Analyse de l'impact de variables environnementales sur les réseaux plantes-pollinisateurs à l'aide d'auto-encodeurs variationnels pour graphes bipartites

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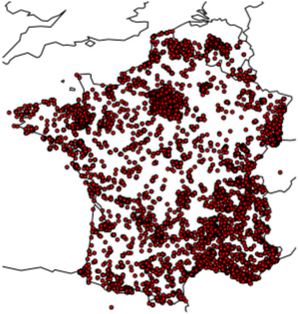
Outline

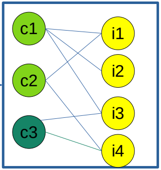
Context



- Citizen science program dataset from 2010 to today
- More than 580 000 entries of plant-pollinator interactions
- Timed observation sampling

From dataset to pollination network

Network from dataset



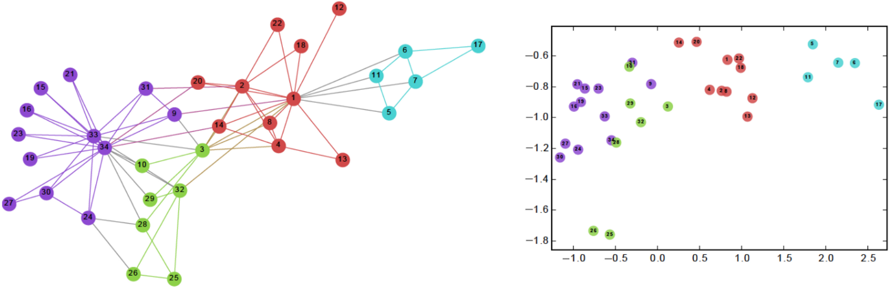
Collection	Plant species	Insect species	Temperature (T)	Date (D)
1	1	1	10°C	03/03/2020
1	1	2	10°C	03/03/2020
1	1	3	10°C	03/03/2020
2	1	1	20°C	08/08/2020
2	1	4	20°C	08/08/2020
3	2	3	10°C	04/04/2020
3	2	4	10°C	04/04/2020

Features from dataset

Features for collection nodes only.
T_{c1}= 10°C
T_{c2}= 20°C
D_{c1}= 03/03/2020
Plant species is also a feature encoded with {0,1}.

Double goal

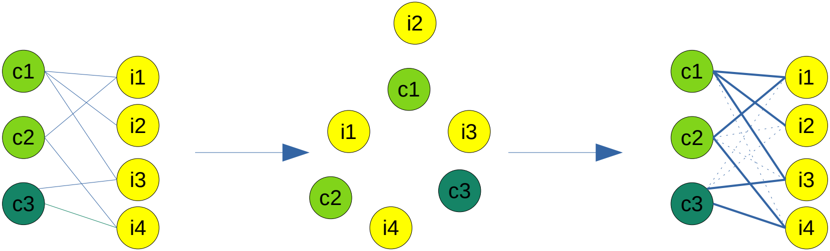
- Embedding : represent nodes and features with $Z \in \mathbb{R}^d$.
- Fairness : Z independent of S.



(picture from https ://towardsdatascience.com/overview-of-deep-learning-on-graph-embeddings-4305c10ad4a4)

Bipartite adaptation of VGAE

$$\underset{\in(\mathcal{G},E,V)}{B, X_1, X_2} \xrightarrow[\text{encoder}(GCN)]{q(Z_1,Z_2|X_1,X_2,B)} \underset{\in\mathbb{R}^d}{Z_1, Z_2} \xrightarrow[\text{decoder}(distance)]{p(B|Z_1,Z_2)} \underset{\in\mathbb{R}^{n_1\times n_2}}{\widehat{B}}$$



Hilbert-Schmidt Independence Criterion

- $X \in \mathcal{X}$ compact with kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$
- $Y \in \mathcal{Y}$ compact with kernel $L : \mathcal{Y} \times \mathcal{Y} \to \mathbb{R}$

$$\begin{aligned} HSIC(X,Y) = ||C_{X,Y}||^2 \\ &= \mathbb{E}_{XYX'Y'}[K(X,X')L(Y,Y')] + \mathbb{E}_{XX}[K(X,X')]\mathbb{E}_{YY'}[L(Y,Y')] \\ &- 2\mathbb{E}_{XY}[\mathbb{E}_{X'}[K(X,X')]\mathbb{E}_{Y'}[L(Y,Y')]]. \end{aligned}$$

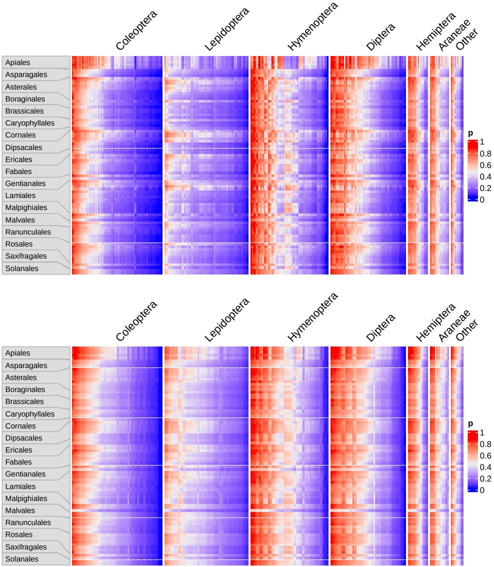
- $K(x_i,x_j) = e^{-\frac{||x_i-x_j||^2}{2\sigma^2}} \implies (HSIC(X,Y) = 0 \iff X \perp Y)$ (Gretton et al., 2005).
- HSIC test : if $X \perp Y$, $n \times \widehat{HSIC} \sim \frac{x^{\alpha-1}e^{-\frac{x}{\beta}}}{\beta^\alpha \Gamma(\alpha)}$ (Gretton et al., 2007)

Loss with HSIC

- Reconstruction loss from (Kipf and Welling, 2016)
- HSIC (Gretton et al., 2005) as a penalty to have independence
- Variational lower bound $\mathcal{L}$:

$$\begin{aligned}\mathcal{L}(W_1, W_2) = \mathbb{E}_{q(Z_1,Z_2|X_1,X_2,B)}[\log p(B|Z_1, Z_2)] \\ -KL[q_1(Z_1|X_1, B)||p_1(Z_1)] \\ -KL[q_2(Z_2|X_2, B)||p_2(Z_2)] \\ +\delta RFF\ HSIC(\mu_1, S)\end{aligned}$$

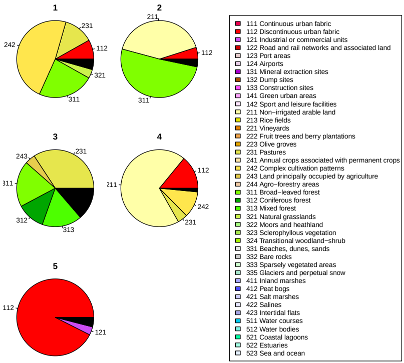
Estimated probabilities of connection between plants and insects on the Spipoll data set, BVGAE is on the top and the fair-BVGAE is on the bottom.



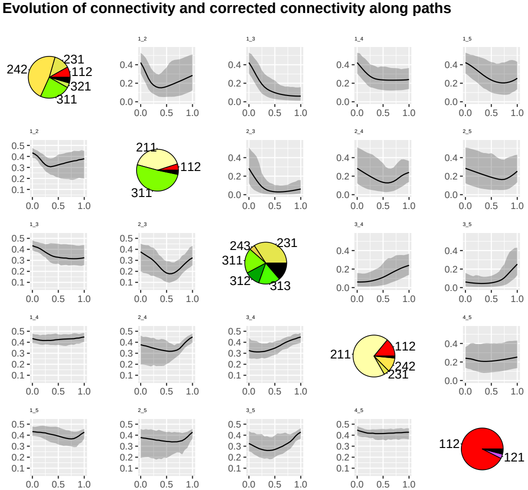
Outline

Work in progress

Typical landscape at places of sampling.



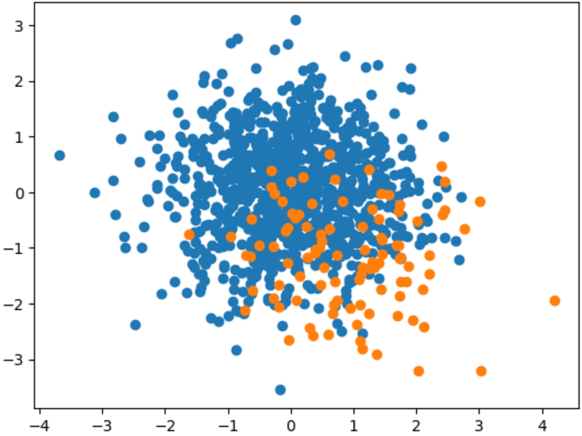
Work in progress



- We try to predict how changing the landscape changes the structure $f(X, B)$ of the network.
- This goal is achieved by changing the input value X.
- Accounting for sampling bias changes the results.

Is this truly interpretable ?

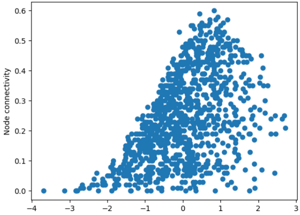
Simulation setting



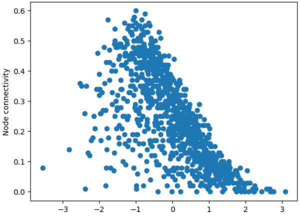
Simulated latent space

- We simulate $x_1, x_2, x_3 \overset{\text{iid}}{\sim} \mathcal{N}(0,1)$ and $y_1, y_2 \overset{\text{iid}}{\sim} \mathcal{N}(1,1)$.
- We generate a network depending on x_1, x_2 (in blue) and y_1, y_2 (in orange).
- Goal : observe the change of connectivity in the network.

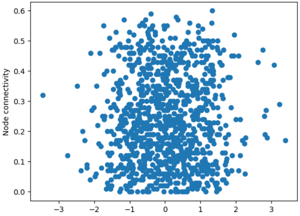
Simulation setting



x_1

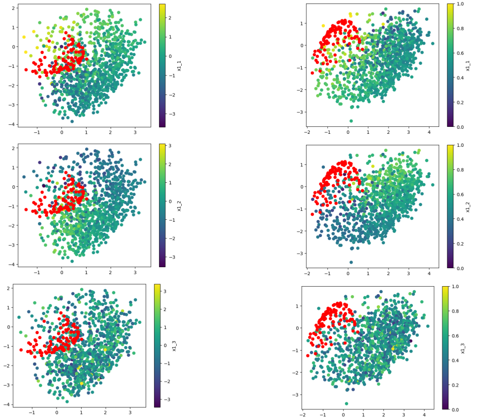


x_2



x_3

Were the covariates useful ?



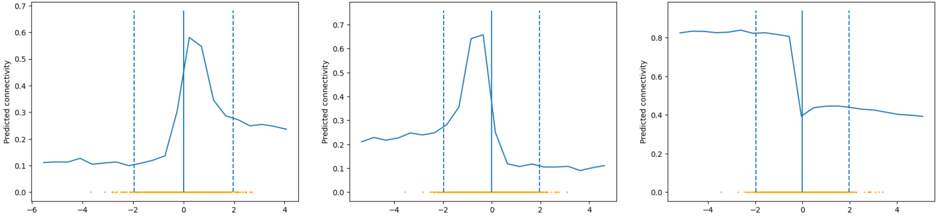
Latent space of f_0 Latent space of f

- Train $f_0(X, B)$ with $X = I_{n_1}$
- Train $f(X, B)$ with $X = [x_1, x_2, x_3]$

- f_0 AUC : 0.821 ± 0.012
- f AUC : 0.822 ± 0.013

Connectivity prediction

- Predict the connectivity : $f(X, B)$.
- Change the input X to see the effect.



x_1 x_2 x_3

Changing x_1 and x_2 yields the correct behavior, but the model is sensitive to x_3, which has no relationship with the data.

Feature importance

- Feature importance : score ϕ that indicates how much a feature j contributes to a prediction $f(X)$ of the model.

Possible feature importance estimation :

- Shapley values
- Gradient
- Integrated Gradient

Shapley values

- $S \in \{0,1\}^F$ represent a coalition of selected features.
- $X_S = \{X_{i,k} | k \in S\}$ is the submatrix of selected columns.
- $val(S) = \mathbb{E}[f(X)|X_S = x_s] - \mathbb{E}[f(X)]$ captures the marginal contribution of the coalition S

$$\phi_j(val) = \sum_{S \subseteq 1,\dots,F \setminus \{j\}} \frac{|S|!(F-|S|-1)!}{F!}(val(S \cup \{j\}) - val(S))$$

Estimating Shapley values for graphs

Duval and Malliaros (2021)

- let $\mu = (\mathbb{E}[X_1], ..., \mathbb{E}[X_F])$.
- Pick $z \in \{0, 1\}^F$ uniformly at random.
- Let X' such as $X'_j = \begin{cases} X_j & \text{if } z_j = 1 \\ \mu_k & \text{otherwise} \end{cases}$ and predict $f(X')$.
- Construct data set $\mathcal{D} := \{(z, f(X'))\}$.
- Apply weighted linear regression on $\mathcal{D}$, each coefficient corresponds to an estimated Shapley value ϕ_j.

Gradient

For each node i and for each feature j :

$$\phi_{i,j} = \nabla[f(X)]_{i,j}$$

$$\phi_j = \frac{1}{n_1} \sum_{i=1}^{n_1} \phi_{i,j}$$

Integrated gradient 1

- Chose a baseline X'
- For each node i and for each feature j calculate

$$IG_j(x_i) = (x_{i,j} - x'_{i,j}) \times \int_{\alpha=0}^{1} \nabla[f(X' + \alpha(X - X'))]_{i,j} d\alpha$$

- for each feature j fit linear regression on $\{(x_{i,j}, IG_j(x_i))\}$, each slope corresponds to an estimation of ϕ_j

Integrated gradient 2

- Let $g : \mathbb{R}^F \mapsto \mathbb{R}$ such as $g(y_1, ..., y_F) = f(\mathbf{1}.(y_1, ..., y_F)^\top)$
- Chose a baseline y'
- For each feature j calculate

$$IG_j(y) = (y_{i,j} - y'_{i,j}) \times \int_{\alpha=0}^{1} \nabla f(y' + \alpha(y - y'))_j d\alpha$$

Result

Sign : $\phi_1 > 0$ and $\phi_2 < 0$
Magnitude : $|\phi_1| > |\phi_3|$ and $|\phi_2| > |\phi_3|$

	Shapley	Grad	IG1	IG2
sign	0.4	1	1	1
magnitude	0.93	0.86	0.83	0.90

Duval, A. and Malliaros, F. D. (2021). Graphsvx : Shapley value explanations for graph neural networks. CoRR, abs/2104.10482.

Gretton, A., Bousquet, O., Smola, A., and Schölkopf, B. (2005). Measuring Statistical Dependence with Hilbert-Schmidt Norms. In Jain, S., Simon, H. U., and Tomita, E., editors, Algorithmic Learning Theory, Lecture Notes in Computer Science, pages 63–77, Berlin, Heidelberg. Springer.

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Kipf, T. N. and Welling, M. (2016). Variational graph auto-encoders.