AGAE score：通过最优子集筛选算法和遗传算法辅助的集成学习方法建立了一种稳定的新冠患者严重程度打分

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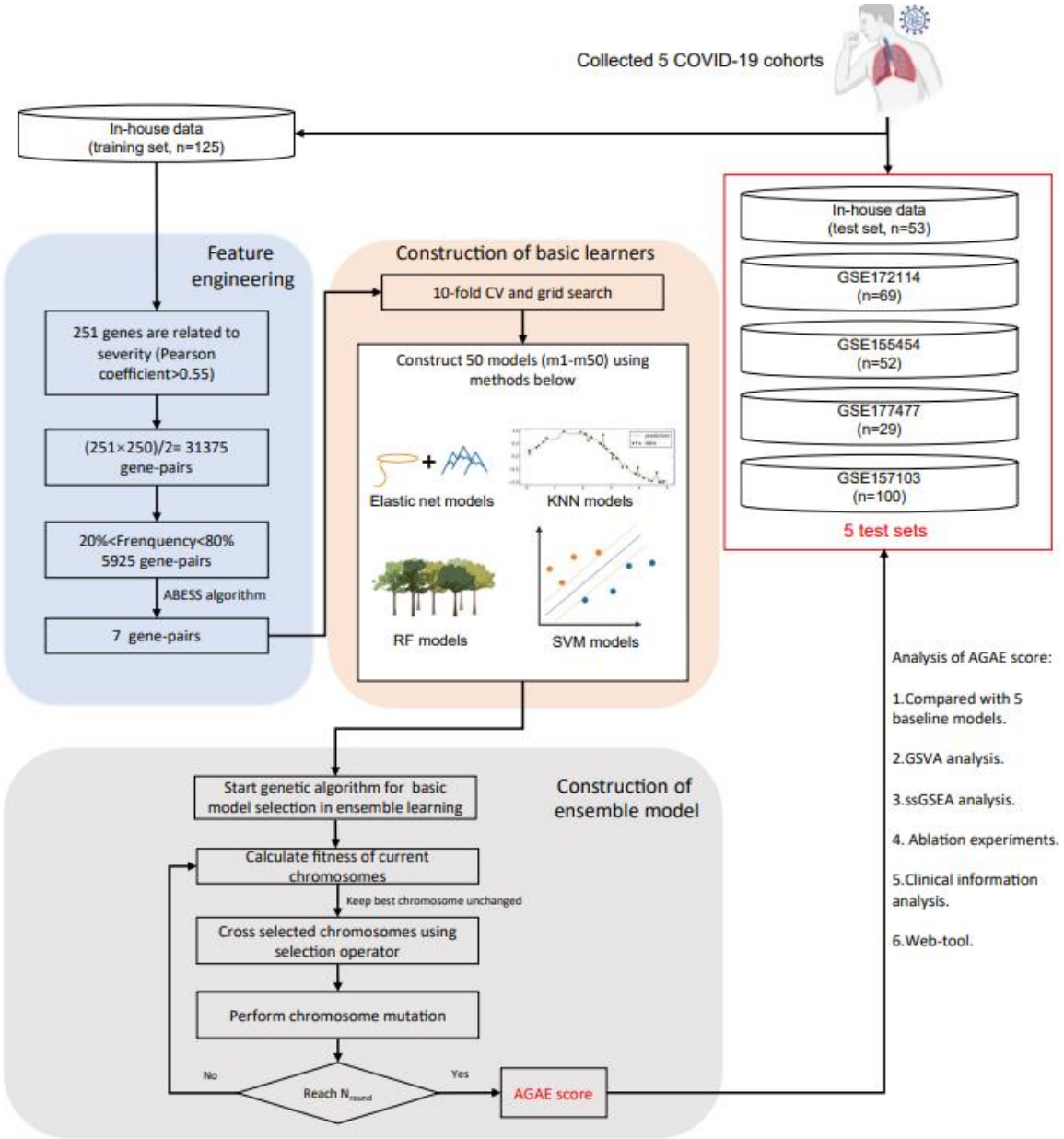


补充图1. AGAE评分的工作流程

(A)

Algorithm 1: The algorithm of AGAE

Input: Training set, $\mathcal{T}_1$.

Output: The trained AGAE score model $\mathcal{M}_{trained}$.

The feature engineering. Select the signaficant genes whose absolute Pearson coefficient with severity level is greater than 0.55 in in $\mathcal{T}_1$. These genes are labelled as $\mathcal{G}_1$;

Pair the genes of $\mathcal{G}_1$ (**Equation 1**) in $\mathcal{T}_1$ set to avoid batch effect and then select the gene-pairs whose frenquency of "1" label is greater than 0.2 and less than 0.8 in the training set and get the gene-pair set $\mathcal{G}_2$;

Perform ABESS algorithm (**Equation 4-11**) on $\mathcal{G}_2$ in $\mathcal{T}_1$ and then get the gene-pair set $\mathcal{G}_3$;

The construction of basic learners. Construct 4 kinds of severity prediction models. Firstly, perform 10-fold CV and grid search in the $\mathcal{T}_1$ set and then built $\mathcal{N}_{gene}$ models using the whole $\mathcal{T}_1$ set and these models are sorted by MSE value in CV from low to high $(m_1 ... m_N)$;

The construction of AGAE score model using genetic algorithm. Set up an ensemble learning model using the m_1 model parameters. Perform the genetic algorithm in the $\mathcal{T}_1$ set. And set the parameters: $\mathcal{N}_{mg}$, $\mathcal{N}_{round}$, $\mathcal{N}_{chromosome}$;

for *training iterations* $i = 1, ..., N_{round}$ **do**

  Compute current fitness value $f(x)$ by **Equation 13** and keep the chromosome with highest fitness unchanged ;

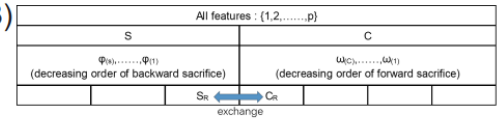
  Selecte chromosomes according to Selection operator (**Equation 14**);

  Cross selected chromosomes ;

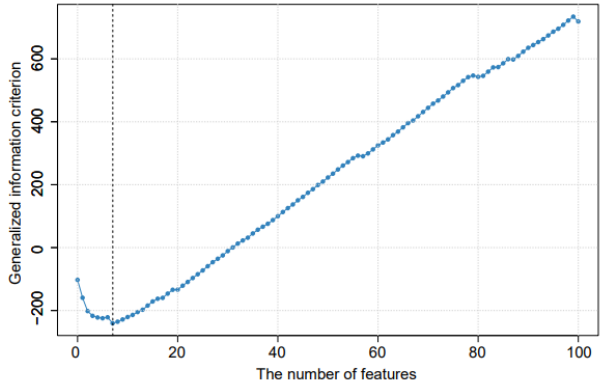
  Generate mutated chromosomes according to $\mathcal{N}_{mg}$ (**Equation 15**);

endfor

(B)



(C)



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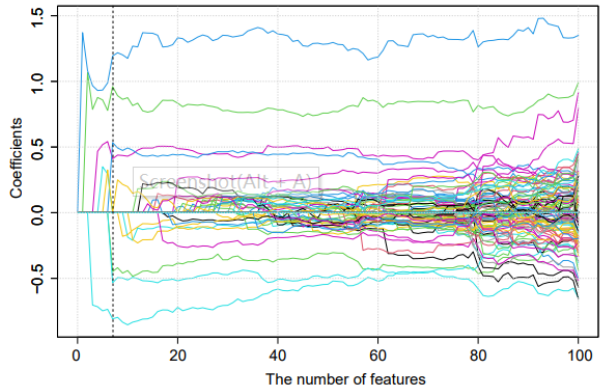

图 1. (A) AGAE 评分算法。 (B) ABESS 算法的图示。 (C) 使用 ABESS 算法选择特征时广义信息准则 (GIC) 的变化。 (D) 选择特征时的特征系数。

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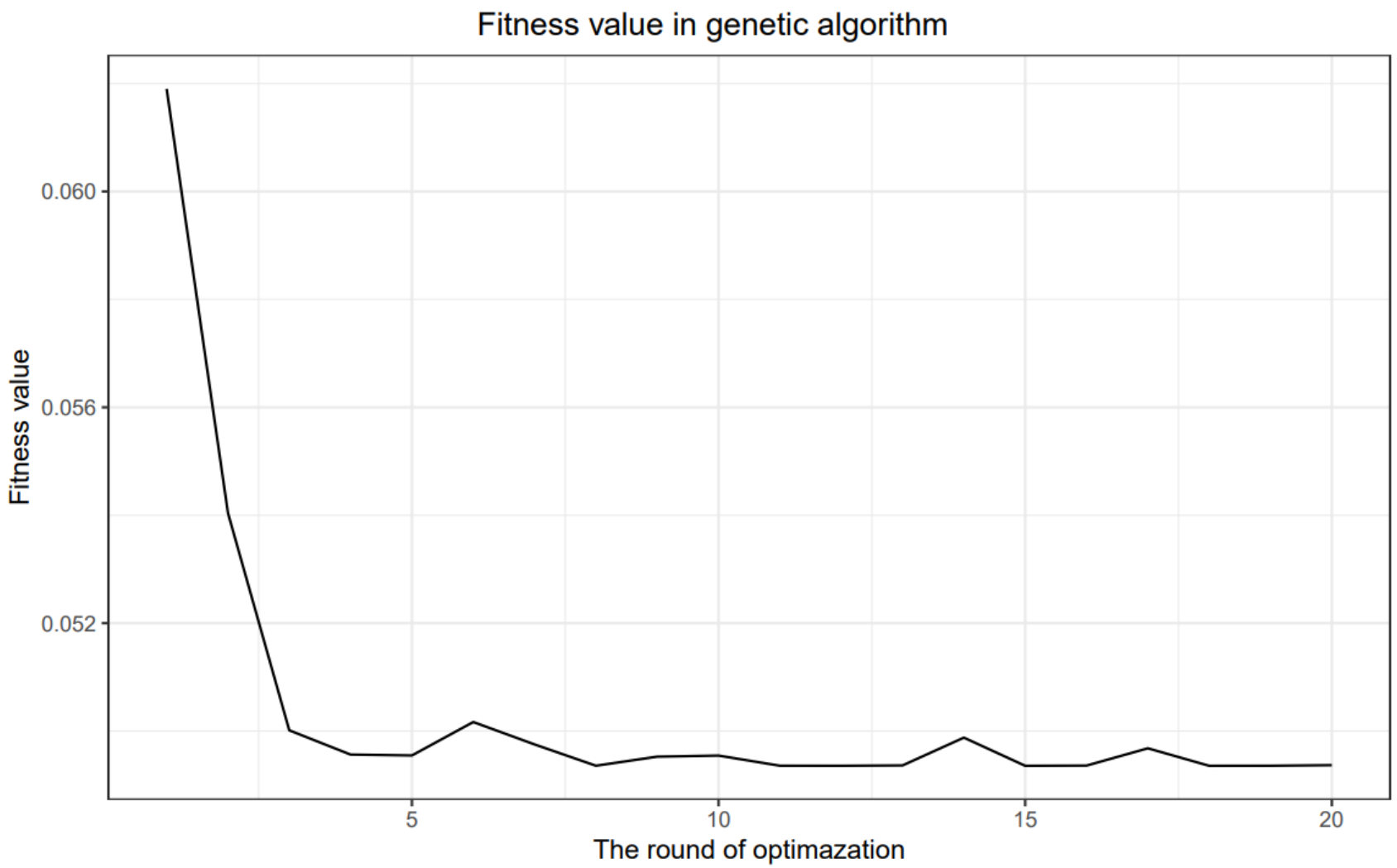

补充图 2. 遗传算法中适应度值的变化。

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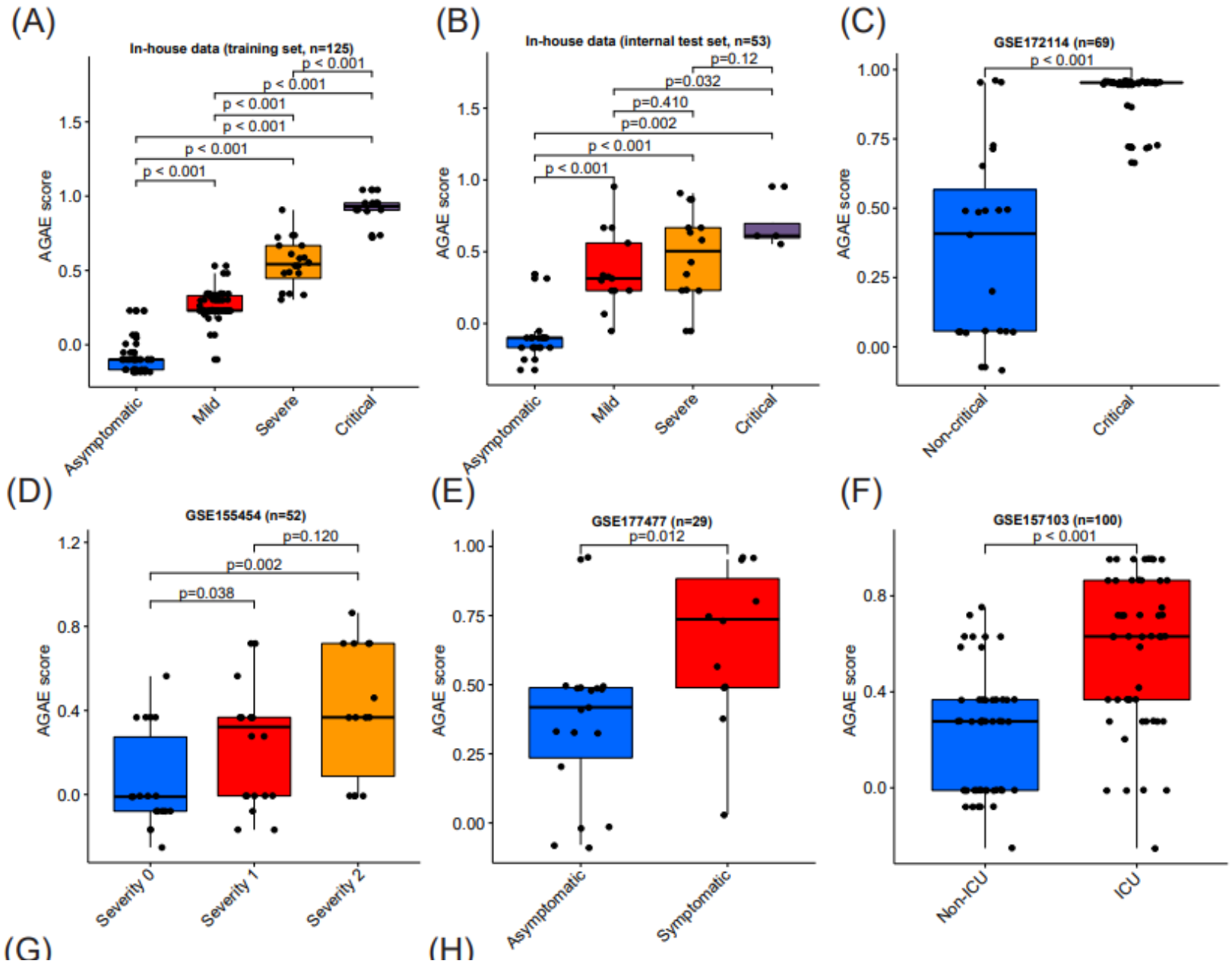

AGAE 得分在训练集和 5 个测试集上的表现。

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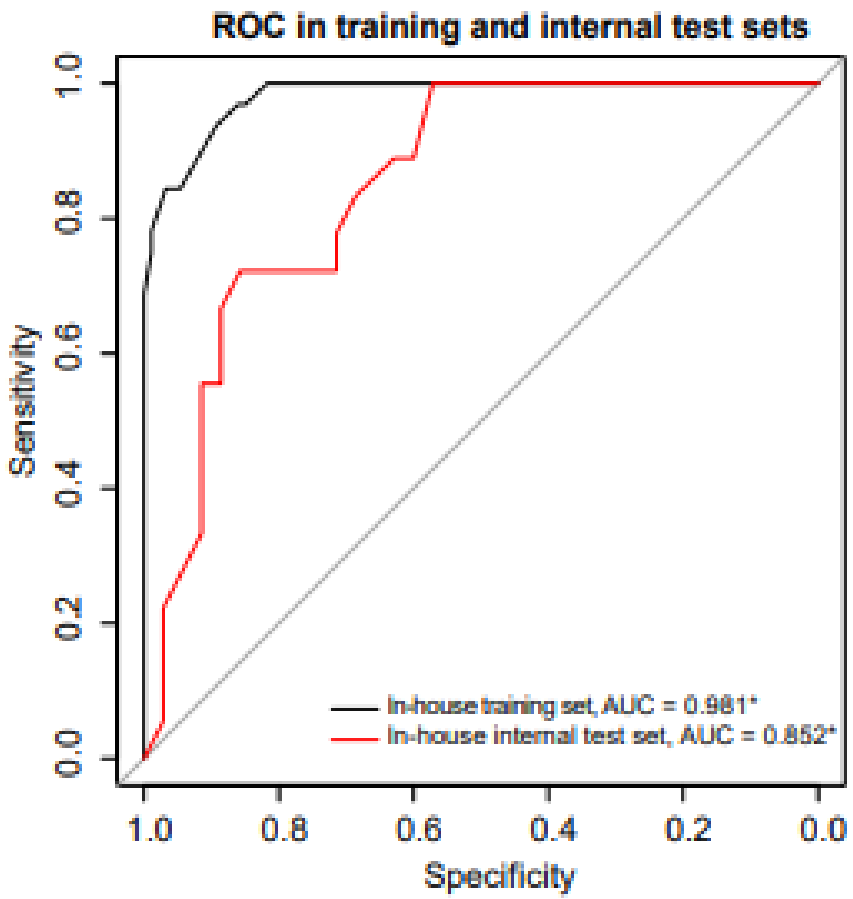

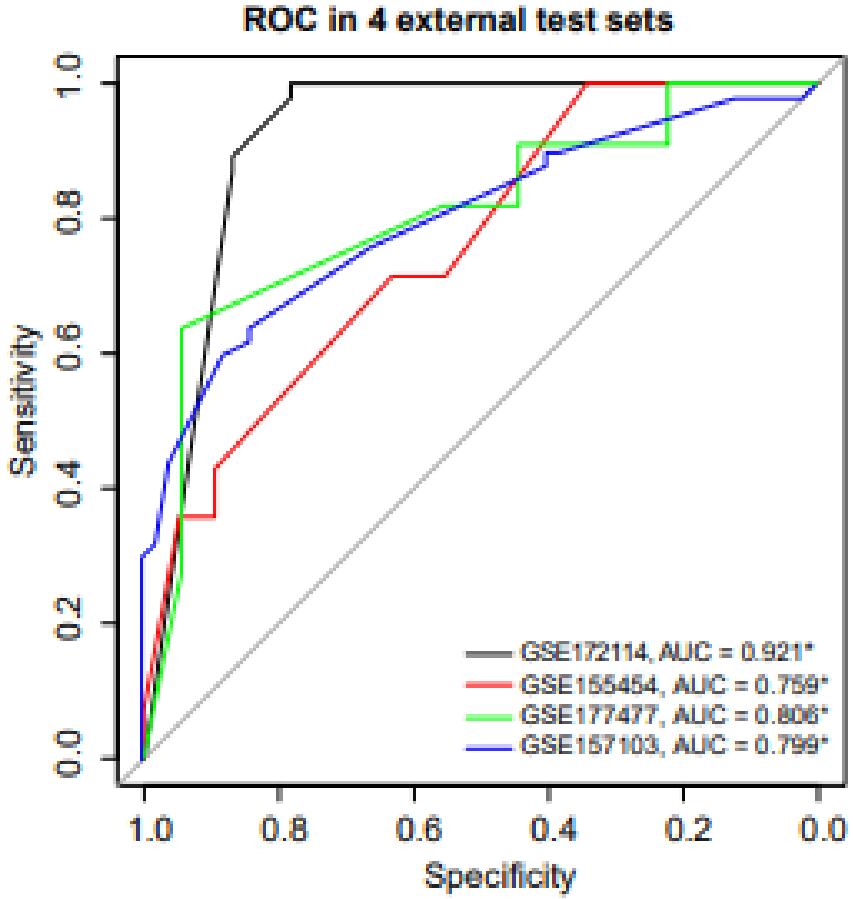

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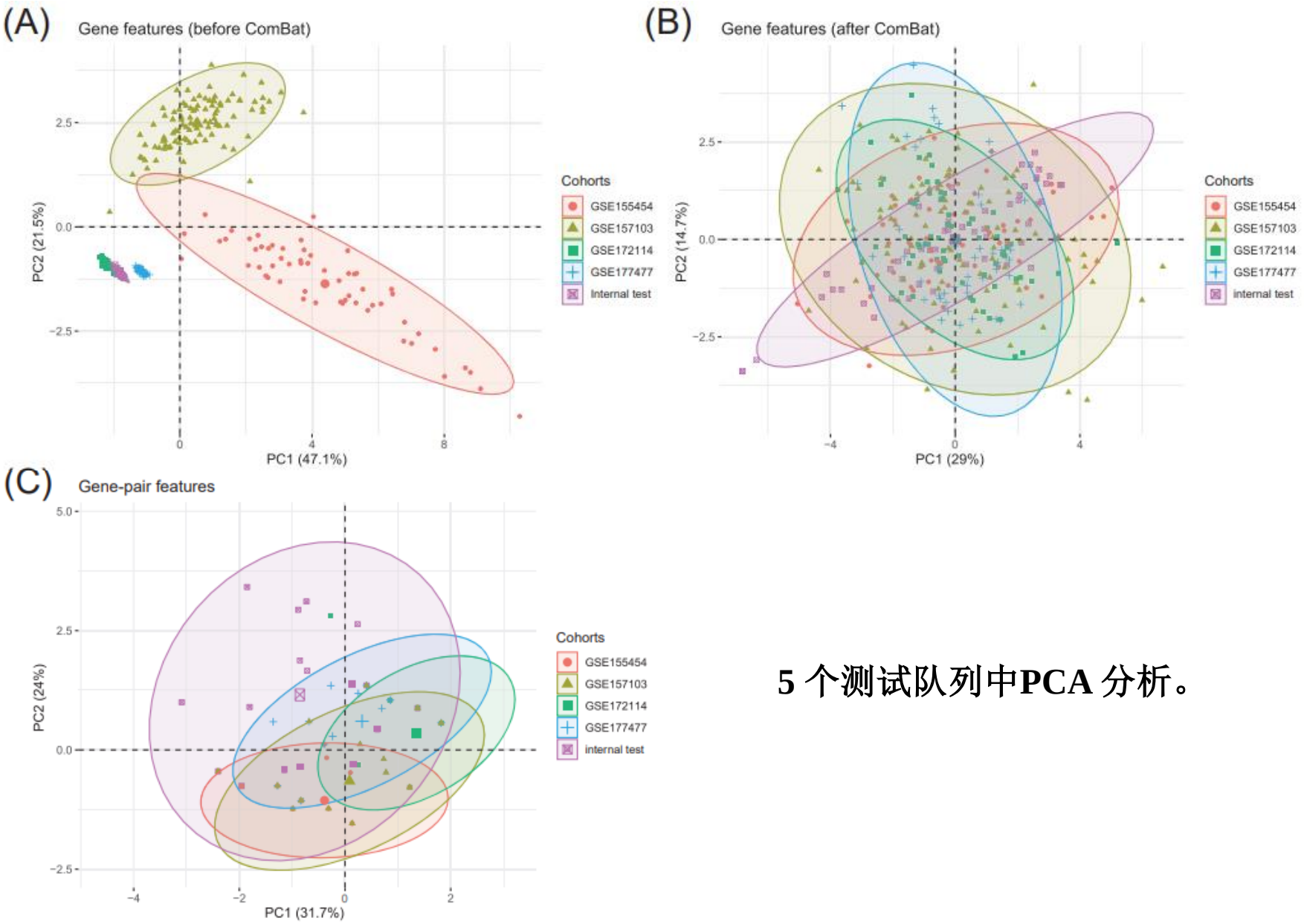

5 个测试队列中PCA 分析。

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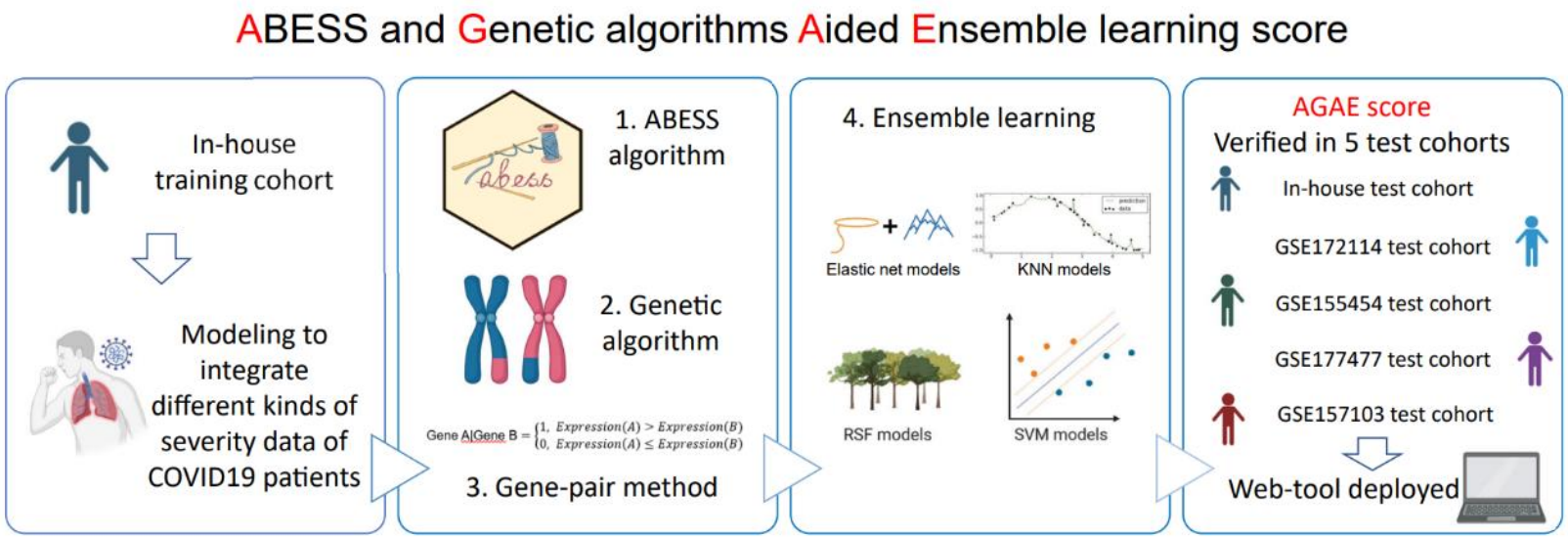
补充表 4. AGAE 评分的 ROC-AUC 和 5 个测试集中的 5 个基线模型。

Models	AGAE score	m3	m21	m30	m32	m6A score
Methods	Ensemble learning	Elastic net	KNN	RF	KNN	LASSO
Internal test set	0.852	0.852	0.814	0.844	0.815	0.692
GSE172114	0.921	0.893	0.921	0.895	0.889	0.508
GSE155454	0.759	0.731	0.688	0.724	0.703	0.590
GSE177477	0.806	0.699	0.745	0.780	0.747	0.727
GSE157103	0.799	0.793	0.791	0.789	0.779	0.743
Average ROC-AUC	0.827	0.794	0.792	0.806	0.787	0.652
p	-	0.076	0.032	0.008	0.002	0.025

总结



•AGAE score是一种基于集成学习的新冠病人疾病严重程度打分，它在5个测试集中的平均ROC-AUC数值达到0.827

•我们提供了我们的内部数据集，这一数据集被划分为训练集和一个内部测试集。
•AGAE score被部署为网站，方便临床工作者使用“https://kwkxbioinfor.shinyapps.io/COVID19/”

•通过消融实验和PCA，我们发现基因配对方法能够有效消除批次效应，最优子集筛选算法和遗传算法能够有效提升模型的准确性和鲁棒性

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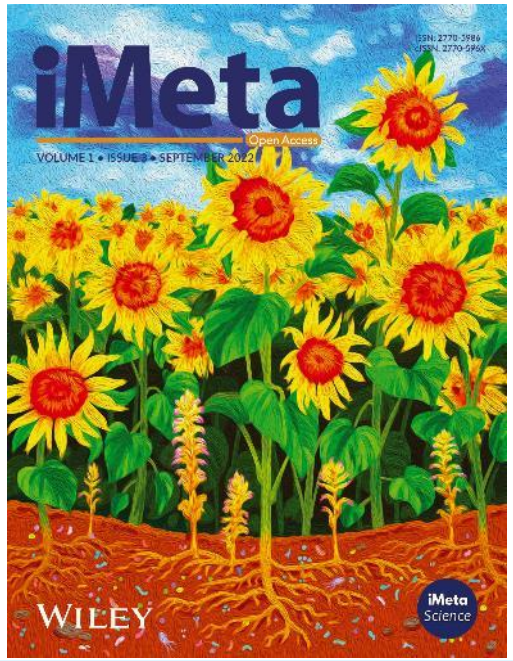

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