Graph Domain Adaptation via Theory-Grounded Spectral Regularization

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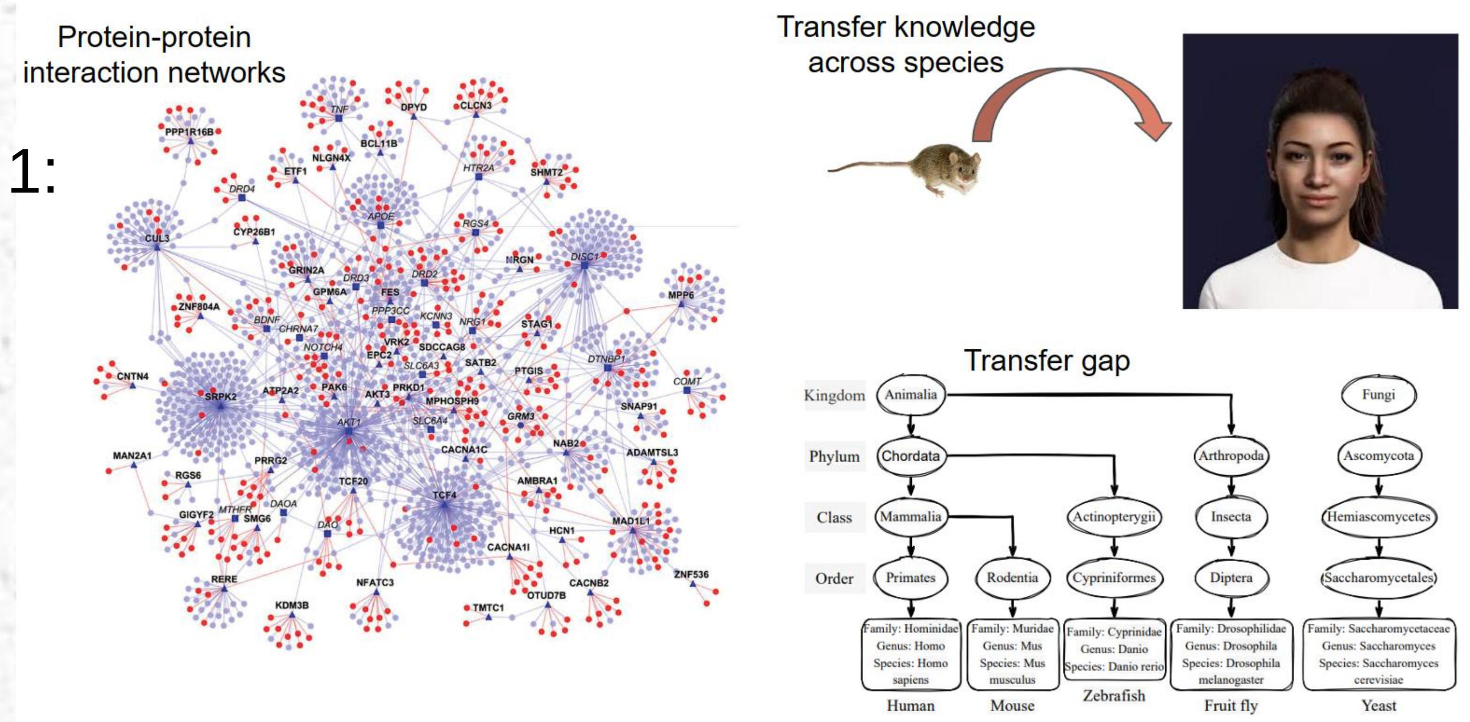
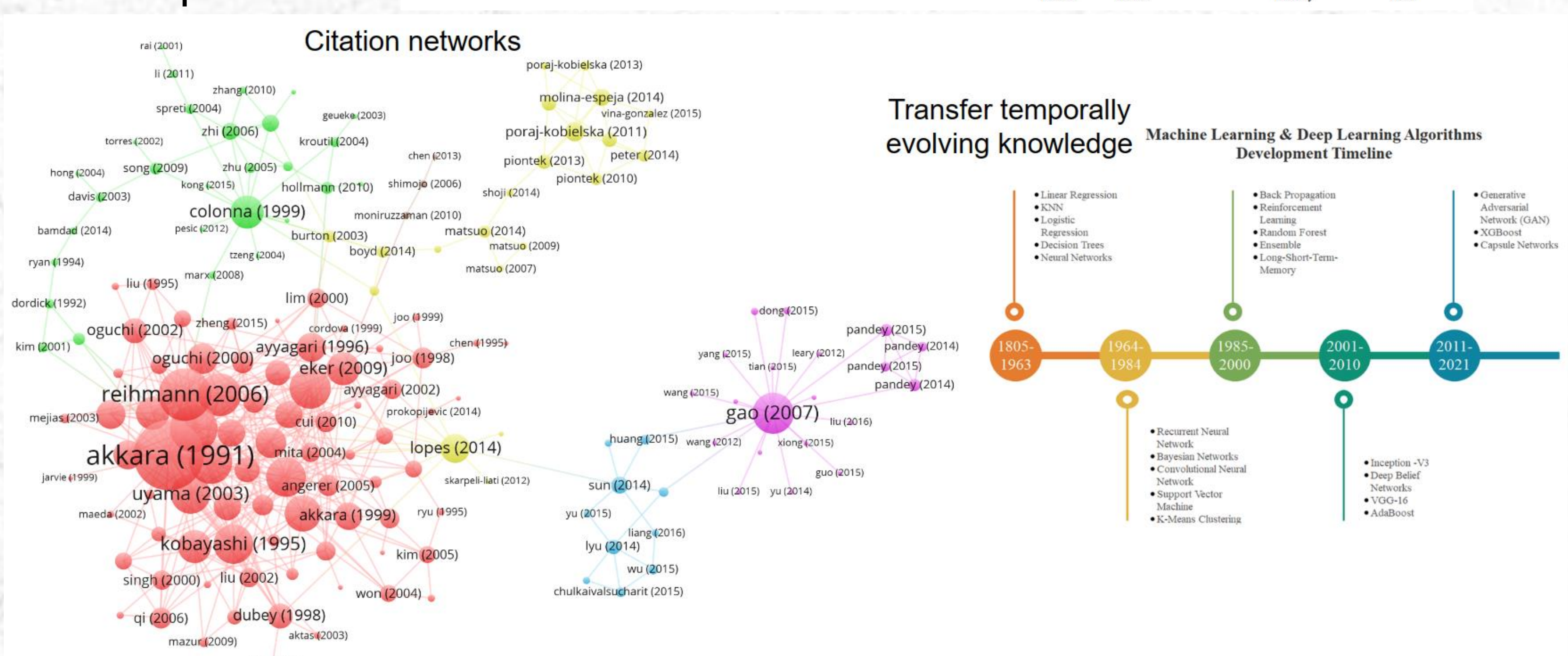
➢ Setup: Graph Learning with Distribution Shifts

Example 1:



Example 2:



➢ Gap: Competitive Transfer Performance with Theoretical Guarantee

- ❖ Graph self-supervised learning: Potential "negative transfer" [1]
- ❖ Transfer algorithms for specific scenarios: Restricted to designated scenarios (e.g. size transfer) [2]
- ❖ Applying domain adaptation methods to graphs: Not specific for graph data, with room to improve [3]

❖ **Question**: How to design algorithms to boost transfer performance across different graph domains, with the grounded theoretical foundation?

➢ References

[1] You et al., "Graph Contrastive Learning with Augmentations", NeurIPS'20. [2] Yehudai et al, "From local structures to size generalization in graph neural networks", ICML'21. [3] Wu et al, "Unsupervised domain adaptive graph convolutional networks", WWW'20

➢ Solution: A theoretical guaranteed, generic, and graph-specific algorithm

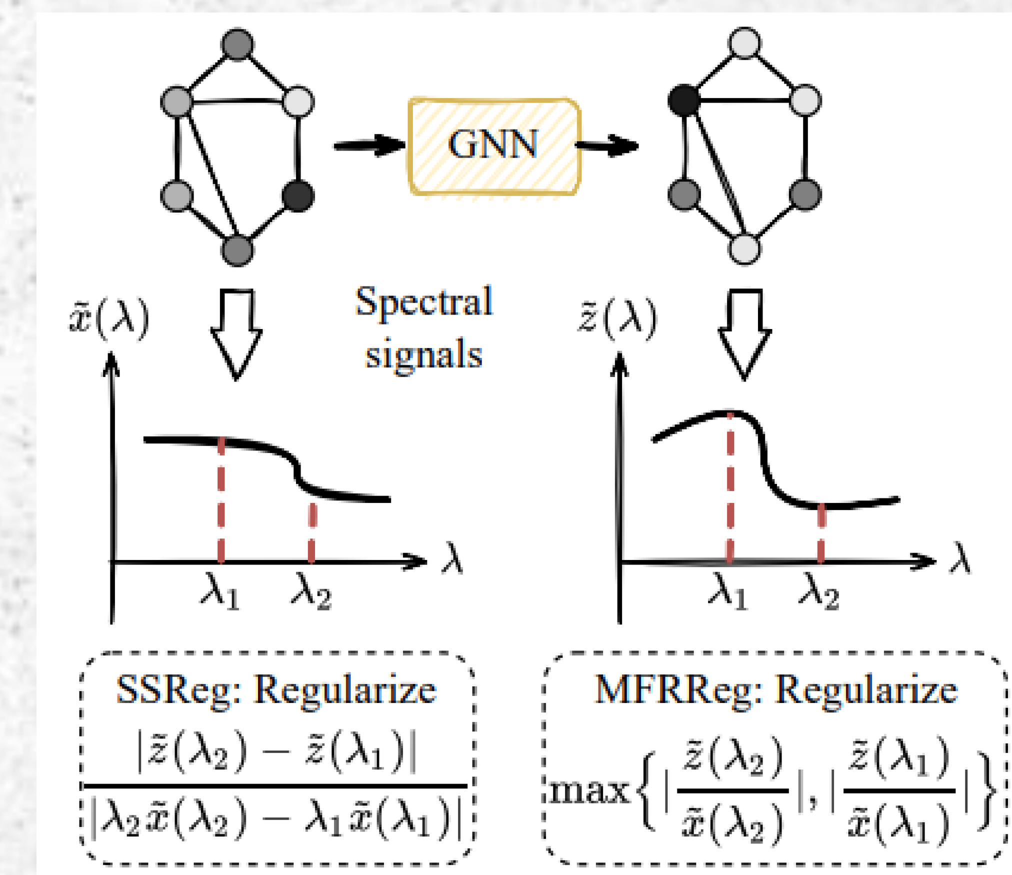
- ❖ Theoretically charactering **graph transfer risk bound** (by combining Eqs. (4-6))
  - Tools: Domain adaptation and spectral graph theory

$$\epsilon_{\mathrm{T}}(h,\hat{h}) \leq \hat{\epsilon}_{\mathrm{S}}(h,\hat{h}) + \sqrt{\frac{4d}{N_{\mathrm{S}}}\log(\frac{eN_{\mathrm{S}}}{d}) + \frac{1}{N_{\mathrm{S}}}\log(\frac{1}{\delta})} + 2C_f C_g W_1\Big(\mathbb{P}_{\mathrm{S}}(G), \mathbb{P}_{\mathrm{T}}(G)\Big) + \omega, \quad (4)$$

$$\|f(G_1) - f(G_2)\|_2 \leq C_\lambda (1 + \tau\sqrt{N_G}) \|A_1 - P^* A_2 P^{*\mathsf{T}}\|_{\mathrm{F}} + \mathcal{O}(\|A_1 - P^* A_2 P^{*\mathsf{T}}\|_{\mathrm{F}}^2) + \max\Big\{|\mathcal{S}(\Lambda_2)|\Big\} \|X_1 - P^* X_2\|_{\mathrm{F}}, \quad (5)$$

$$C_f = \max\Big\{C_\lambda K_1 + \varepsilon K_2, |\mathcal{S}(\lambda^*)|\Big\}, \quad (6)$$

  - Analysis: We identify important GNN properties related to the bound:
    - ○ **Spectral smoothness** (SS) and **maximum frequency response** (MFR)
    - ○ More importantly, SS relates to **node transfer** and MFR relates to **link transfer** (see Sec. 4.2)
- ❖ We accordingly propose to regularize SS and MFR to confine the bound



➢ Experiments

Methods	Co-expression: Link transfer ⇒ MFRReg Mouse	Zebrafish	Fruit fly	Yeast	Mean↑	Rank↓
Mashup	48.98±2.34 (5.49±0.32)	51.63±1.81 (5.37±0.33)	50.28±2.20 (5.51±0.17)	46.31±0.63 (4.96±0.05)	43.90 (5.33)	9.0
D-SCRIPT	54.48±3.27 (6.01±0.63)	61.18±1.05 (8.12±1.77)	66.63±1.41 (9.78±0.25)	58.88±0.80 (7.53±0.11)	60.29 (7.86)	7.5
GraphCL	73.09±1.56 (14.98±2.18)	74.19±0.50 (18.76±2.11)	66.80±2.55 (12.12±2.00)	62.41±1.12 (11.32±2.86)	69.12 (14.29)	5.2
Transformer	69.55±0.41 (18.06±0.13)	69.63±0.84 (27.44±1.21)	57.38±1.77 (10.13±1.02)	63.01±1.45 (11.25±1.58)	64.89 (16.72)	5.8
Transformer +GIN	76.35±0.38 (21.91±1.60)	79.29±2.78 (28.07±4.71)	66.54±1.11 (13.48±0.71)	**63.91**±1.55 (11.15±1.11)	71.52 (18.65)	4.0
Transformer +GIN+DA-C	**78.56**±1.55 (22.76±4.42)	**79.46**±2.97 (27.10±3.10)	64.78±1.23 (11.61±2.08)	60.65±3.85 (10.72±2.44)	70.86 (18.04)	4.8
Transformer +GIN+DA-W	77.38±2.54 (23.03±2.98)	79.22±0.89 (26.90±2.03)	**67.78**±0.40 (**13.78**±0.94)	62.43±2.62 (11.59±1.98)	**71.70** (18.82)	**3.6**
Transformer+GIN +DA-W+SSReg	77.57±1.14 (**23.13**±0.64)	79.44±1.21 (**28.97**±2.22)	65.27±1.49 (11.88±0.89)	62.28±1.71 (**13.24**±2.49)	71.14 (**19.30**)	**3.6**
Transformer+GIN +DA-W+MFRReg	**77.63**±1.00 (**23.83**±2.75)	**80.81**±1.27 (**29.04**±0.62)	**68.56**±0.88 (**13.94**±0.47)	**63.74**±0.27 (**16.80**±2.34)	**72.68** (**20.90**)	**1.2**

Methods	Physical: Node transfer ⇒ SSReg Mouse	Zebrafish	Fruit fly	Yeast	Mean↑	Rank↓
Mashup	51.54±3.82 (5.58±0.35)	37.82±3.43 (3.98±0.12)	46.88±6.87 (7.19±3.93)	57.99±2.28 (6.78±0.92)	48.55 (5.88)	9.0
D-SCRIPT	58.22±6.97 (7.03±1.09)	49.58±1.12 (5.02±0.76)	62.97±0.78 (9.61±0.21)	62.43±0.59 (8.56±0.15)	58.30 (7.55)	8.0
GraphCL	76.88±0.42 (31.16±1.43)	79.11±1.14 (41.80±3.20)	81.02±0.98 (38.63±2.30)	71.03±0.30 (14.58±1.16)	77.01 (31.54)	6.0
Transformer	77.65±0.84 (**35.05**±0.92)	75.61±1.86 (**45.13**±3.15)	76.90±1.64 (32.72±2.34)	67.86±0.61 (12.46±1.08)	74.50 (31.34)	5.6
Transformer +GIN	79.77±0.92 (31.23±1.94)	80.85±2.41 (34.29±12.42)	**82.38**±1.13 (**42.40**±2.04)	71.54±0.36 (15.73±0.79)	78.63 (30.91)	4.3
Transformer +GIN+DA-C	80.14±1.86 (34.29±4.12)	**83.58**±1.15 (44.01±4.00)	81.49±1.27 (38.94±2.36)	71.30±0.61 (**16.80**±0.65)	**79.12** (33.51)	3.3
Transformer +GIN+DA-W	80.18±1.38 (34.14±0.85)	80.88±3.08 (41.88±2.15)	81.51±0.36 (42.02±0.69)	**72.66**±0.36 (16.18±2.67)	78.80 (**33.55**)	**3.6**
Transformer+GIN +DA-W+SSReg	**81.20**±0.25 (**35.99**±1.51)	81.69±1.55 (**45.15**±2.07)	**81.79**±0.74 (**43.44**±1.16)	**73.07**±0.30 (**17.39**±1.01)	**79.43** (**35.49**)	**1.3**
Transformer+GIN +DA-W+MFRReg	**80.93**±1.11 (34.63±3.71)	**81.95**±1.77 (43.09±4.19)	80.15±1.07 (35.43±1.60)	72.22±0.67 (16.40±1.12)	78.81 (32.38)	**3.6**

- ❖ PPI link prediction
- ❖ Please refer to the paper for more numerical results (e.g. citation network node classification)

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