An improved cancer diagnosis algorithm for protein mass spectrometry based on PCA and one-dimensional neural network combining ResNet and SENet

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1. Introduction to the basic building blocks of 1DSE-ResCNN

Conv1d is a convolutional layer used for processing one-dimensional data, which extracts local features through one-dimensional convolution kernels. The formula is:

$$y_i = \sum_{k=1}^{K} x_{i+k-1} \cdot w_k + b \quad (1)$$

Where x represents the input sequence, with a length of N; w represents the convolution kernel's weights, with a size of K; b is the bias term; and y_i is the result of the convolution at the i position of the output.

BatchNorm1d is used for batch normalization of one-dimensional data to accelerate model training and improve model stability. By standardizing the features of each batch of data to have a mean close to 0 and variance close to 1, it can reduce the issues of vanishing or exploding gradients. This normalization process allows the model to converge faster and be more robust to different initial conditions. The formula is:

$$\hat{x}^{(i)} = \frac{x^{(i)} - \mu_{batch}}{\sqrt{\sigma_{batch}^{2} + \varepsilon}} \quad (2)$$

$$y^{(i)} = \gamma \cdot \hat{x}^{(i)} + \beta \quad (3)$$

Where $x^{(i)}$ is the i feature of the input; μ_{batch} and σ_{batch} are the mean and variance of the batch, respectively; ε is a small value to prevent division by zero; and γ and β are trainable scaling and shifting parameters.

ReLU is the Rectified Linear Unit activation function, which introduces nonlinearity, allowing the model to fit more complex functions. Compared to the Sigmoid or Tanh activation functions, it effectively avoids the vanishing gradient problem. Additionally, ReLU has high computational efficiency, making it widely used in deep neural networks. Its definition is:

$$f(x) = \max(0, x) \quad (4)$$

Where, when $x > 0$, the output is x; and when $x \leq 0$, the output is 0.

MaxPool1d is a one-dimensional max pooling layer that performs down sampling by taking the maximum value within a local window, reducing the spatial dimensions of the data. This helps lower computational cost and model complexity while retaining important features, thus helping to prevent model overfitting to some extent. The formula is:

$$y_i = \max\left(x_{i:i+K}\right) \quad (5)$$

Where $x_{i:i+K}$ represents the data from the i to the $i+K$ window, and K is the size of the pooling window; y_i is the maximum value within that window.

BCEWithLogitsLoss is a loss function used for binary classification tasks. It combines the Sigmoid activation function with binary cross-entropy loss, making it suitable for calculating loss directly from the model's unnormalized outputs (logits) in classification problems. The formula is:

$$BCEWithLogitsLoss(x,y) = -[y \cdot \log(\sigma(x)) + (1-y) \cdot \log(1-\sigma(x))] \quad (6)$$

Where x represents the logits from the model output; y represents the true labels; and $\sigma(x) = \frac{1}{1+e^{-x}}$ is the Sigmoid function, which converts logits into probability values.

Adam (Adaptive Moment Estimation) is an adaptive optimization algorithm based on first-order and second-order moment estimation, widely used in deep learning. It combines the advantages of momentum optimizers and RMSProp, adjusting the learning rate for each parameter adaptively while using momentum to accelerate convergence. It is suitable for various neural network models.

2. Residual Block Principle

Residual block a key element in the deep ResNet framework. Its purpose is to alleviate the problem of gradient vanishing during network training. The network increases network depth, accelerates neural network training, enhances feature extraction, and thus improves image classification performance. The structure of the residual block is depicted in Fig.S1 (a).

The residual block employs a direct connection that permits the input X to be transmitted directly to the output. This mechanism ensures the integrity of the information within the entire network. When the input is X, the learned feature is ***H(X)***. The objective is to learn the residuals ***F(X) = H(X) - X***. This enables the original learned feature to be expressed as ***F(X) + X***. The rationale for this approach is that residual learning is more straightforward than the original features. Direct learning is a more straightforward approach. When the residuals are zero, the stacking layer performs a constant mapping, which does not degrade the performance of the network. The residuals are not typically zero, allowing the stacked layer to learn new features based on the input features, which further improves network performance.

3. Squeeze-and-Excitation Block Principle

SENet enables the selective emphasis of valuable features and the suppression of less useful ones through global information the squeeze-and-excitation block models channel relationships by introducing a squeeze and an excitation operation. The structure of the squeeze-and-excitation block is depicted in Fig.S1 (b).

In the squeeze phase, a global average pooling operation is applied to the feature maps of each channel to obtain a value for each channel indicating the global importance of that channel. Formally, the statistic $z \in R^c$ is generated by contracting u by the spatial dimension $H \times W$, where the first c element of z is computed as follows:

$$z_c = F_{sq}(u_c) = \frac{1}{H \times W} \sum_{i=1}^{H} \sum_{j=1}^{W} u_c(i,j) \quad (7)$$

As shown in Eq. Formally, the statistic z_c is generated in terms of the spatial size of the channel reduction u (i.e., the average of the feature maps of the channels c). z_c denotes the c statistic and u_c denotes the feature map of channel c with size $H \times W$. (i,j) denotes the value at that position on the feature map. Then the feature map u passes through, $F_{sq}(u_c)$ outputting a global statistics vector of size $1 \times 1 \times c$. This vector aggregates global information in the channel dimension. Subsequently, in the excitation phase, a weight vector of channels is learned through the application of a fully connected layer and a nonlinear activation function. This weight vector is then applied to each channel on the original feature map, to weigh the features of different channels. In this manner, the SE module is capable of adaptively learning the relative importance of each channel and adjusting the channel contributions in the feature map, weighted according to the requirements of the task at hand. This attention mechanism enables the network to concentrate on the most crucial feature channels, thereby enhancing the model's performance.

4. Definition and calculation of cumulative feature information

Cumulative Feature Information is typically used in dimensionality reduction techniques like PCA to measure the amount of original data information retained by selecting the top few principal components. Cumulative feature information helps us understand if the selected principal components effectively preserve significant information from the original data.
The steps to calculate cumulative feature information are as follows:
(1). Eigenvalue Decomposition: Perform eigenvalue decomposition on the covariance matrix of the data to obtain the eigenvalues for each principal component.
(2). Explained Variance Ratio: The variance explained by each principal component can be calculated using the formula:

$$Explained\ Variance\ Ratio = \frac{\lambda_i}{\sum_{i=1}^{n} \lambda_i} \tag{8}$$

where λ_i is the eigenvalue of the i^{th} principal component, representing the amount of variance explained by that component, and n is the total number of components.
(3). Cumulative Variance Ratio: Cumulative feature information refers to the total variance explained by the first k principal components:

$$Cumulative\ Variance\ Ratio = \sum_{i=1}^{k} \frac{\lambda_i}{\sum_{i=1}^{n} \lambda_i} \tag{9}$$

(4). Deciding the Number of Principal Components: By observing the cumulative variance ratio, we can decide how many components to retain. Typically, when the cumulative variance reaches 80% or 90%, it is considered that most of the original information is preserved.

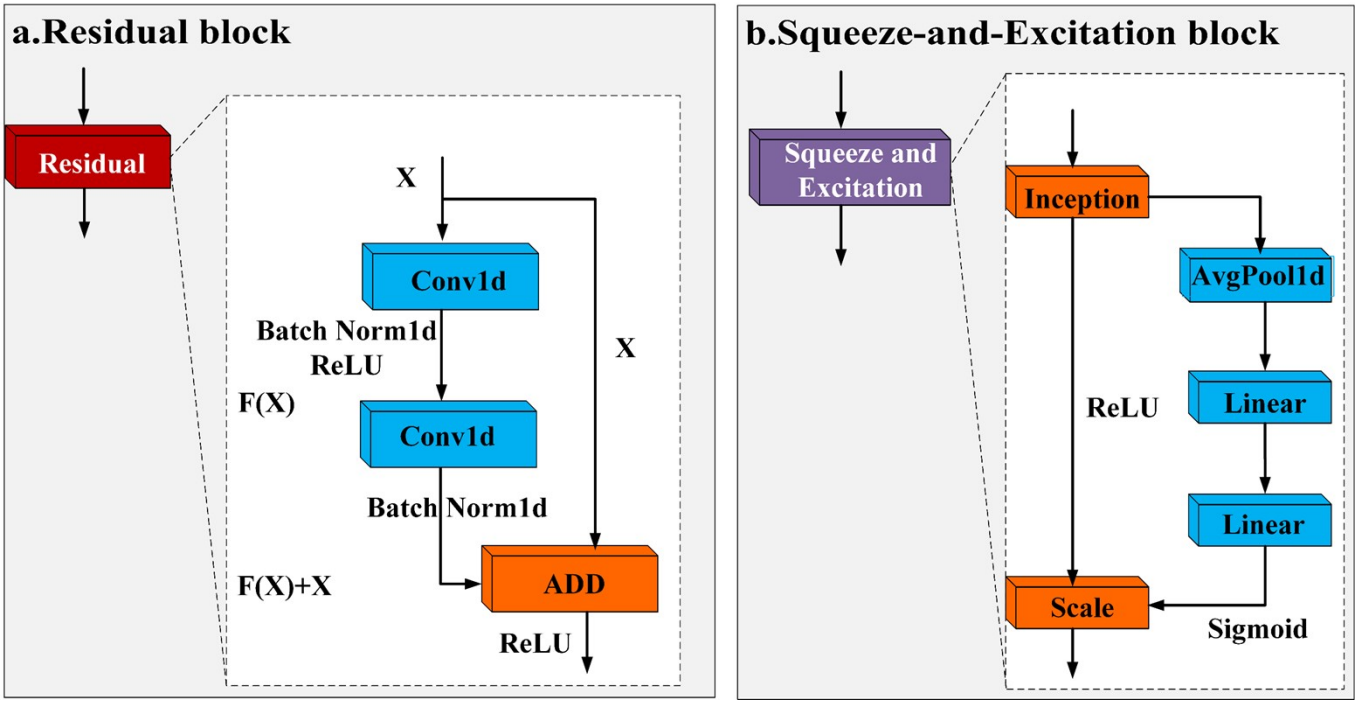

Fig.S1 Structure of Residual Block and Squeeze-and-Excitation block.

Table S1 Principal component analysis dimensionality reduction process

Principal Component Analysis Dimensionality Reduction
Input: The set of sample is $X = \{X^1, X^2, ..., X^M\}$, each with n-dimensional features $X^i = \{x_1^i, x_2^i, ..., x_n^i\}^T$. Each feature x_j has its own eigenvalues. The dimensionality of the low-dimensional spaces is K, $0 \le K \le n$.
1: Centering all samples be de-meaned (decentralized): $x_j = x_j - \frac{1}{n}\sum_{i=1}^{n} x_j$
2: Compute the covariance matrix of the samples: $ConvX = \frac{1}{n} XX^T$
3: Compute the eigenvalues and corresponding eigenvectors of covariance matrix $ConvX$: $ConvX = \Lambda L$, where $\Lambda = diag[\lambda 1, \lambda 2, ..., \lambda n]$ are the eigenvalues of the covariance matrix X, and L are the eigenvectors of the covariance matrix X.
4: Sort the eigenvalues $\Lambda(set\lambda 1 \ge \lambda 2 \ge ... \ge \lambda n \ge 0)$ in descending order, then select the largest K。Next, use the corresponding K eigenvectors as row vectors to form the eigenvector matrix P, and transform the data into a new matrix constructed by K eigenvectors Y.
Output: $Y = PX$ where Y is the matrix after dimensionality reduction.

Table S2 Original information retained after reducing the dimensions of the three datasets (OC_L8, OC_L4, OC_H) to 10, 50, 100, 150, and 200 using PCA (results rounded to two decimal places).

Dataset\Dimension	**Cumulative feature information**				
	10(%)	**50(%)**	**100(%)**	**150(%)**	**200(%)**
OC_L8	83.63	96.87	99.08	99.74	100.00
OC_L4	90.74	98.78	99.66	99.88	99.96
OC_H	36.33	75.49	92.14	97.87	99.71

Table S3 Average accuracy of the 1DSE-ResCNN model over five experiments on a test set of three datasets, reduced to 50, 100, and 200 dimensions using PCA.

Dataset	**Dimension**	**Acc(%)**
OC_L8	200	100.00
	100	100.00
	50	100.00
OC_L4	200	98.998
	100	96.667
	50	95.667
OC_H	200	99.076
	100	95.692
	50	96.308

Abbreviations: Acc, Accuracy.

Table S4 Results of five tests for six models on the test set of ovarian cancer 8-7-02 dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	98.68	98.15	96.30	99.00	98.55
	RF	84.21	78.61	59.26	87.74	80.81
	LR	100.00	100.00	100.00	100.00	100.00
2	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	94.74	94.26	92.59	94.26	94.26
	RF	77.63	68.52	37.04	87.12	69.64
	LR	100.00	100.00	100.00	100.00	100.00
4	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	100.00	100.00	100.00	100.00	100.00
	RF	85.53	79.02	60.00	88.54	81.63
	LR	100.00	100.00	100.00	100.00	100.00
6	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	98.68	97.50	95.00	99.12	98.28
	RF	86.84	78.21	60.00	86.41	81.06
	LR	100.00	100.00	100.00	100.00	100.00
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	93.42	92.25	86.67	94.07	92.98
	RF	72.37	65.00	30.00	84.33	63.78
	LR	100.00	100.00	100.00	100.00	100.00

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.

Table S5 Results of five tests for six models on the test set of ovarian cancer 4-3-02 dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	95.00	95.09	96.42	94.94	94.99
	SVM	95.00	94.87	92.86	95.12	94.97
	KNN	76.67	77.90	96.43	81.25	76.24
	RF	66.67	67.63	82.14	68.89	66.33
	LR	96.66	96.65	96.43	96.65	96.65
2	1DSE-ResCNN	98.33	98.33	96.67	98.39	98.33
	ResNet18	96.67	96.67	96.67	96.67	96.67
	SVM	91.67	91.67	93.33	91.71	91.66
	KNN	71.67	71.67	90.00	75.03	70.68
	RF	75.00	75.00	76.67	75.03	74.99
	LR	91.67	91.67	93.33	91.71	91.66
4	1DSE-ResCNN	98.33	98.39	100.00	98.33	98.33
	ResNet18	93.33	93.21	89.65	93.60	93.30
	SVM	93.33	93.33	93.10	93.33	93.33
	KNN	80.00	80.42	93.10	82.14	79.80
	RF	75.00	75.03	75.86	75.00	74.99
	LR	93.33	93.33	93.10	93.33	93.33
6	1DSE-ResCNN	98.33	97.83	100.00	98.68	98.22
	ResNet18	96.67	97.30	94.59	96.00	96.53
	SVM	95.00	95.12	94.59	94.44	94.75
	KNN	91.67	89.95	97.30	92.50	90.94
	RF	80.00	82.14	72.97	80.42	79.80
	LR	95.00	95.12	94.59	94.44	94.75
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	95.00	95.05	93.55	95.00	94.99
	SVM	93.33	93.33	93.55	93.33	93.33
	KNN	86.67	86.43	93.55	87.43	86.53
	RF	76.67	77.20	61.29	79.85	76.24
	LR	91.67	91.71	90.32	91.67	91.66

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.

Table S6 Results of five tests for six models on the test set of high-resolution ovarian cancer dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	98.46	98.21	100.00	98.68	98.42
	SVM	93.85	93.29	97.30	94.23	93.66
	KNN	78.46	75.00	100.00	86.27	75.38
	RF	93.85	93.29	97.29	94.23	93.66
	LR	95.38	94.64	100.00	96.25	95.22
2	1DSE-ResCNN	96.92	96.30	100.00	97.50	96.79
	ResNet18	93.85	92.59	100.00	95.24	93.50
	SVM	90.77	88.89	100.00	93.18	90.09
	KNN	81.54	77.78	100.00	88.00	78.90
	RF	92.31	90.74	100.00	94.19	91.81
	LR	90.77	88.89	100.00	93.18	90.09
4	1DSE-ResCNN	98.46	98.21	100.00	98.68	98.42
	ResNet18	95.38	94.64	100.00	96.25	94.64
	SVM	92.31	91.07	100.00	94.05	91.94
	KNN	75.38	71.43	100.00	84.91	71.11
	RF	90.77	89.29	100.00	93.02	90.25
	LR	92.31	91.07	100.00	94.05	91.93
6	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	95.38	95.59	100.00	95.59	95.38
	SVM	89.23	89.28	90.32	89.20	89.22
	KNN	69.23	70.59	100.00	80.39	66.97
	RF	95.38	95.59	100.00	95.59	95.38
	LR	92.31	92.36	93.55	92.28	92.30
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	96.92	96.88	100.00	97.14	96.88
	SVM	95.38	95.31	100.00	95.83	95.37
	KNN	70.77	70.31	100.00	81.73	67.71
	RF	96.92	96.88	100.00	97.14	96.92
	LR	95.38	95.31	100.00	95.83	95.37

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.

Table S7 Results of five tests for six models on the train set of ovarian cancer 8-7-02 dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	96.61	95.31	90.62	97.48	96.25
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
2	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	97.18	96.09	92.19	97.88	96.89
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
4	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	97.18	96.21	92.42	97.84	96.93
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
6	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	97.74	97.18	94.37	98.18	97.62
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	97.18	95.90	91.80	97.93	96.80
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.

Table S8 Results of five tests for six models on the train set of ovarian cancer 4-3-02 dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	90.00	89.87	94.44	90.36	89.94
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
2	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	90.00	90.00	98.57	91.21	89.93
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
4	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	86.43	86.29	95.77	87.80	86.29
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
6	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	87.14	87.59	92.06	87.22	87.12
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	94.29	94.37	100.00	94.81	94.28
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.

Table S9 Results of five tests for six models on the train set of high-resolution ovarian cancer dataset, reduced to 200 dimensions using PCA. (The datasets were randomly split into training and testing sets at a 7:3 ratio using five random seeds (0, 2, 4, 6, 8). Each random seed corresponds to a completely different data split, resulting in five independent experiments. The results are rounded to two decimal places).

Random seed	Model	Acc(%)	Sen(%)	Spe(%)	Pre(%)	F1(%)
0	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	84.77	82.84	100.00	89.25	83.62
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
2	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	86.75	85.29	100.00	90.29	86.00
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
4	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	83.44	81.34	100.00	88.53	81.34
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
6	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	78.81	73.77	100.00	86.89	73.77
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00
8	1DSE-ResCNN	100.00	100.00	100.00	100.00	100.00
	ResNet18	100.00	100.00	100.00	100.00	100.00
	SVM	100.00	100.00	100.00	100.00	100.00
	KNN	79.47	75.40	100.00	86.97	75.40
	RF	100.00	100.00	100.00	100.00	100.00
	LR	100.00	100.00	100.00	100.00	100.00

Abbreviations: Acc, Accuracy; Pre, Precision; Sen, Sensitivity; Spe, Specificity; F1, F1-Scores.