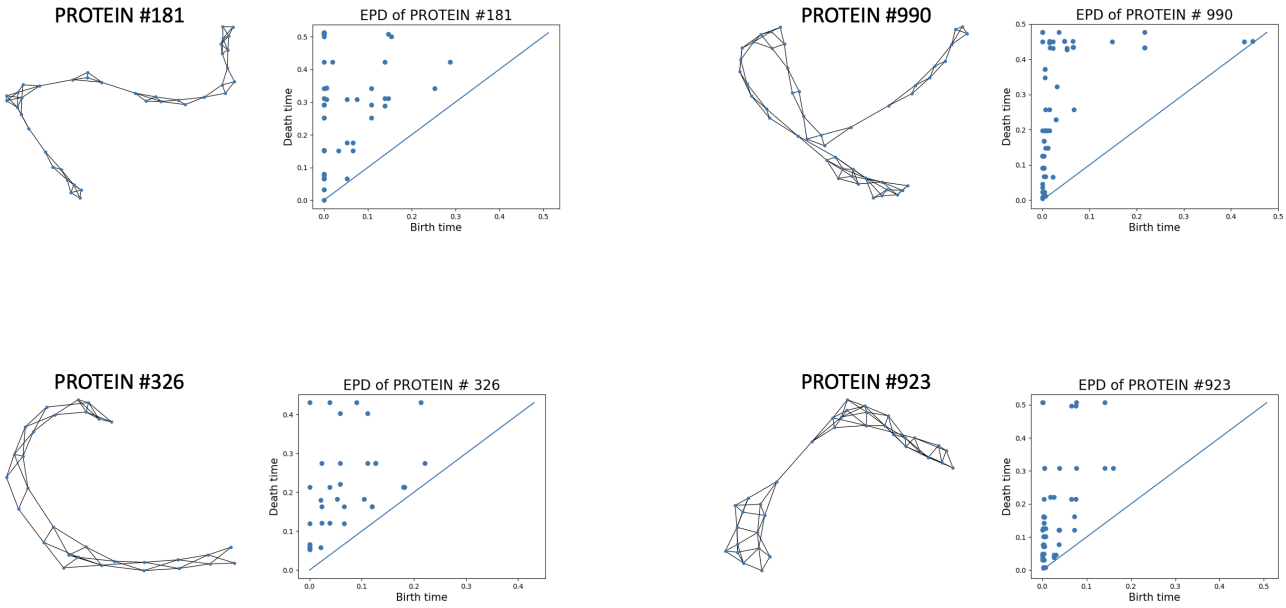
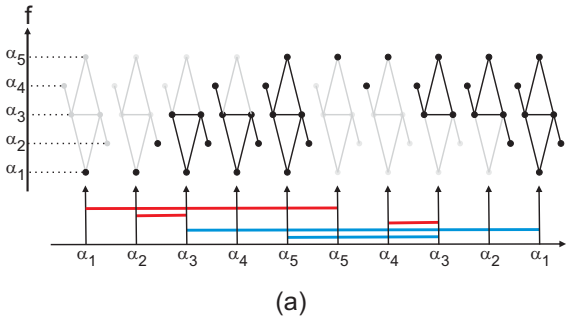


Figure 1: Proteins structures and EPDs in PROTEINS dataset.



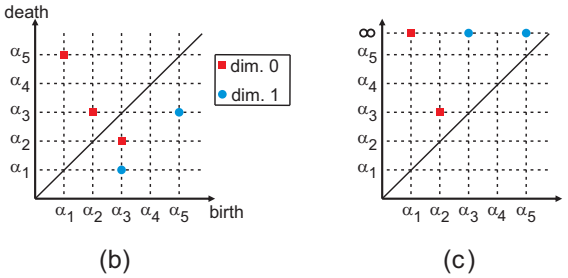


Figure 2: Comparison between persistence homology (PH) and extended persistence homology (EPH) in graphs.

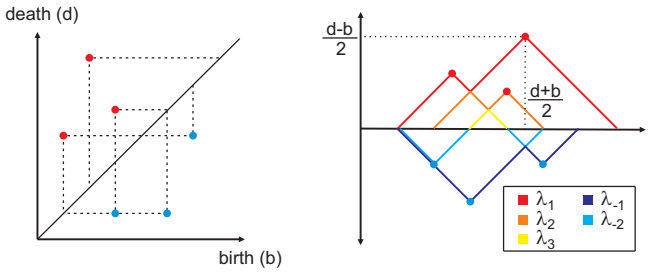


Figure 3: Construction of an extended persistence landscape.

Table 1: The main symbols and definitions in this paper.

Notation	Definition
$\mathcal{G}$	an attribute graph
$\mathcal{V}$	a set of nodes
$\mathcal{E}$	a set of edges
$\boldsymbol{X}$	a node feature matrix
$\boldsymbol{A}$	an adjacency matrix
$\boldsymbol{D}$	a degree matrix corresponding to $\boldsymbol{A}$
N	the number of nodes
F	the dimension of node features
Υ	number of graphs in a set of graphs
b_ρ and d_ρ	a birth time and death time for a topological feature ρ
$\mathscr{K}$	an abstract simplicial complex
$\mathcal{G}_{\nu_j}$	a subgraph with a scale parameter ν_j in a sequence of nested subgraphs
ω	a edge-weight function
$\mathcal{T}(\cdot)$/$\mathcal{T}_i(\cdot)$/$\mathcal{T}_i'(\cdot)$	graph data augmentations
f_{ENCODER}	a shared encoder for graph representation learning
$\text{sim}(\cdot,\cdot)$	a similarity function
$\tilde{\boldsymbol{H}}_i$ and $\tilde{\boldsymbol{H}}_i'$	learned representations of the two augmented graph $\tilde{\mathcal{G}}_i$ and $\tilde{\mathcal{G}}_i'$
$\tilde{\boldsymbol{Z}}_i$ and $\tilde{\boldsymbol{Z}}_i'$	latent extended topological representations of the two augmented graph $\tilde{\mathcal{G}}_i$ and $\tilde{\mathcal{G}}_i'$
$\mathcal{Q}$	number of sublevel filtration functions
$\mathfrak{F}_q$	the q-th sublevel filtration
$\Psi(\cdot)$	a extended topological layer (ETL)
$\tilde{\boldsymbol{\Xi}}$	extended topological features based on a augmented graph $\tilde{\mathcal{G}}$
$\boldsymbol{\Omega}(\cdot)$	a function which extracts extended persistence features
f_{CNN}	the convolutional neural network
ϕ_{MAX}	the global max-pooling layer
$\ell_{i,\text{G}}$	graph contrastive loss for a graph $\mathcal{G}_i$ (in Figure 1 of the main body, for the sake of simplicity, we use ℓ_{G} denotes $\ell_{i,\text{G}}$)
$\ell_{i,\text{T}}$	topological contrastive loss for a graph $\mathcal{G}_i$ (in Figure 1 of the main body, for the sake of simplicity, we use ℓ_{T} denotes $\ell_{i,\text{T}}$)
ℓ	the final training objective function
ζ	a temperature hyperparameter
α and β	hyperparameters which balance the contribution of graph and topological contrastive losses
$\mathscr{K}(\mathcal{G}_{\nu_j})$	the simplicial complex associated to the graph $\mathcal{G}_{\nu_j}$
Λ_i	generating function of extended persistence homology
$\lambda_k(\mathcal{G})$	k^{th} landscape fuction of graph $\mathcal{G}$
$\Lambda_p(\text{EDg}_1, \text{EDg}_2)$	ℓ_p-norm between extended persistence diagrams EDg_1 and EDg_2
$\Lambda_p(\text{EM}_1, \text{EM}_2)$	ℓ_p-norm between extended persistence modules EM_1 and EM_2
$d_B(\text{EDg}_1, \text{EDg}_2)$	bottleneck distance between extended persistence diagrams EDg_1 and EDg_2
$d_I(\text{EM}_1, \text{EM}_2)$	interleaving distance between extended persistence modules EM_1 and EM_2
EDg	extended persistence diagram
EPI	extended persistence image
EPL	extended persistence landscape
EM	persistence module