

Supplementary Materials for

Multimodal contrastive learning for spatial gene expression prediction using histology images

Supplementary Notes

1. Evaluation metrics

We use Pearson Correlation Coefficient (PCC), Mean Squared Error (MSE), and Mean Absolute Error (MAE) to evaluate the proposed method against baselines.

$$\text{PCC} = \frac{\text{Cov}(\mathbf{X}_{\text{observed}}, \mathbf{X}_{\text{pred}})}{\text{Var}(\mathbf{X}_{\text{observed}}) \times \text{Var}(\mathbf{X}_{\text{pred}})} \quad (1)$$

where $\text{Cov}()$ is the covariance, and $\text{Var}()$ is the variance.

$$\text{MSE} = \frac{1}{N} \sum_{i=1}^N (\mathbf{X}_{\text{observed}} - \mathbf{X}_{\text{pred}})^2 \quad (2)$$

$$\text{MAE} = \frac{1}{N} \sum_{i=1}^N |\mathbf{X}_{\text{observed}} - \mathbf{X}_{\text{pred}}| \quad (3)$$

$\mathbf{X}_{\text{observed}}$ and \mathbf{X}_{pred} are the observed and predicted gene expression, respectively. In the assessment of spatial clustering performance, we employ the Adjusted Rand Index (ARI) to measure the correlation between the clustering outcomes and the actual pathological annotation regions. The ARI can be mathematically expressed as follows:

$$\text{ARI} = \frac{\sum_{ij} \binom{n_{ij}}{2} - \frac{[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}]}{\binom{n}{2}}}{\frac{1}{2} [\sum_i \binom{a_i}{2} + \sum_j \binom{b_j}{2}] - \frac{[\sum_i \binom{a_i}{2} \sum_j \binom{b_j}{2}]}{\binom{n}{2}}} \quad (4)$$

where a_i and b_j are the number of samples appearing in the i -th predicted cluster and the j -th true cluster, respectively. n_{ij} means the number of overlaps between the i -th predicted cluster and the j -th true cluster.

Supplementary Figures

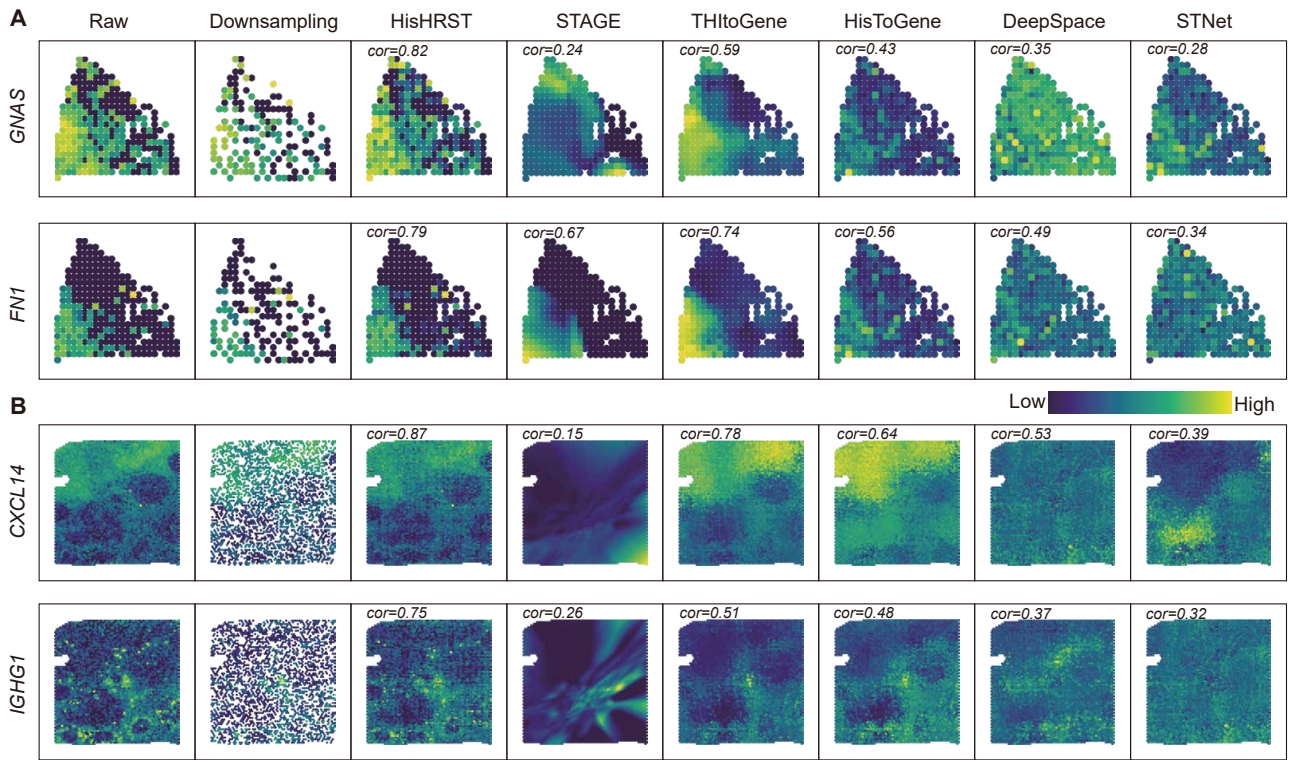


Figure S1. (A) Visualizing the gene expression pattern recovery performance of HisHRST, STAGE, THItGene, HisToGene, DeepSpace, and STNet on *GNAS* and *FN1* marker genes on the HER2+ dataset. (B) Visualizing the recovery performance of gene expression patterns for *CXCL14* and *IGHG1* marker genes using the same methods on the IDC dataset.

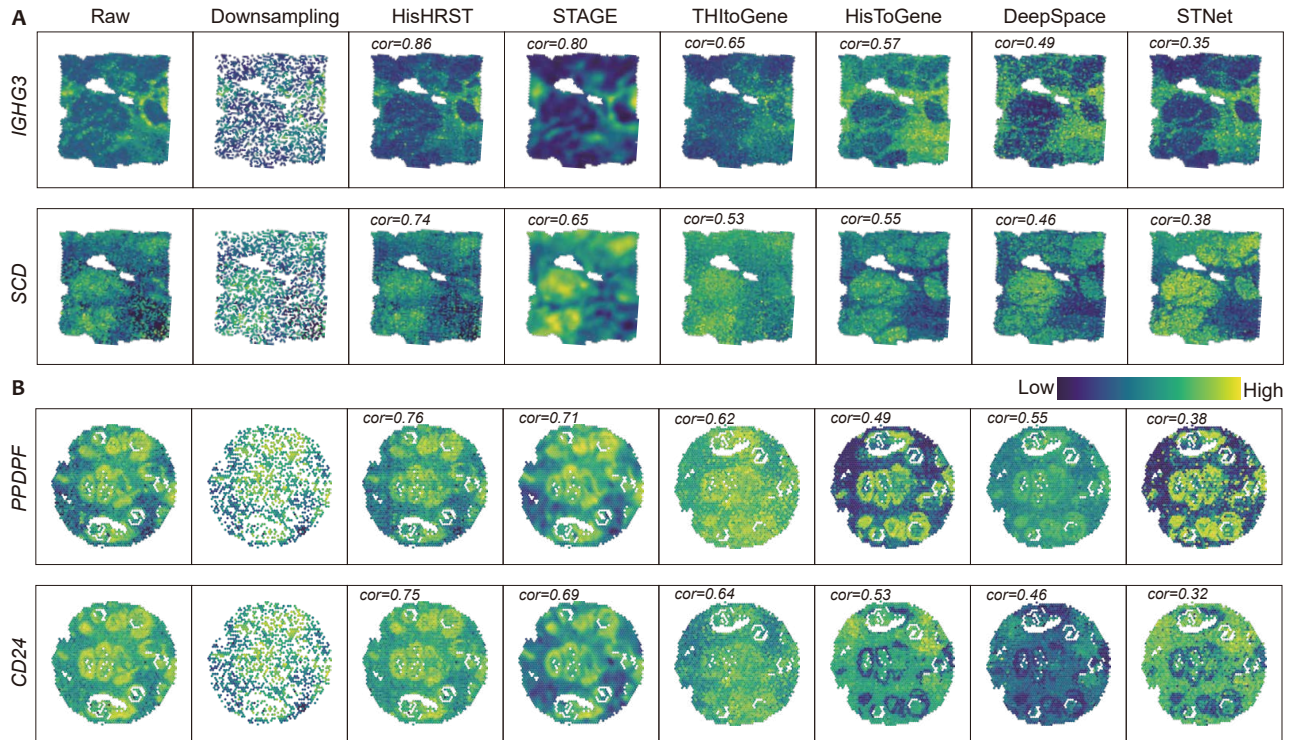


Figure S2. (A) Visualizing the gene expression pattern recovery performance of HisHRST, STAGE, THItGene, HisToGene, DeepSpace, and STNet on *IGHG3* and *SCD* marker genes on the BC1 dataset. (B) Visualizing the recovery performance of gene expression patterns for *PPDPF* and *CD24* marker genes using the same methods on the BC2 dataset.