

Dataset	GOOD-HIV	GOOD-PCBA	GOOD-ZINC	GOOD-CMNIST
Graph/Node	Graph	Graph	Graph	Graph
Input(X)	Molecule	Molecule	Molecule	Image-conveted graphs
Prediction(Y)	HIV replications	Bioassays	Constrained Solubility	Digit numbers
Domain selection	Scaffold/Size	Scaffold/Size	Scaffold/Size	Color
# domains	19,089/151	113,760/192	129,959/33	7 (10)
# examples	41,127	437,929	249,455	70,000
Source	Real-world	Real-world	Real-world	Semi-artificial
Task	Binary-classification	Multi-task binary classification	Regression	Multi-class classification
Metric	ROC-AUC	Average Precision	MAE	Accuracy
Example domain	Scaffold	Size	Scaffold	Color
Shift type	Covariate	Concept	Covariate	Concept
# environments	10/1/1	3/1/1	10/1/1	3/1/1
Train example				
Test example				
Dataset	GOOD-Motif	GOOD-Cora	GOOD-Arxiv	GOOD-CBAS
Graph/Node	Graph	Node	Node	Node
Input(X)	Motif-base graphs	Scientific publications	Arrive papers	A BA-house graph
Prediction(Y)	Motifs	Publication classes	Subject areas	Node roles
Domain selection	Base/Size	Word/Degree	Time/Degree	Color
# domains	5 (3)/5 (3)	218/102	35/547	7 (4)
# examples	30,000	19,793	169,343	700
Source	Synthesis	Real-world	Real-world	Synthetic
Task	Multi-class classification	Multi-class classification	Multi-class classification	Multi-class classification
Metric	Accuracy	Accuracy	Accuracy	Accuracy
Example domain	Base	Degree	Time	Color
Shift type	Covariate	Concept	Covariate	Concept
# environments	3/1/1	3/1/1	10/1/1	3/1/1
Train example				
Test example				