Inferring higher-order co-occurrence patterns and **simplicial complexes** from presence/absence data

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How to infer higher-order co-occurrence patterns and simplicial complexes from presence/absence data?

By using log-linear models and hypothesis testing!

	Site 1	Site 2	Site 3	Site 4	Site 5
Species A	1	0	1	1	0
Species B	1	1	0	1	0
Species C	0	0	0	0	1

Step 1 : Fill a contingency table for each pair

	Site 1	Site 2	Site 3	Site 4	Site 5
Species A	1	0	1	1	0
Species B	1	1	0	1	0

→

Contingency table : Count how many times a specific presence/absence situation appeared in the data.

	Species $B = 0$	Species $B = 1$	Total
Species A $= 0$	$x_{00} = 1$	$x_{01} = 1$	$x_{0+} = 2$
Species A $= 1$	$x_{10} = 1$	$x_{11} = 2$	$x_{1+} = 3$
Total	$x_{+0} = 2$	$x_{+1} = 3$	$N = 5$

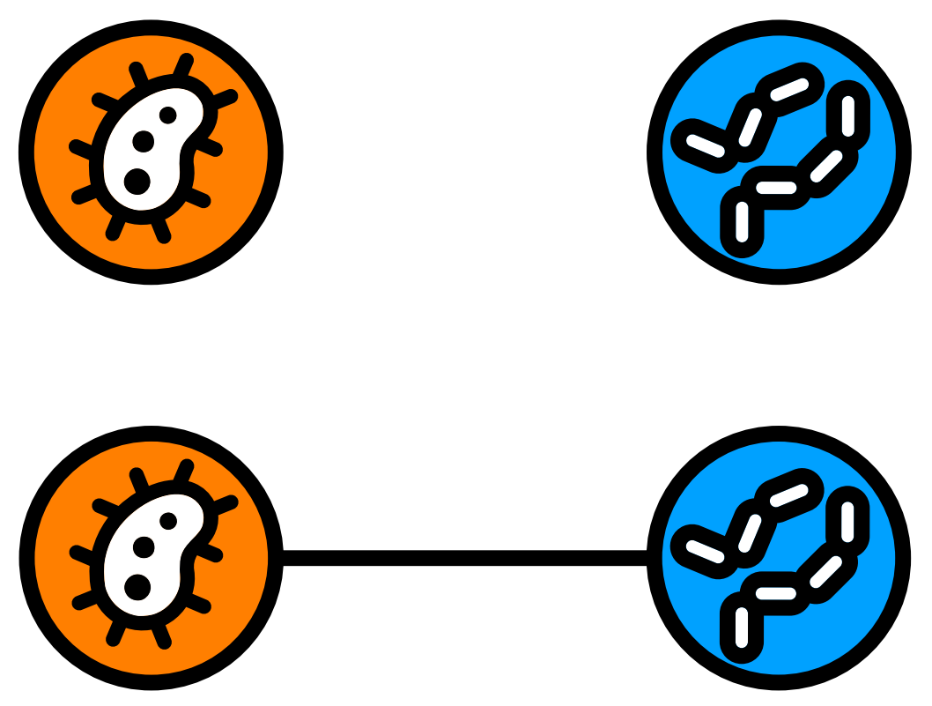
Step 2 : Set hypotheses and corresponding log-linear models

H_0 : Species i and j occur independently.

$$\log(m_{ij}) = u + u_i^A + u_j^B$$

H_1 : Species i and j are correlated.

$$\log(m_{ij}) = u + u_i^A + u_j^B + u_{ij}^{AB}$$



Contingency tables are instances of a **multinomial distribution**. The log-likelihood of the distribution is given by

$$\log\left(\frac{N!}{\prod_{ij} x_{ij}!}\right) + \sum_{i,j} x_{ij}\log(m_{ij}) - N\log(N),$$

N is the total number of observations;
x_{ij} are the cell entries in the contingency table;
m_{ij} are the expected counts in the multinomial distribution.

Step 3 : Find expected values under H_0

We rewrite the log-likelihood of the sampling distribution as

$$\log\left(\frac{N!}{\prod_{ij} x_{ij}!}\right) + \sum_{ij} x_{ij}\left(u + u_i^A + u_j^B\right) - N\log(N),$$

and design an iterative procedure to find the maximum likelihood estimates.

	Species $B = 0$	Species $B = 1$
Species A $= 0$	$\hat{m}_{00}$	$\hat{m}_{01}$
Species A $= 1$	$\hat{m}_{10}$	$\hat{m}_{11}$

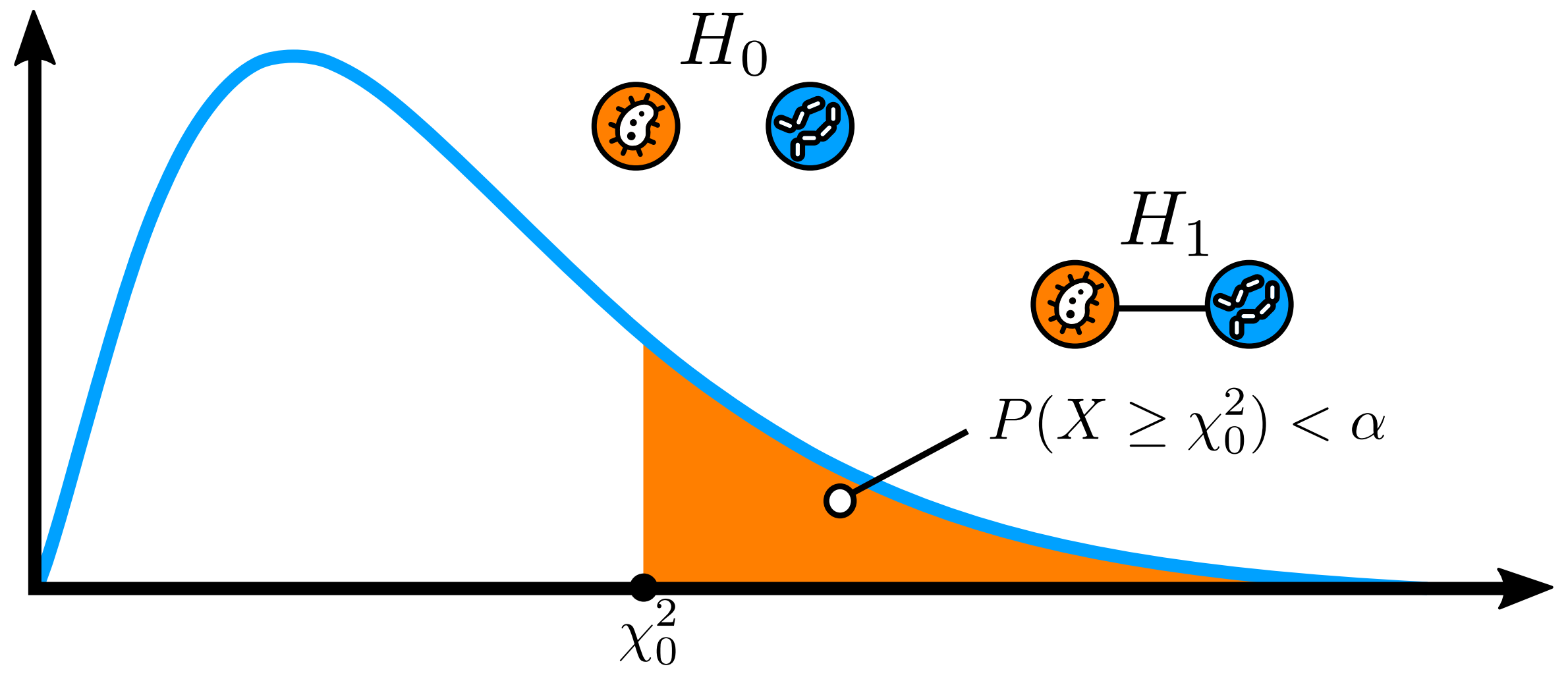
$\hat{m}_{ij}$ maximum likelihood estimates under H_0

Step 4 : Test H_0 using χ^2 statistics

Using the χ_0^2 statistics, we measure how close our observations are from the expected values under H_0. We compute the statistics with

$$\chi_0^2 = \sum_{i,j} \frac{(x_{ij} - \hat{m}_{ij})^2}{\hat{m}_{ij}}.$$

We reject the hypothesis with a significance level α if the probability of drawing χ_0^2 from a χ^2 distribution is smaller than α.

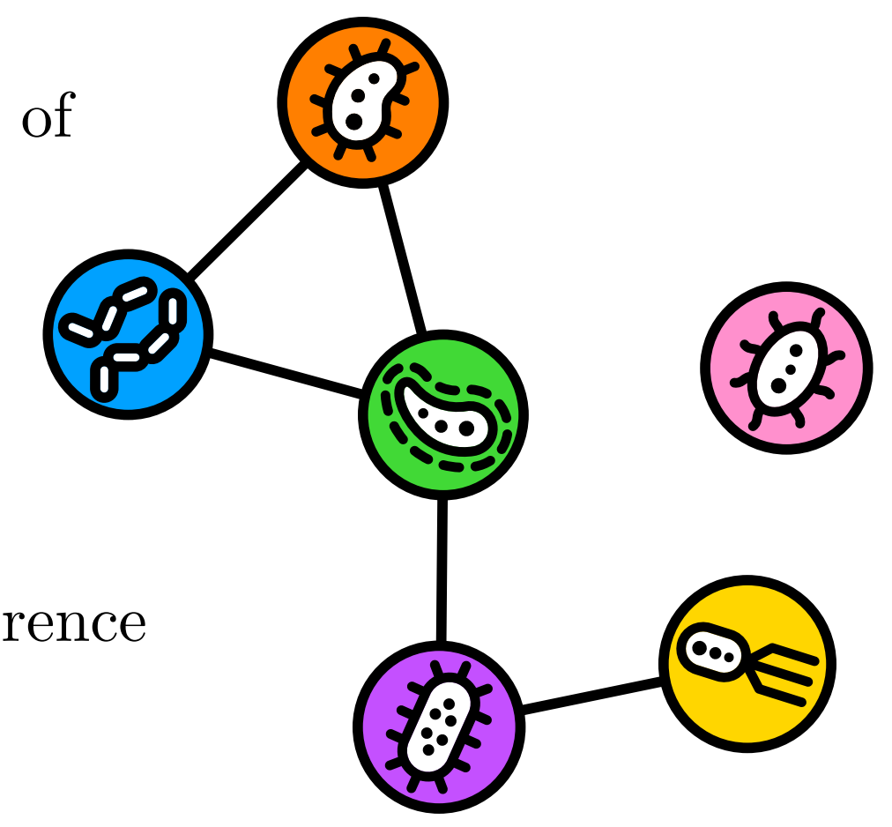


Step 5 : Repeat for each pair

By repeating for each pair, we infer a **network** of statistically significant co-occurrences!

Nodes : Observed species

Links : Probabilistic dependencies in the occurrence



When the **number of observations is low**, the statistics is not distributed as a χ^2distribution and step 4 **will not give an accurate result**.

In that case we **need to** generate the **exact distribution** of the statistics for each pair.

Step 6 : Repeat for each triple with higher-order log-linear models

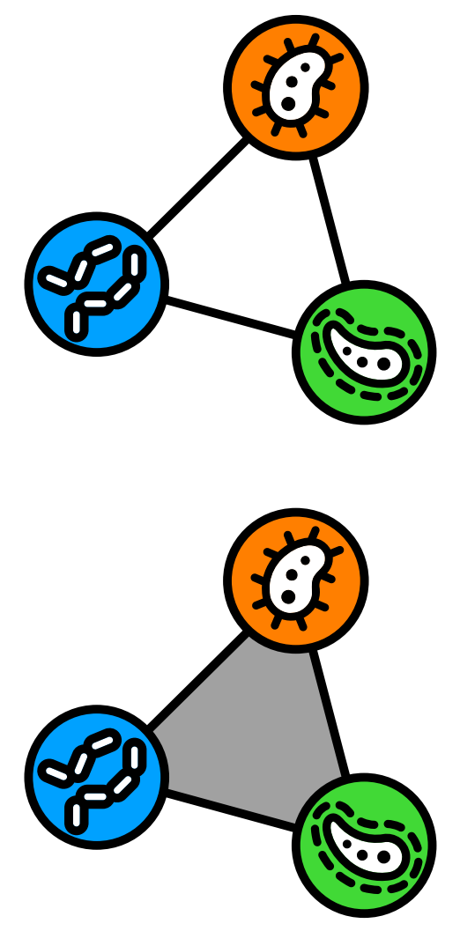
The **only extra steps** are to find the **new log-likelihood** and set the **appropriate hypotheses.**

H_0: Species i, j and k are dependent through pairwise dependencies.

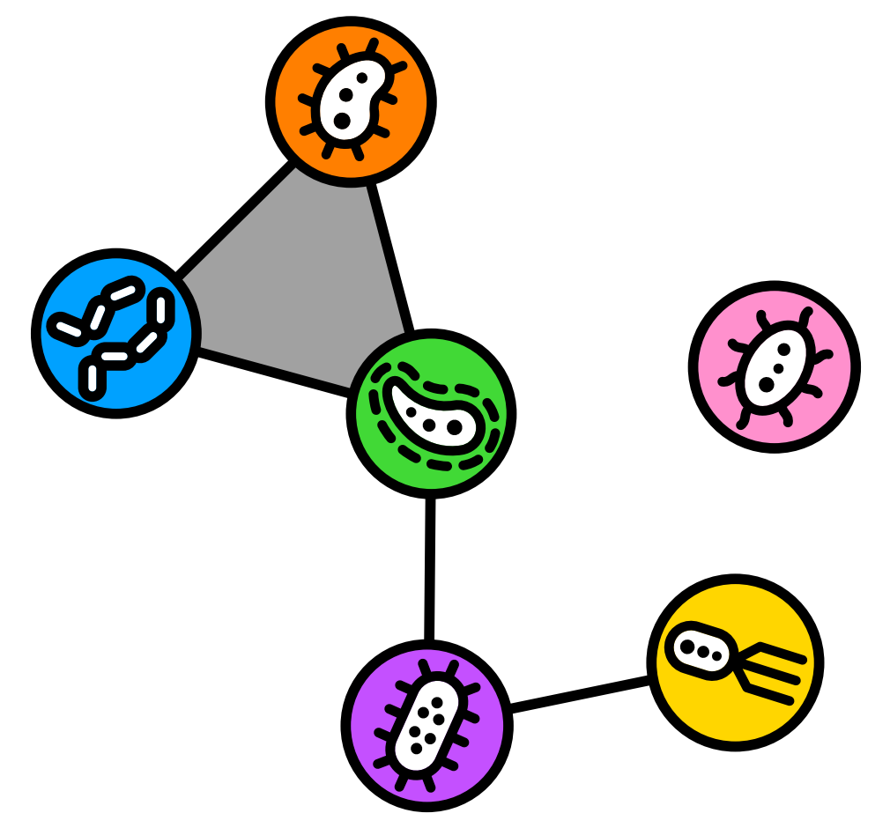
$$\log(m_{ijk}) = u + u_i^A + u_j^B + u_k^C + u_{ij}^{AB} + u_{ik}^{AC} + u_{jk}^{BC}$$

H_1: Species i, j and k form a higher-order co-occurrence pattern.

$$\log(m_{ijk}) = u + u_i^A + u_j^B + u_k^C + u_{ij}^{AB} + u_{ik}^{AC} + u_{jk}^{BC} + u_{ijk}^{ABC}$$



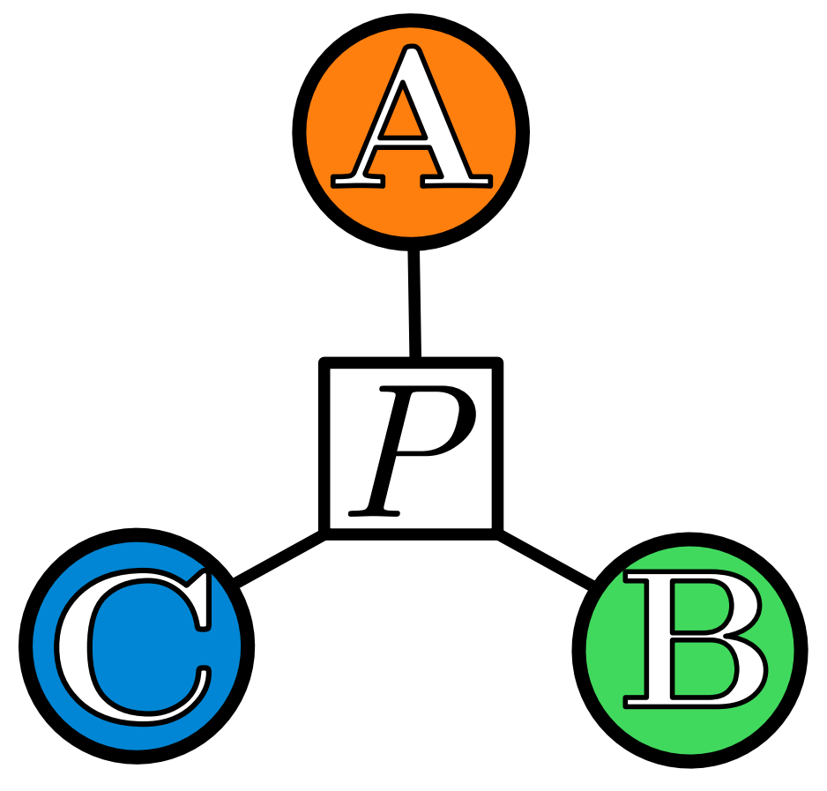
We obtain a **simplicial complex** with **higher-order co-occurrence patterns!**



Repeat this procedure for the highest possible order!

Validation of the inference method with a generative model

A **factor graph** is a bipartite graph that encodes the relationship between random variables via factor nodes. The probability of drawing a particular state for a set of random variables linked to the factor node is determined by the factor [2].



With $A, B, C \in \{0,1\}$,

$$P(A,B,C) = \frac{e^{-\beta H(A,B,C)}}{Z},$$

Z is the partition function.

We design each factor such that its logarithm can be mapped to a log-linear model. For the previous factor graph, we could choose

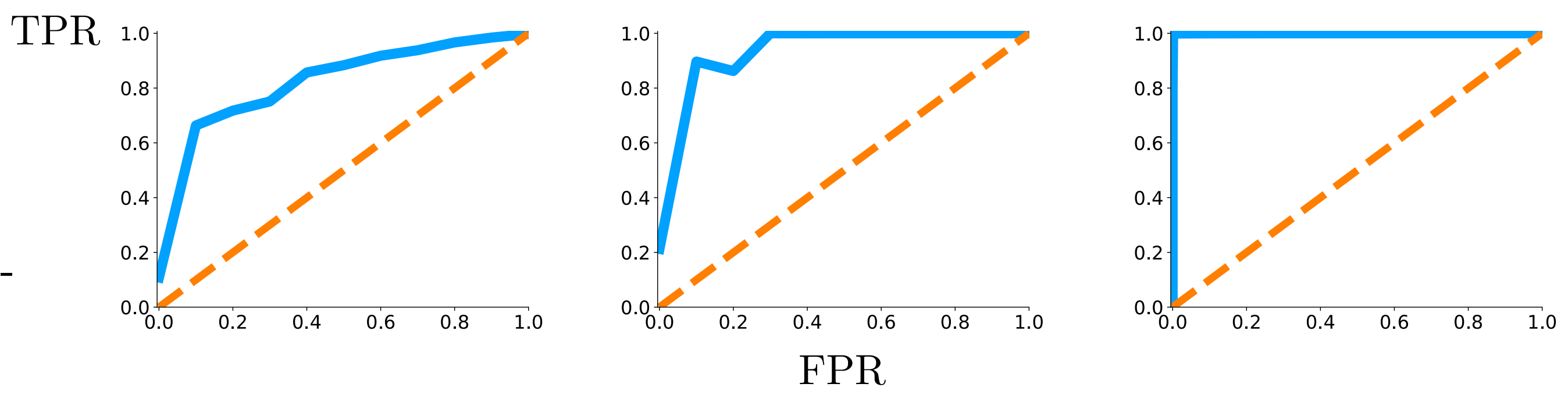
$$H(A,B,C) = \omega_1 ABC + \omega_2 AB(1-C) + \ldots + \omega_{n-1}B + \omega_n C,$$

where $\omega_1, \ldots, \omega_n$ are real numbers.

Using a **Metropolis-Hasting** sampling scheme and the total distribution of the factor graph, one can generate **synthetic observations**.

	Instance 1	Instance 2	Instance 3	Instance 4	Instance 5	...
A	1	0	1	1	0	...
B	1	1	0	1	0	...
C	0	0	0	0	1	...
⋮	⋮	⋮	⋮	⋮	⋮	⋱

The inferred simplicial complex is then compared with the original factor graph



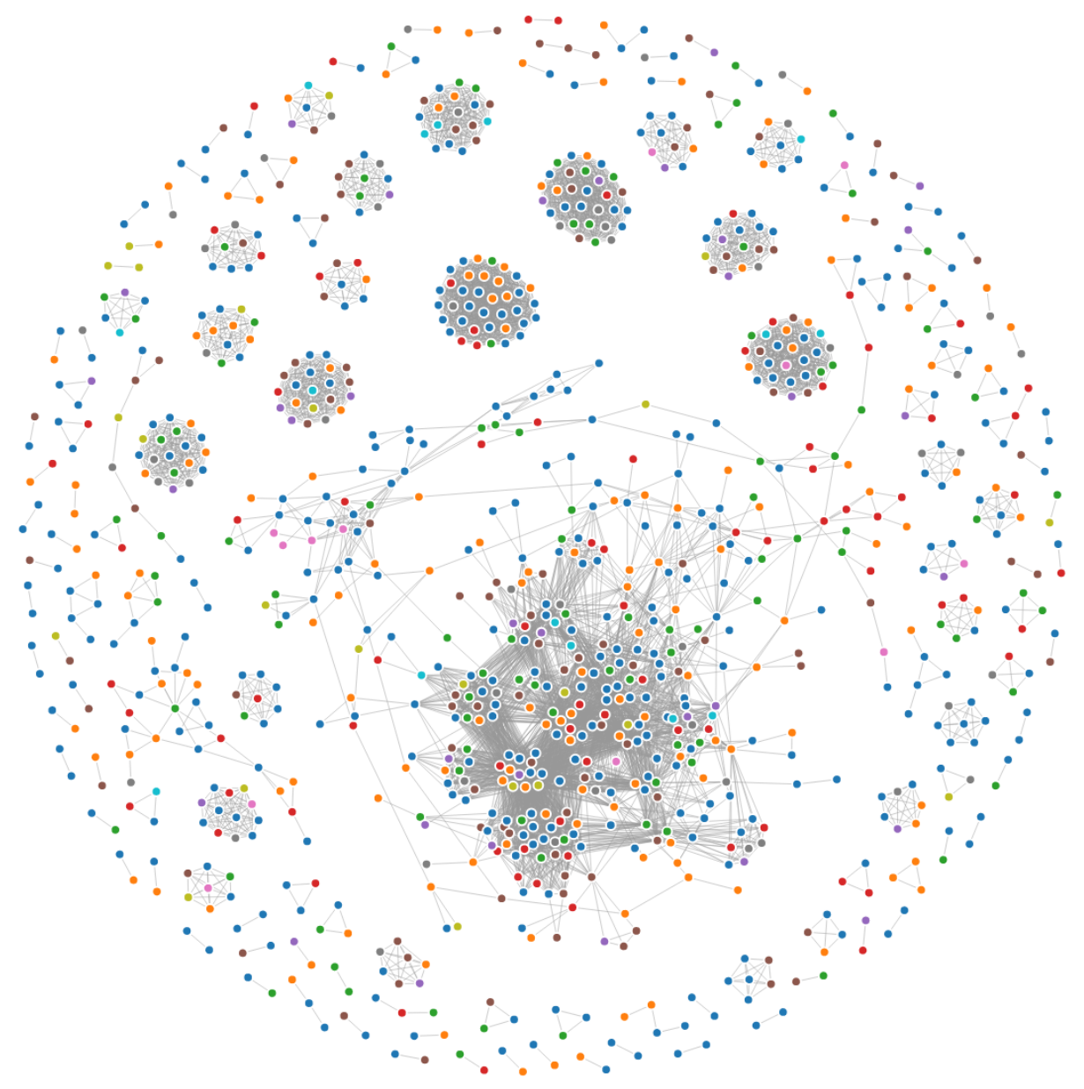
ROC curves of the inferred links for 500 (left), 1000 (middle) and 2500 (right) instances with α varying from 0 to 1. The original factor graph corresponds to the simplicial complex shown in step 6.

Results on two real datasets

Datasets generously provided by Warwick Vincent (Université Laval), Jérôme Compte (INRS, Québec Canada), and Daniel Fortin (Université Laval)

38 thermokarsts (ponds created by the thawing of permafrost) in Northern Québec, Canada, were sampled. The identified **microorganisms** were separated in 2611 taxonomic groups.

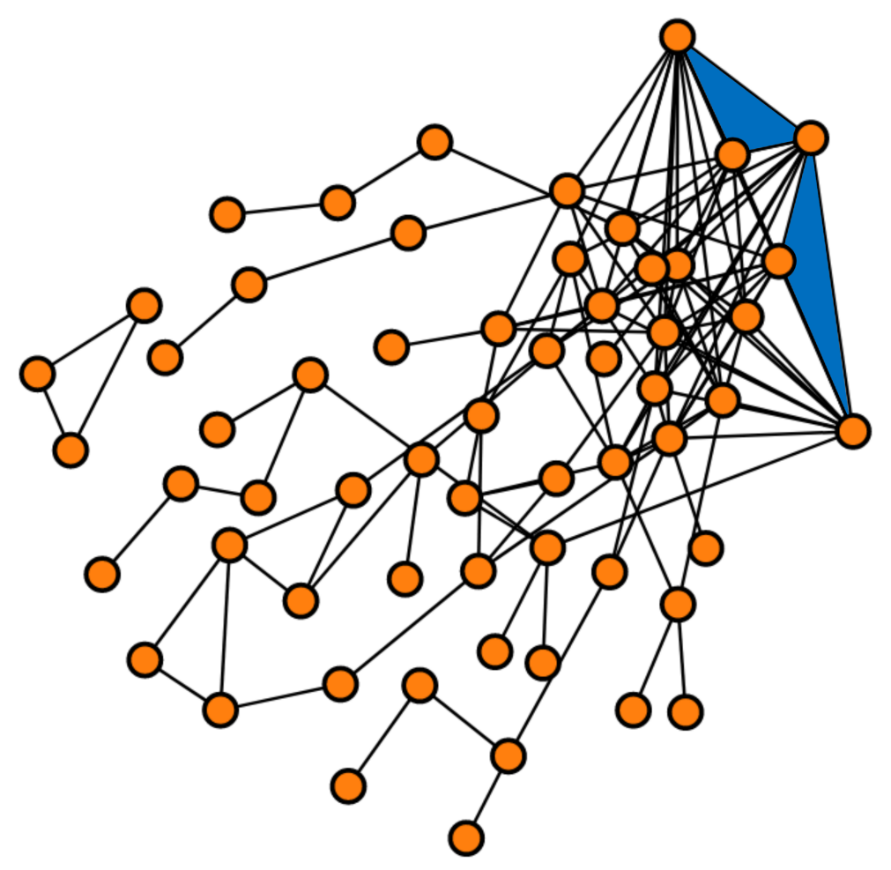
Co-occurrence network of microorganisms in thermokarsts using the exact distribution and a significance level $\alpha = 0.001$



Independent taxons : 1591
Number of 1-simplices : 6589
Number of 2-simplices : 0

Finding 2-simplices with 38 observations is a hard problem since, in some cases, the maximum likelihood estimates do not exist.

185 sites in the forests of the Côte-Nord, Québec, Canada were sampled. **70 bird species** were identified.



Co-occurrence patterns of nesting birds using the exact distribution and a significance level $\alpha = 0.01$

Independent species : 11
Number of 1-simplices : 123
Number of 2-simplices : 2

With 185 observations and the exact distribution of the statistics, we were able to find higher-order co-occurrence patterns!