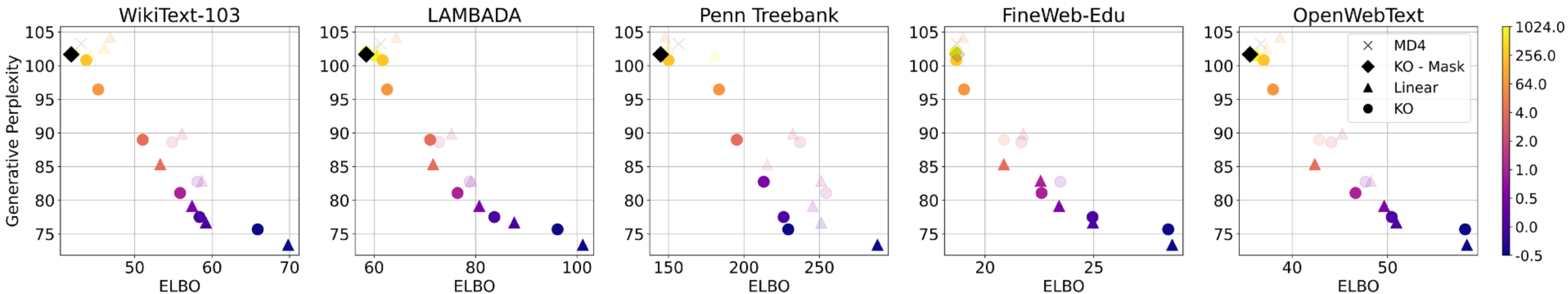


Text experiments

● Kinetic optimal
▲ Linear



Source = mask

Source = data statistics

* ELBO is computed with our bound

Crystalline Material Experiment

Method	NFE	Validity (%) \uparrow		Coverage (%) \uparrow		Property \downarrow		Stability Rate (%) \uparrow
		Structural	Composition	Recall	Precision	wdist (ρ)	wdist (N_{el})	
CDVAE (Xie et al., 2021)	5000	100.00	86.70	99.15	99.49	0.688	0.278	1.57
DiffCSP (Jiao et al., 2023)	1000	100.00	83.25	99.71	99.76	0.350	0.125	5.06
FlowMM (Miller et al., 2024)	1000	96.85	83.19	99.49	99.58	0.239	0.083	4.65
CrystalLLM (70B) (Gruver et al., 2024)	–	99.6	95.4	85.8	98.9	0.81	0.44	5.28
Autoregressive	–	86.43	89.33	63.31	99.74	0.088	0.030	1.99
Perm. invariant DFM - Mask w/ Cubic	250	94.40	84.40	98.25	99.40	0.244	0.144	6.90
Perm. invariant DFM - Mask w/ Kinetic Optimal	250	95.79	88.50	90.11	99.29	0.542	0.154	7.02