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Template based Graph Neural Network with Optimal Transport Distances

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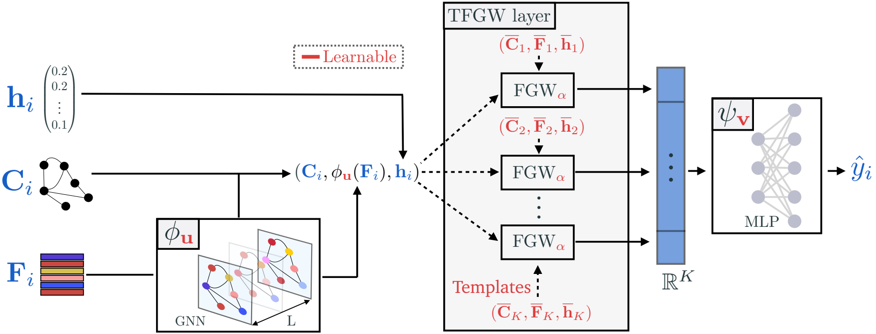
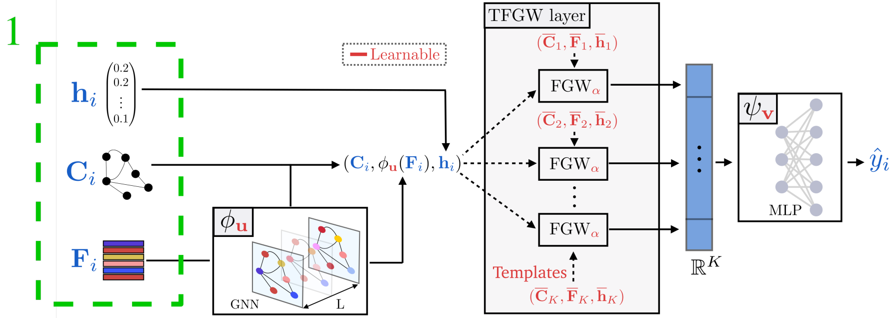


- **TFGW: A novel pooling layer derived from OT distances.**
- Leading to new end-to-end GNN models for graph-level tasks.
- 4 main components where learnable parameters are illustrated in red.



1. Modeling graphs as discrete distributions

- $\boldsymbol{h}_i$: probability vector modeling nodes relative importance.
- $\boldsymbol{C}_i$: node relationship matrix *e.g* adjacency, shortest-path, laplacian, etc.
- $\boldsymbol{F}_i$: node feature matrix.

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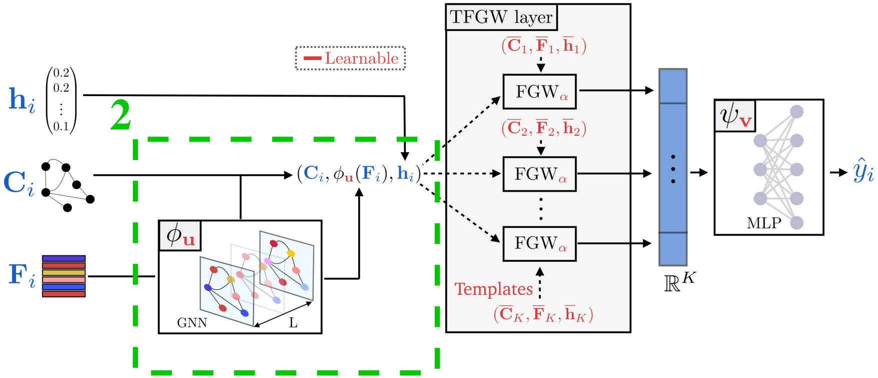
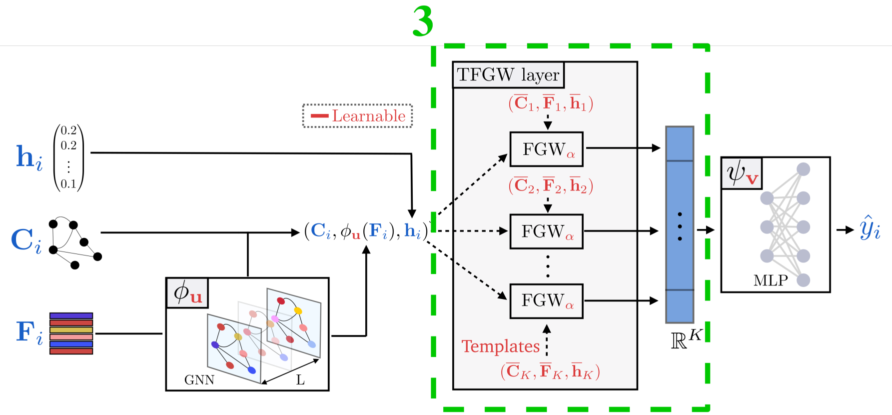


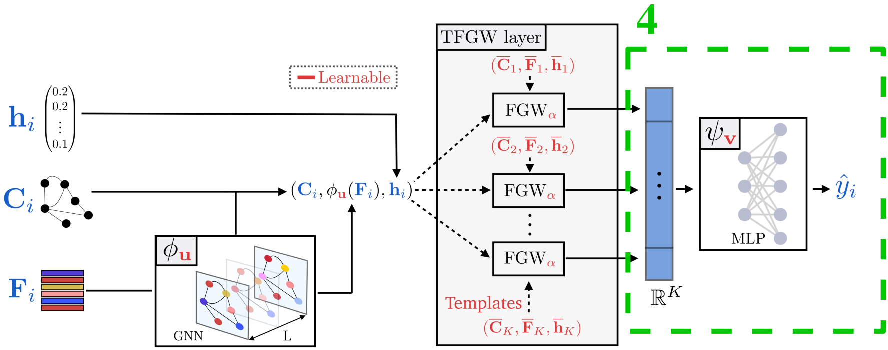
2. Node embeddings

- $\phi_{\boldsymbol{u}}$: Spatial GNN of L layers parameterized by $\boldsymbol{u}$ *e.g* GIN, GAT, etc.
- Promotes discriminant features on the nodes $\phi_{\boldsymbol{u}}(\boldsymbol{F}_i)$



3. Template-based Fused Gromov-Wasserstein pooling

- FGW_α: OT distance resulting from a soft graph matching problem.
- $\alpha \in [0;1]$: relative importance between structure $\boldsymbol{C}_i$ and node features $\phi_{\boldsymbol{u}}(\boldsymbol{F}_i)$.
- $\{\overline{\boldsymbol{C}}_k, \overline{\boldsymbol{F}}_k, \overline{\boldsymbol{h}}_k\}$: FGW distances to K templates used as graph representation.



4. Final MLP for predictions

- $\psi_{\boldsymbol{v}}$: MLP with non-linearities fed with the distance embeddings.
- $\hat{y}_i$: final prediction for graph-level tasks.

Numerical experiments

	MUTAG	PTC	ENZYMES	PROTEIN	NCI1	IMDB-B	IMDB-M	COLLAB
Best competitor accuracy (%)	OTGNN 92.1	OTGNN 68.0	FGW 72.2	OTGNN 78.0	WWL 85.7	WWL 71.6	WWL 52.6	WWL 81.4
TFGW+GIN (ours) accuracy gain	96.4 **+4.3**	72.4 **+4.4**	75.1 **+2.9**	82.9 **+4.9**	88.1 **+2.4**	78.3 **+6.7**	56.8 **+4.2**	84.3 **+2.9**

- **Better Generalization**: TFGW+GIN outperforms best competitor among benchmarked SOTA GNN and Kernel models.
- **Enhanced Expressivity** beyond Weisfeiler-Lehman Isomorphism tests.
- **Sensitivity analysis**:
  - TFGW > Other pooling (GIN & GAT).
  - Flexible choice of input structure C_i.

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Thank you for your attention.

Let's meet at the poster session !