成果一.

我院王勇研究员与合作者的论文 ClusterMatch aligns single-cell RNAsequencing data at the multi-scale cluster level via stable matching 被 BIOINFORMATICS 接收发表。

摘要: Motivation Unsupervised clustering of single-cell RNA sequencing (scRNA-seq) data holds the promise of characterizing known and novel cell type in various biological and clinical contexts. However, intrinsic multi-scale clustering resolutions poses challenges to deal with multiple sources of variability in the high-dimensional and noisy data.Results We present ClusterMatch, a stable match optimization model to align scRNA-seq data at the cluster level. In one hand, ClusterMatch leverages the mutual correspondence by canonical correlation analysis and multi-scale Louvain clustering algorithms to identify cluster with optimized resolutions. In the other hand, it utilizes stable matching framework to align scRNA-seq data in the latent space while maintaining interpretability with overlapped marker gene set. Through extensive experiments, we demonstrate the efficacy of ClusterMatch in data integration, cell type annotation, and cross-species/timepoint alignment scenarios. Our results show ClusterMatch's ability to utilize both global and local information of scRNA-seq data, sets the appropriate resolution of multi-scale clustering, and offers interpretability by utilizing marker genes. Availability and implementation The code of ClusterMatch software is freely available at https://github.com/AMSSwanglab/ClusterMatch. 论文链接: http://dx.doi.org/10.1093/bioinformatics/btae480

#### 成果二.

我院孙六全研究员与合作者的论文 Factor-augmented transformation models for interval-censored failure time data 被 BIOMETRICS 接收发表。

摘要: Interval-censored failure time data frequently arise in various scientific studies where each subject experiences periodical examinations for the occurrence of the failure event of interest, and the failure time is only known to lie in a specific time interval. In addition, collected data may include multiple observed variables with a certain degree of correlation, leading to severe multicollinearity issues. This work proposes a factor-augmented transformation model to analyze interval-censored failure time data while reducing model dimensionality and avoiding multicollinearity elicited by multiple correlated covariates. We provide a joint modeling framework by comprising a factor analysis model to group multiple observed variables into a few latent factors and a class of semiparametric transformation models with the augmented factors to examine their and other covariate effects on the failure event. Furthermore, we propose a nonparametric maximum likelihood estimation approach and develop a computationally stable and reliable expectation-maximization algorithm for its implementation. We establish the asymptotic properties of the proposed estimators and conduct simulation studies to assess the empirical performance of the proposed method. An application to the Alzheimer's Disease Neuroimaging Initiative (ADNI) study is provided. An R package ICTransCFA is also available for practitioners. Data used in preparation of this article were obtained from the ADNI database. 论文链接: <u>http://dx.doi.org/10.1093/biomtc/ujae078</u>

### 成果三.

我院骆顺龙研究员与合作者的论文 No-broadcasting of magic states 被 PHYSICAL REVIEW A 接收发表。

摘要: From both intuitive and physical perspectives, it is generally recognized that within a resource theory framework, free operations cannot broadcast a resource state due to their inability to generate resource from free states. In the stabilizer formalism of fault-tolerant quantum computation, the basic ingredients of the corresponding resource theory consist of stabilizer states as free states and stabilizer operations as free operations. The celebrated Gottesman-Knill theorem shows that quantum advantages over classical computation come from the magic (nonstabilizer) resource, such as magic states or non-Clifford gates. In this work, we prove that broadcasting of any magic state via stabilizer operations is impossible, which is reminiscent of the no-broadcasting theorems for noncommuting states or quantum correlations. We further derive a trade-off relation between the magic resource consumed in the initial system and that gained in the target system. These results characterize magic states in the stabilizer formalism from the broadcasting angle, and may have implications for distributed quantum computation and quantum secret sharing.

论文链接: <u>http://dx.doi.org/10.1103/PhysRevA.110.012462</u>

#### 成果四.

我院吴凌云研究员与合作者的论文 Reverse network diffusion to remove indirect noise for better inference of gene regulatory networks 被 BIOINFORMATICS 接收发表。

摘要: Motivation Gene regulatory networks (GRNs) are vital tools for delineating regulatory relationships between transcription factors and their target genes. The boom in computational biology and various biotechnologies has made inferring GRNs from multi-omics data a hot topic. However, when networks are constructed from gene expression data, they often suffer from false-positive problem due to the transitive effects of correlation. The presence of spurious noise edges obscures the real gene interactions, which makes downstream analyses, such as detecting gene function modules and predicting disease-related genes, difficult and inefficient. Therefore, there is an urgent and compelling need to develop network denoising methods to improve the accuracy of GRN inference. Results In this study, we proposed a novel network denoising method named REverse Network Diffusion On Random walks (RENDOR). RENDOR is designed to enhance the accuracy of GRNs afflicted by indirect effects. RENDOR takes noisy networks as input, models higher-order indirect interactions between genes by transitive closure, eliminates false-positive effects using the inverse network diffusion method, and produces refined networks as output. We conducted a comparative assessment of GRN inference accuracy before and after denoising on

simulated networks and real GRNs. Our results emphasized that the network derived from RENDOR more accurately and effectively captures gene interactions. This study demonstrates the significance of removing network indirect noise and highlights the effectiveness of the proposed method in enhancing the signal-to-noise ratio of noisy networks. Availability and implementation The R package RENDOR is provided at https://github.com/Wu-Lab/RENDOR and other source code and data are available at https://github.com/Wu-Lab/RENDOR-reproduce

论文链接: <u>http://dx.doi.org/10.1093/bioinformatics/btae435</u>

## 成果五.

我院黄飞敏研究员与合作者的论文 UNIQUENESS OF COMPOSITE WAVE OF SHOCK AND RAREFACTION IN THE INVISCID LIMIT OF NAVIER-STOKES EQUATIONS 被 SIAM JOURNAL ON MATHEMATICAL ANALYSIS 接 收发表。

摘要: The uniqueness of entropy solution for the compressible Euler equations is a fundamental and challenging problem. In this paper, the uniqueness of a composite wave of shock and rarefaction of one-dimensional compressible Euler equations is proved in the inviscid limit of compressible Navier-Stokes equations. Moreover, the relative entropy around the original Riemann solution consisting of shock and rarefaction under the large perturbation is shown to be uniformly bounded by the framework developed in [M. J. Kang and A. F. Vasseur, Invent. Math., 224 (2021), pp. 55--146]. The proof contains two new ingredients: (1) a cut-off technique and the expanding property of rarefaction are used to overcome the errors generated by the viscosity related to inviscid rarefaction; (2) the error terms concerning the interactions between shock and rarefaction are controlled by the compressibility of shock, the decay of derivative of rarefaction, and the separation of shock and rarefaction as time increases.

论文链接: <u>http://dx.doi.org/10.1137/23M156584X</u>

# 成果六.

我院张世华研究员与合作者的论文 Whole brain alignment of spatial transcriptomics between humans and mice with BrainAlign 被 NATURE COMMUNICATIONS 接收发表。

摘要: The increasing utilization of mouse models in human neuroscience research places higher demands on computational methods to translate findings from the mouse brain to the human one. In this study, we develop BrainAlign, a self-supervised learning approach, for the whole brain alignment of spatial transcriptomics (ST) between humans and mice. BrainAlign encodes spots and genes simultaneously in two separated shared embedding spaces by a heterogeneous graph neural network. We demonstrate that BrainAlign could integrate cross-species spots into the embedding space and reveal the conserved brain regions supported by ST information, which facilitates the detection of homologous regions between humans and mice. Genomic analysis further

presents gene expression connections between humans and mice and reveals similar expression patterns for marker genes. Moreover, BrainAlign can accurately map spatially similar homologous regions or clusters onto a unified spatial structural domain while preserving their relative positions.

论文链接: <u>http://dx.doi.org/10.1038/s41467-024-50608-2</u>