Supplementary materials

1 Model setting

In our scATAC-seq framework, the encoder consists of a four-layer feedforward network with layer sizes of 3200, 1600, 800 and 400 neurons, yielding a 32-dimensional latent representation. The decoder and classifiers take this 32-dimensional embedding as input directly, without any intervening hidden layers. Training is performed with mini-batches of 64 samples over 3000 epochs, using the AdamW optimizer (learning rate = 0.0002, weight decay = 5×10^{-4}).

2 Metric definitions

$Kappa$ is a minor-class sensitive method to provide a thorough evaluation on classification performance. $F1\_SCORE$, computed by averaging precision rate over recall rate for every type, applies to multi-classification scenarios and is equivalent to accuracy for binary classification. Finally, ACC measures the overall proportion of correctly classified samples. These metrics are mathematically formulated in Equations (13)-(16) below.

$$\text{Jaccard} = \frac{1}{N}\sum_{i=1}^{N}\frac{|Y_i \cap \hat{Y}_i|}{|Y_i \cup \hat{Y}_i|} \tag{1}$$

$$Kappa = \frac{p_o - p_e}{1 - p_e} \tag{2}$$

$$\text{F1\_SCORE} = \frac{1}{K}\sum_{k=1}^{K}\frac{2 \cdot TP_k}{2 \cdot TP_k + FP_k + FN_k} \tag{3}$$

$$ACC = \frac{\sum_{k=1}^{K} TP_k}{N} \tag{4}$$

Specifically:

- N: Total samples
- Y_i: Ground truth set for sample i
- $\hat{Y}_i$: Predicted set for sample i
- $|\cdot|$: Set cardinality
- $\cap/\cup$: Set intersection/union
- p_o: Observed agreement (accuracy)
- p_e: Expected chance agreement
- K: Total classes
- TP_k: True positives for class k
- FP_k: False positives for class k
- FN_k: False negatives for class k

where detailed calculations can be found in [1], [2], [3].

References

[1] Jaccard, P. (1902). Distribution de la flore alpine. *Bulletin de la Société Vaudoise des Sciences Naturelles*, 38, 69-130. 2

[2] Van Rijsbergen, C. J. (2004). *The geometry of information retrieval*. Cambridge University Press. 2

[3] Cohen, J. (1960). A coefficient of agreement for nominal scales. *Educational and Psychological Measurement*, 20(1), 37-46.