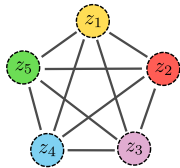


Markov Random Field



$$G = (V, E)$$

Inference of Max-marginal Probabilities

for all candidate molecules

$$p_{\max}(z_3 = 4) = \max_{\{\mathbf{z}' \in \mathcal{Z} \mid z'_3 = 4\}} p(\mathbf{z}')$$

Ranked Candidates for each MS feature

using their max-marginal probabilities

