the following experiments.

Moreover, as shown in Figure 2, our method DLovasz is almost always better than the others in terms of predicted accuracy. It is not surprising that both RW and Hub outperform Glasso and NS since RW and Hub are specifically designed for scale-free or hub networks.

In Figure 1, we also plot the log-log degree distribution for the true network and the networks estimated by DLovasz, RW and Glasso. Both DLovasz and RW fit well with the power-law distribution while Glasso does not, which confirms that both DLovasz and RW indeed favor scale free networks.

![Figure 3. Visualization of the hub network. The network consists of 1643 nodes and 3996 edges. For visualization purpose we remove the connected component with size less than or equal to 4. We also highlight the hubs in the network, where hub is defined as nodes such that their degrees are at least 30.](image3.png)

![Figure 4. Simulation for the Gaussian Graphical Models on a hub network, where $n = 806$ and $p = 1643$. X-axis is the number of predicted edges and Y-axis is the number of correctly predicted edges.](image4.png)
Figure 1. This figure shows the log-log degree distribution for (1) true network (2) DLovasz (3) RW and (4) Glasso. Linear relationship is expected since the true network is scale-free. The Glasso’s distribution violates most the assumption since there is a point around (2,0).

5.2. Performance on Hub Networks

We also tested our method on a hub network, i.e. the network containing a few nodes with much larger degrees. See Figure 3 for a visualization, where larger dots indicate the hub nodes. The data is obtained from DREAM5 dataset 1, in which a simulated gene expression data with 806 samples and a ground truth edge set are provided. Please refer to (Marbach et al., 2012) for more details. The result in Figure 4 shows that our method outperforms all the others, although our method is not specifically designed for hub networks.

5.3. Gene Expression Data

To further test our method, we applied it to a Saccharomyces cerevisiae genome expression data set in DREAM5, which contains 805 samples and 4511 genes. The ground truth edge set consists of 3902 edges. See (Marbach et al., 2012) for a detailed description of the data. After removing the 0-degree nodes in the ground truth, there are 1081 genes (i.e., \( p = 1081 \)). We determine the hyper parameters of all the methods such that they output exactly the same number of edges. As shown in Figure 5, our method obtains much higher accuracy than the other methods.

We choose the values of the hyper-parameters such that each method predicts 4000 edges. The degree distributions of the resultant networks are shown in Figure 6. As shown in this figure, our estimated network is more similar to a scale free network. Further, our method detects 8 hubs (with degree > 40), two (gadX and gadE) of which are known to play important functions. In particular, gadX is a transcriptional regulator of glutamic acid decarboxylase system, regulating biofilm formation (Hodges et al., 2010); gadE is a regulator involved in the regulation of several genes required in the maintenance of pH homeostasis (Hommais et al., 2004).

6. Conclusions

We have presented a novel node-specific prior to study the inference of scale-free networks, which are widely used to model social and biological networks. Our prior not only favors a desirable global node degree distribution, but also takes into consideration the relative strength of all the possible edges adjacent to the same node and the estimated degree of each individual node. To fulfill this, we have developed a ranking-based algorithm to dynamically modeling the degree distribution of a given network. The optimization problem resulting from our prior is quite challenging.
We have developed a novel ADMM algorithm to solve it. We have demonstrated the superior performance of our prior through simulations and two DREAM5 datasets. Our prior greatly outperforms the others in terms of the number of correctly predicted edges, especially on the real gene expression data.

The idea presented in this paper can potentially be useful to other degree-constrained network inference problem. In particular, it might be applied to infer protein residue-residue interaction network from a multiple sequence alignment, for which we may predict the degree distribution of each residue using a supervised machine learning method.

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