Continual Learning on Graphs: Challenges, Solutions, and Opportunities



Dacheng TAO
Dongjin SONG
Xikun ZHANG

THE UNIVERSITY OF SYDNEY
UCONN UNIVERSITY OF CONNECTICUT

Agenda

- Background (10 min)
- Motivation of Continual Graph Learning (CGL) (10 min)
- Problem setup of CL and CGL (20 min)
- CL techniques & CGL techniques (30 min)
- Evaluation Metrics & CGL benchmarks (10 min)
- Future opportunities (10 min)
- Q&A

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- **Background**
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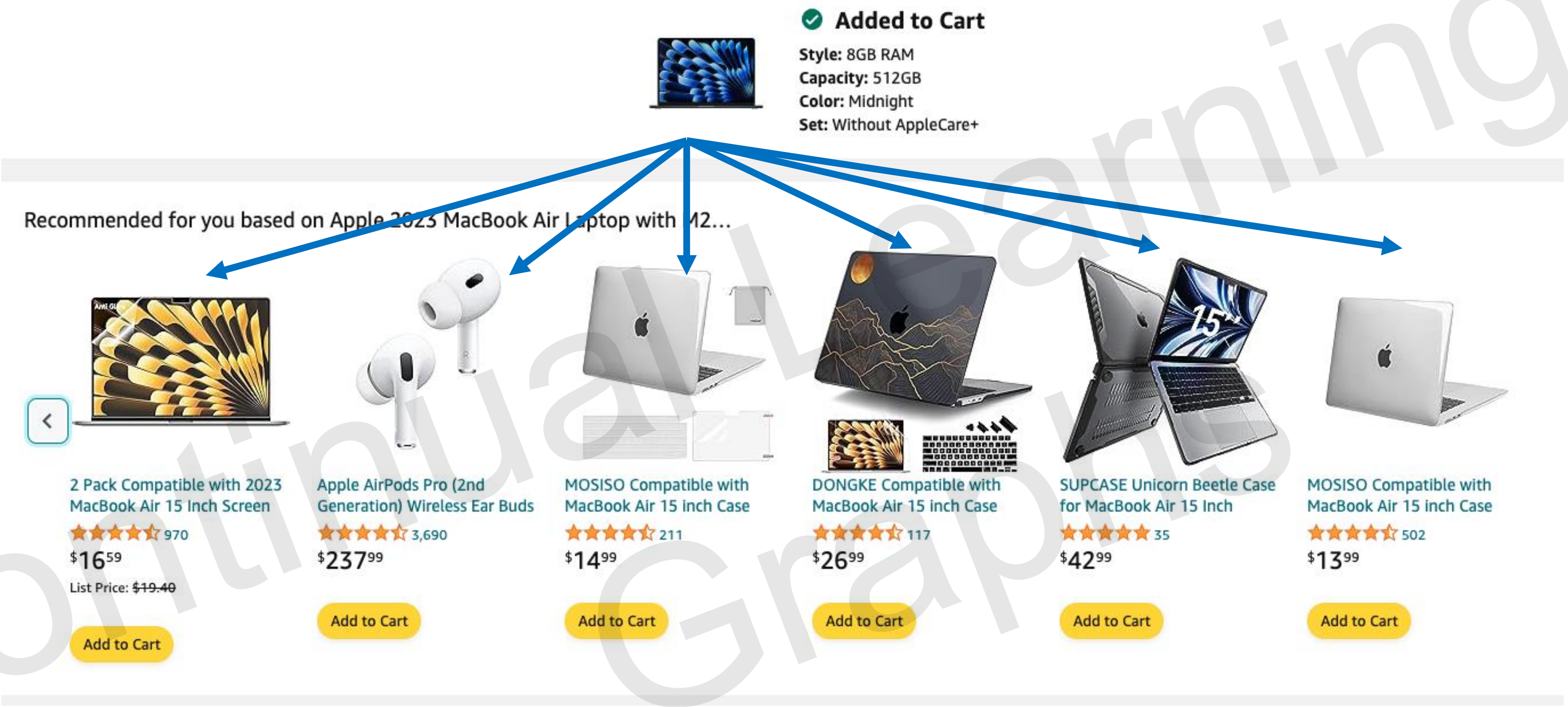
Background - Graphs

Social networks

https://visiblenetworklabs.com/2023/01/06/social-network-analysis-for-foundations/

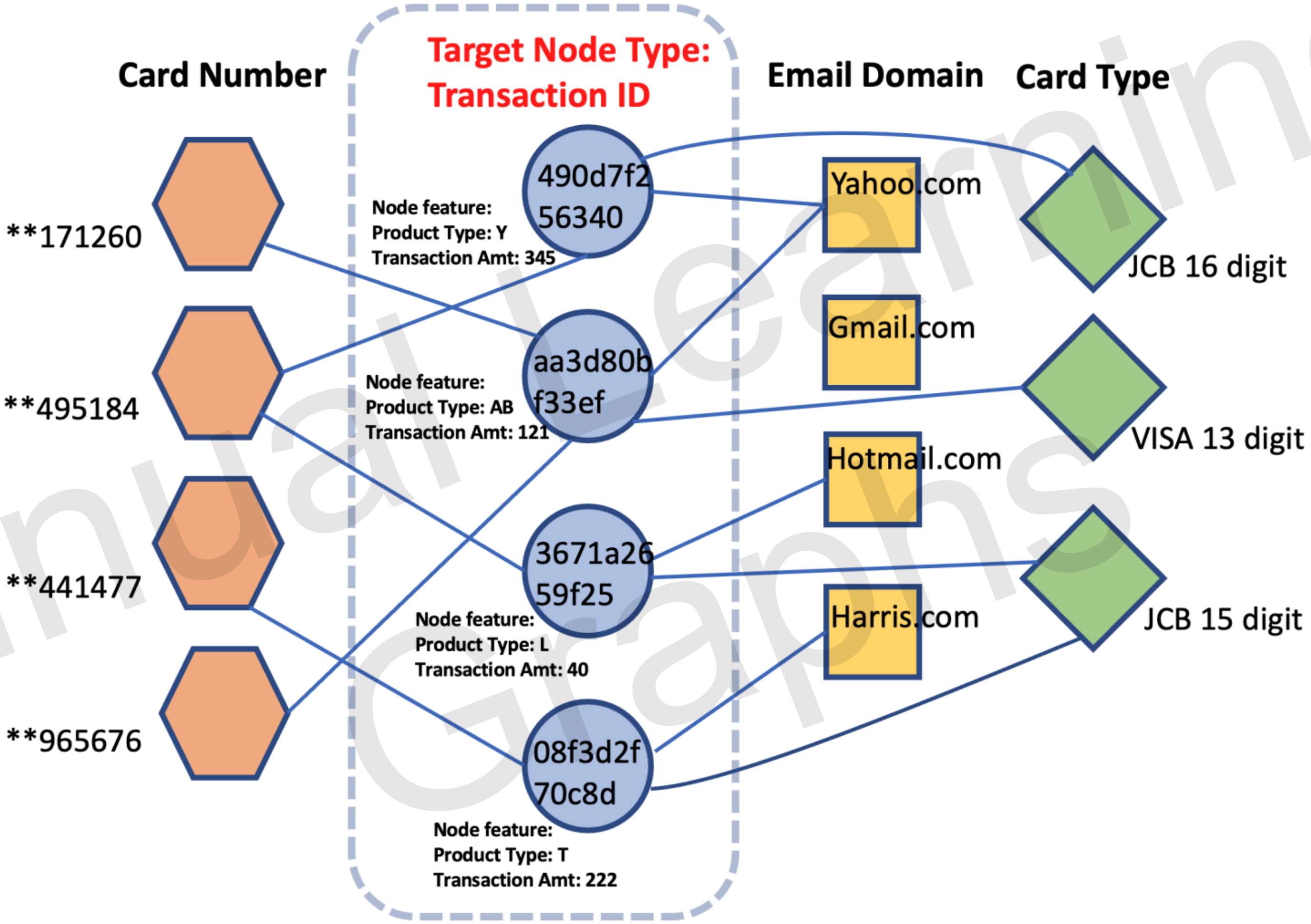
Background - Graphs



Amazon co-purchasing networks

Top right: https://aws.amazon.com/blogs/machine-learning/detect-financial-transaction-fraud-using-a-graph-neural-network-with-amazon-sagemaker/

Background - Graphs

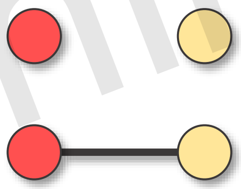


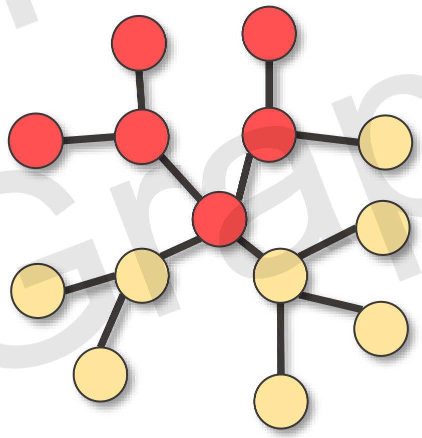
Financial transaction networks

Background - Graphs

Graphs consist of

- Nodes (or vertices)
- Edges (or links) connecting nodes





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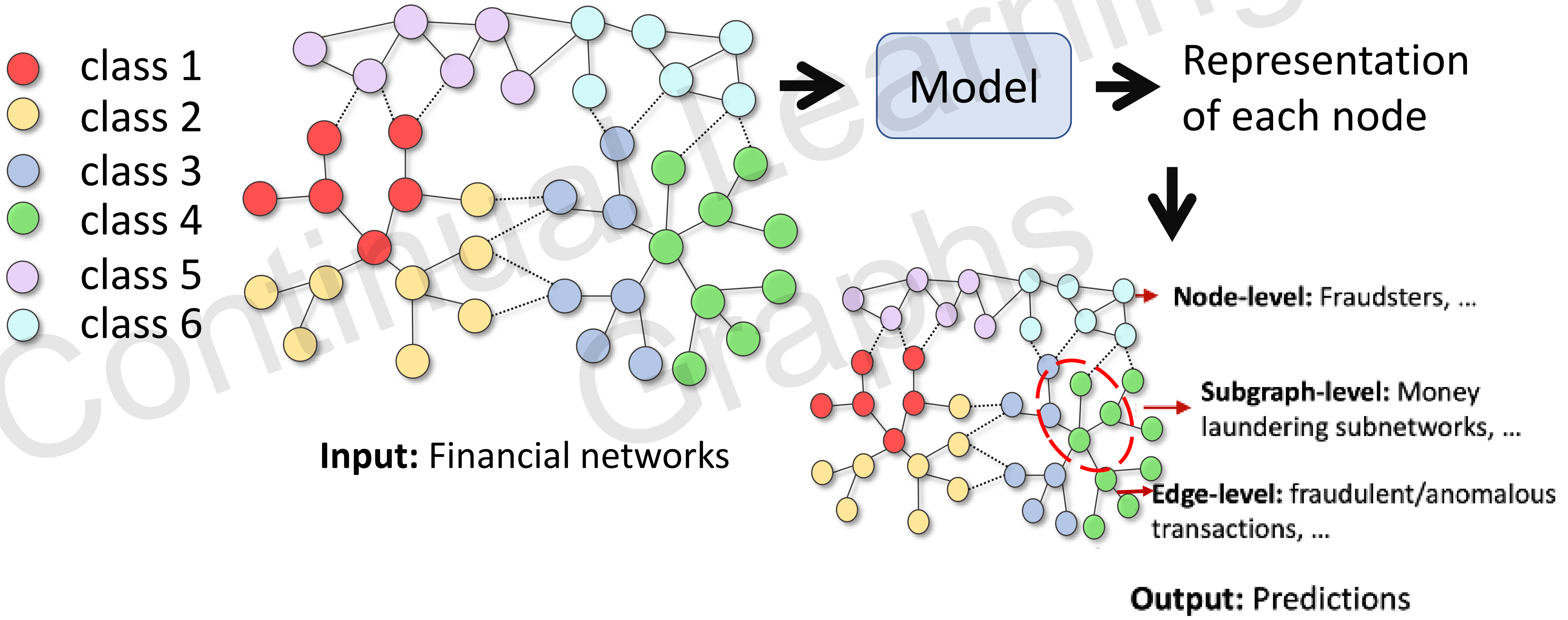

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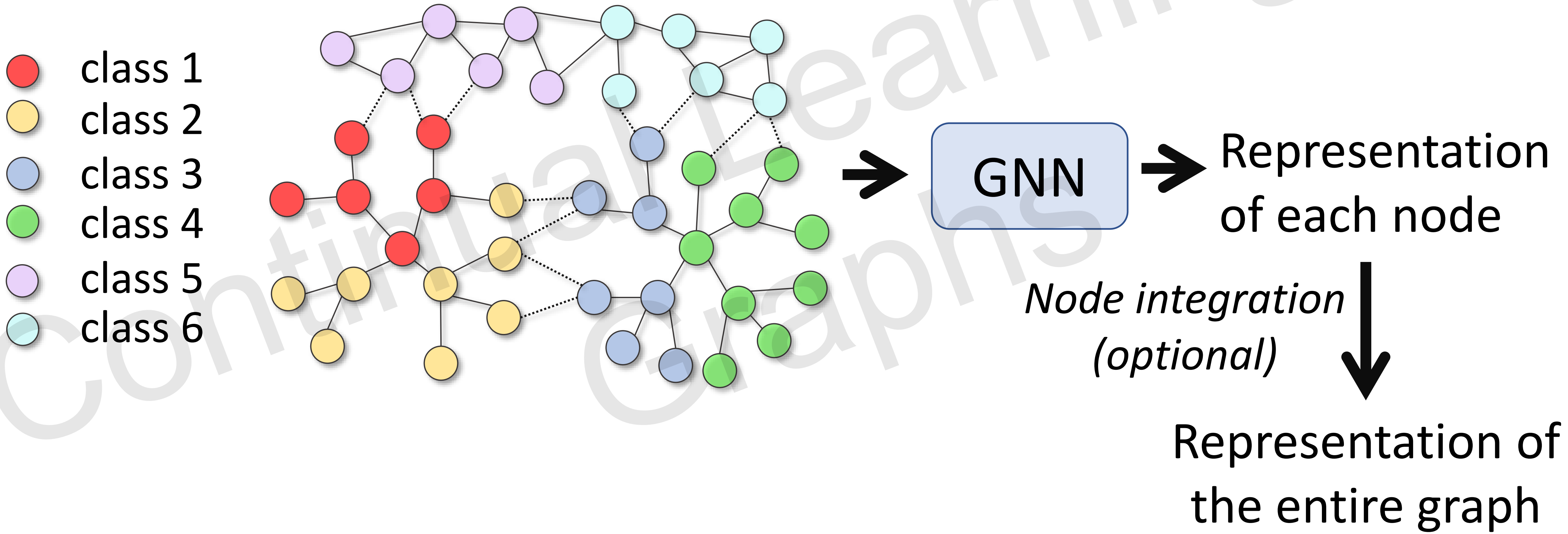
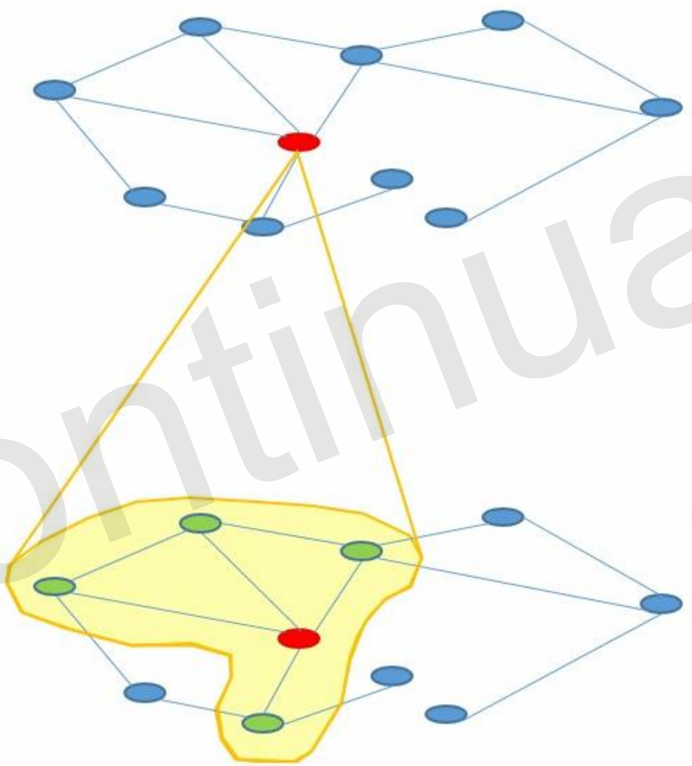


Background

Message Passing Neural Network (MPNN)



Message function

$$m_v^{t+1} = \sum_{w \in \boxed{N(v)}} \boxed{M_t}(h_v^t, h_w^t, e_{vw})$$

Neighbours of *v*

$$h_v^{t+1} = \boxed{U_t}(h_v^t, m_v^{t+1})$$

Node update function

$$\hat{y} = \boxed{R}(\{h_v^T \mid v \in G\}).$$

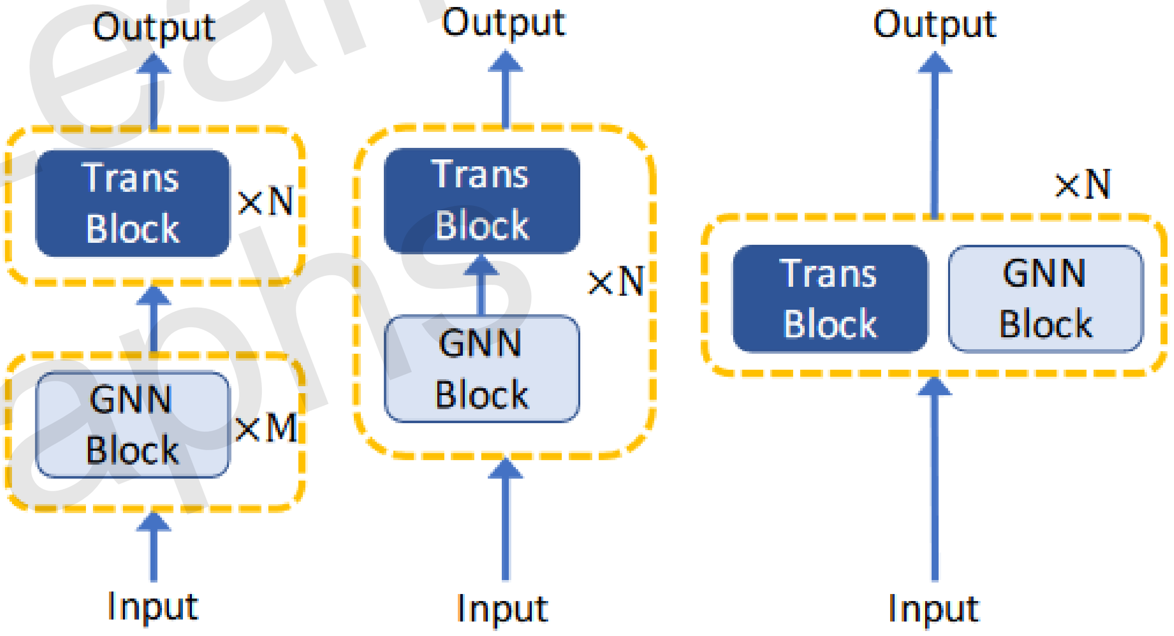
Readout function

Gilmer, Justin, et al. "Neural message passing for quantum chemistry." International conference on machine learning. PMLR, 2017.

Background

Graph transformers

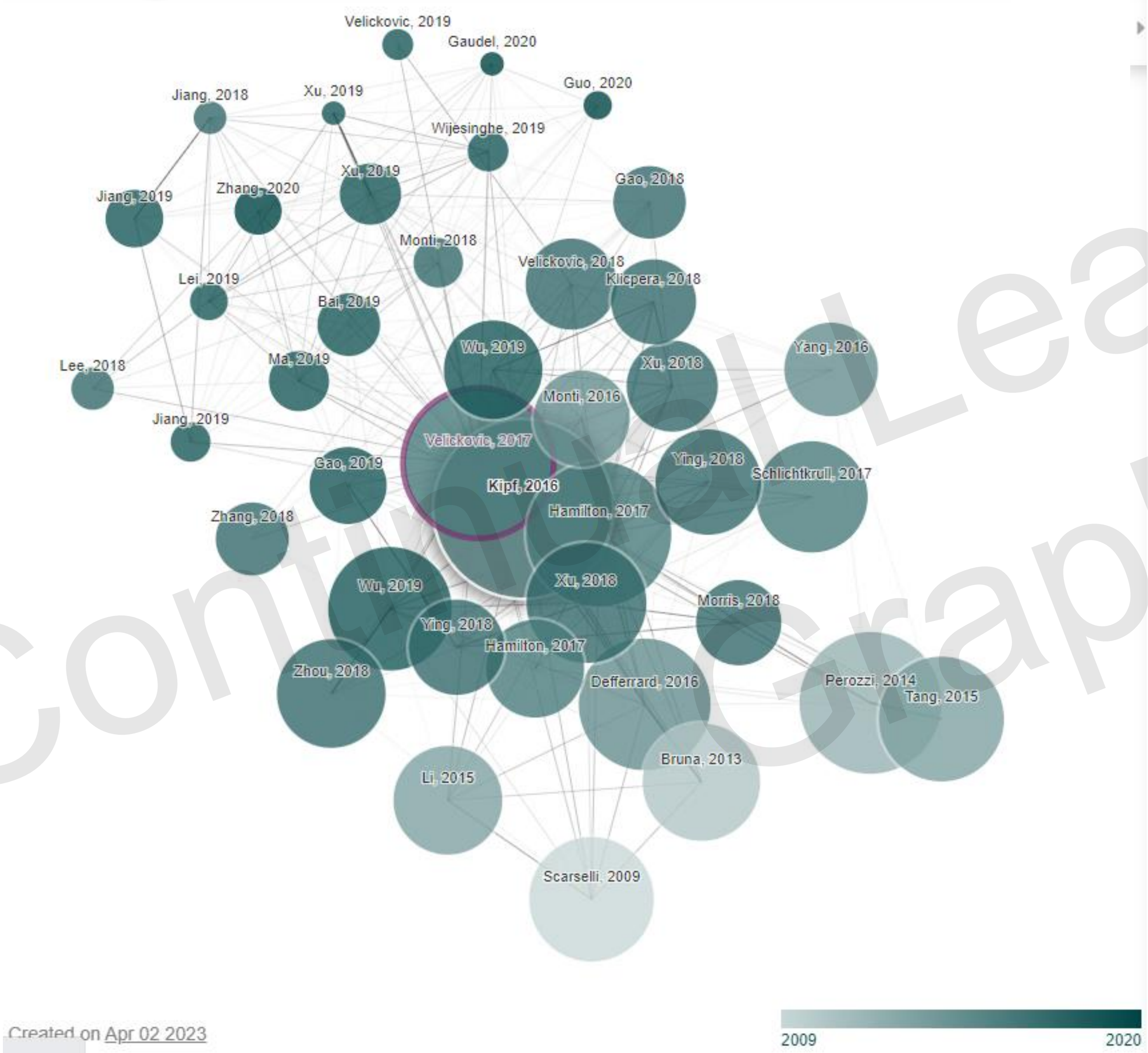
- GNNs as Auxiliary Modules in Transformer
- Improved Positional Embeddings from Graphs
- Improved Attention Matrices from Graphs



(a) Before Trans (b) Alternatively (c) Parallel

Min, Erxue, et al. "Transformer for graphs: An overview from architecture perspective." arXiv preprint arXiv:2202.08455 (2022).

Background

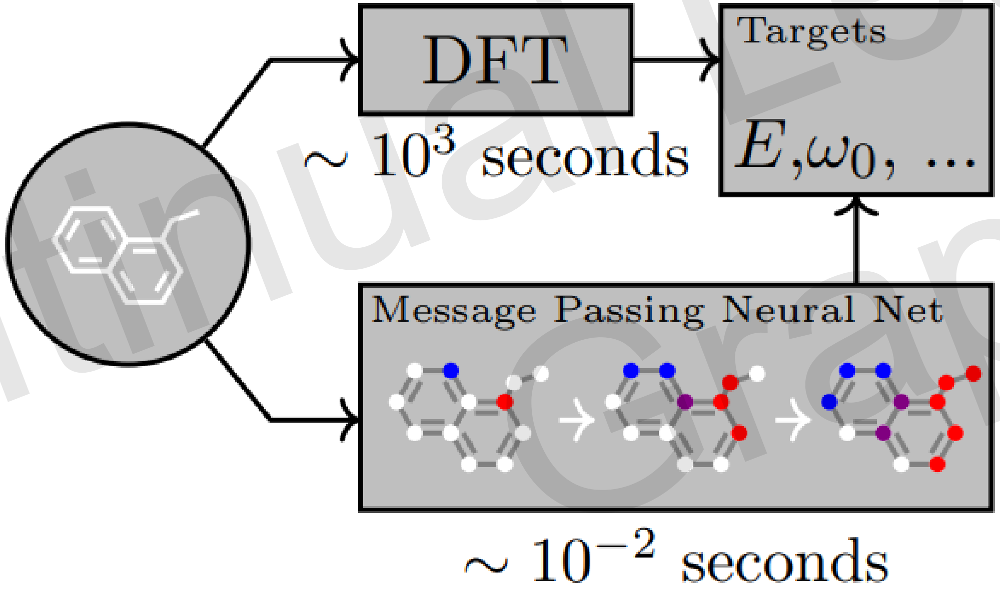


Popular node-level task:
Node classification on
Citation network

https://www.connectedpapers.com/

Background

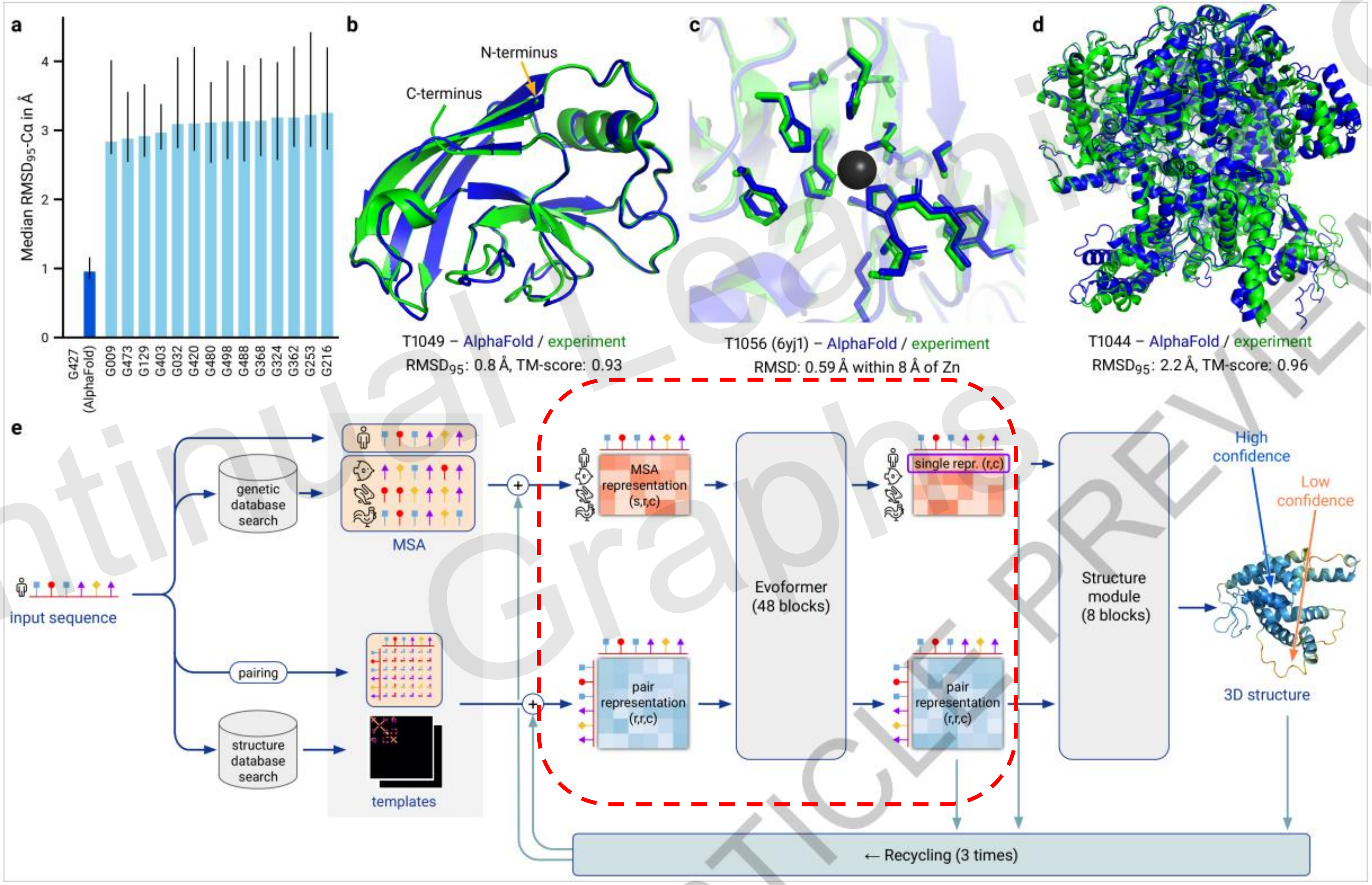
Message Passing Neural Network (MPNN)



Popular graph-level task: Molecule property prediction

Gilmer, Justin, et al. "Neural message passing for quantum chemistry." International conference on machine learning. PMLR, 2017.

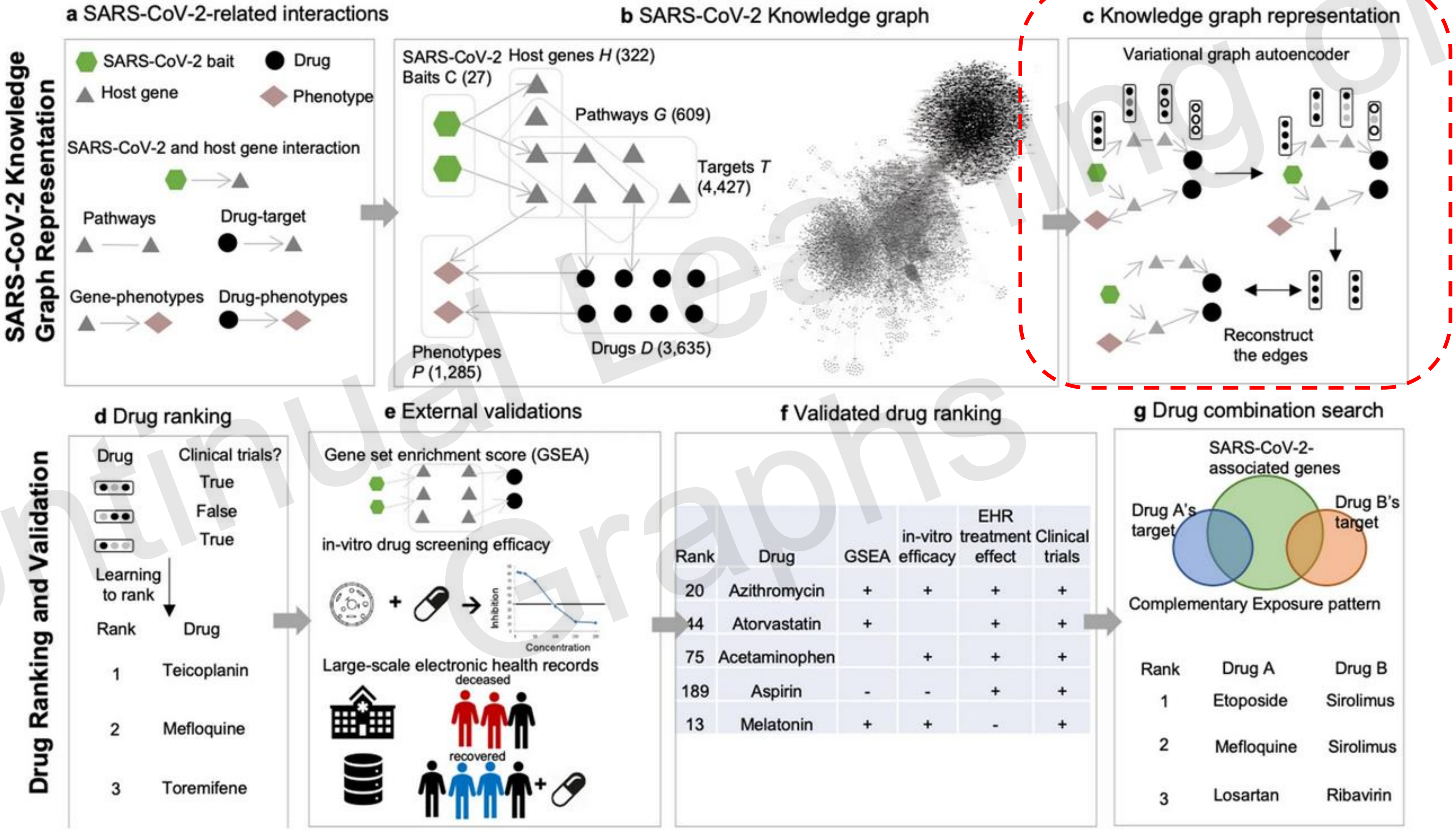
Background AlphaFold2 (Protein structure prediction)



Jumper, John, et al. "Highly accurate protein structure prediction with AlphaFold." *Nature* 596.7873 (2021): 583-589.

Background

Drug discovery

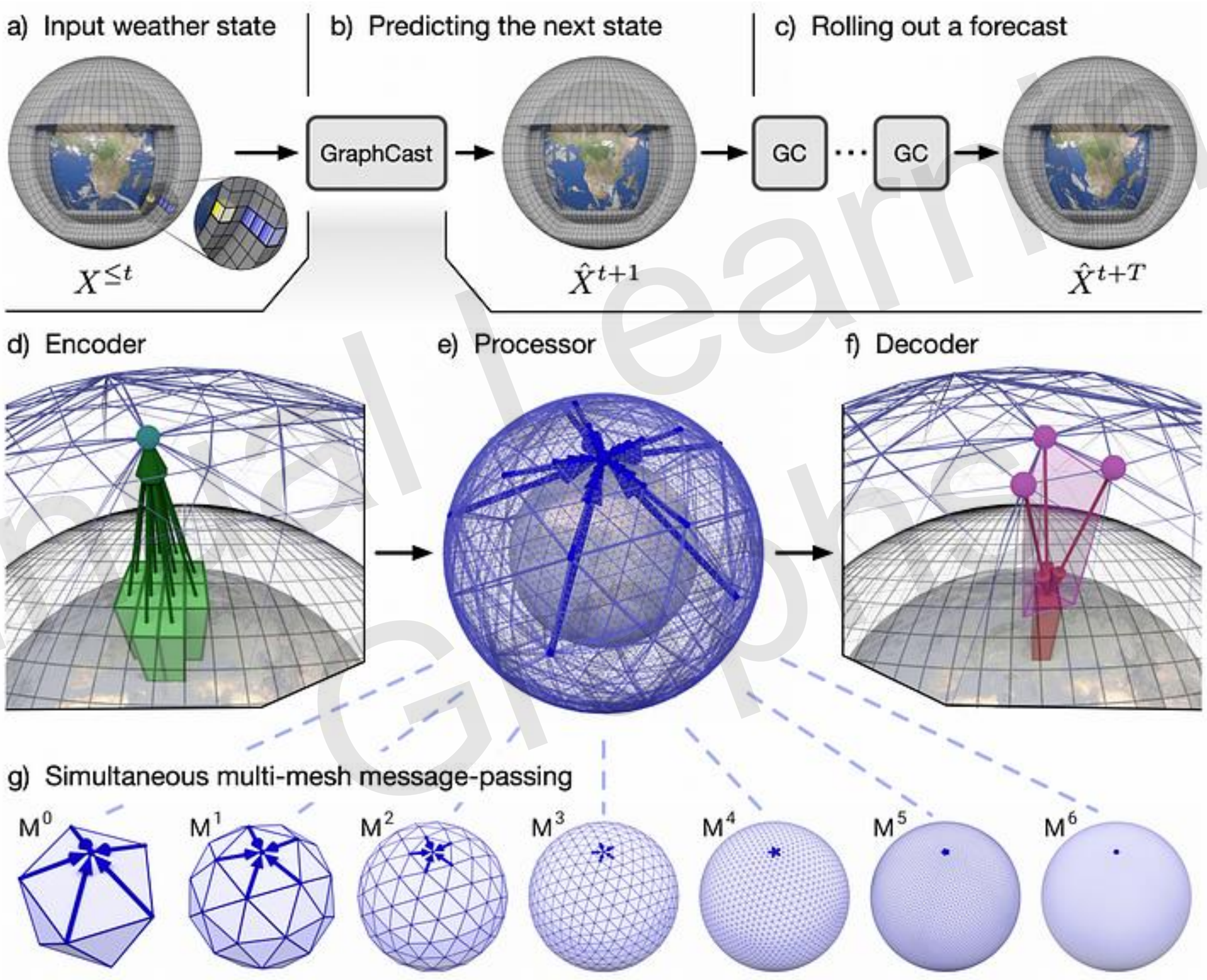


Rank	Drug	GSEA	in-vitro efficacy	EHR treatment effect	Clinical trials
20	Azithromycin	+	+	+	+
44	Atorvastatin	+		+	+
75	Acetaminophen		+	+	+
189	Aspirin	-	-	+	+
13	Melatonin	+	+	-	+

Rank	Drug A	Drug B
1	Etoposide	Sirolimus
2	Mefloquine	Sirolimus
3	Losartan	Ribavirin

Hsieh, Kanglin, et al. "Drug repurposing for COVID-19 using graph neural network and harmonizing multiple evidence." Scientific reports 11.1 (2021): 23179.

Background GraphCast (Weather forecasting)



Lam, Remi, et al. "GraphCast: Learning skillful medium-range global weather forecasting." arXiv preprint arXiv:2212.12794 (2022).

Agenda

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- Problem setup of CL and CGL
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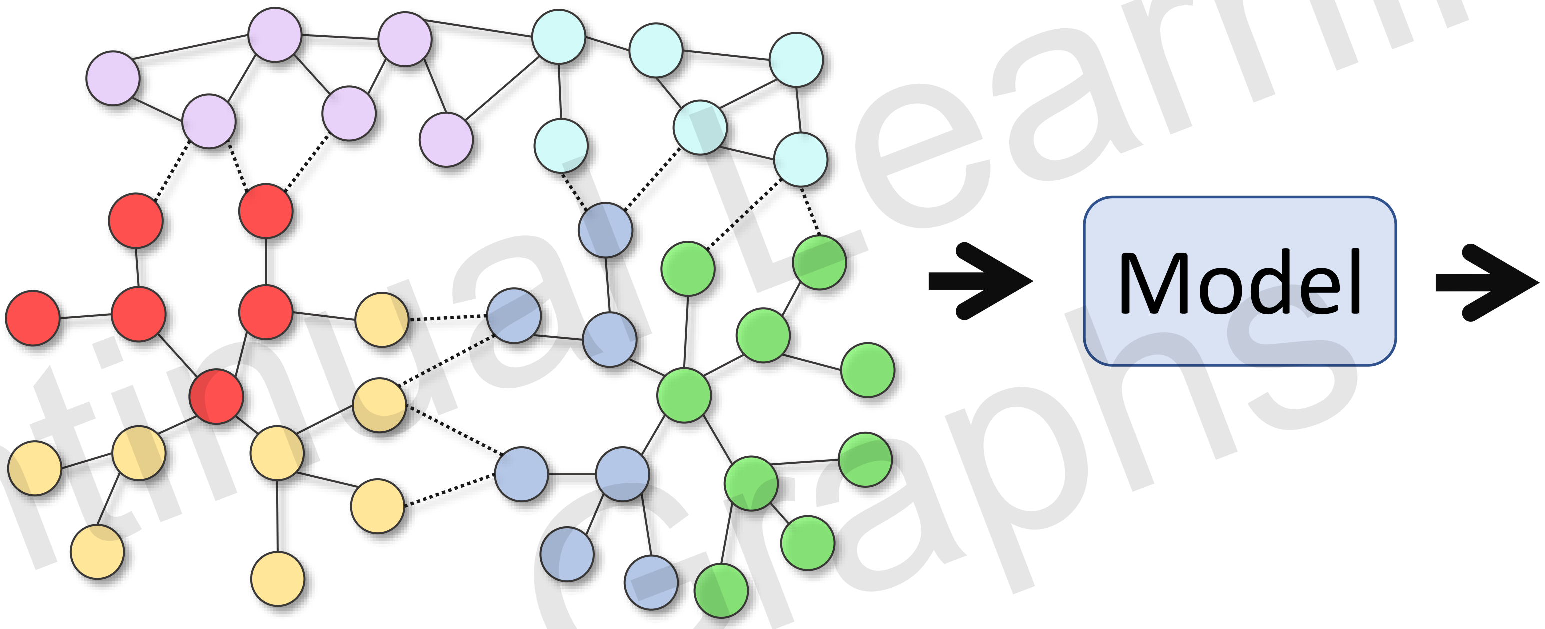
Motivation

Learning on static graphs

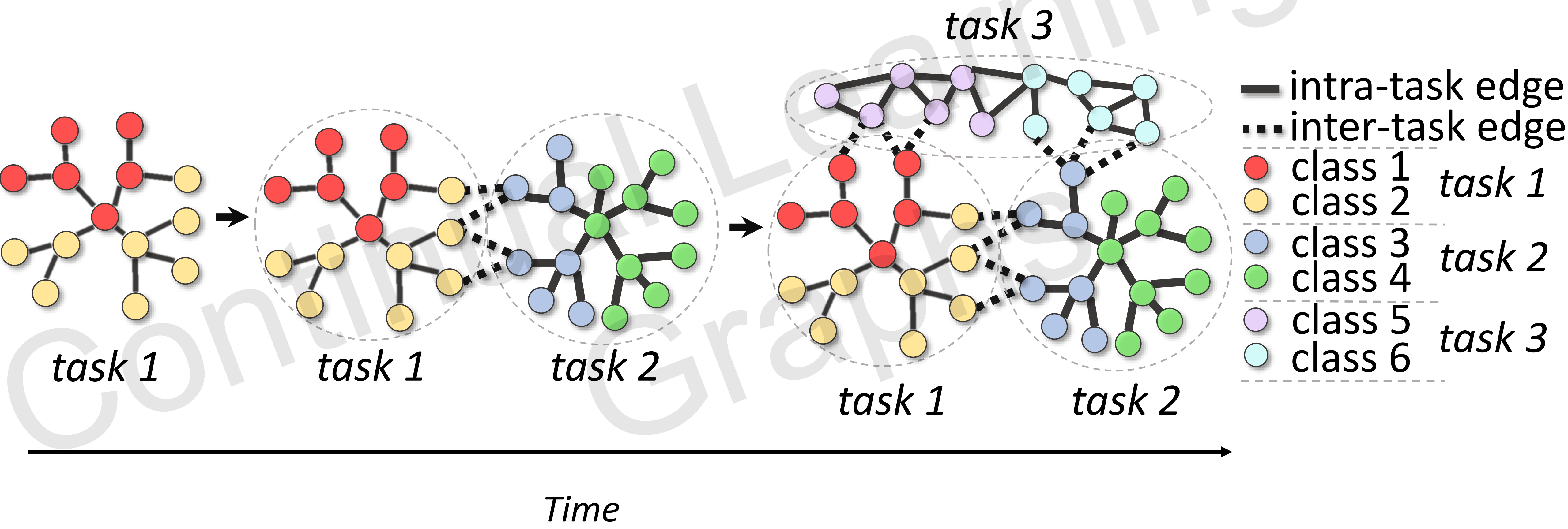
- class 1
- class 2
- class 3
- class 4
- class 5
- class 6



Representation of each node

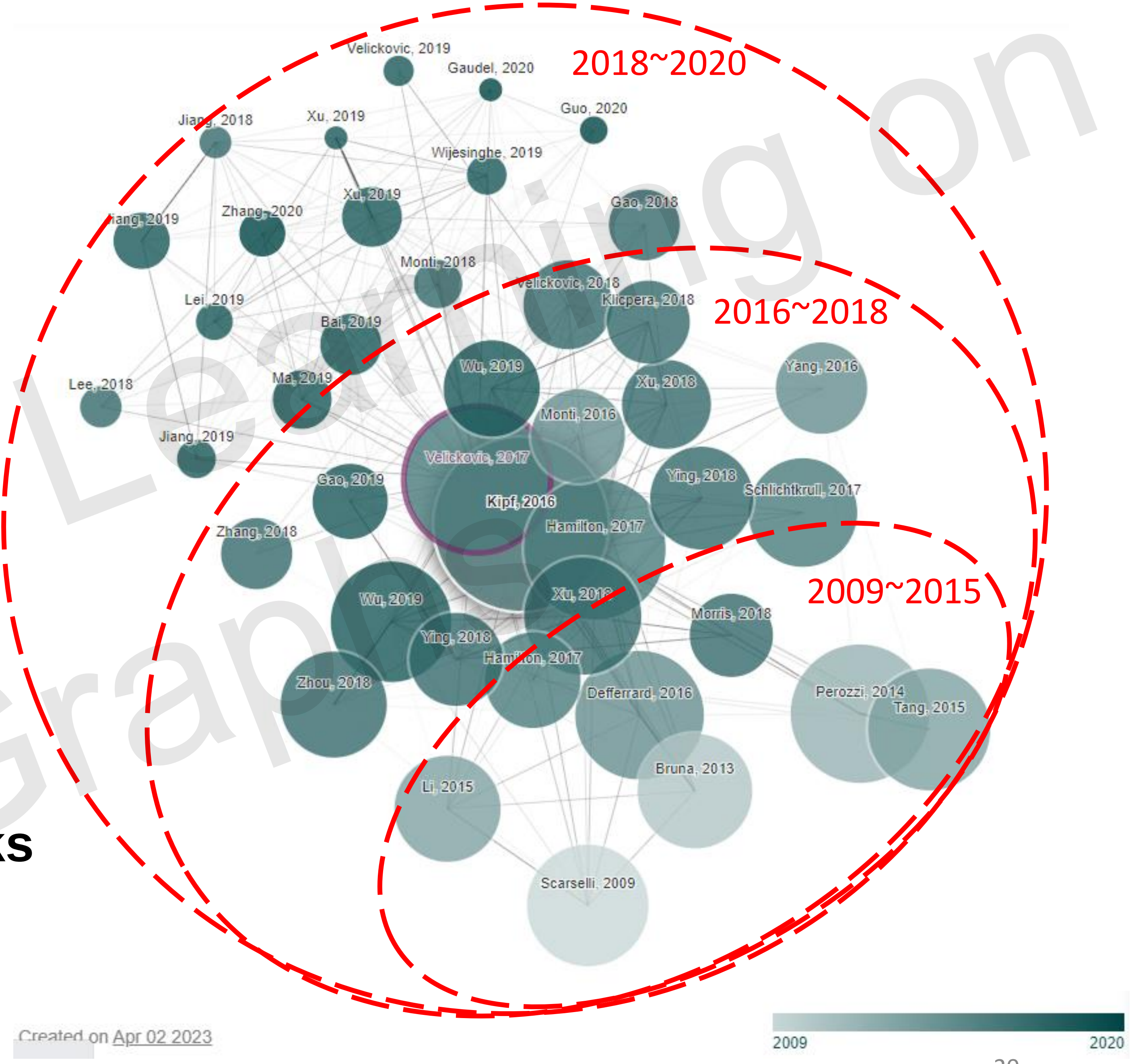
Motivation

Real-world graphs are expanding all the time



Motivation

Graphs are growing



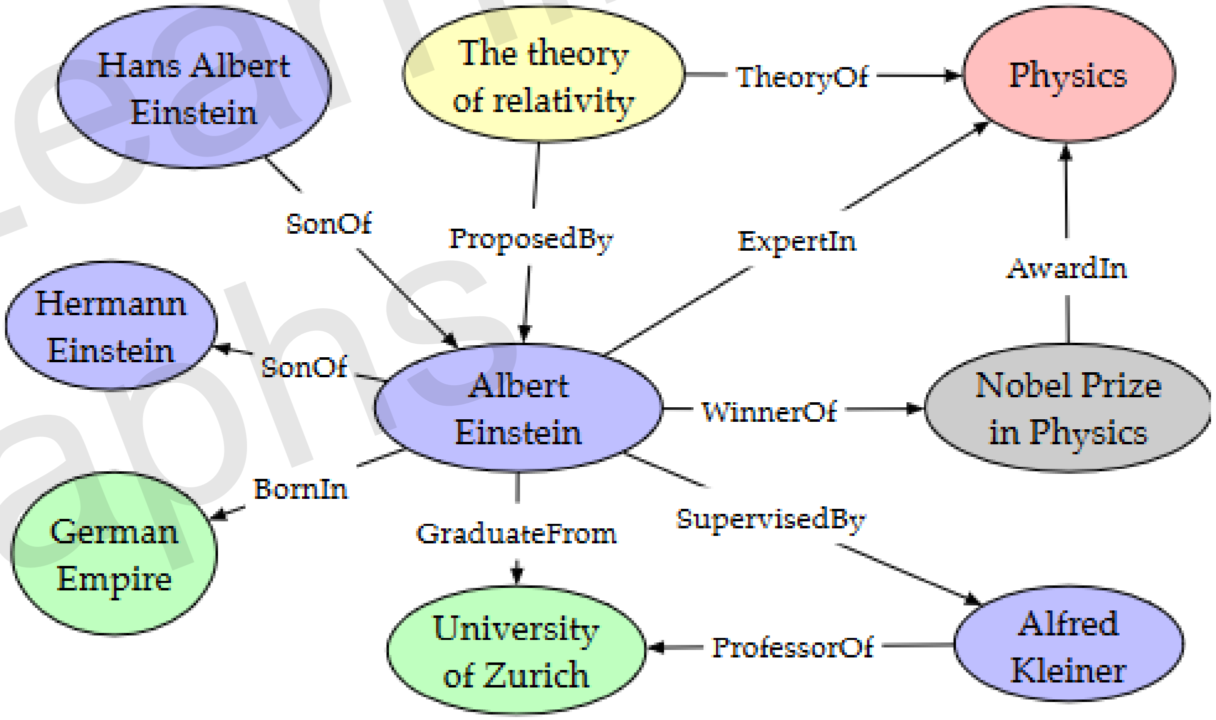
Academic social networks expand with time

https://www.connectedpapers.com/

Motivation

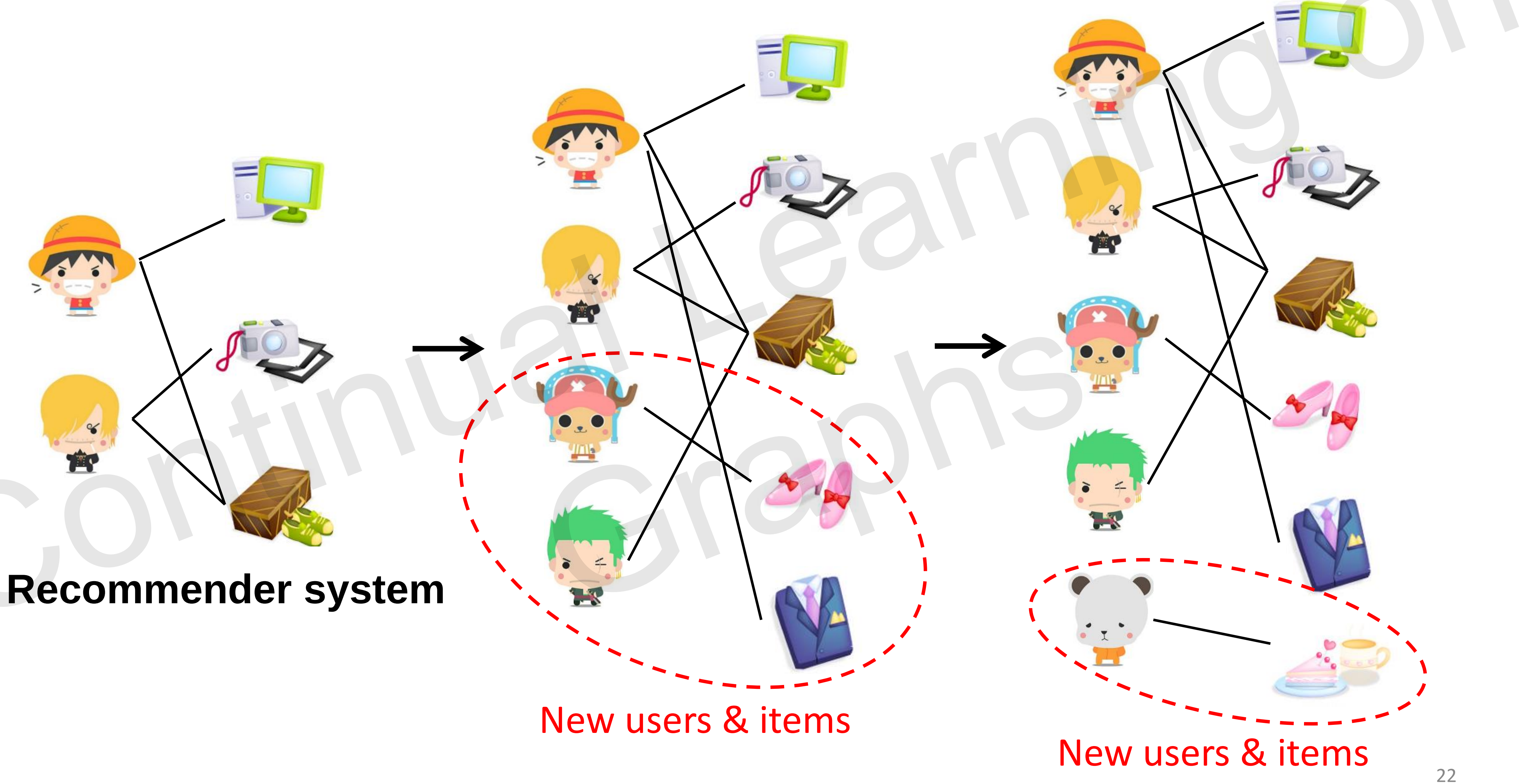
Knowledge graph grows with time

(Albert Einstein, **BornIn**, German Empire)
(Albert Einstein, **SonOf**, Hermann Einstein)
(Albert Einstein, **GraduateFrom**, University of Zurich)
(Albert Einstein, **WinnerOf**, Nobel Prize in Physics)
(Albert Einstein, **ExpertIn**, Physics)
(Nobel Prize in Physics, **AwardIn**, Physics)
(The theory of relativity, **TheoryOf**, Physics)
(Albert Einstein, **SupervisedBy**, Alfred Kleiner)
(Alfred Kleiner, **ProfessorOf**, University of Zurich)
(The theory of relativity, **ProposedBy**, Albert Einstein)
(Hans Albert Einstein, **SonOf**, Albert Einstein)



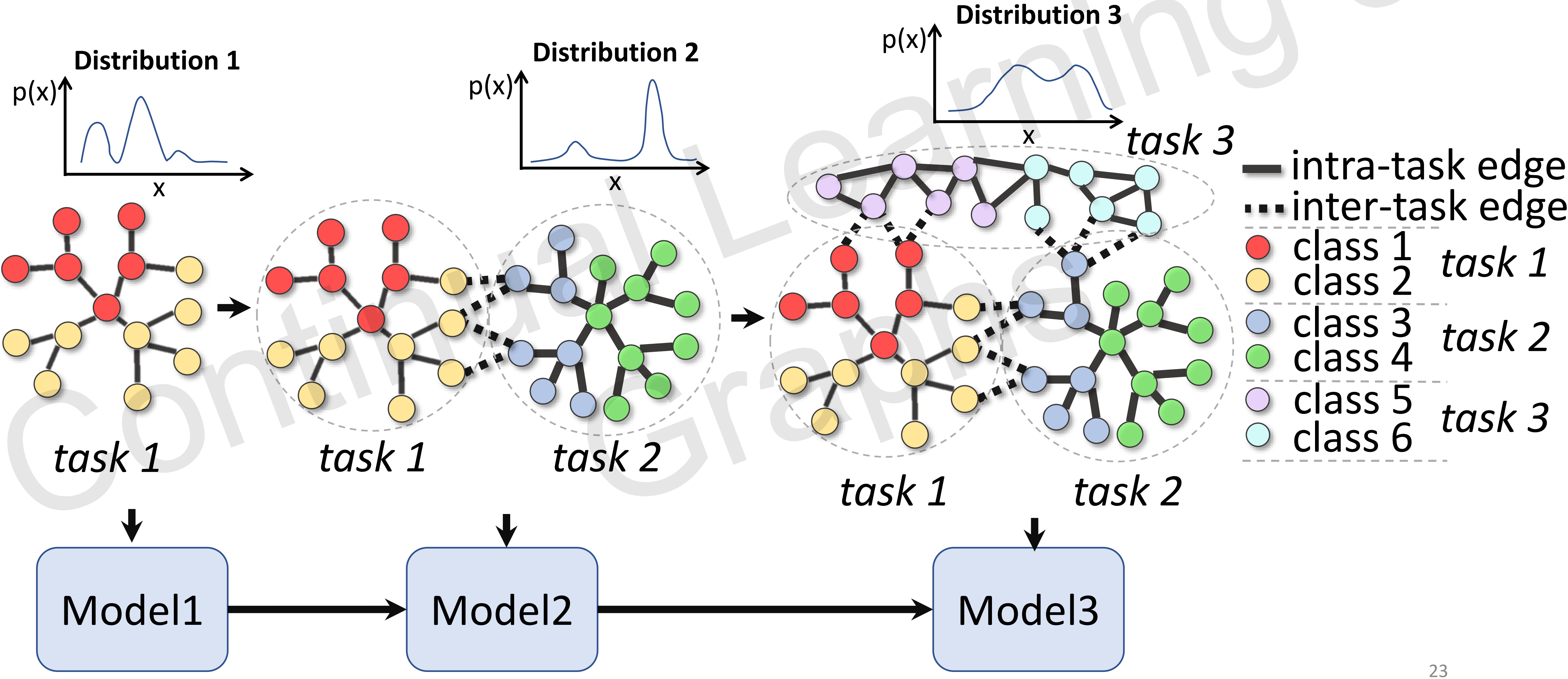
Ji, Shaoxiong, et al. "A survey on knowledge graphs: Representation, acquisition, and applications." IEEE transactions on neural networks and learning systems 33.2 (2021): 494-514

Motivation



Motivation

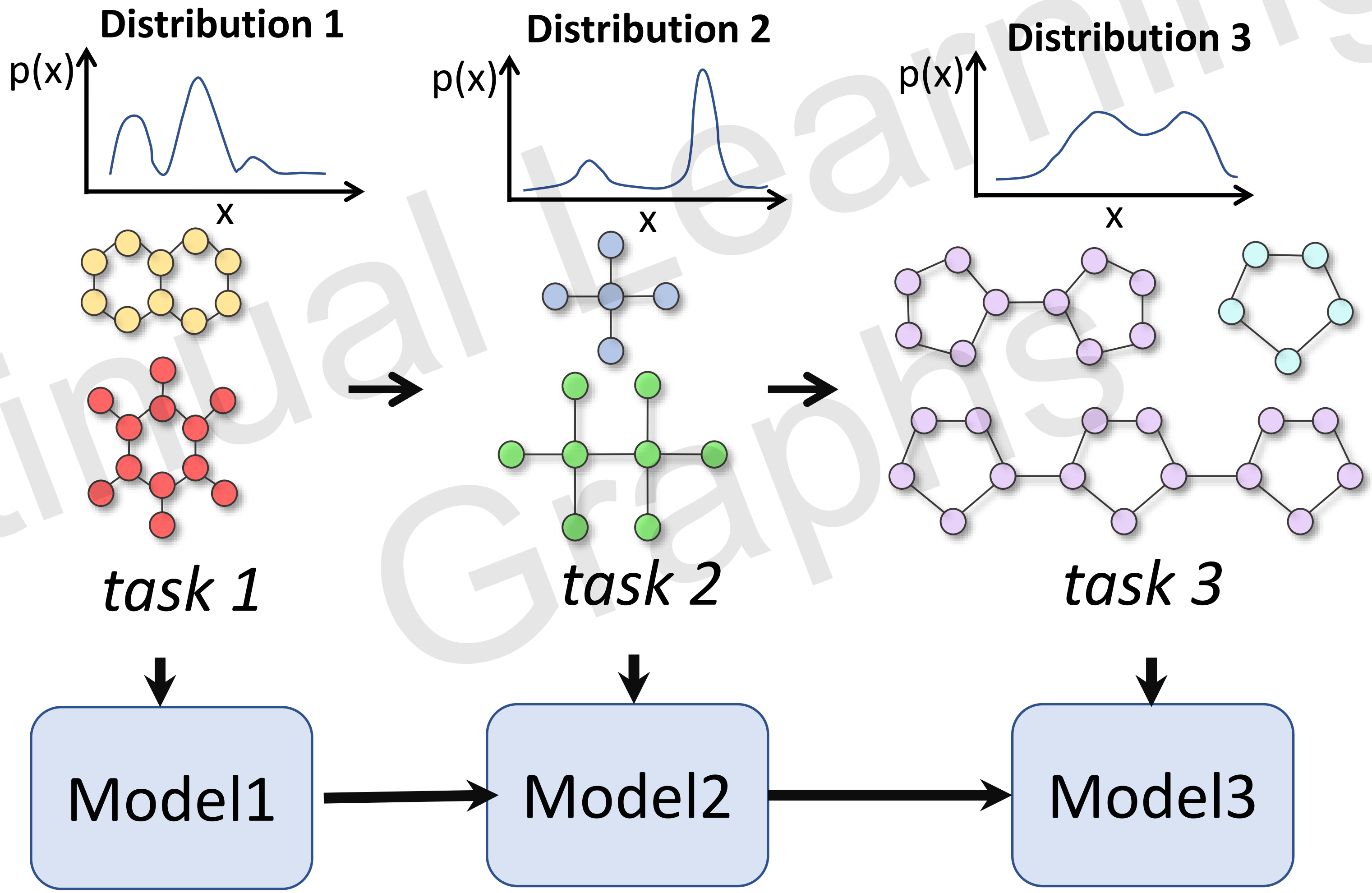
Model has to adapt



Motivation

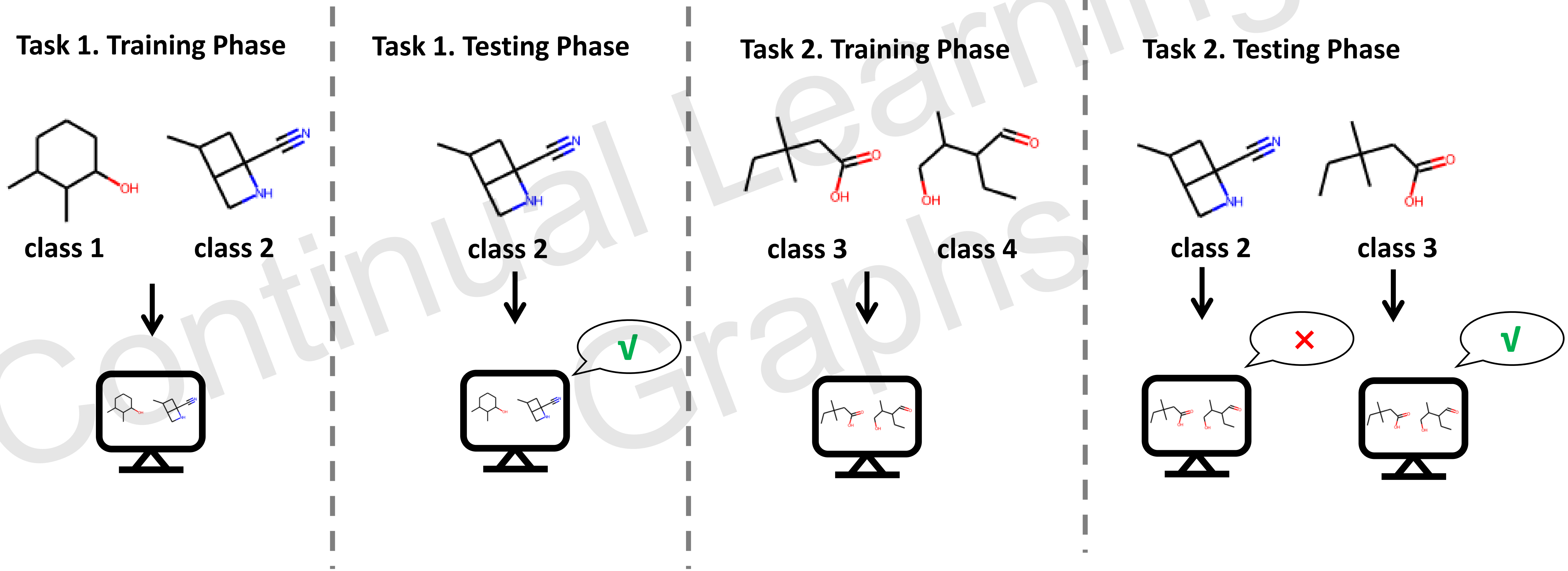
Realistic continual learning scenario

G-CGL: Graph level prediction, multiple graphs



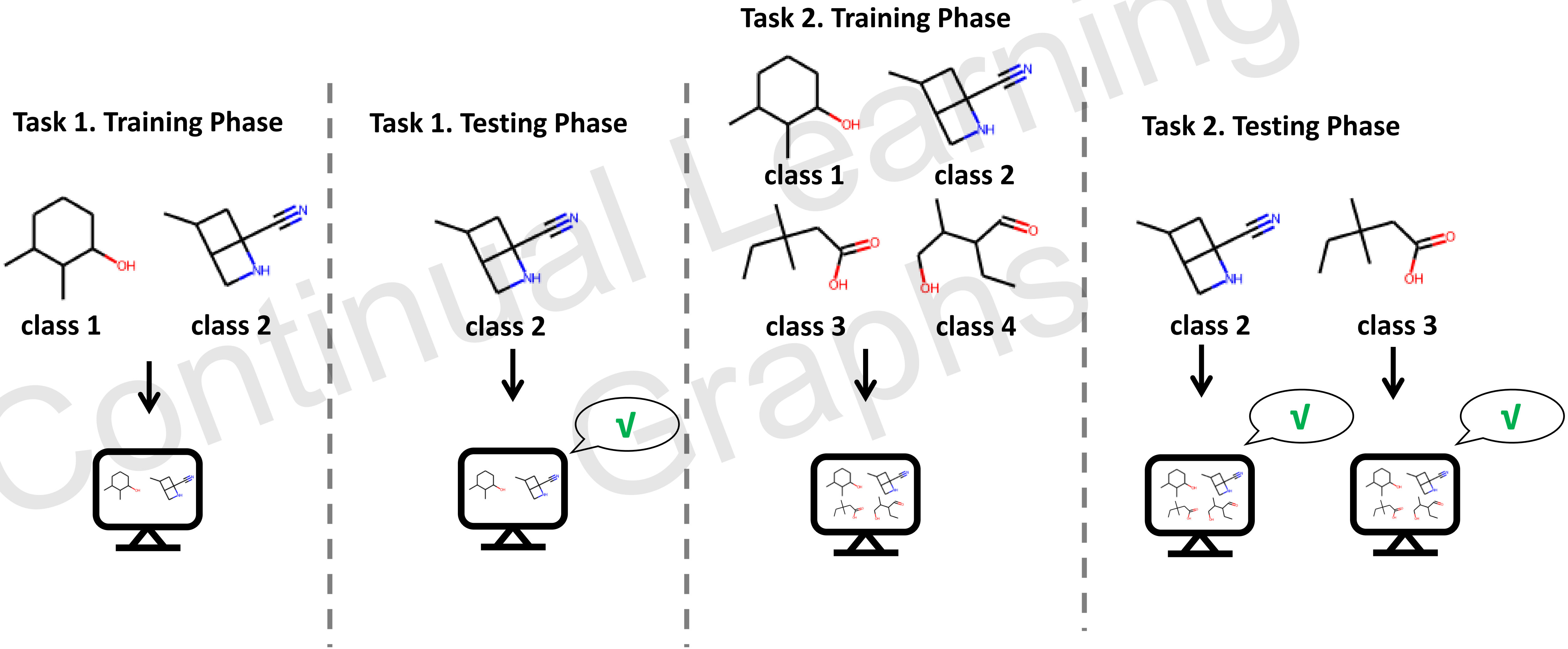
Motivation

Catastrophic forgetting



Motivation

Can we just retrain over all data?



Motivation

Retraining is computationally impractical

Scale	Name	#Nodes	#Edges*
Medium	ogbn-products	2,449,029	61,859,140
Medium	ogbn-proteins	132,534	39,561,252
Small	ogbn-arxiv	169,343	1,166,243
Large	ogbn-papers100M	111,059,956	1,615,685,872
Medium	ogbn-mag	1,939,743	21,111,007

Scale	Name	#Nodes	#Edges*
Medium	ogbl-ppa	576,289	30,326,273
Small	ogbl-collab	235,868	1,285,465
Small	ogbl-ddi	4,267	1,334,889
Medium	ogbl-citation2	2,927,963	30,561,187
Medium	ogbl-wikikg2	2,500,604	17,137,181
Small	ogbl-biokg	93,773	5,088,434
Medium	ogbl-vessel*	3,538,495	5,345,897

Scale	Name	#Graphs	#Nodes per graph	#Edges per graph*
Small	ogbg-molhiv	41,127	25.5	27.5
Medium	ogbg-molpcba	437,929	26.0	28.1
Medium	ogbg-ppa	158,100	243.4	2,266.1
Medium	ogbg-code2	452,741	125.2	124.2

Task category	Name	#Graphs	#Total nodes	#Total edges
Node-level	MAG240M	1	244,160,499	1,728,364,232
Link-level	WikiKG90Mv2	1	91,230,610	601,062,811
Graph-level	PCQM4Mv2	3,746,619	52,970,652	54,546,813

Hu, Weihua, et al. "Open graph benchmark: Datasets for machine learning on graphs." *Advances in neural information processing systems* 33 (2020): 22118-22133.

Motivation

Objectives

- Enough plasticity to adapt to new tasks (including new topologies)
- Minimal forgetting on previous tasks (topologies)
- If possible, positive cross task transfer

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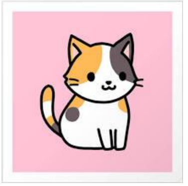
Problem Setup - CL

Basic concept: tasks

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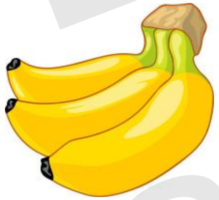
Task 1

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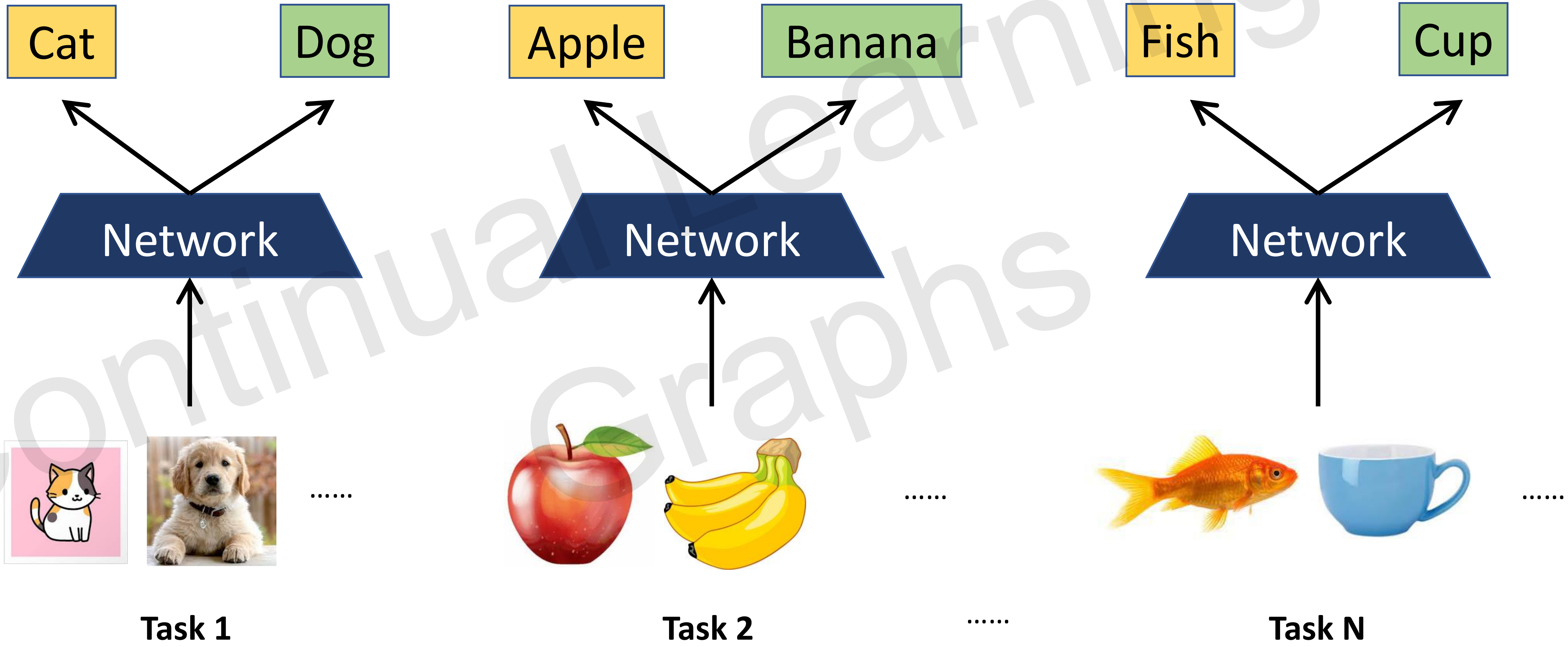
Task 2


......

Task N

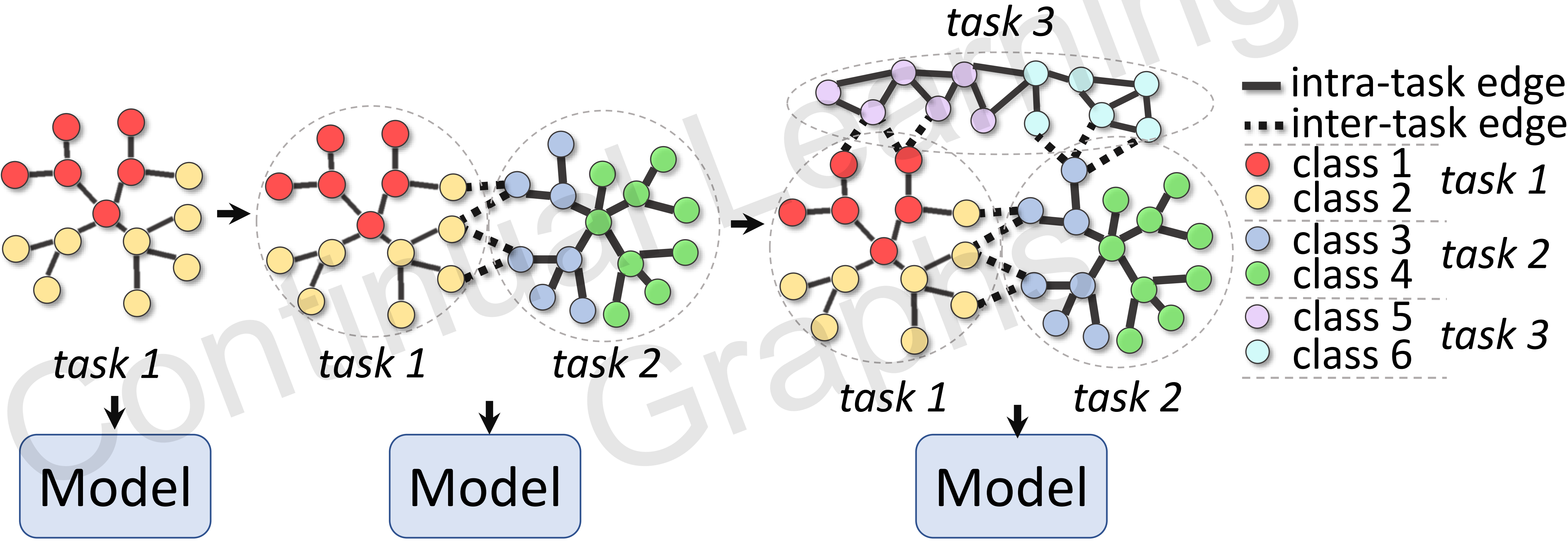
Problem Setup - CL

Commonly adopted task constructions



Problem Setup - CGL

Realistic continual learning scenario



Problem Setup - CGL

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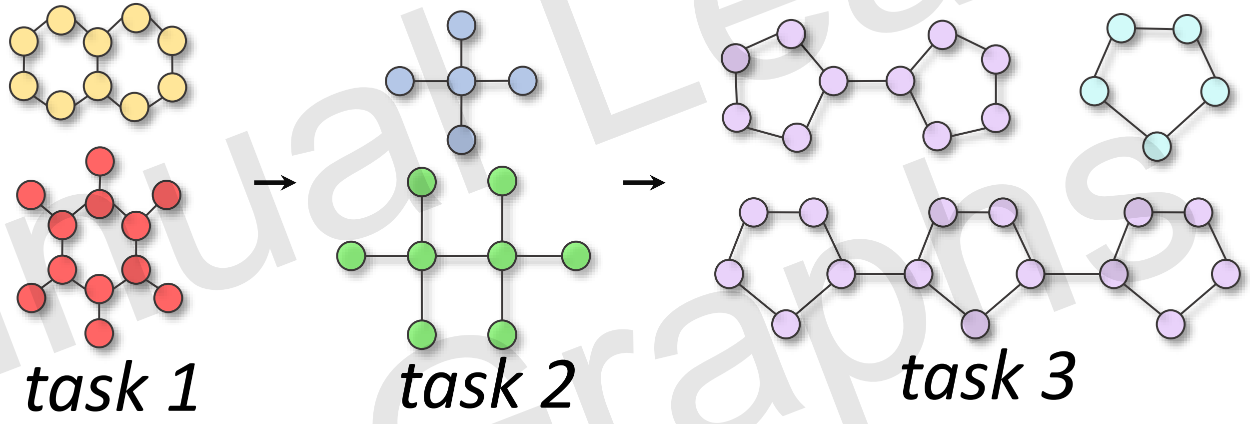
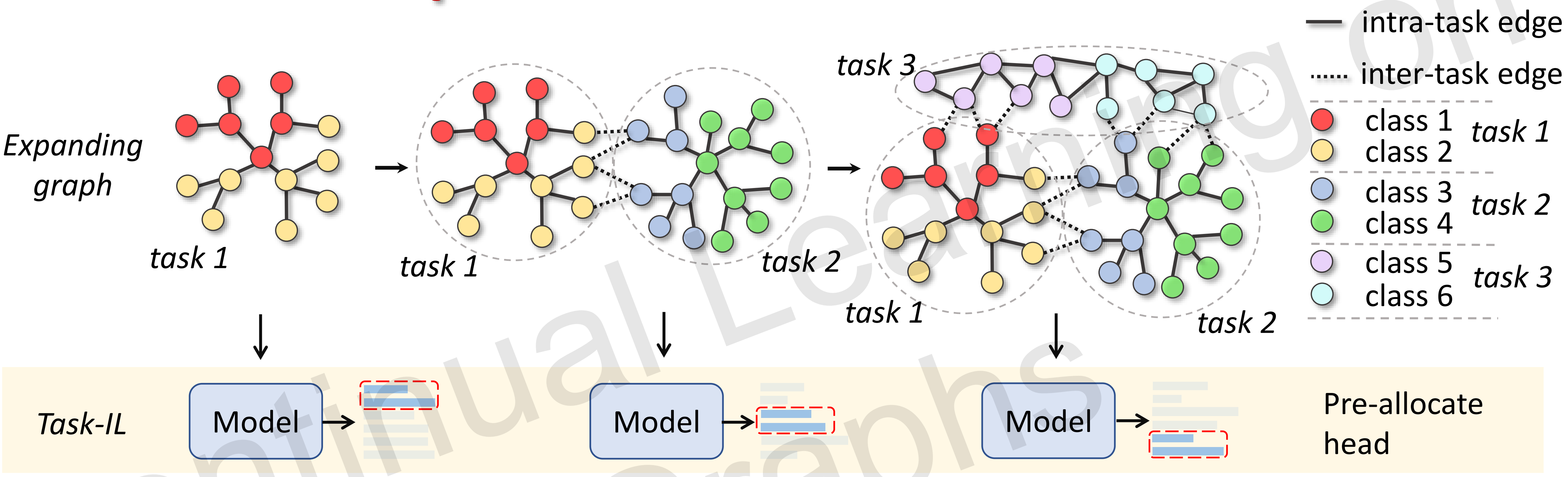
G-CGL: Graph level prediction, multiple graphs



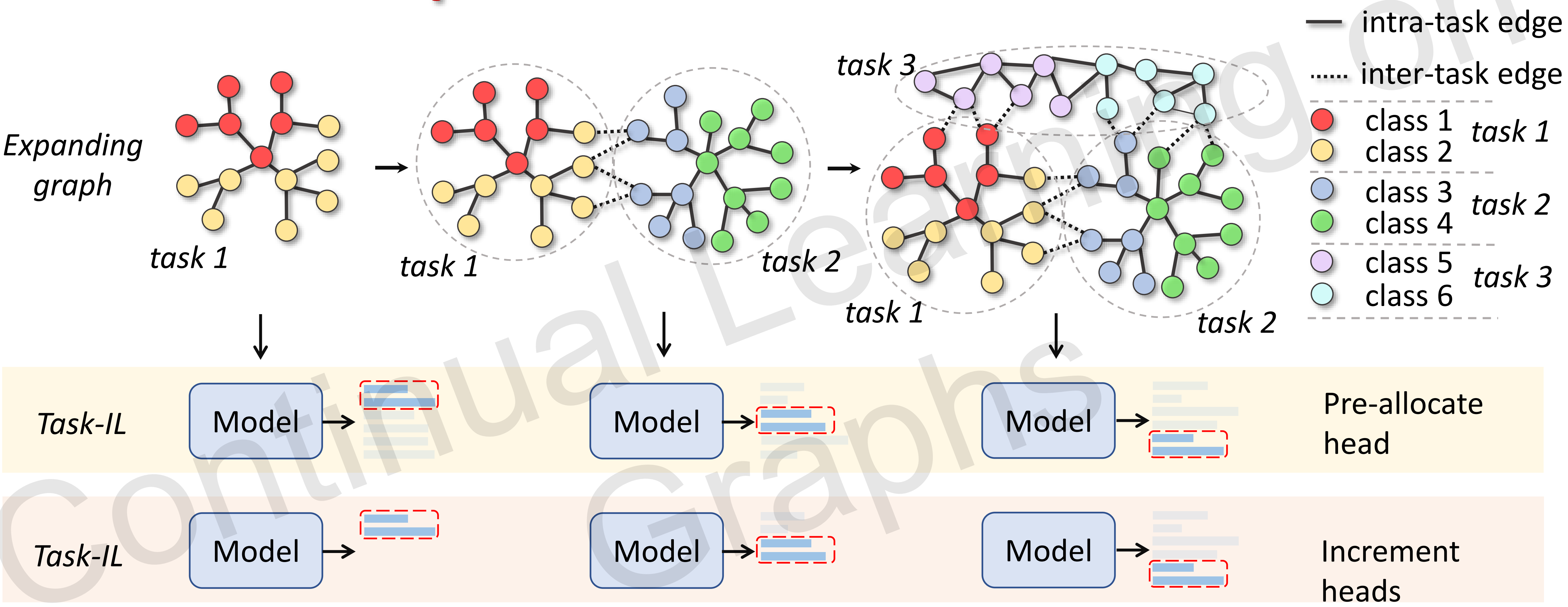
- Node- or graph-level tasks?

Problem Setup – CGL Task IL & Node-level task



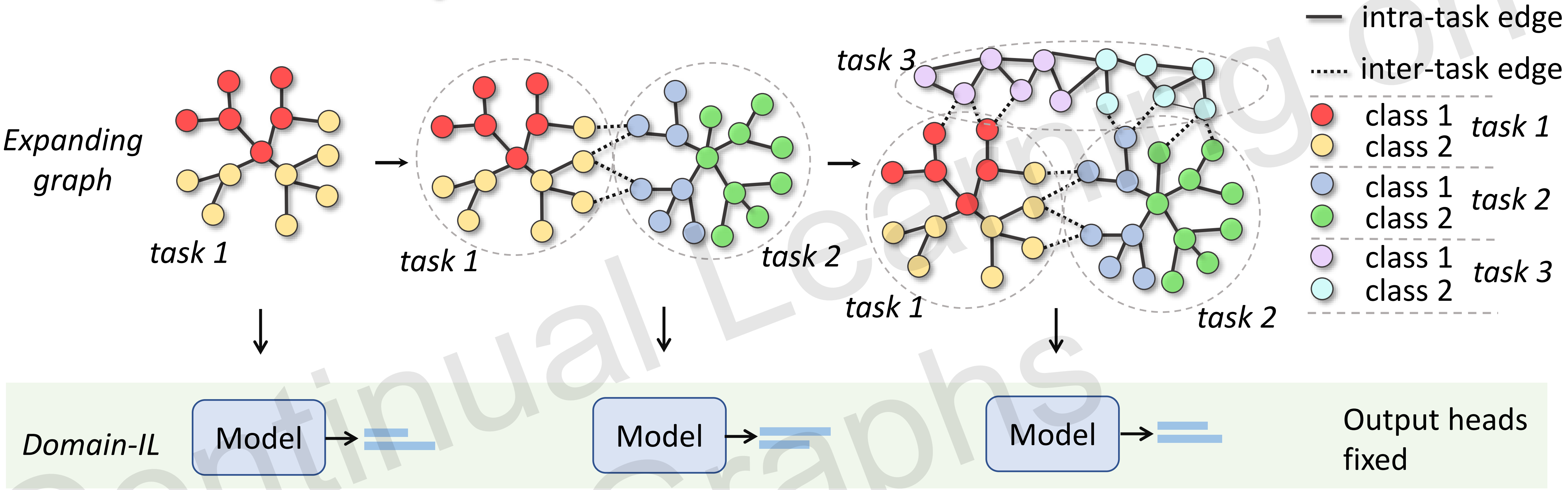
Activate task-specific heads

Problem Setup – CGL Task IL & Node-level task

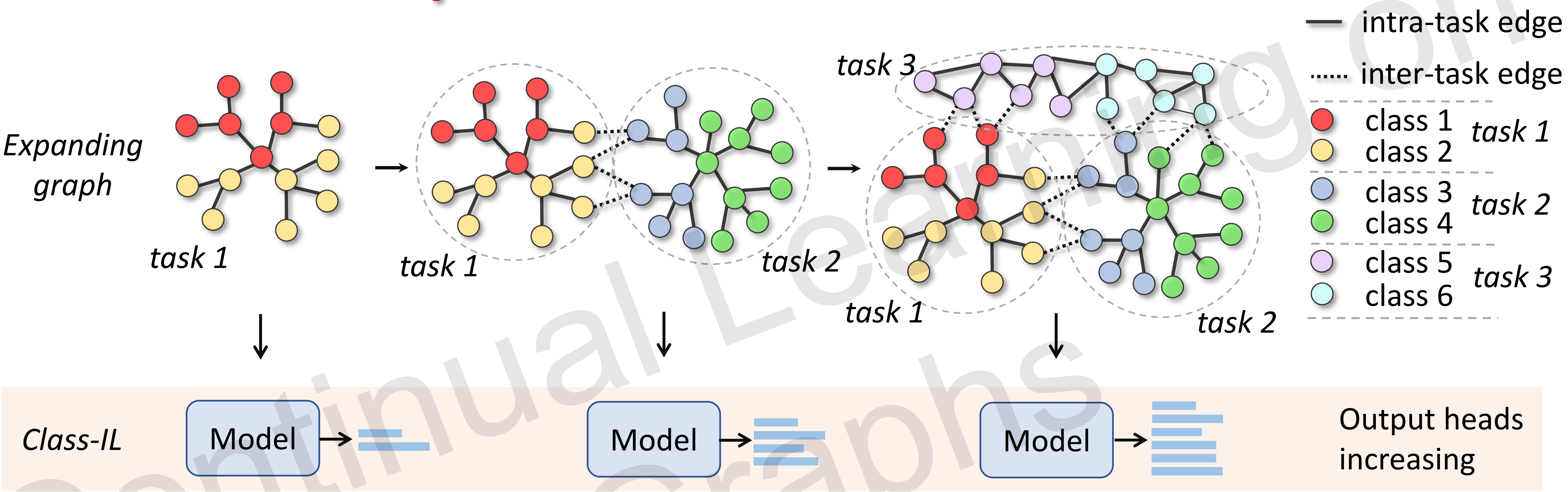


Activate task-specific heads

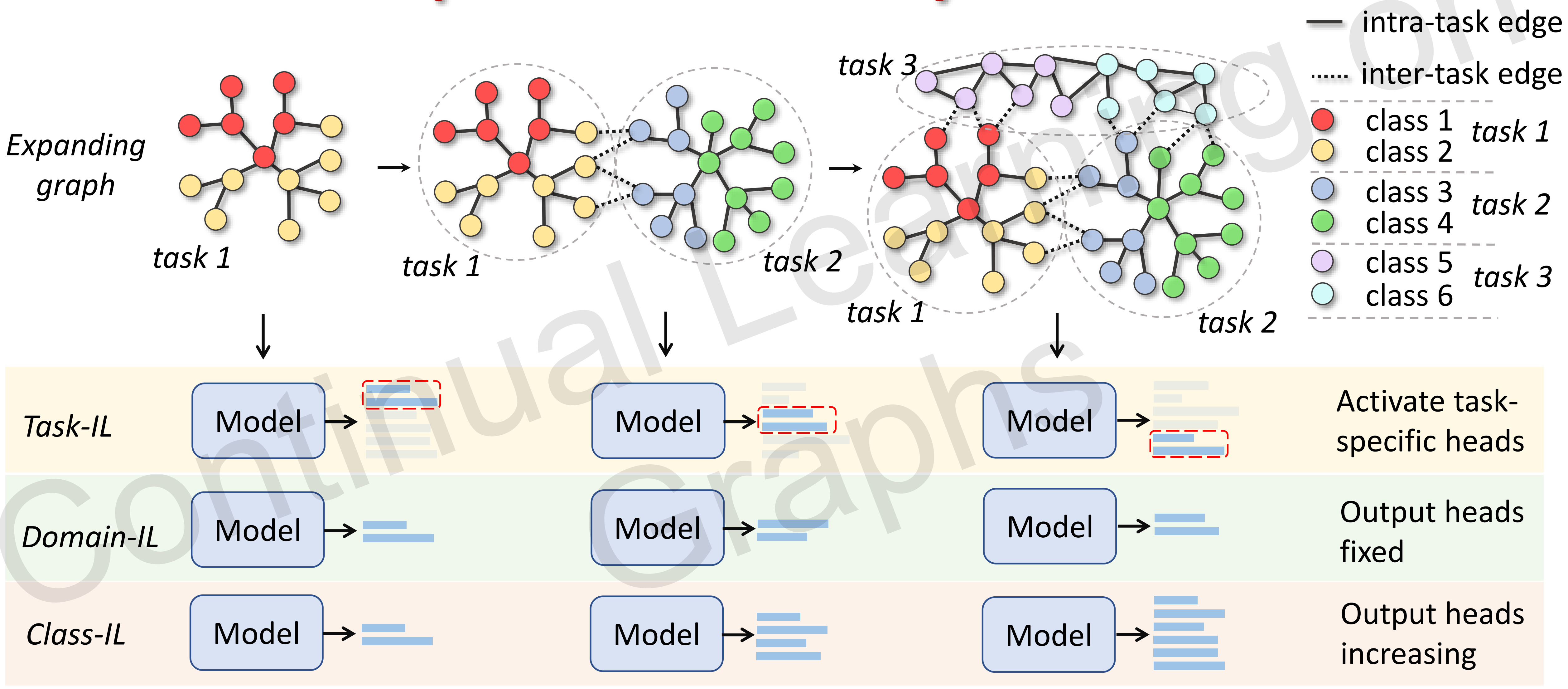
Problem Setup – CGL Domain IL & Node-level task



Problem Setup – CGL Class IL & Node-level task



Problem Setup – CGL Summary of Three Scenarios



Problem Setup – CGL Challenges

Difficulty: Plasticity-stability dilemma

- Plasticity: adapting to new tasks
- Stability: maintaining performance on old tasks
- **Catastrophic forgetting**: models adapting well to new tasks while forgetting old tasks severely

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CL & CGL Techniques

Rough Categories

- **Regularization:** Penalize changes to the model via regularizations
- **Parameter-isolation:** Separate parameters for new and old tasks (partially or entirely)
- **Memory-replay:** Replay data from existing/old tasks while adapting the model to new ones

CL & CGL Techniques

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CL Techniques Elastic weight consolidation (EWC, regularization based)

Basic loss for learning the currently given task

$$\mathcal{L}(\theta) = \boxed{\mathcal{L}_B(\theta)} + \boxed{\sum_i \frac{\lambda}{2} F_i(\theta_i - \theta^*_{A,i})^2}$$

Regularization term for minimizing the forgetting problem

$\boldsymbol{\lambda}$:balances the contribution of the old tasks

$\boldsymbol{F_i}$:Parameter importance to task A (measured by Fisher information)

Kirkpatrick, James, et al. "Overcoming catastrophic forgetting in neural networks." Proceedings of the national academy of sciences 114.13 (2017): 3521-3526.

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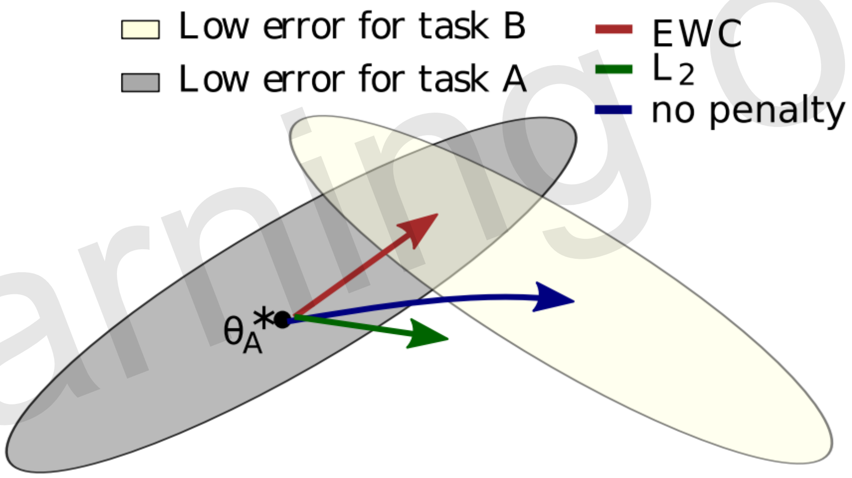

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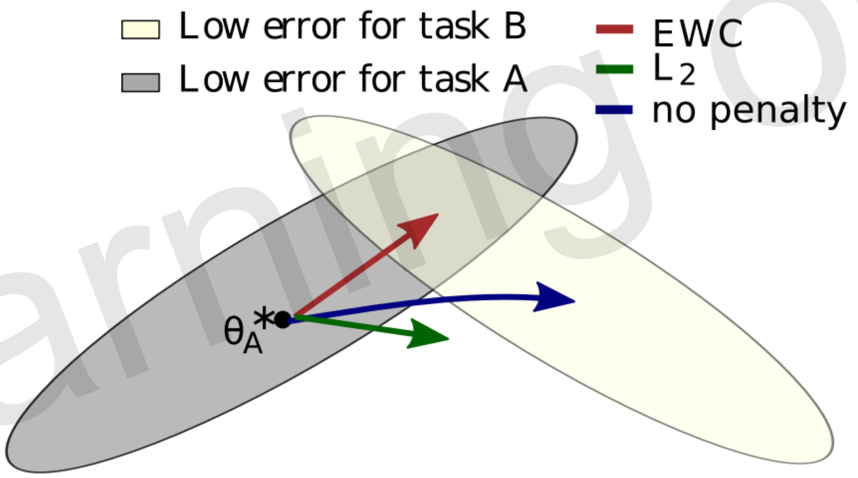

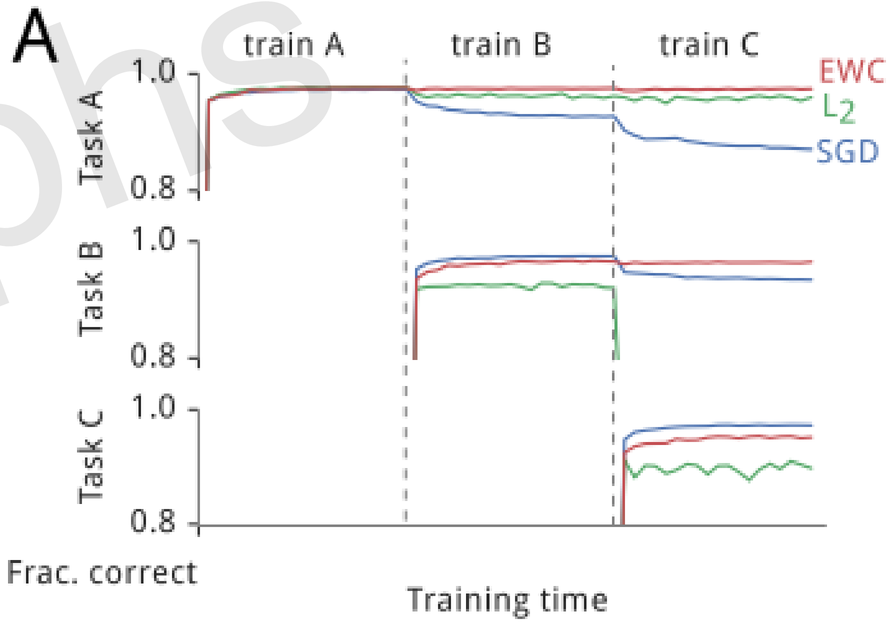

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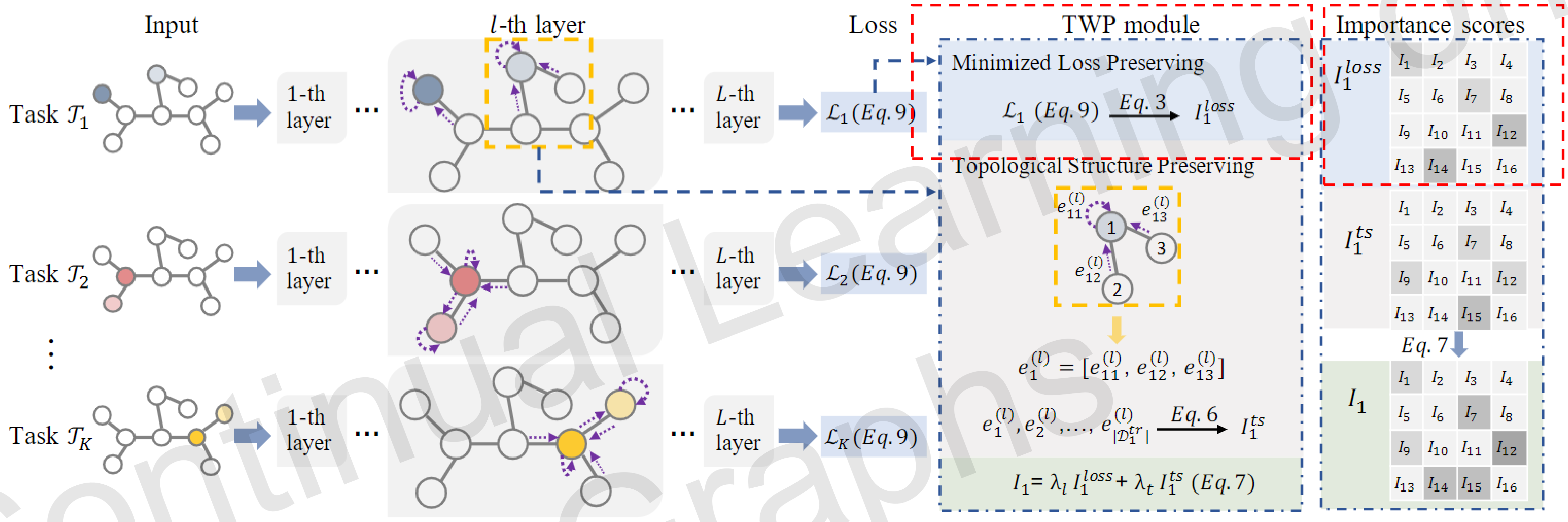
CGL Techniques Topology-aware Weight Preserving (TWP, regularization based)



Minimized Loss Preserving

$$\mathcal{L}(X_k^{tr}; W + \Delta W) - \mathcal{L}(X_k^{tr}; W) \approx \sum_m f_m(X_k^{tr})\Delta \boldsymbol{w}_m$$

$$f_m(X_k^{tr}) = \frac{\partial \mathcal{L}}{\partial \boldsymbol{w}_m} \qquad \boxed{I_k^{loss} = [\|f_m(X_k^{tr})\|]}$$

importance score (loss)

Liu, Huihui, Yiding Yang, and Xinchao Wang. "Overcoming catastrophic forgetting in graph neural networks." *Proceedings of the AAAI conference on artificial intelligence*. Vol. 35. No. 10. 2021.

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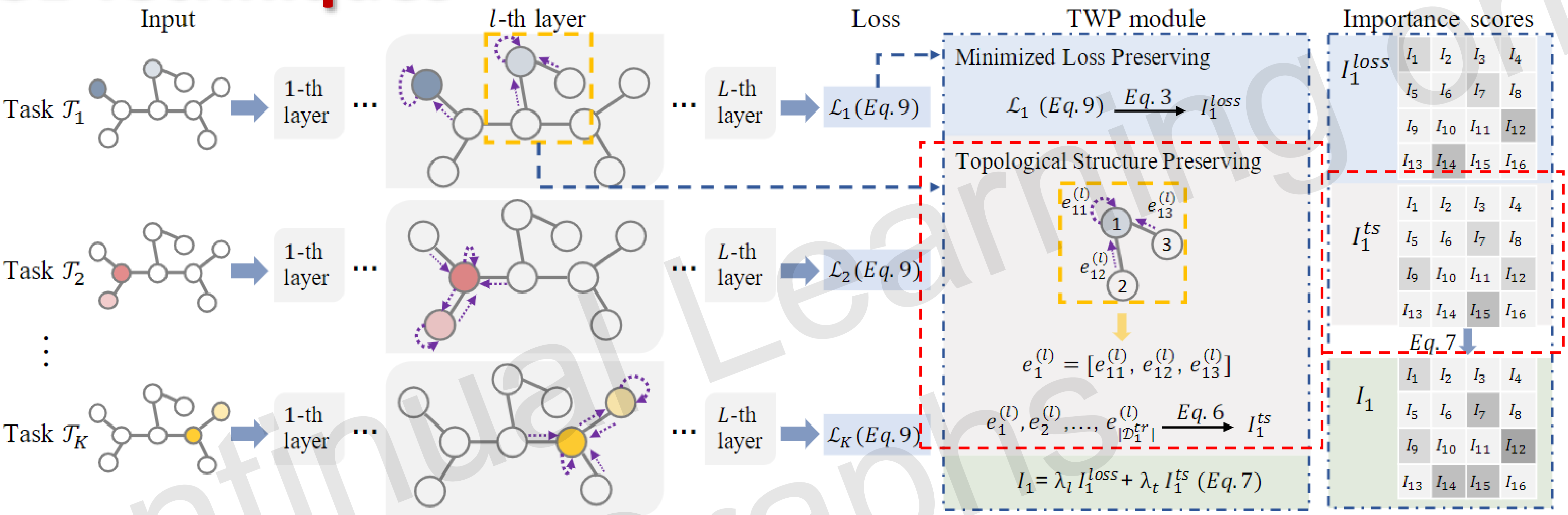


Topological Structure Preserving

$$e_{ij}^{(l)} = a(\boldsymbol{H}_{i,j}^{(l-1)}; W^{(l)})$$

(for GAT)

Embedding of i and j

$$e_{ij}^{(l)} = (\boxed{\boldsymbol{h}_i^{(l-1)}W^{(l)}})^{\mathrm{T}}\tanh(\boxed{\boldsymbol{h}_j^{(l-1)}W^{(l)}})$$

(for any GNN)

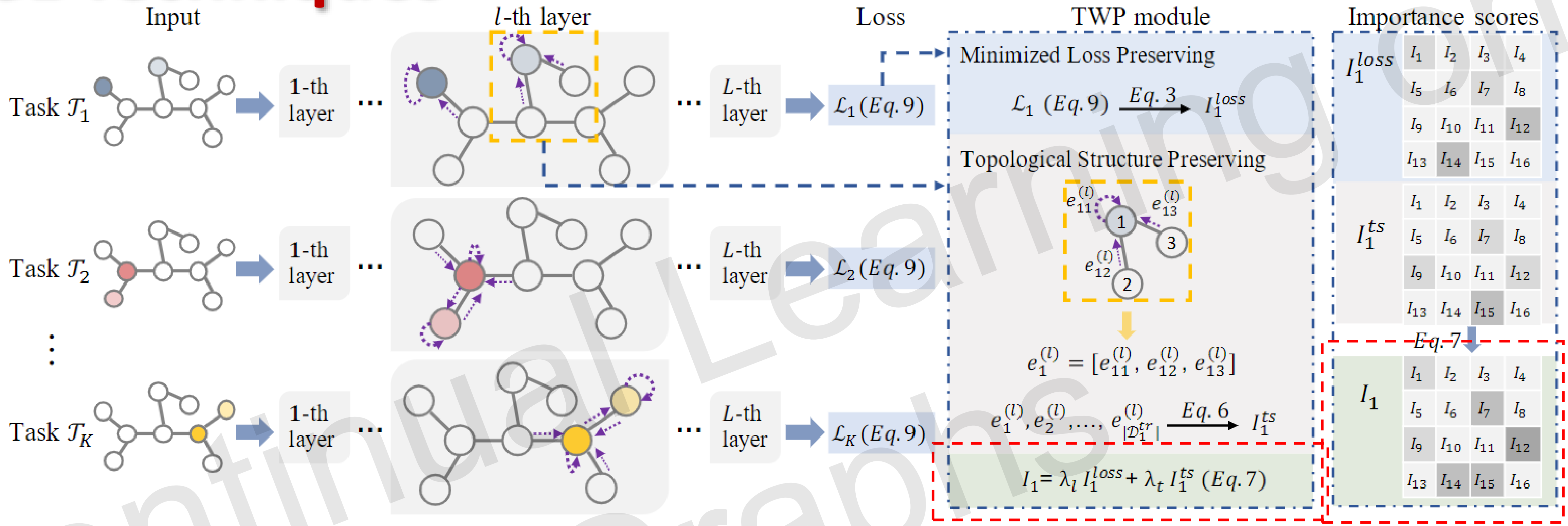
$$g_m(\boldsymbol{H}^{(l-1)}) = \frac{\partial\left(\left|[e_1^{(l)}, \dots, e_{|\mathcal{D}_k^{tr}|}^{(l)}]\right|_2^2\right)}{\partial \boldsymbol{w}_m}$$

$$\boxed{I_k^{ts} = [\|g_m(\boldsymbol{H}_k^{(l-1)})\|]}$$

importance score (topology)

Liu, Huihui, Yiding Yang, and Xinchao Wang. "Overcoming catastrophic forgetting in graph neural networks." *Proceedings of the AAAI conference on artificial intelligence*. Vol. 35. No. 10. 2021.

CGL Techniques Topology-aware Weight Preserving (TWP, regularization based)



$$\boxed{I_k = \lambda_l I_k^{loss} + \lambda_t I_k^{ts}}$$

importance score (total)

$$\mathcal{L}'_{k+1}(W) = \mathcal{L}_{k+1}^{new}(W) + \boxed{\sum_{n=1}^{k} I_n \otimes (W - W_n^*)^2}$$

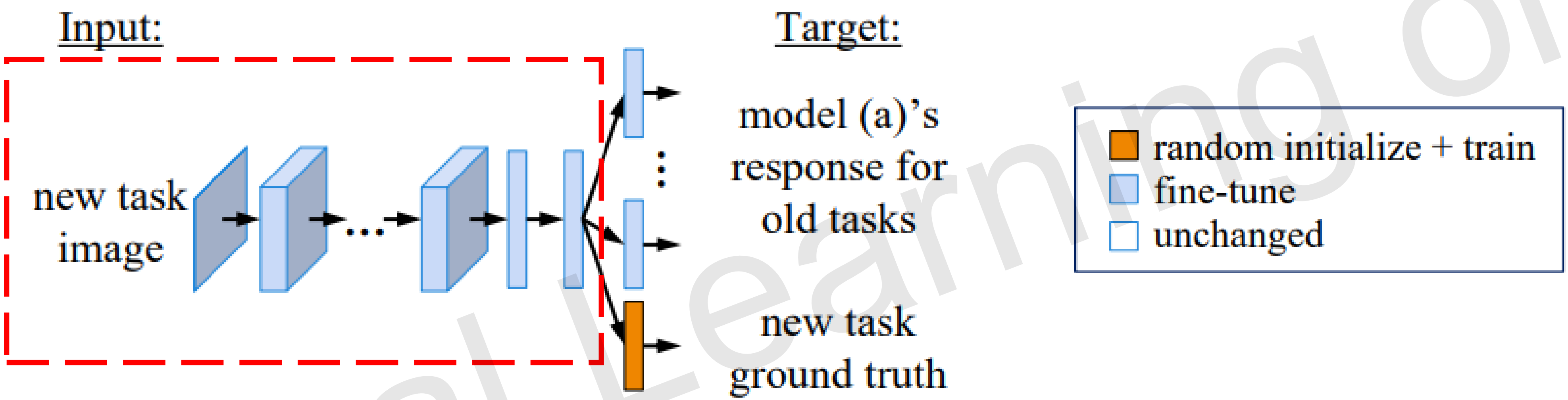
regularization

$$\mathcal{L}_{k+1}(W) = \mathcal{L}'_{k+1}(W) + \beta \| I_{k+1} \|_1$$

Liu, Huihui, Yiding Yang, and Xinchao Wang. "Overcoming catastrophic forgetting in graph neural networks." *Proceedings of the AAAI conference on artificial intelligence*. Vol. 35. No. 10. 2021.

CL Techniques

Learning without forgetting (LwF, regularization based)



Start with:

θ_s: shared parameters

θ_o: task specific parameters for each old task

X_n, Y_n: training data and ground truth on the new task

Initialize:

$Y_o \leftarrow \mathrm{CNN}(X_n, \theta_s, \theta_o)$ // *compute output of old tasks for new data*

$\theta_n \leftarrow \mathrm{RANDINIT}(|\theta_n|)$ // *randomly initialize new parameters*

Train:

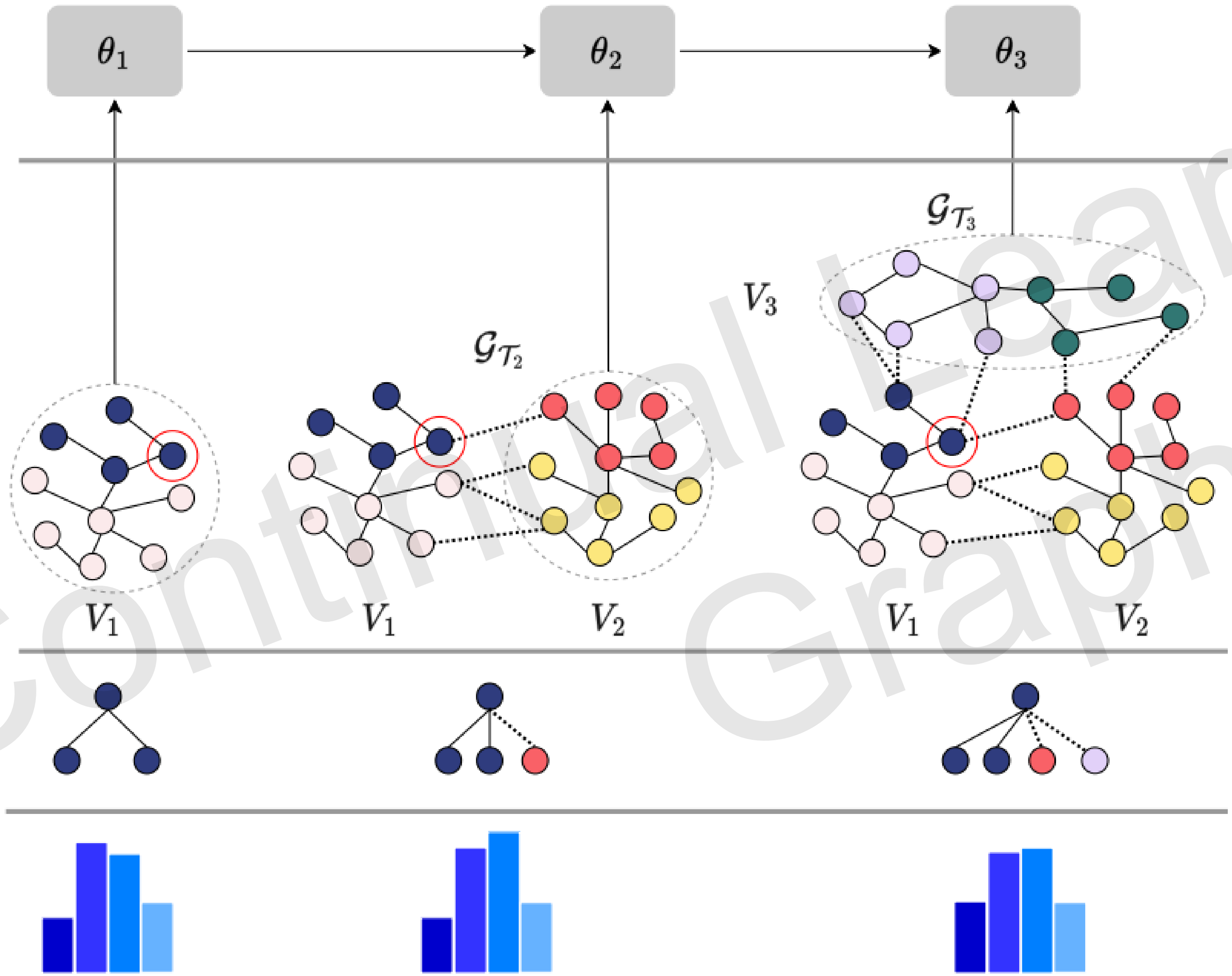
Define $\hat{Y}_o \equiv \mathrm{CNN}(X_n, \hat{\theta}_s, \hat{\theta}_o)$ // *old task output*

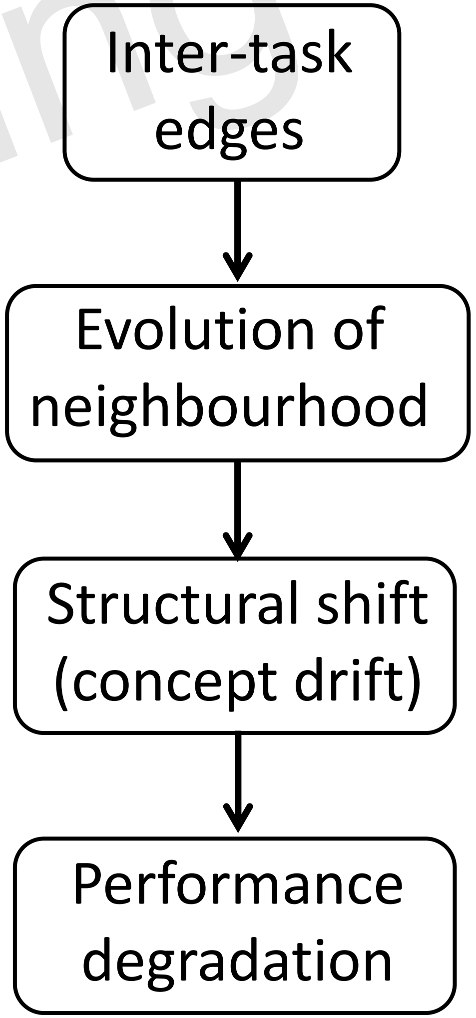
Define $\hat{Y}_n \equiv \mathrm{CNN}(X_n, \hat{\theta}_s, \hat{\theta}_n)$ // *new task output*

$$\theta_s^*,\ \theta_o^*,\ \theta_n^* \leftarrow \underset{\hat{\theta}_s, \hat{\theta}_o, \hat{\theta}_n}{\mathrm{argmin}} \left(\lambda_o \mathcal{L}_{old}(Y_o, \hat{Y}_o) + \mathcal{L}_{new}(Y_n, \hat{Y}_n) + \mathcal{R}(\hat{\theta}_s, \hat{\theta}_o, \hat{\theta}_n) \right)$$

Li, Zhizhong, and Derek Hoiem. "Learning without forgetting." IEEE transactions on pattern analysis and machine intelligence 40.12 (2017): 2935-2947.

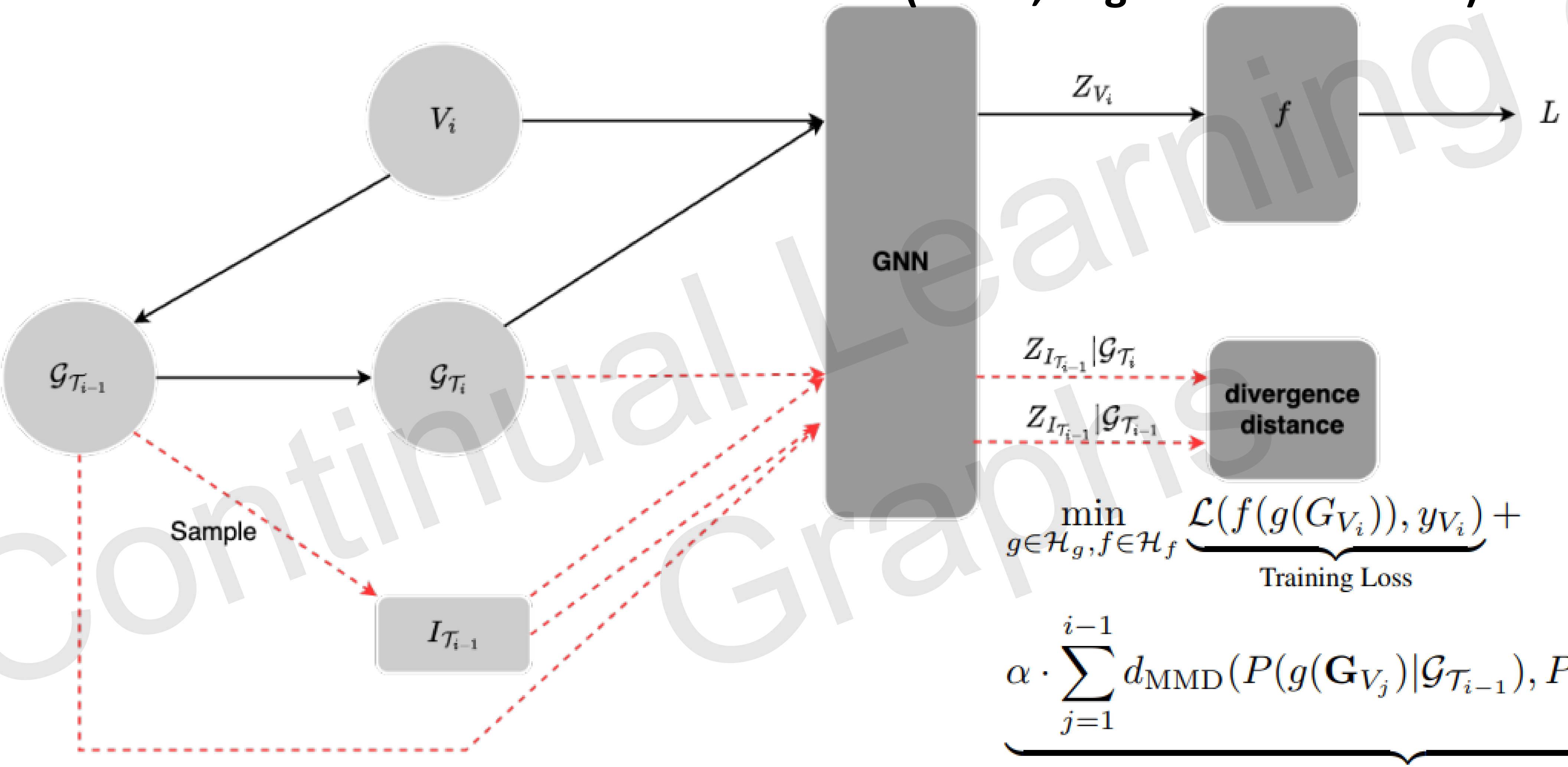
CGL Techniques Towards Robust Graph Incremental Learning on Evolving Graphs (SSRM, Regularization based)





Su, Junwei, et al. "Towards Robust Graph Incremental Learning on Evolving Graphs." International Conference on Machine Learning. PMLR, 2023, pp. 32 728–32 748.

CGL Techniques Towards Robust Graph Incremental Learning on Evolving Graphs (SSRM, Regularization based)



$$\min_{g\in\mathcal{H}_g, f\in\mathcal{H}_f} \underbrace{\mathcal{L}(f(g(G_{V_i})), y_{V_i})}_{\text{Training Loss}} + \underbrace{\alpha \cdot \sum_{j=1}^{i-1} d_{\mathrm{MMD}}(P(g(\mathbf{G}_{V_j})|\mathcal{G}_{\mathcal{T}_{i-1}}), P(g(\mathbf{G}_{V_j})|\mathcal{G}_{\mathcal{T}_i}))}_{\text{Structural Shift Mitigation}} + \underbrace{\beta \cdot d_{\mathrm{MMD}}(P(g(\mathbf{G}_{V_j})|\mathcal{G}_{\mathcal{T}_{i-1}}), P(g(\mathbf{G}_{V_i})|\mathcal{G}_{\mathcal{T}_i}))}_{\text{Structural Shift Mitigation}}$$

Su, Junwei, et al. "Towards Robust Graph Incremental Learning on Evolving Graphs." International Conference on Machine Learning. PMLR, 2023, pp. 32 728–32 748.

CL & CGL Techniques

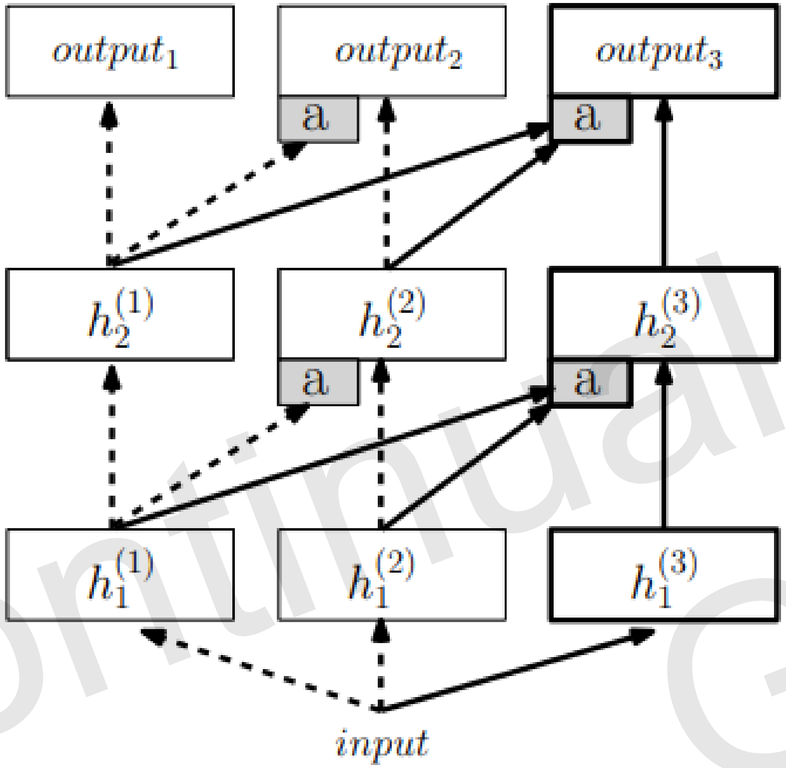
Rough Categories

- **Regularization:** Penalize changes to the model via regularizations

- **Parameter-isolation:** Separate parameters for new and old tasks (partially or entirely)

- **Memory-replay:** Replay data from existing/old tasks while adapting the model to new ones

CL Techniques Progressive neural network (Parameter isolation based)



$$h_i^{(k)} = f\left(\underbrace{W_i^{(k)} h_{i-1}^{(k)}}_{\text{From current task}} + \underbrace{\sum_{j<k} U_i^{(k:j)} h_{i-1}^{(j)}}_{\text{From previous tasks}}\right)$$

$W_i^{(k)}$ weight matrix of layer i of column k

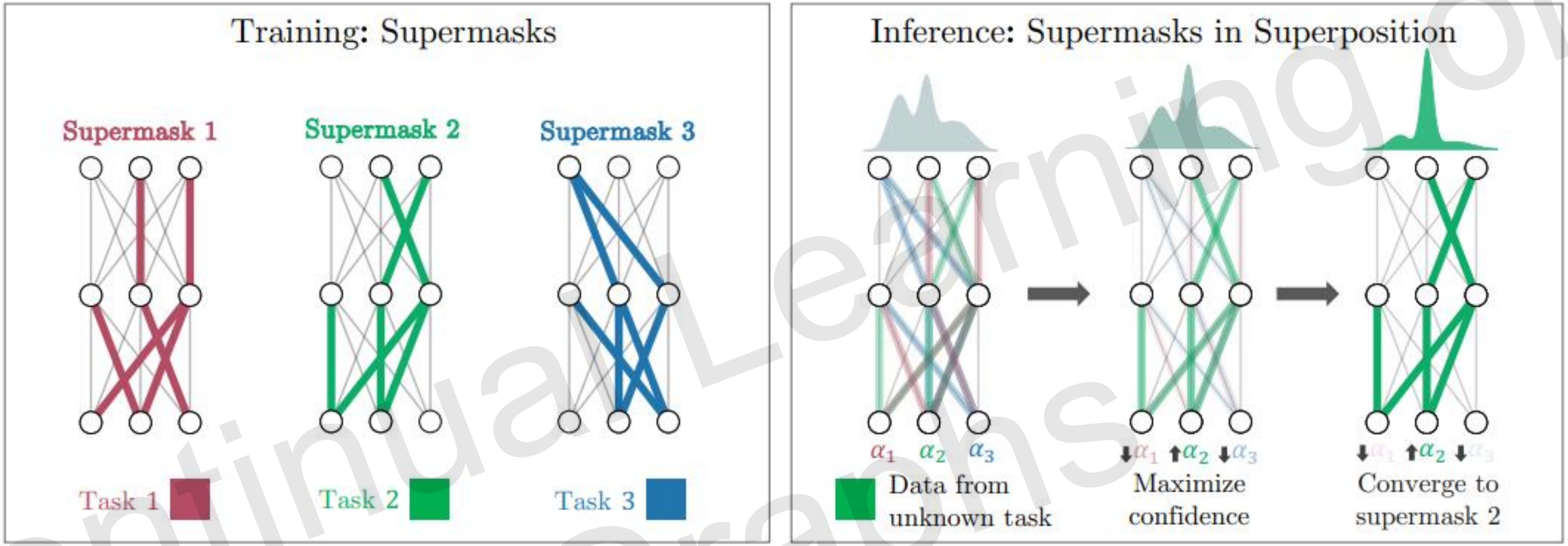
$U_i^{(k:j)}$ layer $i-1$ of column j, to layer i of column k

$$f(x) = \max(0, x)$$

Separate branch for each task

Rusu, Andrei A., et al. "Progressive neural networks." arXiv preprint arXiv:1606.04671 (2016).

CL Techniques Supermasks in Superposition (Parameter isolation based)



Learn a Supermask atop the backbone for each task: $\mathbf{p} = f\left(\mathbf{x}, W \odot M\right)$

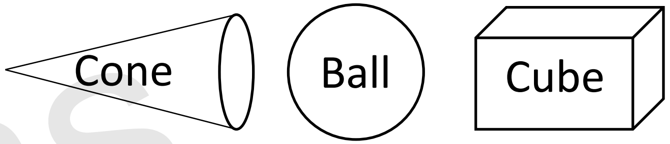
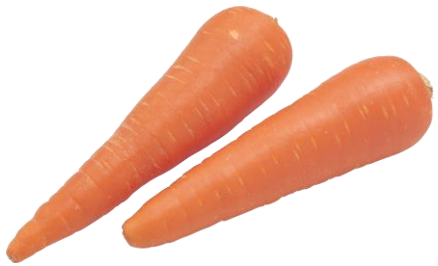
Without task indicators: $\mathbf{p}(\alpha) = f\left(\mathbf{x}, W \odot \left(\sum_{i=1}^{k} \alpha_i M^i\right)\right)$ $\quad \arg\max_i \left(-\frac{\partial \mathcal{H}\left(\mathbf{p}\left(\alpha\right)\right)}{\partial \alpha_i}\right)$

Wortsman, Mitchell, et al. "Supermasks in superposition." Advances in Neural Information Processing Systems 33 (2020): 15173-15184.

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

Motivation: Inspired by human cognition process, <u>Different representations</u> of data in different classes may be better represented by <u>different combinations</u> of a shared <u>pool of basic features</u>

Basic feature types:	**<u>Color</u>**	**<u>Shape</u>**
Basic feature instances (prototypes):	Orange Red Green	
Objects (combinations of basic feature prototypes):	 Green Ball	 Red Ball;  Orange Cone
Class (higher level hierarchy):	**Fruits**	**Vegetables**

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

Graph nodes (e.g. people in social network, papers in citation networks) should also be decomposable.

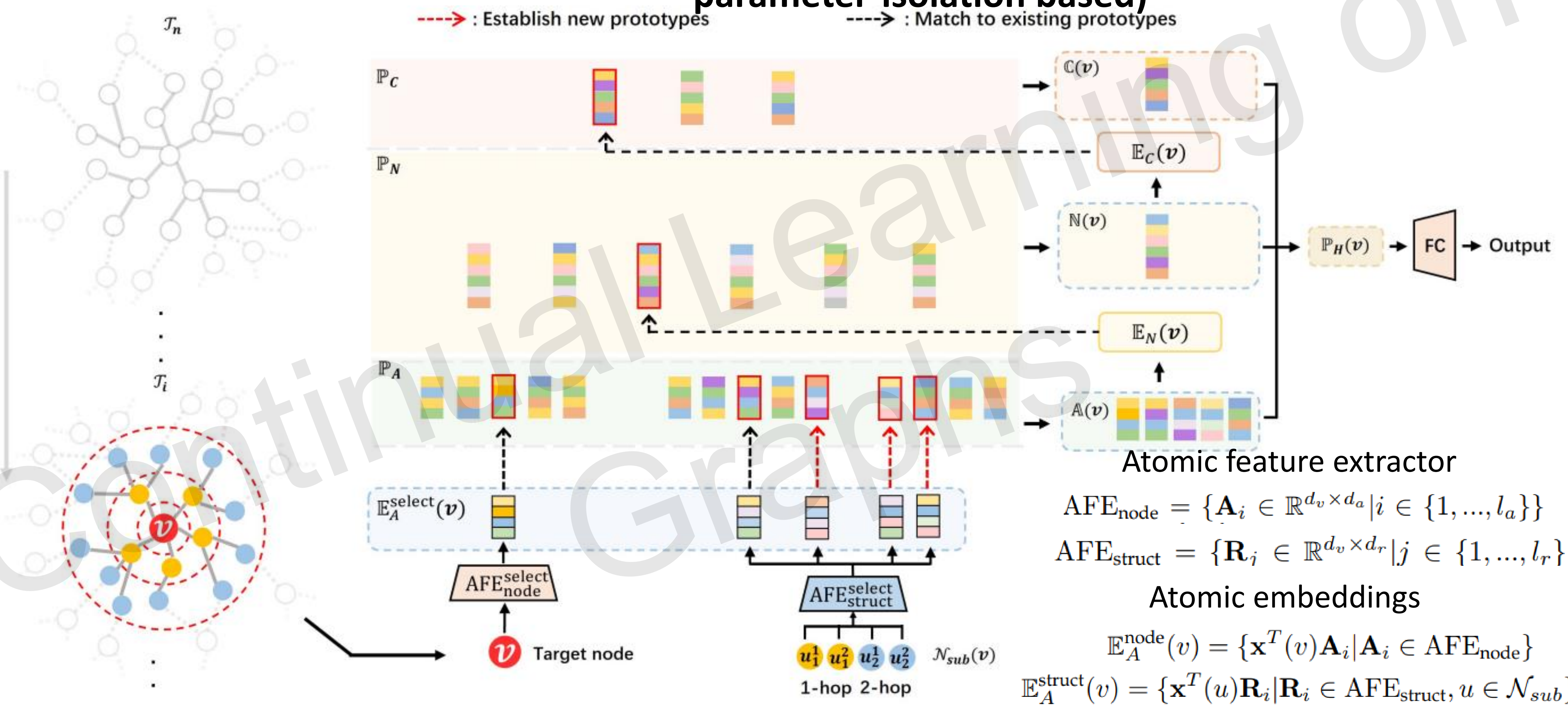
Sharing basic representations → **model parameters change less across tasks** → **Less forgetting**

Analogy	Our design
Basic feature types (color, shape)	**Atomic feature extractor (AFE)**
Basic feature instances (orange, red, green, etc.)	**Atom prototype (A-Prototype)**
Objects (watermelon, tomato, etc.)	**Node-level prototype (N-Prototype)**
Class (fruit, vegetable)	**Class-level prototype (C-Prototype)**

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)



Atomic feature extractor

$$\mathrm{AFE}_{\text{node}} = \{\mathbf{A}_i \in \mathbb{R}^{d_v \times d_a} | i \in \{1, \dots, l_a\}\}$$

$$\mathrm{AFE}_{\text{struct}} = \{\mathbf{R}_j \in \mathbb{R}^{d_v \times d_r} | j \in \{1, \dots, l_r\}\}$$

Atomic embeddings

$$\mathbb{E}_A^{\text{node}}(v) = \{\mathbf{x}^T(v)\mathbf{A}_i | \mathbf{A}_i \in \mathrm{AFE}_{\text{node}}\}$$

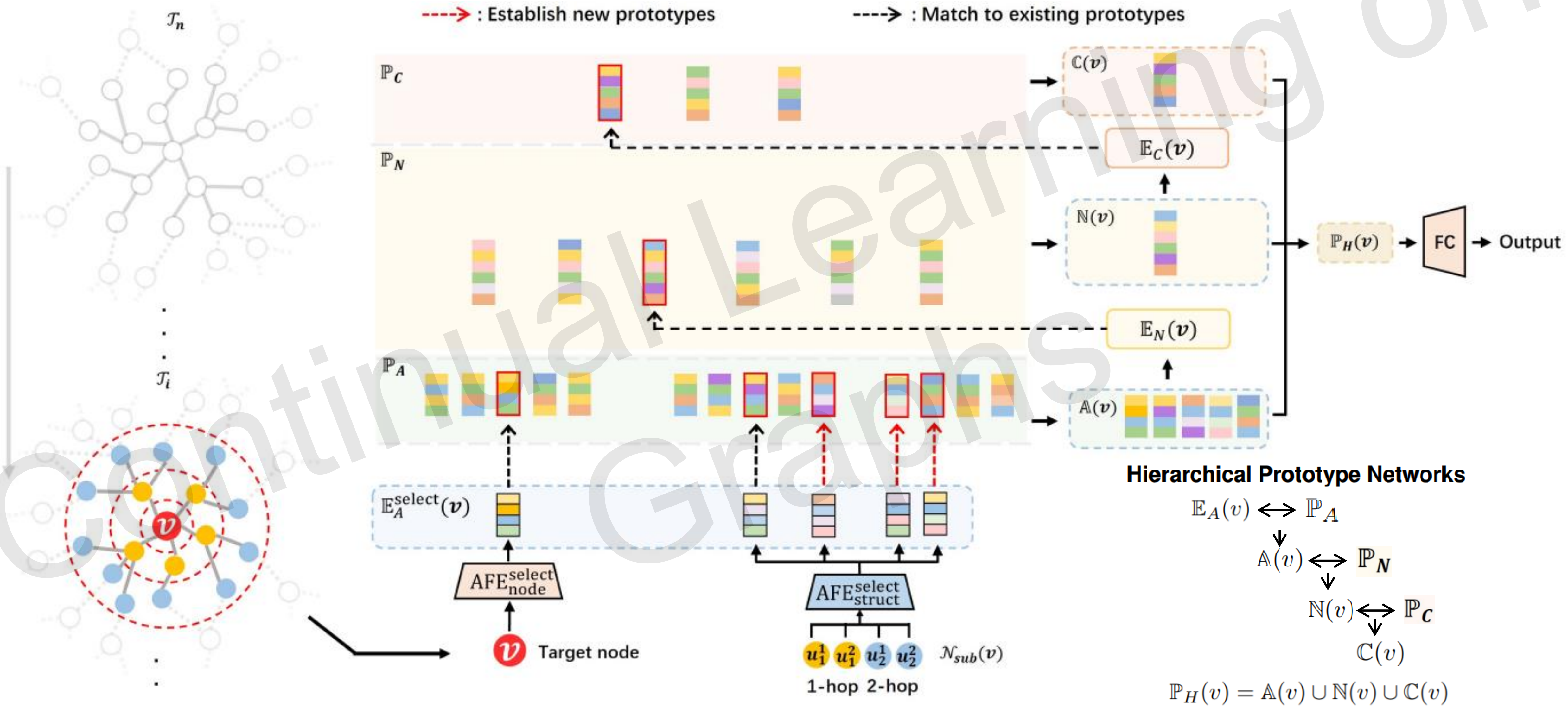
$$\mathbb{E}_A^{\text{struct}}(v) = \{\mathbf{x}^T(u)\mathbf{R}_i | \mathbf{R}_i \in \mathrm{AFE}_{\text{struct}}, u \in \mathcal{N}_{sub}\}$$

$$\mathbb{E}_A(v) = \mathbb{E}_A^{\text{node}}(v) \cup \mathbb{E}_A^{\text{struct}}(v)$$

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)



Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

- Theoretical justification of the capability to overcome forgetting

Theorem 2 (Task distance preserving). *For HPNs trained on consecutive tasks $\mathcal{T}^p$ and $\mathcal{T}^{p+1}$. If $l_a d_a + l_r d_r \geqslant (l_r + 1)d_v$ and $\mathbf{W}$ is column full rank, then as long as $t_A < \lambda_{\min}(l_r + 1)\mathbf{dist}(\mathbb{V}_p, \mathbb{V}_{p+1})$, learning on $\mathcal{T}^{p+1}$ will not modify representations HPNs generate for data from $\mathcal{T}^p$, i.e., catastrophic forgetting is avoided.*

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

C.L.T.	Base	Cora		Citeseer		Actor		OGB-Arxiv		OGB-Products	
		AM/%	FM/%	AM/%	FM/%	AM/%	FM /%	AM/%	FM /%	AM/%	FM /%
None	GCN	63.5±1.9	-42.3±0.4	64.5±3.9	-7.7±1.6	43.6±3.6	-9.1±2.9	56.8±4.3	-19.8±3.2	45.2±5.6	-27.8±7.1
	GAT	71.9±3.8	-33.1±2.3	66.8±0.9	-19.6±0.3	53.1±2.7	-4.3±1.6	54.3±3.5	-21.7±4.6	44.9±6.9	-30.3±5.2
	GIN	68.3±2.3	-35.4±3.4	57.7±2.3	-36.4±0.3	45.5±2.3	-8.9±2.8	53.2±6.5	-23.5±8.1	43.1±7.4	-31.4±8.8
EWC [24]	GCN	63.1±1.2	-42.7±1.6	54.4±4.2	-30.3±0.9	44.3±1.1	-7.1±1.4	72.1±2.4	-9.1±1.9	66.7±0.5	-8.4±0.4
	GAT	72.2±1.5	-32.2±1.6	65.7±2.5	-19.7±2.3	54.2±2.5	-2.5±1.5	73.2±1.1	-10.8±2.1	67.9±1.0	-9.6±1.3
	GIN	69.6±2.6	-28.5±2.8	57.9±3.4	-36.3±2.4	47.6±2.1	-7.2±1.6	74.1±1.7	-8.3±2.0	67.3±2.3	-13.6±1.5
LwF [23]	GCN	76.1±1.4	-21.3±2.4	67.0±0.2	-8.3±2.7	49.7±2.5	-3.6±1.4	69.9±3.9	-12.1±2.8	66.3±2.5	-11.8±3.4
	GAT	70.8±2.8	-34.6±4.1	66.1±4.1	-18.9±1.5	52.8±2.7	-6.2±2.2	68.9±4.4	-13.6±3.3	65.1±4.1	-13.2±2.9
	GIN	74.1±2.7	-23.3±0.8	63.1±1.9	-16.5±2.2	49.7±2.6	-4.1±1.5	71.4±4.8	-15.9±5.6	65.9±4.0	-10.7±3.1
GEM [27]	GCN	75.7±3.0	-6.5±4.4	41.8±2.6	-31.9±1.4	52.7±3.1	+3.9±2.9	75.4±1.7	-13.6±0.5	71.3±1.7	-10.5±0.9
	GAT	69.8±3.0	-26.1±2.6	71.3±2.2	+9.0±1.5	54.3±3.6	-2.0±0.9	76.6±0.7	-11.3±0.4	70.4±0.8	-10.9±1.6
	GIN	80.2±3.3	-2.0±4.2	49.7±0.5	-24.5±0.9	45.2±2.8	-11.1±1.5	77.3 ±2.1	-11.2±1.6	76.5±3.3	-7.2±2.5
MAS [59]	GCN	65.5±1.9	-21.4±3.7	59.5±3.1	-0.1±2.4	50.7±2.4	-1.5±0.8	69.8±0.4	-18.8±0.9	62.0±1.1	-17.9±1.9
	GAT	84.7±0.7	-5.6±2.0	69.1±1.1	-4.8±3.3	53.7±2.6	-1.6±0.8	70.6±1.3	-16.7±1.6	64.4±2.3	-14.5±3.2
	GIN	76.7±2.6	-4.0±3.6	65.2±3.9	+0.0±2.0	51.6±2.6	-0.6±1.3	65.3 ±2.9	-17.0±2.3	61.4±3.8	-20.9±2.9
ERGN. [60]	GCN	63.5±2.4	-42.3±0.7	54.2±3.9	-30.3±1.9	52.4±3.3	+0.6±1.4	63.3±1.7	-18.1±0.9	60.7±2.8	-26.6±3.3
	GAT	71.1±2.5	-34.3±1.0	65.5±0.3	-20.4±3.9	51.4±2.2	-7.2±3.2	63.5±2.4	-19.5±1.9	61.3±1.7	-25.1±0.8
	GIN	68.3±0.4	-35.4±0.4	57.7±3.1	-36.4±1.3	42.7±3.9	-13.0±2.1	69.2±1.8	-11.8±1.4	61.8±4.7	-23.4±7.9
TWP [18]	GCN	68.9±0.9	-5.7±1.5	60.5±3.8	-0.3±4.4	50.6±2.0	-4.8±1.1	75.6±0.3	-10.4±0.5	69.9±0.4	-9.0±1.1
	GAT	81.3±3.2	-14.4±1.5	69.8±1.5	-8.9±2.6	54.0±1.8	-2.1±1.9	75.8±0.5	-5.9±0.3	69.3±2.3	-8.9±1.5
	GIN	73.7±3.2	-3.9 ±2.6	68.9±0.7	-2.4±1.9	49.9±1.9	-3.6±2.0	76.6±1.8	-11.3±1.1	69.9±1.4	-10.3±2.7
Join.	GCN	93.7± 0.5	-	78.9±0.4	-	57.0±0.9	-	77.2±0.8	-	72.9±1.2	-
	GAT	93.9± 0.9	-	79.3±0.8	-	57.1±0.9	-	81.8±0.3	-	73.7±2.4	-
	GIN	93.2± 1.2	-	78.7±0.9	-	56.9±0.6	-	82.3±1.9	-	77.9±2.1	-
HPNs		**93.7±1.5**	**+0.6±1.0**	**79.0±0.9**	**-0.6±0.7**	**56.8±1.4**	**-0.9±0.9**	**85.8± 0.7**	**+0.6±0.9**	**80.1±0.8**	**+2.9±1.0**

Comparison with State-of-the-arts

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

- Theoretical upper bound on the number of prototypes

Theorem 1 (Upper bounds on numbers of prototypes). *Given the notations defined in HPNs, the upper bound on the number of A-prototypes n_a can be given by*

$$n_A \leqslant (l_a + l_r) \max_N S(d_a, N, 1 - t_A), \tag{14}$$

and the upper bounds on the number of N-prototypes and the C-prototypes are:

$$n_N \leqslant \max_N S(d_n, N, 1 - t_N) \tag{15}$$

$$n_C \leqslant \max_N S(d_c, N, 1 - t_C) \tag{16}$$

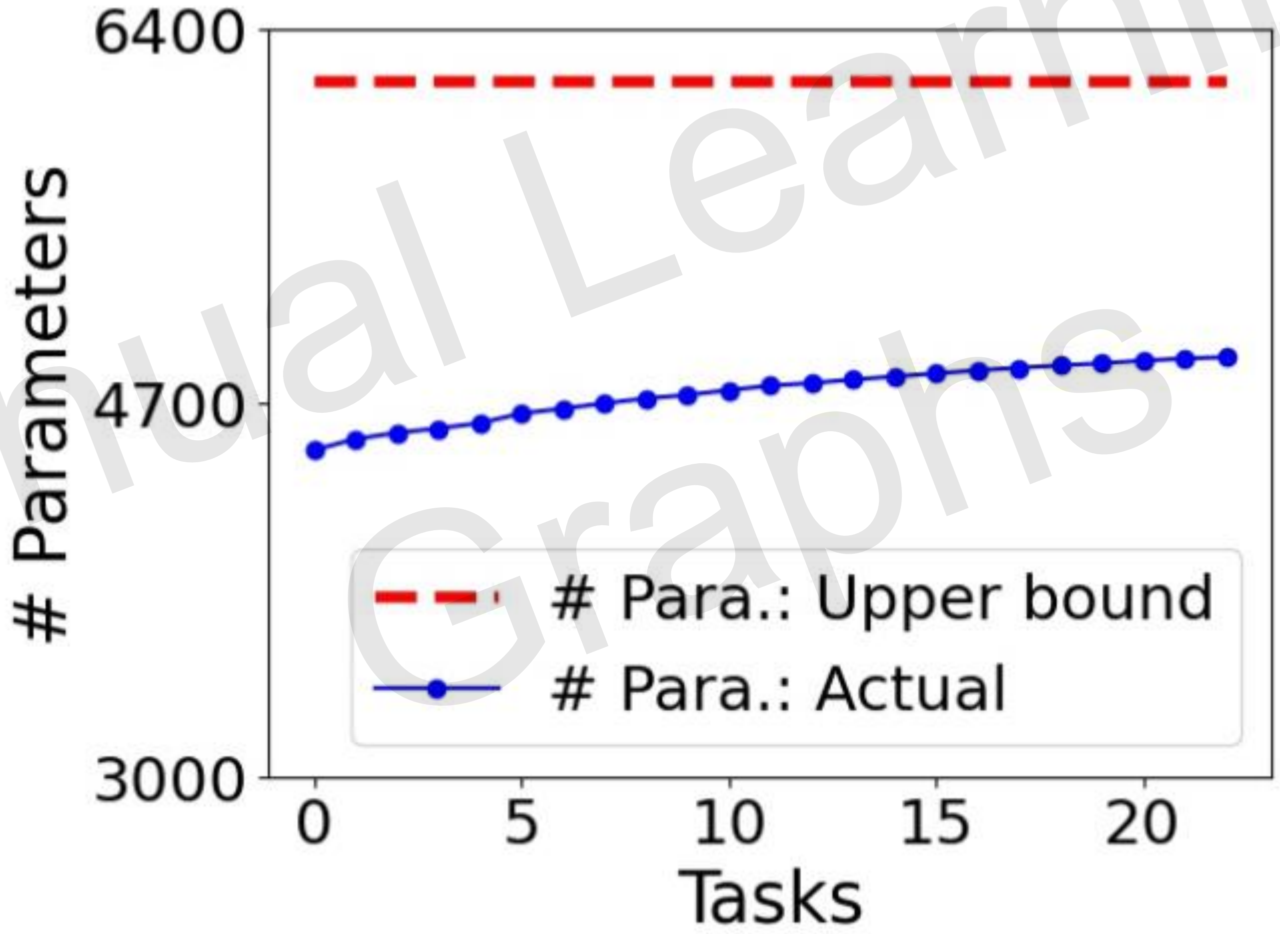
where $S(n, N, t)$ is the spherical code defined on a n dimensional hypersphere .

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Hierarchical prototype networks for continual graph representation learning." *IEEE Transactions on Pattern Analysis and Machine Intelligence* (2022).

CGL Techniques

Hierarchical prototype networks (HPNs, parameter-isolation based)

- Theoretical upper bound on the number of prototypes



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CL & CGL Techniques

Rough Categories

- **Regularization:** Penalize changes to the model via regularizations
- **Parameter-isolation:** Separate parameters for new and old tasks (partially or entirely)
- **Memory-replay:** Replay data from existing/old tasks while adapting the model to new ones

CL Techniques Tiny Episodic Memories (memory replay based)

Algorithm 1 Experience Replay for Continual Learning.

procedure ER($\mathcal{D}$, mem_sz, batch_sz, lr)
  $\mathcal{M} \leftarrow \{\} *$ mem_sz ▷ Allocate memory buffer of size mem_sz
  $n \leftarrow 0$ ▷ Number of training examples seen in the continuum

Memory replay

  for $t \in \{1, \cdots, T\}$ **do**
    for $B_n \overset{K}{\sim} \mathcal{D}_t$ **do** ▷ Sample without replacement a mini-batch of size K from task t
      $B_{\mathcal{M}} \overset{K}{\sim} \mathcal{M}$ ▷ Sample a mini-batch from $\mathcal{M}$
      $\theta \leftarrow SGD(B_n \cup B_{\mathcal{M}}, \theta, \mathrm{lr})$ ▷ Single gradient step to update the parameters by stacking current minibatch with minibatch from memory
      $\mathcal{M} \leftarrow \texttt{UpdateMemory}(\text{mem\_sz}, t, n, B_n)$ ▷ Memory update, see §4
      $n \leftarrow n +$ batch_sz ▷ Counter update

Memory update

  return $\theta, \mathcal{M}$

Chaudhry, Arslan, et al. "On tiny episodic memories in continual learning." *arXiv preprint arXiv:1902.10486* (2019).

CL Techniques Tiny Episodic Memories (memory replay based)

Algorithm 2 Reservoir sampling update. mem_sz is the number of examples the memory can store, t is the task id, n is the number of examples observed so far in the data stream, and B is the input mini-batch.

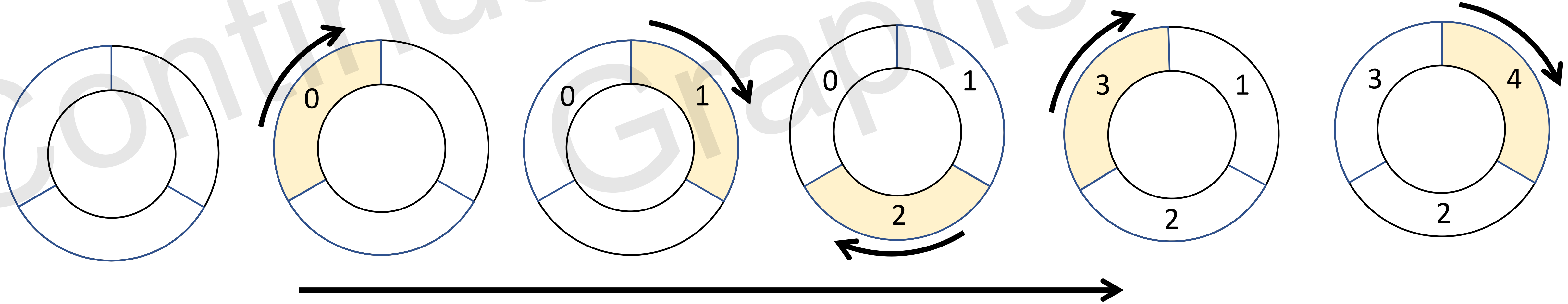
```
procedure UPDATEMEMORY(mem_sz, t, n, B)
    j ← 0
    for (x, y) in B do
        M ← |𝓜|                              ▷ Number of samples currently stored in the memory
        if M < mem_sz then
            𝓜.append(x, y, t)
        else
            i = randint(0, n + j)
            if i < mem_sz then
                𝓜[i] ← (x, y, t)            ▷ Overwrite memory slot.
        j ← j + 1
    return 𝓜
```


Chaudhry, Arslan, et al. "On tiny episodic memories in continual learning." *arXiv preprint arXiv:1902.10486* (2019).

CL Techniques Tiny Episodic Memories (memory replay based)

Algorithm 3 Ring buffer.

procedure UPDATEMEMORY(mem_sz, t, n, B)
  for ($\mathbf{x}$, y) in B **do**
    # Assume FIFO stacks $\mathcal{M}[t][y]$ of fixed size are already initialized
    $\mathcal{M}[t][y]$.append($\mathbf{x}$)
  return $\mathcal{M}$



Chaudhry, Arslan, et al. "On tiny episodic memories in continual learning." *arXiv preprint arXiv:1902.10486* (2019).

CL Techniques

Tiny Episodic Memories (memory replay based)

Algorithm 4 K-Means. Memory is populated using samples closest (in feature space) to sequential K-Means centroids.

procedure UPDATEMEMORY(mem_sz, t, n, B)

    # Assume array $\mathcal{M}[t][y]$ of fixed size is already initialized

    # Assume K centroids c_j are already initialized

    # Assume cluster counters n_j are already initialized to 0

    for $(\mathbf{x}, y)$ in B **do**

        $j \leftarrow \text{argmin}_{j \in \{1, \cdots, K\}} ||\phi_\theta(\mathbf{x}) - c_j||$ Choose the closest cluster

        $n_j \leftarrow n_j + 1$

        $c_j \leftarrow c_j + \frac{1}{n_j} * (\phi_\theta(\mathbf{x}) - c_j)$ Update the cluster center

        $d = ||\phi_\theta(\mathbf{x}) - c_j||$

        if $d < \mathcal{M}[t][y][j]$.get_dst() **then** ▷ Store the current example if it is closer to the centroid

            $\mathcal{M}[t][y][j] \leftarrow (\mathbf{x}, d)$

    return $\mathcal{M}$

CL Techniques Tiny Episodic Memories (memory replay based)

Algorithm 5 Mean of Features. Store examples that are closest to the running average feature vector.

procedure UPDATEMEMORY(mem_sz, t, n, B)
    # Assume heaps $\mathcal{M}[t][y]$ of fixed size are already initialized
    # Assume average features $f[t][y]$ are already initialized
    # Assume moving average decay hyper-parameter (α) is given
    for $(\mathbf{x}, y)$ in B **do**
        $f[t][y] \leftarrow \alpha * f[t][y] + (1 - \alpha) * \phi_\theta(\mathbf{x})$ Update the running average
        $d = ||\phi_\theta(\mathbf{x}) - f[t][y]||$
        if $\mathcal{M}[t][y]$.find_max() $> d$ **then**   ▷ Store the current example if it is closer to the center
            $\mathcal{M}[t][y]$.delete_max()
            $\mathcal{M}[t][y]$.insert($\mathbf{x}; d$)
    return $\mathcal{M}$

Chaudhry, Arslan, et al. "On tiny episodic memories in continual learning." *arXiv preprint arXiv:1902.10486* (2019).

CL Techniques Gradient episodic memory (GEM, memory replay based)

Loss of the stored data:

$$\ell(f_\theta, \mathcal{M}_k) = \frac{1}{|\mathcal{M}_k|} \sum_{(x_i,k,y_i)\in \boxed{\mathcal{M}_k}} \ell(f_\theta(x_i,k), y_i)$$

Memory buffer storing representative data from an old task k

When observing a new triplet (x,y,t):

$$\begin{aligned} \text{minimize}_\theta \quad & \ell(f_\theta(x,t), y) \\ \text{subject to} \quad & \ell(f_\theta, \mathcal{M}_k) \le \ell(f_\theta^{t-1}, \mathcal{M}_k) \text{ for all } k < t \end{aligned}$$

$$\langle g, g_k \rangle := \left\langle \frac{\partial \ell(f_\theta(x,t), y)}{\partial \theta}, \frac{\partial \ell(f_\theta, \mathcal{M}_k)}{\partial \theta} \right\rangle \ge 0, \text{ for all } k < t.$$

Lopez-Paz, David, and Marc'Aurelio Ranzato. "Gradient episodic memory for continual learning." Advances in neural information processing systems 30 (2017).

CL Techniques Gradient episodic memory (GEM, memory replay based)

Loss of the stored data:

$$\ell(f_\theta, \mathcal{M}_k) = \frac{1}{|\mathcal{M}_k|} \sum_{(x_i,k,y_i)\in \boxed{\mathcal{M}_k}} \ell(f_\theta(x_i, k), y_i)$$

Memory buffer storing representative data from an old task k

When observing a new triplet (x,y,t):

$$\begin{aligned} \text{minimize}_\theta \quad & \ell(f_\theta(x,t), y) \\ \text{subject to} \quad & \ell(f_\theta, \mathcal{M}_k) \leq \ell(f_\theta^{t-1}, \mathcal{M}_k) \text{ for all } k < t \end{aligned}$$

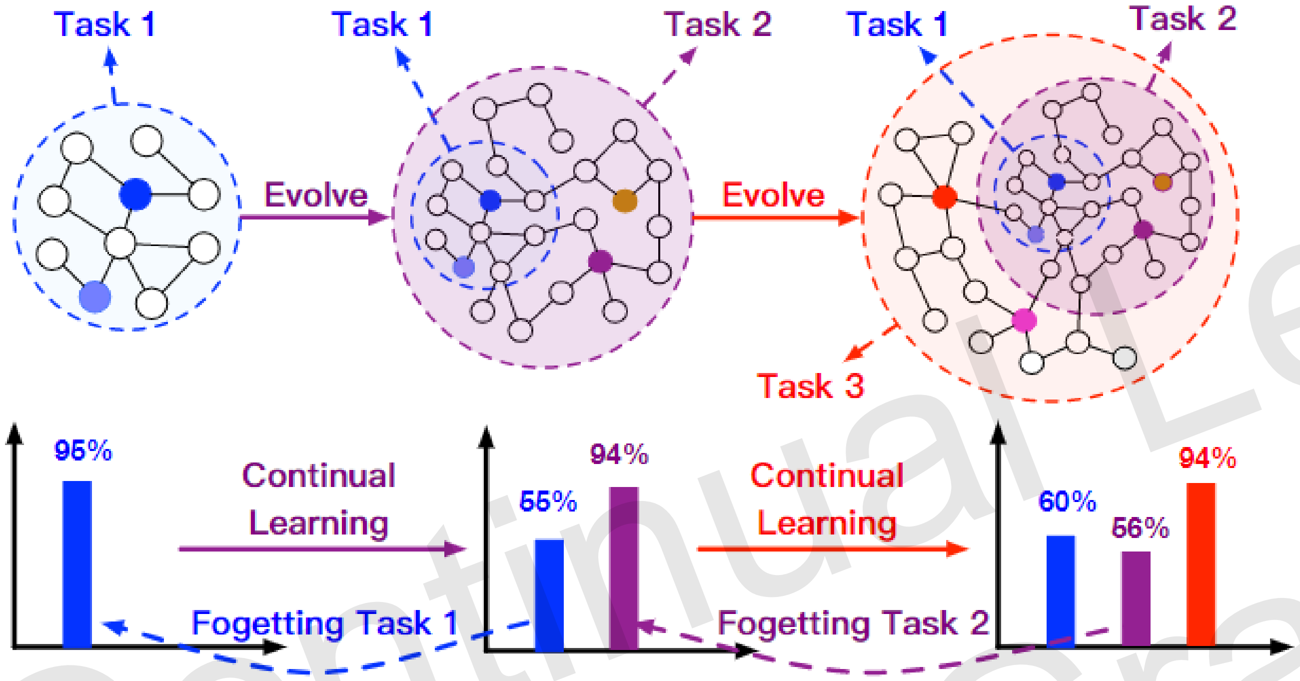
$$\langle g, g_k \rangle := \left\langle \frac{\partial \ell(f_\theta(x,t), y)}{\partial \theta}, \frac{\partial \ell(f_\theta, \mathcal{M}_k)}{\partial \theta} \right\rangle \geq 0, \text{ for all } k < t.$$

Aim: Find directions in the parameter space that are favourable for all tasks

Lopez-Paz, David, and Marc'Aurelio Ranzato. "Gradient episodic memory for continual learning." Advances in neural information processing systems 30 (2017).

CGL Techniques

Experience Replay Graph Neural Networks (ER-GNN, memory replay based)



Original loss:

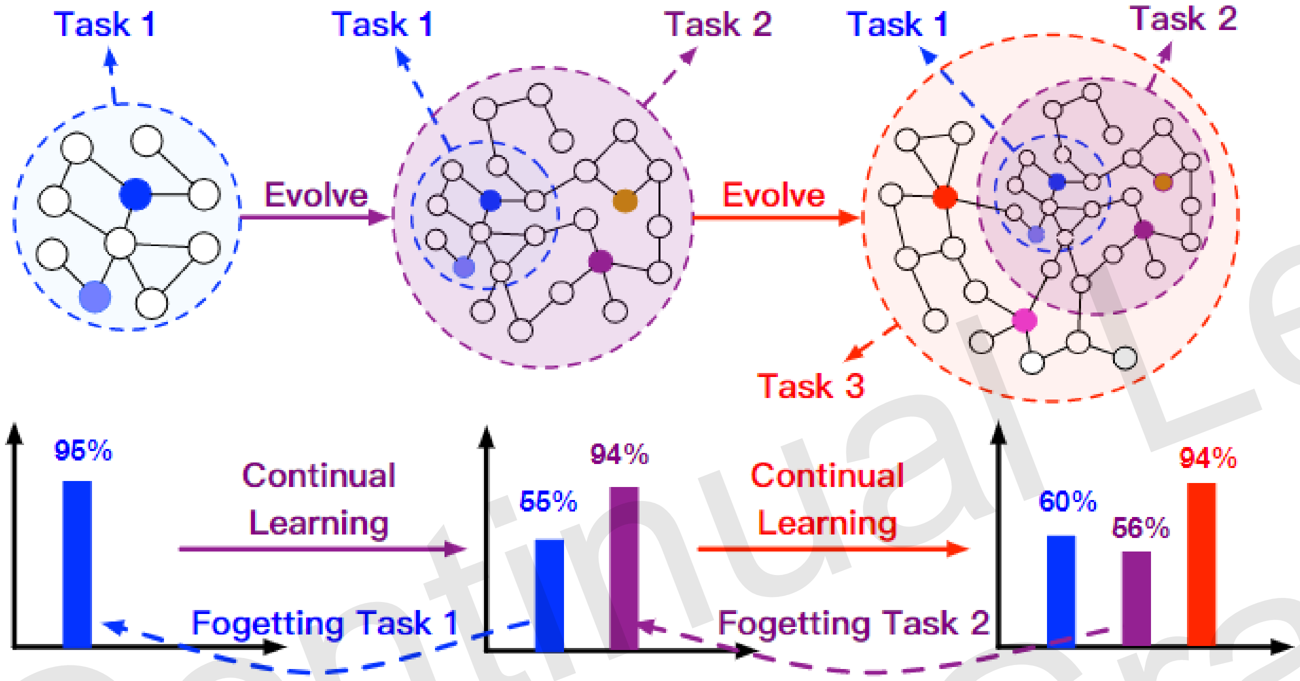
$$\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}) = -\Big(\sum_{(\boldsymbol{x_i}, y_i)\in\mathcal{D}} (y_i \log f_{\boldsymbol{\theta}}(\boldsymbol{x_i}) + (1-y_i)\log(1-f_{\boldsymbol{\theta}}(\boldsymbol{x_i})))\Big)$$

Store representative nodes
(without topological information)

Zhou, Fan, and Chengtai Cao. "Overcoming catastrophic forgetting in graph neural networks with experience replay." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. No. 5. 2021.

CGL Techniques

Experience Replay Graph Neural Networks (ER-GNN, memory replay based)



Store representative nodes
(without topological information)

Original loss:

$$\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}) = -\Big(\sum_{(\boldsymbol{x_i}, y_i)\in\mathcal{D}} (y_i \log f_{\boldsymbol{\theta}}(\boldsymbol{x_i}) + (1-y_i)\log(1-f_{\boldsymbol{\theta}}(\boldsymbol{x_i})))\Big)$$

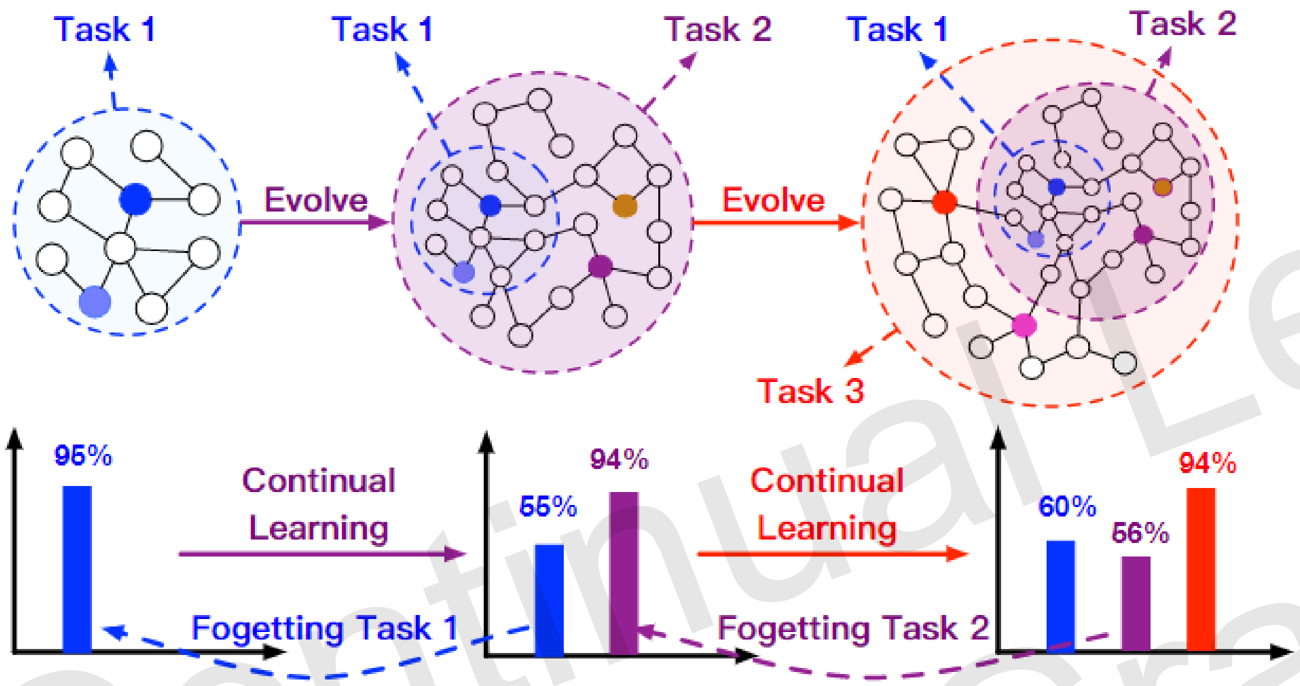
Loss with memory buffer:

$$\mathcal{L}'_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}, B) = \beta\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}) + (1-\beta)\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, B)$$

Zhou, Fan, and Chengtai Cao. "Overcoming catastrophic forgetting in graph neural networks with experience replay." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. No. 5. 2021.

CGL Techniques

Experience Replay Graph Neural Networks (ER-GNN, memory replay based)



Store representative nodes
(without topological information)

Original loss:

$$\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}) = -\left(\sum_{(\boldsymbol{x_i}, y_i) \in \mathcal{D}} (y_i \log f_{\boldsymbol{\theta}}(\boldsymbol{x_i}) + (1 - y_i) \log(1 - f_{\boldsymbol{\theta}}(\boldsymbol{x_i})))\right)$$

Loss with memory buffer:

$$\mathcal{L}'_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}, B) = \beta \mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}) + (1 - \beta) \mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, B)$$

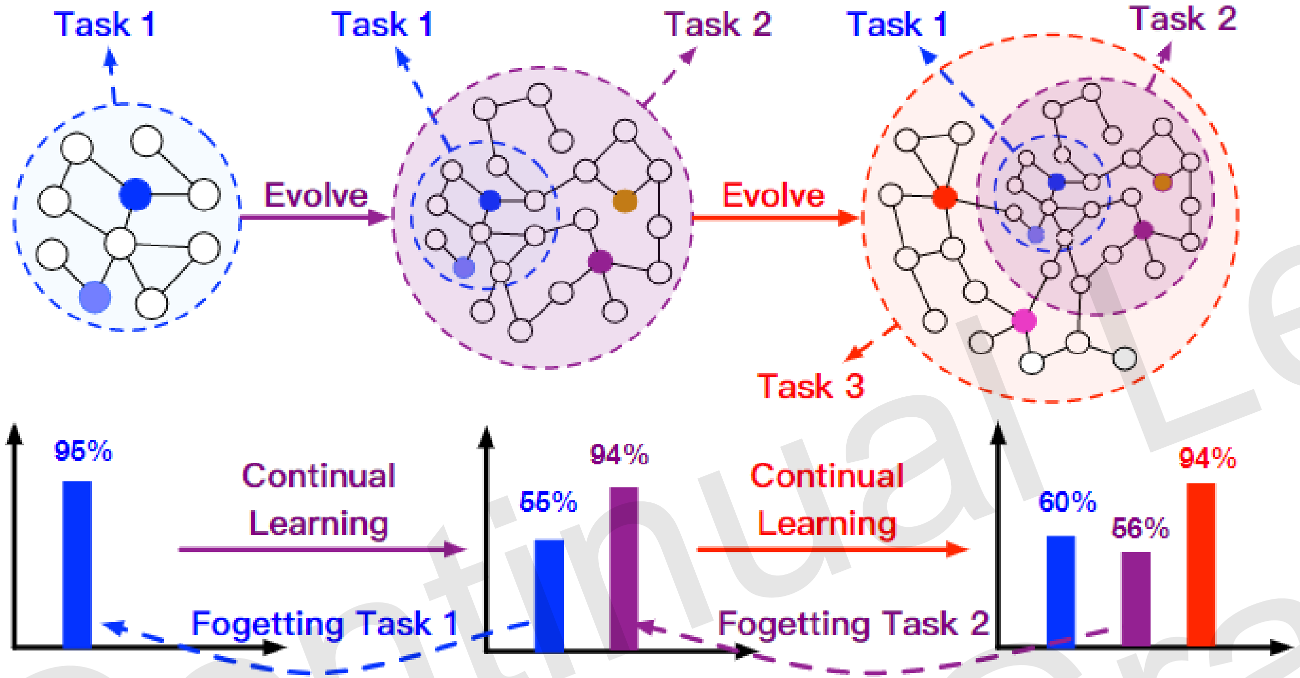
Objective:

$$\boldsymbol{\theta} = \arg\min_{\boldsymbol{\theta} \in \Theta} (\mathcal{L}'_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}, B))$$

Zhou, Fan, and Chengtai Cao. "Overcoming catastrophic forgetting in graph neural networks with experience replay." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. No. 5. 2021.

CGL Techniques

Experience Replay Graph Neural Networks (ER-GNN, memory replay based)



Store representative nodes
(without topological information)

Original loss:

$$\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}) = -\Big(\sum_{(\boldsymbol{x_i}, y_i)\in\mathcal{D}} (y_i \log f_{\boldsymbol{\theta}}(\boldsymbol{x_i}) + (1-y_i)\log(1-f_{\boldsymbol{\theta}}(\boldsymbol{x_i})))\Big)$$

Loss with memory buffer:

$$\mathcal{L}'_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}, B) = \beta\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}) + (1-\beta)\mathcal{L}_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, B)$$

Objective:

$$\boldsymbol{\theta} = \arg\min_{\boldsymbol{\theta}\in\Theta}(\mathcal{L}'_{\mathcal{T}_i}(f_{\boldsymbol{\theta}}, \mathcal{D}_i^{\text{tr}}, B))$$

Balance the contribution:

$$\beta = |B|/(|\mathcal{D}_i^{\text{tr}}| + |B|)$$

$|\mathcal{D}_i^{\text{tr}}|$: Size of training set of the current task

$|B|$: Size of training set of the memory buffer

Zhou, Fan, and Chengtai Cao. "Overcoming catastrophic forgetting in graph neural networks with experience replay." *Proceedings of the AAAI Conference on Artificial Intelligence*. Vol. 35. No. 5. 2021.

CGL Techniques Sparsified Subgraph Memory (SSM, memory replay based)

GNNs generate node representations based on multi-hop neighborhood

↓

Applying memory replay to graphs requires storing multi-hop neighbors

↓

L-hop neighbors grow in $O(d^L)$, d is average degree

↓

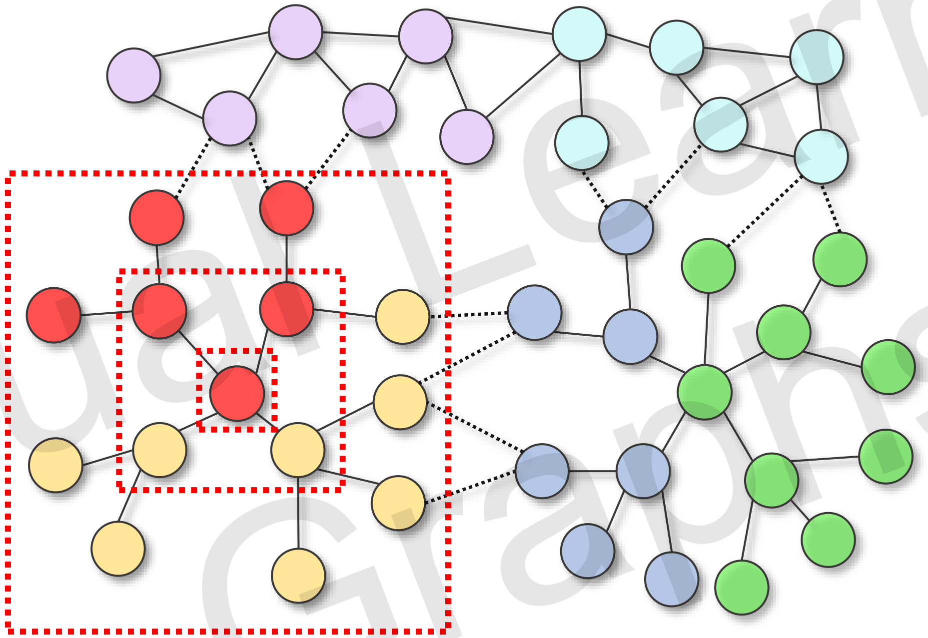
Memory explosion problem

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." *2022 IEEE International Conference on Data Mining (ICDM)*. IEEE, 2022.

CGL Techniques **Sparsified Subgraph Memory (SSM, memory replay based)**

- GNNs typically require no less than 2-hop computation subgraphs (i.e. at least two layers)

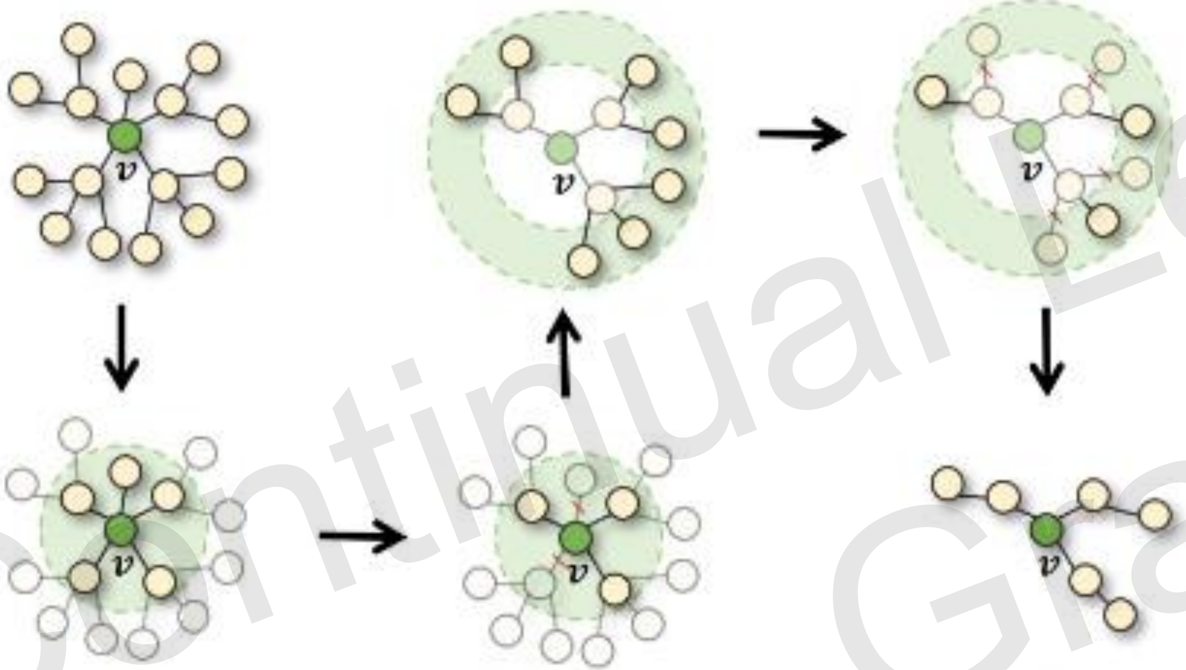
Exponentially growing computation subgraph



- Size of a computation subgraph grows in $O(d^L)$, d is average degree, L is number of hops
- Memory explosion (e.g. $d = 492$ in Reddit dataset)

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." *2022 IEEE International Conference on Data Mining (ICDM)*. IEEE, 2022.

CGL Techniques Sparsified Subgraph Memory (SSM, memory replay based)

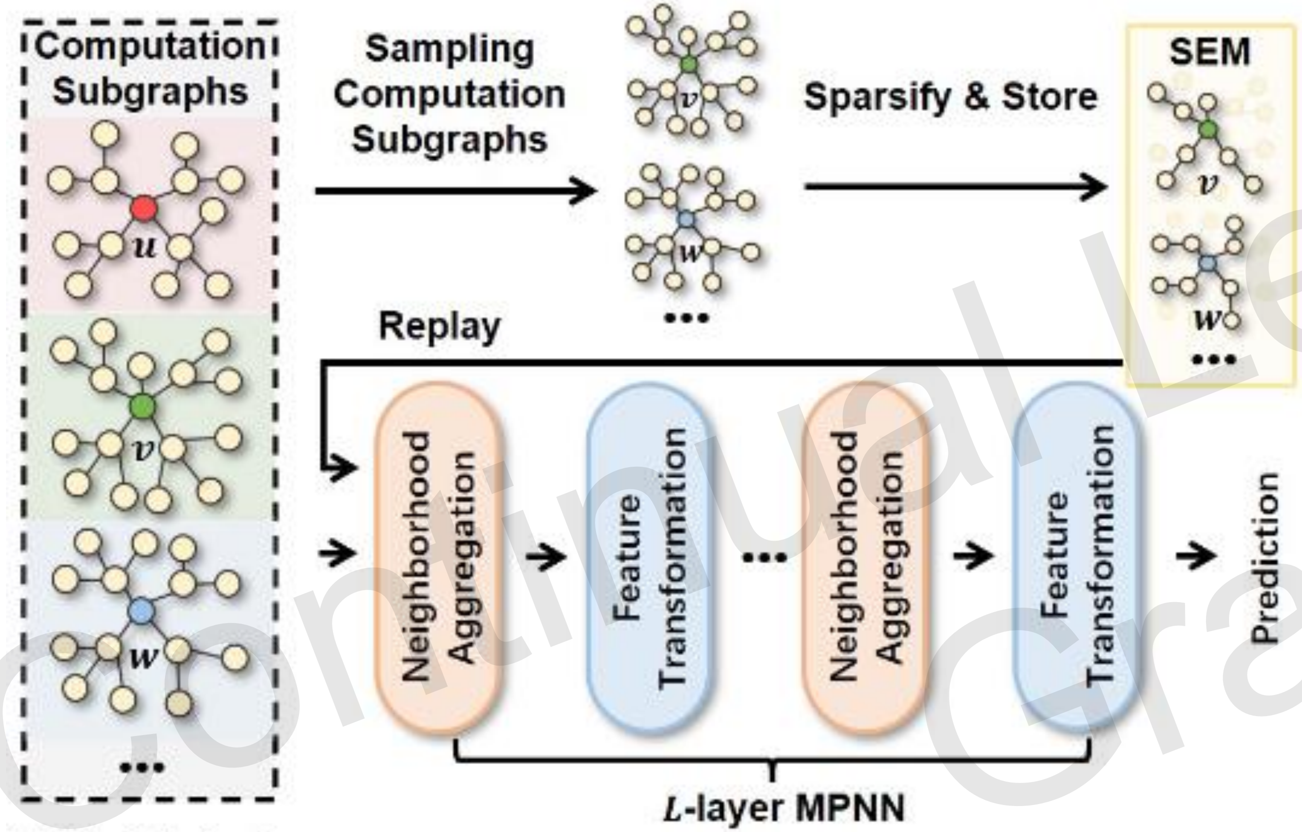


(b) Subgraph sparsification

- Sparsify hop by hop
- First selected a fixed number of 1-hop neighbors
- Then selected a fixed number of 2-hop neighbors (must be connected to selected 1-hop neighbors)
- Any sampling strategy can be used

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." *2022 IEEE International Conference on Data Mining (ICDM)*. IEEE, 2022.

CGL Techniques Sparsified Subgraph Memory (SSM, memory replay based)



(a) Model pipeline

- Each node has a computation subgraph, size is $O(d^L)$
- Selected a fixed number of computations to store
- Sparsify each selected computation subgraph into a fixed number of nodes, size reduces to $O(1)$
- Plug and play, easy to use in any GNNs

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." *2022 IEEE International Conference on Data Mining (ICDM)*. IEEE, 2022.

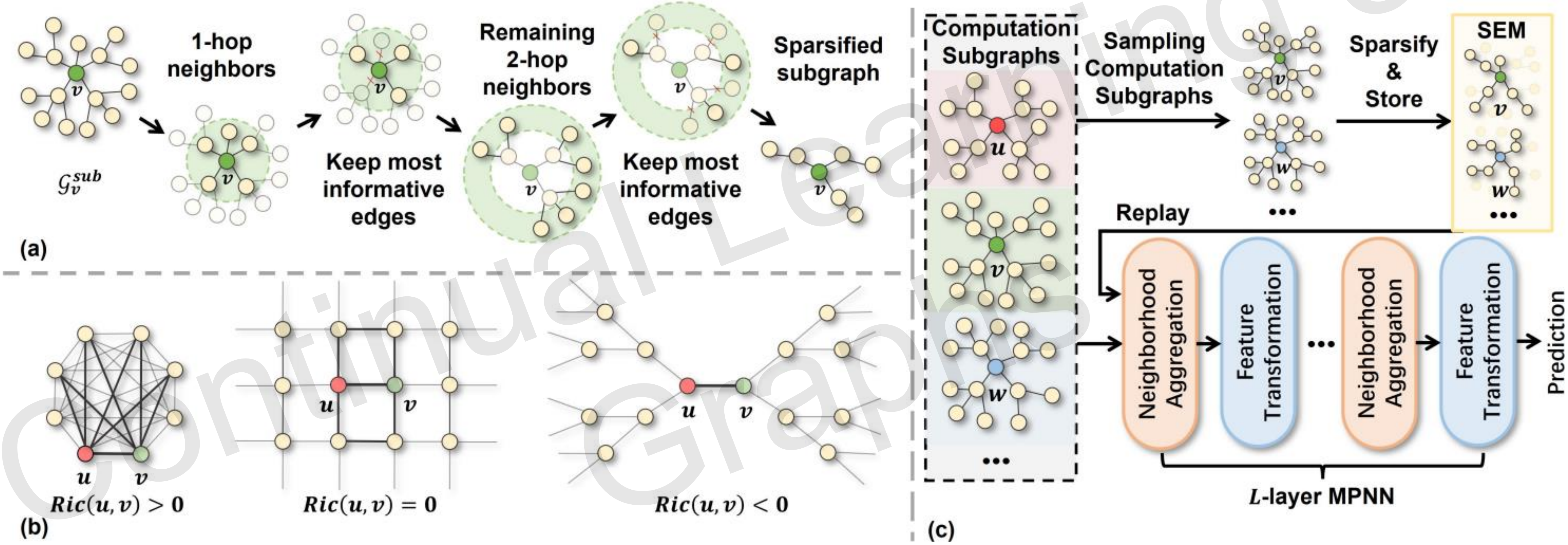
CGL Techniques
Sparsified Subgraph Memory (SSM, memory replay based)

Continual learning techniques	CoraFull		OGB-Arxiv		Reddit		OGB-Products	
	AA/% ↑	AF/% ↑	AA/% ↑	AF /% ↑	AA/% ↑	AF /% ↑	AA/% ↑	AF /% ↑
Fine-tune	3.5±0.5	-95.2±0.5	4.9±0.0	-89.7±0.4	5.9±1.2	-97.9±3.3	3.4±0.8	-82.5±0.8
EWC [19]	52.6±8.2	-38.5±12.1	8.5±1.0	-69.5±8.0	10.3±11.6	-33.2±26.1	23.8±3.8	-21.7±7.5
MAS [2]	12.3±3.8	-83.7±4.1	4.9±0.0	-86.8±0.6	13.1±2.6	-35.2±3.5	16.7±4.8	-57.0±31.9
GEM [7]	8.4±1.1	-88.4±1.4	4.9±0.0	-89.8±0.3	28.4±3.5	-71.9±4.2	5.5±0.7	-84.3±0.9
TWP [27]	62.6±2.2	-30.6±4.3	6.7±1.5	-50.6±13.2	13.5±2.6	-89.7±2.7	14.1±4.0	-11.4±2.0
LwF [20]	33.4±1.6	-59.6±2.2	9.9±12.1	-43.6±11.9	86.6±1.1	-9.2±1.1	48.2±1.6	-18.6±1.6
ER-GNN [9]	34.5±4.4	-61.6±4.3	30.3±1.5	-54.0±1.3	88.5±2.3	-10.8±2.4	56.7±0.3	-33.3±0.5
Joint (Not under continual setting)	81.2±0.4	-3.3±0.8	51.3±0.5	-6.7±0.5	97.1±0.1	-0.7±0.1	71.5±0.1	-5.8±0.3
SEM-uniform (Ours)	73.0±0.3	-14.8±0.5	47.1±0.5	-11.7±1.5	94.3±0.1	-1.4±0.1	62.0±1.6	-9.9±1.3
SEM-degree (Ours)	**75.4±0.1**	-9.7±0.0	**48.3±0.5**	-10.7±0.3	**94.4±0.0**	-1.3±0.0	**63.3±0.1**	-9.6±0.3

Comparison under the challenging class-IL

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." *2022 IEEE International Conference on Data Mining (ICDM)*. IEEE, 2022.

CGL Techniques **Ricci Curvature-Based Graph Sparsification**



Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Ricci Curvature-Based Graph Sparsification for Continual Graph Representation Learning." IEEE Transactions on Neural Networks and Learning Systems (2023).

CGL Techniques

Ricci Curvature-Based Graph Sparsification

Continual learning techniques	CoraFull		OGB-Arxiv		Reddit		OGB-Products	
	AA/% ↑	AF/% ↑	AA/% ↑	AF /% ↑	AA/% ↑	AF /% ↑	AA/% ↑	AF /% ↑
Fine-tune	3.5±0.5	-95.2±0.5	4.9±0.0	-89.7±0.4	5.9±1.2	-97.9±3.3	7.6±0.7	-88.7±0.8
EWC [25]	52.6±8.2	-38.5±12.1	8.5±1.0	-69.5±8.0	10.3±11.6	-33.2±26.1	23.8±3.8	-21.7±7.5
MAS [27]	6.5±1.5	-92.3±1.5	4.8±0.4	-72.2±4.1	9.2±14.5	-23.1±28.2	16.7±4.8	-57.0±31.9
GEM [7]	8.4±1.1	-88.4±1.4	4.9±0.0	-89.8±0.3	11.5±5.5	-92.4±5.9	4.5±1.3	-94.7±0.4
TWP [38]	62.6±2.2	-30.6±4.3	6.7±1.5	-50.6±13.2	8.0±5.2	-18.8±9.0	14.1±4.0	-11.4±2.0
LwF [26]	33.4±1.6	-59.6±2.2	9.9±12.1	-43.6±11.9	86.6±1.1	-9.2±1.1	48.2±1.6	-18.6±1.6
ER-GNN [9]	34.5±4.4	-61.6±4.3	21.5±5.4	-70.0±5.5	82.7±0.4	-17.3±0.4	48.3±1.2	-45.7±1.3
SSM-uniform [23]	73.0±0.3	-14.8±0.5	47.1±0.5	-11.7±1.5	94.3±0.1	-1.4±0.1	62.0±1.6	-9.9±1.3
SSM-degree [23]	75.4±0.1	-9.7±0.0	48.3±0.5	-10.7±0.3	94.4±0.0	-1.3±0.0	63.3±0.1	-9.6±0.3
Joint (Not under continual setting)	81.2±0.4	-	51.3±0.5	-	97.1±0.1	-	71.5±0.1	-
SEM-curvature (Ours)	**77.7±0.8**	-10.0±1.2	**49.9±0.6**	-8.4±1.3	**96.3±0.1**	-0.6±0.1	**65.1±1.0**	-9.5±0.8

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Ricci Curvature-Based Graph Sparsification for Continual Graph Representation Learning." IEEE Transactions on Neural Networks and Learning Systems (2023).

CGL Techniques Rough Categories

	Pros:	Cons:
• **Regularization:** Penalize changes to model parameters via regularizations	• Good stability on old tasks • Suitable for different architectures	• Poor plasticity for new tasks
• **Parameter-isolation:** Separate parameters for new and old tasks (partially or entirely)	• Good stability and plasticity	• Memory usage • May not fit different architectures • Computation burden
• **Memory-replay:** Replay old task data to the model when learning new ones	• Good stability and plasticity • Suitable for different architectures	• Memory usage • Computation burden

Agenda

- Background
- Motivation of Continual Graph Learning
- Problem setup of CL and CGL
- CL techniques & CGL techniques
- **Evaluation Metrics & CGL benchmarks**
- Future opportunities

Evaluation Metrics

Performance Matrix: model's performance (accuracy, f1 score, etc.) after learning each task, the most thorough metric

$$M^p \in R^{T\times \mathrm{T}}$$

T: number of tasks in the sequence

$M_{i,j}^p$: Performance on task j after learning from task 1 to i

Evaluation Metrics

Performance Matrix: model's performance (accuracy, f1 score, etc.) after learning each task, the most thorough metric

$$M^p \in R^{T\times \mathrm{T}}$$

T: number of tasks in the sequence

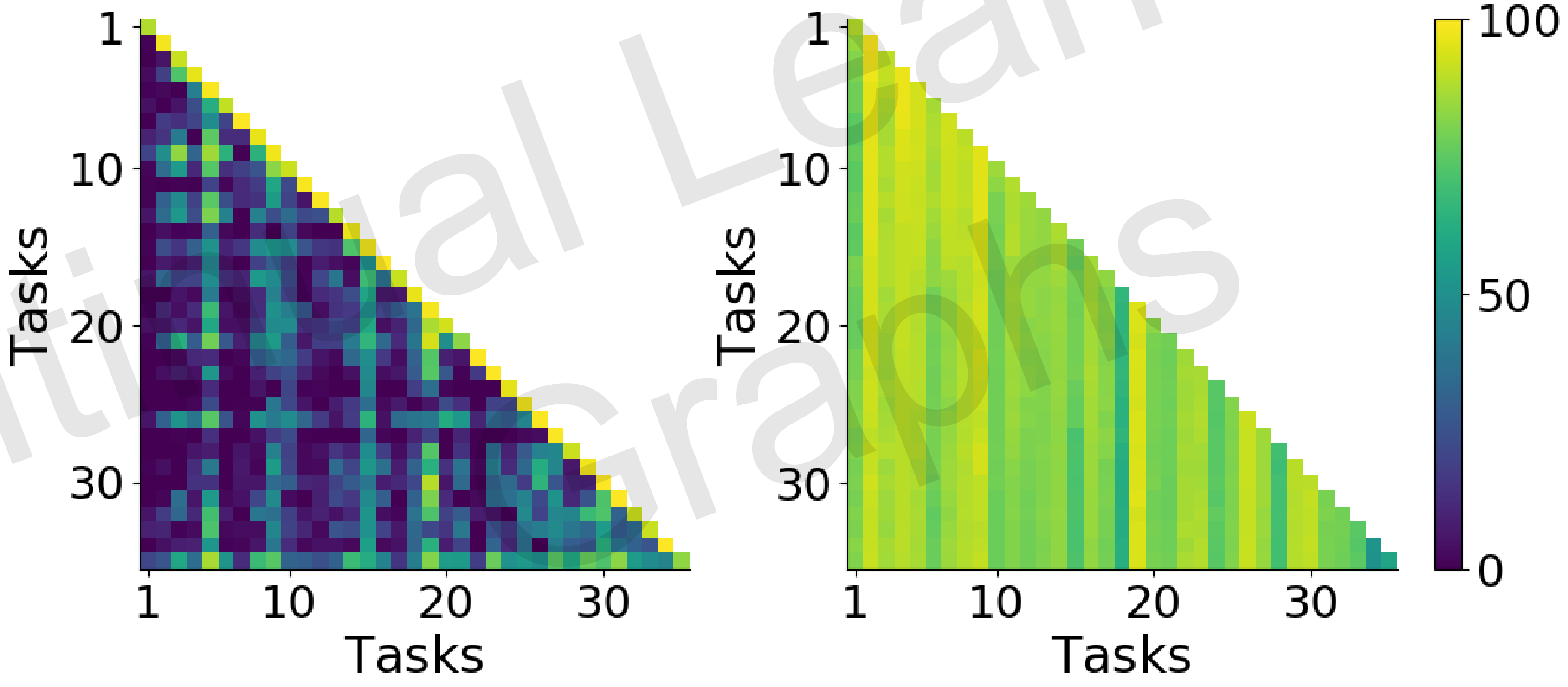
$M^p_{i,j}$: Performance on task j after learning from task 1 to i

An example

	T1	**T2**	**T3**
T1	100%		
T2	90%	98%	
T3	60%	70%	99%

Evaluation Metrics

Can be visualized



Evaluation Metrics

Average Performance (AP): Performance (e.g. accuracy, f1 score) averaged over currently learnt tasks, applicable after learning each task:

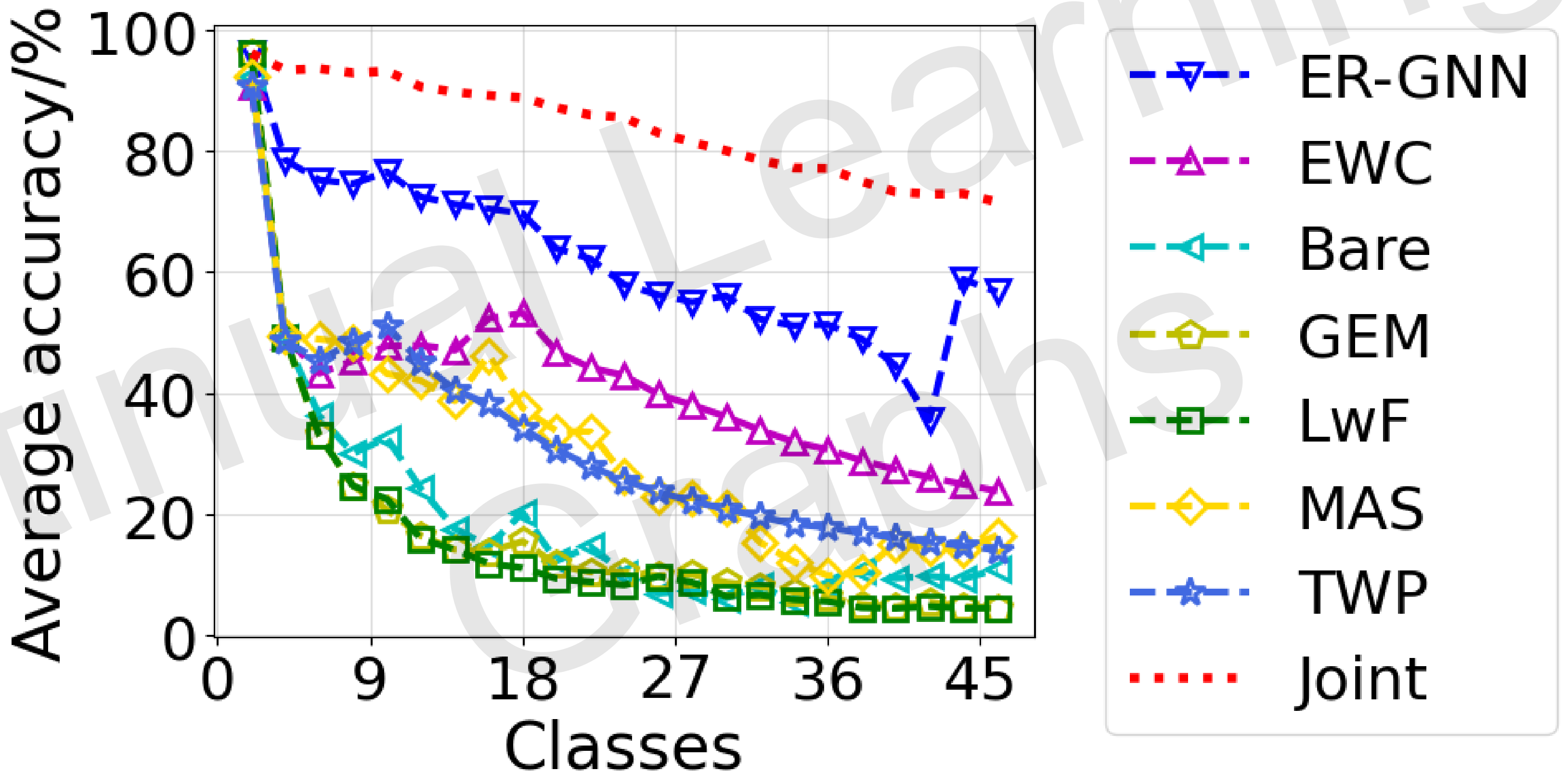
$$\left\{\frac{\sum_{j=1}^{i} \mathrm{M}_{i,j}^{p}}{i} \middle| i = 1, \ldots, T\right\}$$

	T1	T2	T3
T1	100%		
T2	90%	98%	
T3	60%	70%	99%

$$\frac{(60\%+70\%+99\%)}{3} = 76.3\%$$

Evaluation Metrics

Learning dynamics (curve of AP)



Evaluation Metrics

Average Forgetting (AF): Performance decrease averaged over all learnt tasks, applicable from the second task

Forgetting on task i

$$\left\{ \frac{\sum_{j=1}^{i-1} \left(\boxed{\mathrm{M}^{p}_{i,j} - \mathrm{M}^{p}_{j,j}} \right)}{i-1} \middle| i = 2, \ldots, T \right\}$$

	T1	T2	T3
T1	100%		
T2	90%	98%	
T3	60%	70%	99%

$$\frac{(60\%-100\%)+(70\%-98\%)}{3-1} = -29\%$$

Evaluation Metrics

Average Forgetting (AF) another definition: Performance decrease averaged over all learnt tasks, applicable from the second task

$$f_j = \max_{k=1,\ldots,i-1}(M^p_{k,j} - M^p_{i,j})$$

AF after each task $\{\frac{\sum_{j=1}^{i-1} f_j}{i-1} | i = 2, \ldots, T\}$

	T1	T2	T3
T1	75%		
T2	90%	98%	
T3	60%	70%	99%

$\frac{(60\%-90\%)+(70\%-98\%)}{3-1}$=-24%

Evaluation Metrics

Forward transfer

Benefit from learning on all the (j-1) tasks before j

performance on task j with random model initialization

$$\frac{\sum_{j=2}^{T}\left(\boxed{\mathrm{M}^{p}_{j-1}}_{,j} - \boxed{\bar{b}_j}\right)}{T-1}$$

CGL Benchmarks

Continual Graph Learning Benchmark

CGLB: Benchmark Tasks for Continual Graph Learning

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

Continual Graph Learning Benchmark

N-CGL

G-CGL

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

N-CGL

Datasets for Task-IL & Class-IL

CoraFull-CL: Classification on new classes of articles

Arxiv-CL: Classification on new classes of articles

Reddit-CL: Classification on new classes of communities

Products-CL: Classification on new classes of products

G-CGL

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

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Reddit-CL: Classification on new classes of communities

Products-CL: Classification on new classes of products

G-CGL

Datasets for Task-IL

Datasets for Class-IL

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

N-CGL

Datasets for Task-IL & Class-IL

CoraFull-CL: Classification on new classes of articles
Arxiv-CL: Classification on new classes of articles
Reddit-CL: Classification on new classes of communities
Products-CL: Classification on new classes of products

G-CGL

Datasets for Task-IL

SIDER-tIL: Prediction on new molecule properties
Tox21-tIL: Prediction on new molecule properties
Aromaticity-CL: Classification on new classes of molecules

Datasets for Class-IL

Aromaticity-CL: Classification on new classes of molecules

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

Table 1: The detailed statistics of the constructed benchmark datasets for N-CGL.

Benchmark datasets	CoraFull-CL	Arxiv-CL	Reddit-CL	Products-CL
Data source	CoraFull [34]	OGB-Arxiv[1]	Reddit [17]	OGB-Products[2]
Learning scenario	task-IL & class-IL	task-IL & class-IL	task-IL & class-IL	task-IL & class-IL
# nodes	19,793	169,343	227,853	2,449,028
# edges	130,622	1,166,243	114,615,892	61,859,036
# classes	70	40	40	46
# tasks	35	20	20	23
average # nodes per task	660	8,467	11,393	122,451
average # edges per task	4,354	58,312	5,730,794	2,689,523

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

Table 2: The detailed statistics of the constructed benchmark datasets for G-CGL.

Benchmark datasets	SIDER-tIL	Aromaticity-CL	Tox21-tIL
Data source	SIDER [53]	PubChemBioAssayAromaticity [54]	Tox21 [3]
Learning scenario	task-IL	task-IL & class-IL	task-IL
# graphs	1,427	3,868	7,831
# nodes	48,006	115,061	145,459
# edges	100,912	253,018	302,190
# classes	27	30	12
# tasks	27	15	12
average # graphs per task	53	155	653
average # nodes per task	1,778	7,671	12,122
average # edges per task	3,737	16,868	25,183

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

Benchmark results

1. Task-IL & Class-IL
2. Node-level & Graph-level
3. W/WO Inter-task edges
4. Comparisons among different baselines
5. Visualization results

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks

CGLB Continual Graph Learning Benchmark

Toolkit

1. Continual learning pipelines
2. Implementations of different baselines
3. Visualization tools

https://github.com/QueuQ/CGLB

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Cglb: Benchmark tasks for continual graph learning." *Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track*. 2022.

CGL Benchmarks (Graph-Level)

Catastrophic Forgetting in Deep Graph Networks: an Introductory Benchmark for Graph Classification

	MNIST	CIFAR10	OGBG-PPA
Size	70000	60000	158100
Node Attrs.	3	5	0
Edge Attrs.	0	0	7
Classes	10	10	37
Avg $\|\mathcal{V}_g\|$	70,57	117,63	243,4
Avg $\|\mathcal{E}_g\|$	564,63	941,07	2266,1
Data Split	55K/5K/15K	45K/5K/15K	49%/29%/22%
Class Split	2+2+2+2+2	2+2+2+2+2	17+5+5+5+5

[diningphil/continual_learning_for_graphs (github.com)](https://github.com/diningphil/continual_learning_for_graphs)

Carta, Antonio, et al. "Catastrophic forgetting in deep graph networks: an introductory benchmark for graph classification." *arXiv preprint arXiv:2103.11750* (2021).

Survey Paper

Continual Learning on Graphs: Challenges, Solutions, and Opportunities

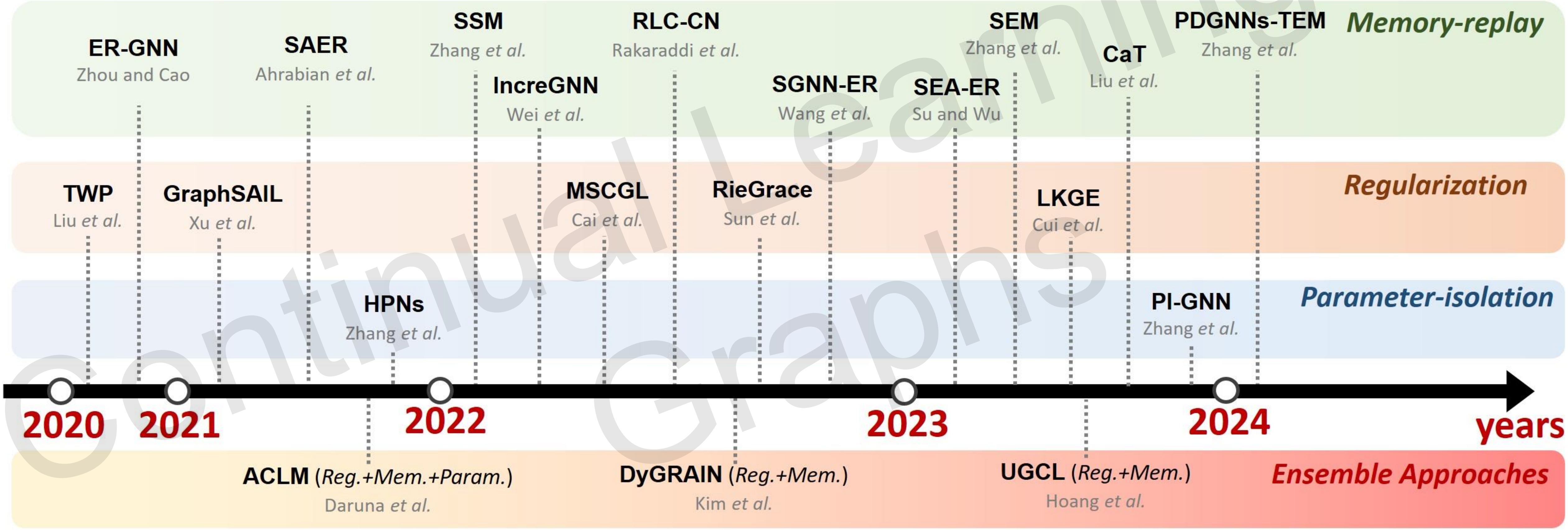
Method	Applications	Task Granularity	Technique	Characteristics
TWP [2]	General	Node/Graph	Reg.	Preserve the topology learnt from previous tasks
RieGrace [71]	General	Node	Reg.	Maintain previous knowledge via knowledge distillation
GraphSAIL [72]	Recommender Systems	Node	Reg.	Local and global structure preservation, node information preservation
MSCGL [73]	General	Node	Reg.	Parameter changes orthogonal to previous parameters
LKGE [74]	Knowledge Graph	Node	Reg.	Alleviating forgetting issue with l2 regularization
ER-GNN [75]	General	Node	Mem.	Replay representative nodes
SSM [76]	General	Node	Mem.	Replay representative sparsified computation subgraphs
SEM [77]	General	Node	Mem.	Sparsify computation subgraphs based on information bottleneck
PDGNNs-TEM [78]	General	Node	Mem.	Replay representative topology-aware embeddings
IncreGNN [79]	General	Node	Mem.	Replay nodes according to their influence
RLC-CN [80]	General	Node	Mem.	Model structure adaption and dark experience replay
SGNN-ER [81]	General	Node	Mem.	Model retraining with generated fake historical data
SAER [82]	Recommender System	Node	Mem.	Buffer the representative user-item pairs based on reservoir sampling
SEA-ER [83]	General	Node	Mem.	Minimize the structural difference between the memory buffer and the original graph
CaT [84]	General	Node	Mem.	Train the model solely on balanced condensed graphs from all tasks
HPNs [3]	General	Node	Para.	Extracting and storing basic features to encourage knowledge sharing across tasks, model expanding to accommodate new patterns
PI-GNN [85]	General	Node	Para.	Separate parameters for encoding stable and changed graph parts
DyGRAIN [86]	General	Node	Mem.+Reg.	Alleviate catastrophic forgetting and concept shift of previous task nodes via memory replay and knowledge distillation
ACLM [87]	Knowledge Graph	Node	Mem.+Reg.+Para.	Adapting general CL techniques to CGL tasks
UGCL [88]	General	Node/Graph	Mem.+Reg.	Memory replay & local/global structure preservation

https://arxiv.org/abs/2402.11565

https://github.com/UConn-DSIS/Survey-of-Continual-Learning-on-Graphs

Survey Paper

Continual Learning on Graphs: Challenges, Solutions, and Opportunities



https://arxiv.org/abs/2402.11565
https://github.com/UConn-DSIS/Survey-of-Continual-Learning-on-Graphs

Agenda

- Background on Graph Representation Learning
- Motivation of Continual Graph Learning
- Problem setup of CL and CGL
- CL techniques & CGL techniques
- Evaluation Metrics & CGL benchmarks
- **Future opportunities**

Future Opportunities

- Trade-off between Effectiveness and Space Complexity
- Task-free CGL
- Extension to other Modalities (Heterogeneous graphs)
- Extension to more graph related tasks
- Into large models, on large graphs

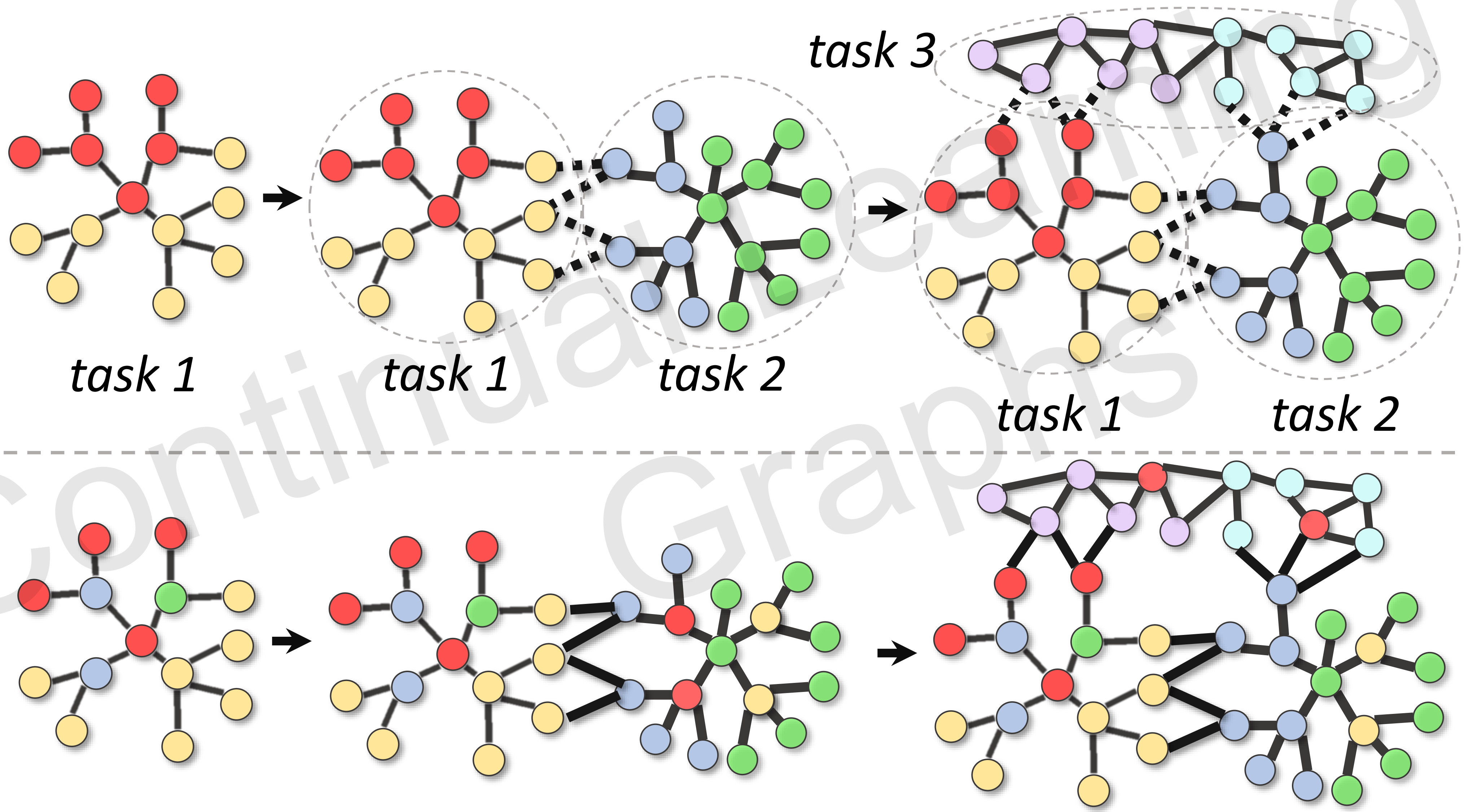
Future Opportunities

Trade-off between Effectiveness and Space/Computation Complexity

- **Regularization:** No extra memory buffer. Poor plasticity for new tasks.
- **Parameter-isolation:** Extra memory consumption for network expansion. Good performance.
- **Memory-replay:** Extra memory consumption for representative data. Good performance.

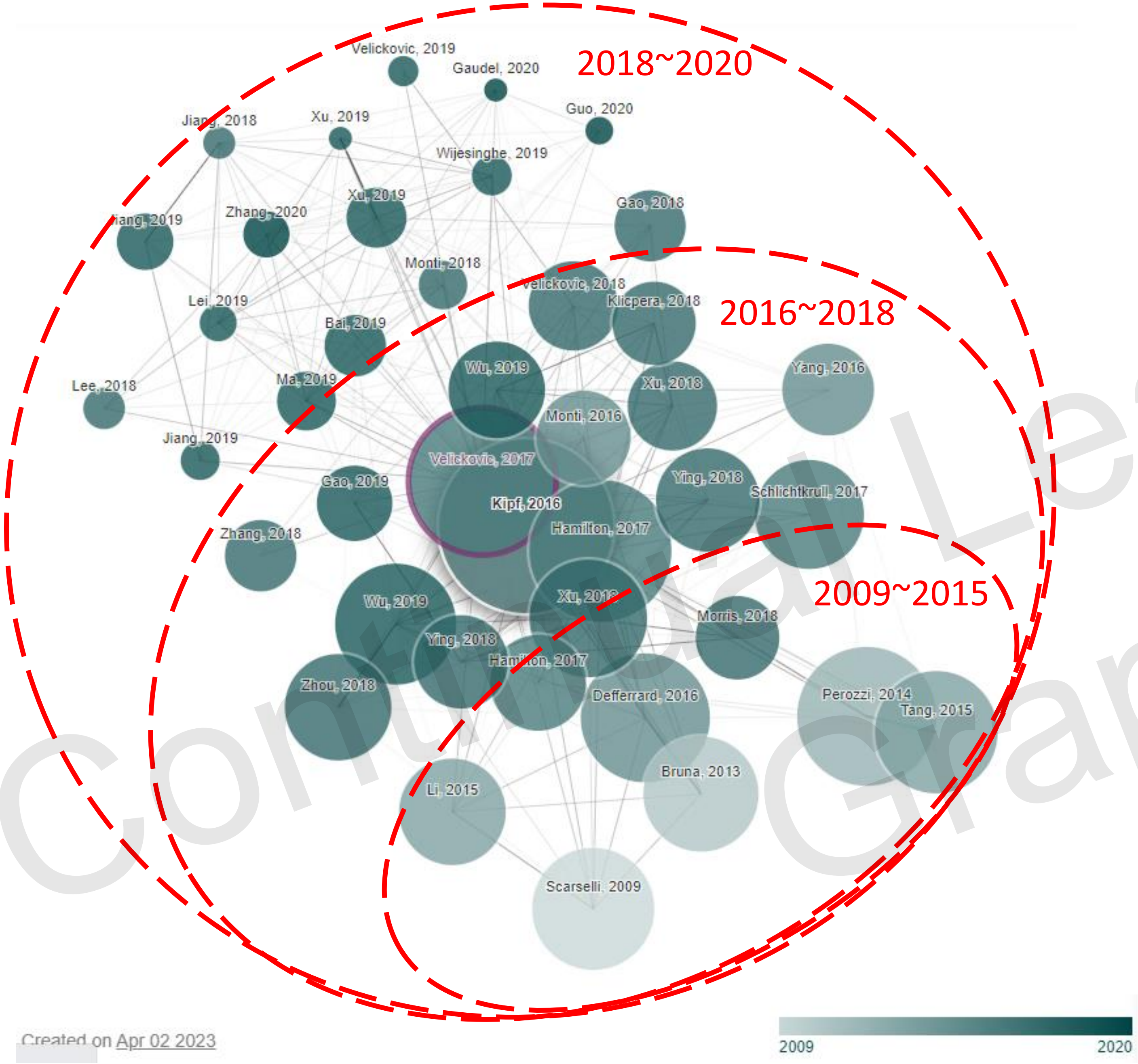
Future Opportunities

Task-free CGL



Explicit Task Boundaries

Implicit Task Boundaries

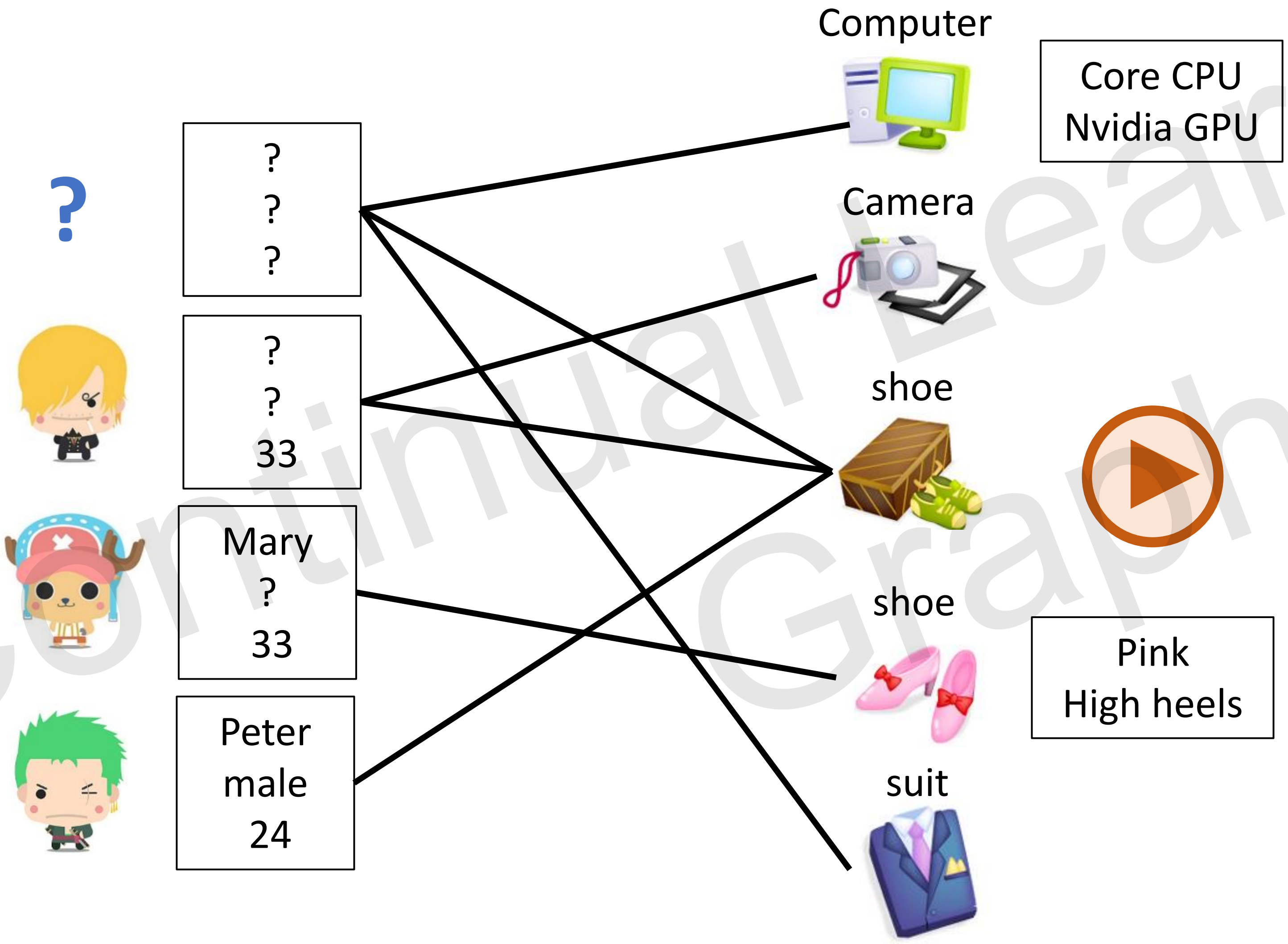


- Research may focus on different topics in different years.
- Papers on new and old topics are blended without clear boundaries.
- When to treat the new data as new tasks?
- Techniques from other areas may help!

https://www.connectedpapers.com/

Future Opportunities

Extension to other Modalities (Heterogeneous graphs)

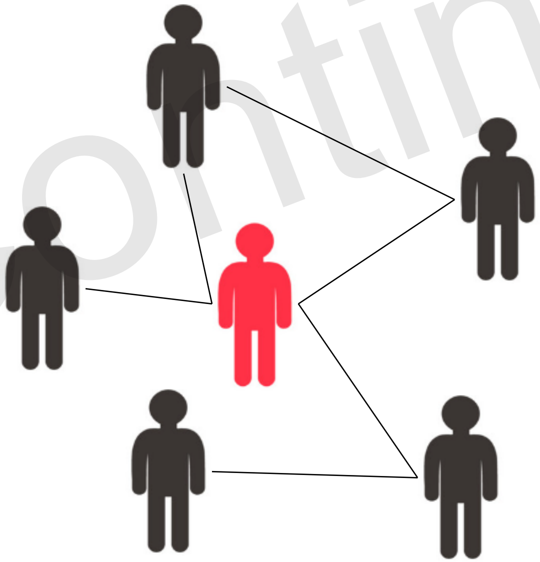


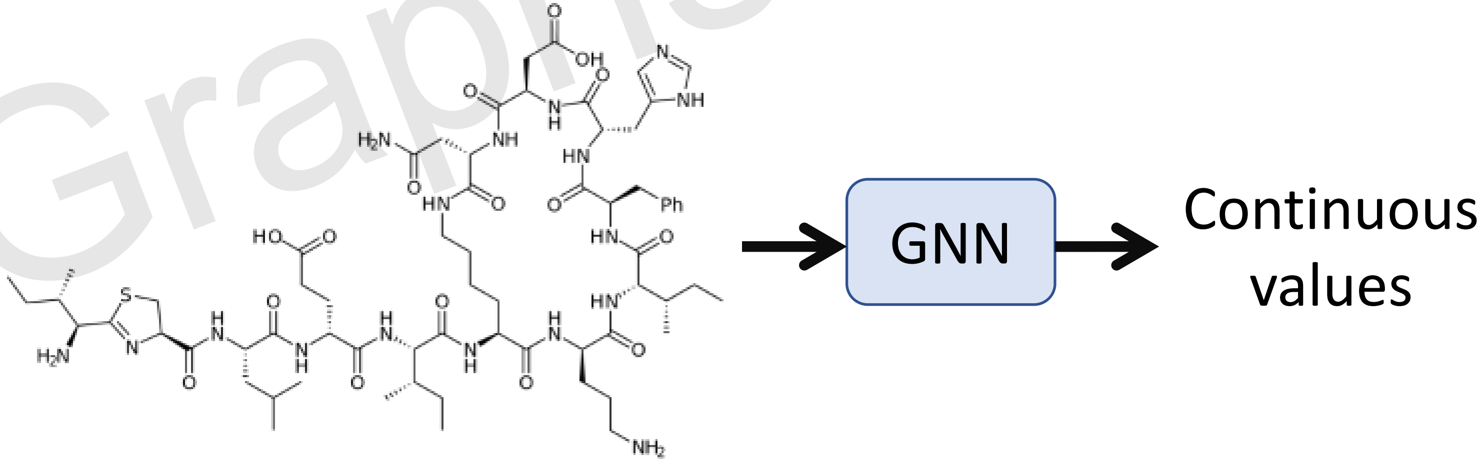
- **Different Modalities**
- **Different number of modalities**
- **Can learning on one modality benefit the others?**

Future Opportunities

Extension to more graph related tasks

- **Anomaly detection**
- **Graph/Node regression**
- **Etc.**

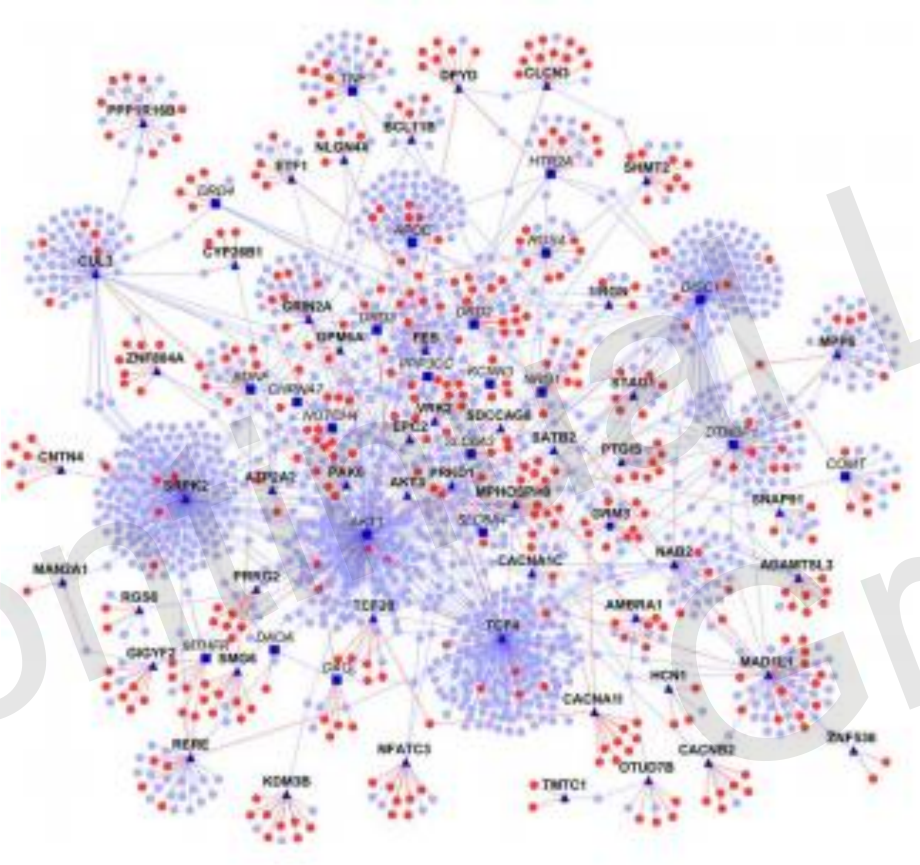




Molecules

Future Opportunities

Into large models, on large graphs



- **Graphs could grow to be very large gradually**
- **Models can also grow accordingly**

https://www.genengnews.com/insights/protein-protein-interactions-get-a-new-groove-on/

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Gilmer, Justin, et al. "Neural message passing for quantum chemistry." International conference on machine learning. PMLR, 2017.
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For understanding the basic logic of GNNs

Parisi, German I., et al. "Continual lifelong learning with neural networks: A review." Neural networks 113 (2019): 54-71.
https://www.sciencedirect.com/science/article/pii/S0893608019300231

For an overview of continual learning

Van de Ven, Gido M., and Andreas S. Tolias. "Three scenarios for continual learning." arXiv preprint arXiv:1904.07734 (2019).
https://arxiv.org/abs/1904.07734

For an understanding of different incremental scenarios

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "CGLB: Benchmark tasks for continual graph learning." Thirty-sixth Conference on Neural Information Processing Systems Datasets and Benchmarks Track. 2022.
https://openreview.net/forum?id=5wNiiIDynDF

For an overview of CGL settings and challenges

Key References

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Continual Learning on Graphs: Challenges, Solutions, and Opportunities." arXiv preprint arXiv:2402.11565 (2019).
https://arxiv.org/abs/2402.11565

A comprehensive survey on CGL research

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Sparsified Subgraph Memory for Continual Graph Representation Learning." 2022 IEEE International Conference on Data Mining (ICDM). IEEE, 2022.
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A CGL module for preserving both nodal and topological information

Zhang, Xikun, Dongjin Song, and Dacheng Tao. "Ricci curvature-based graph sparsification for continual graph representation learning." IEEE Transactions on Neural Networks and Learning Systems (2023)..
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A CGL module for preserving nodal information


Q&A
2024