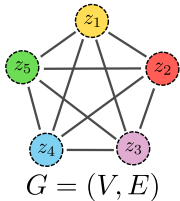


Markov Random Field



Inference of Max-marginal Probabilities (for all candidate molecules and features)

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

Ranked Candidates of MS features (max-marginal probabilities)

