Original Article: Liver, Pancreas, and Biliary Tract

Machine-learning Approach for the Development of a Novel Predictive Model for the Diagnosis of Hepatocellular Carcinoma

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Running Head

Development of a HCC predictive model

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None of the authors have any competing interest.

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The seven authors are justifiably credited with authorship, according to the authorship criteria.

In detail: MS – conception, design, analysis and interpretation of data, drafting of the manuscript, final approval given; KM－analysis and interpretation of data, final approval given; SK－analysis and interpretation of data, final approval given;

RT – analysis and interpretation of data, critical revision of manuscript, final approval given; SS – collection and assembly of data, final approval given; KK – critical revision of manuscript, final approval given; YY– critical revision of manuscript, final approval given

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Data Availability Statement

The datasets generated during the current study are available from the corresponding author on reasonable request.

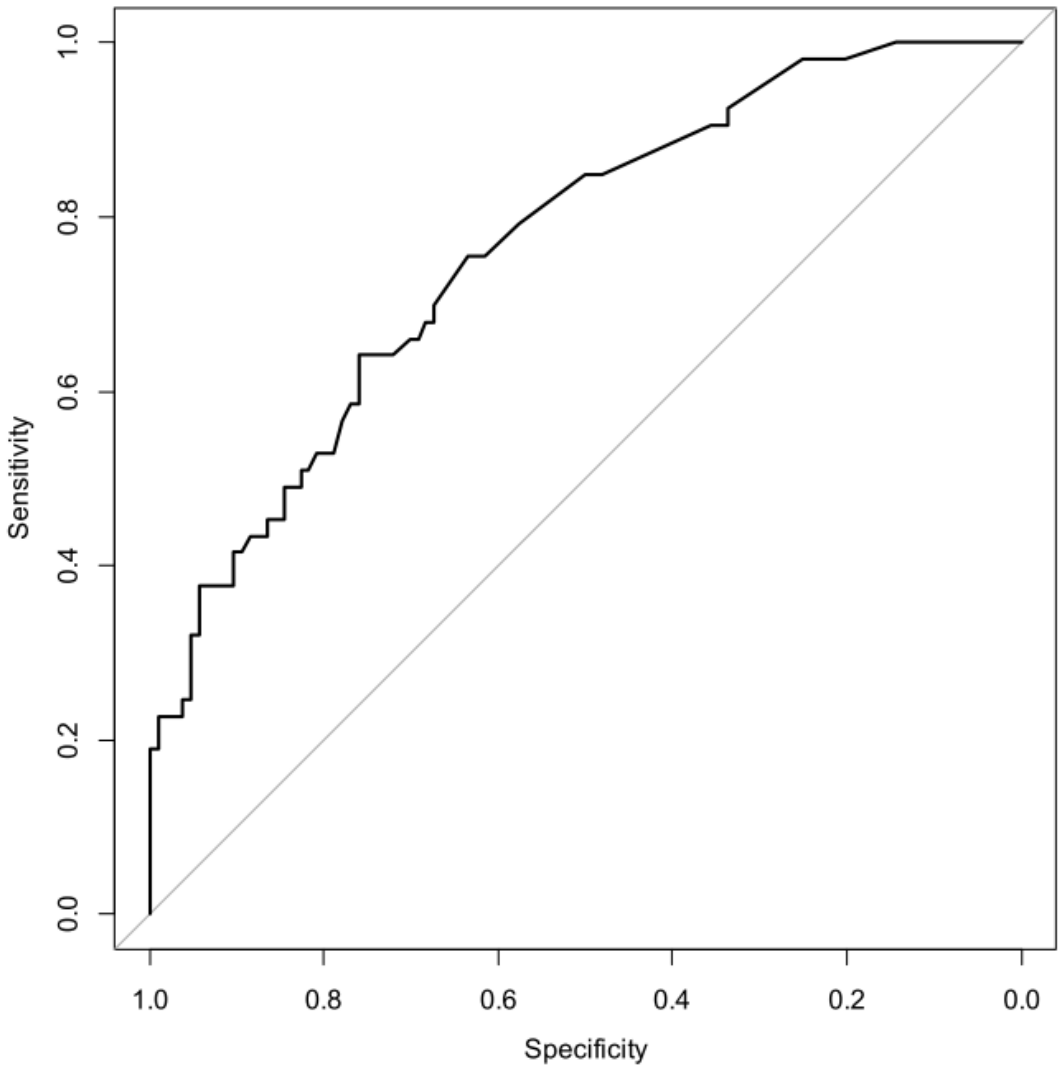
Supplementary Table 1. The detailed process of searching for the optimal hyperparameters

Classifiers	Details of hyperparameter searching
L1 penalized logistic regression model	lambda was searched from 1e-01 to 1e-10 (1e-01, 1e-02, 1e-03, 1e-04, 1e-05, 1e-06, 1e-07, 1e-08, 1e-09, 1e-10)
L2 penalized logistic regression model	lambda was searched from 1e-01 to 1e-10 (1e-01, 1e-02, 1e-03, 1e-04, 1e-05, 1e-06, 1e-07, 1e-08, 1e-09, 1e-10)
Elastic net penalized Logistic regression model	alpha was searched from 0.1 to 0.9 (at intervals of 0.1) lambda was searched from 1e-01 to 1e-10 (1e-01, 1e-02, 1e-03, 1e-04, 1e-05, 1e-06, 1e-07, 1e-08, 1e-09, 1e-10)
RBF Support vector machine	C was searched from 1.0 to 5.0 (at intervals of 0.1) sigma was searched from 0.001 to 0.1 (at intervals of 0.001)
Gradient Boosting	1st step max_depth was searched from 1.0 to 5.0 (at intervals of 1.0) min_child was searched from 0.001 to 0.1 (at intervals of 0.001) nround was searched from 200, 300, 500, and 1000 2nd step Using the optimal hyperparameters derived in the 1st step colsample_bytree was searched from 0.5 to 1.0 (at intervals of 0.1) subsample was searched from 0.5 to 1.0 (at intervals of 0.1) 3rd step Using the optimal hyperparameters derived in the 1st and 2nd steps, eta was searched from 0.01 to 0.15 (at intervals of 0.01) 4th step Using the optimal hyperparameters derived in the 1st, 2nd, and 3rd steps, Gamma was searched from 0.0 to 0.15 (at intervals of 0.01)
Random Forest	mtry was searched from 1.0 to 10.0 (at intervals of 1.0) ntree was searched from 100, 200, 300, 500, and 1000
Neural Network	size was searched from 1.0 to 10.0 (at intervals of 1.0) decay was searched from 0.1 to 1.0 (at intervals of 0.1)
Deep Learning	epochs was searched from 10 to 100 (at intervals of 10) batch_size was searched from 10 to 30 (at intervals of 10)

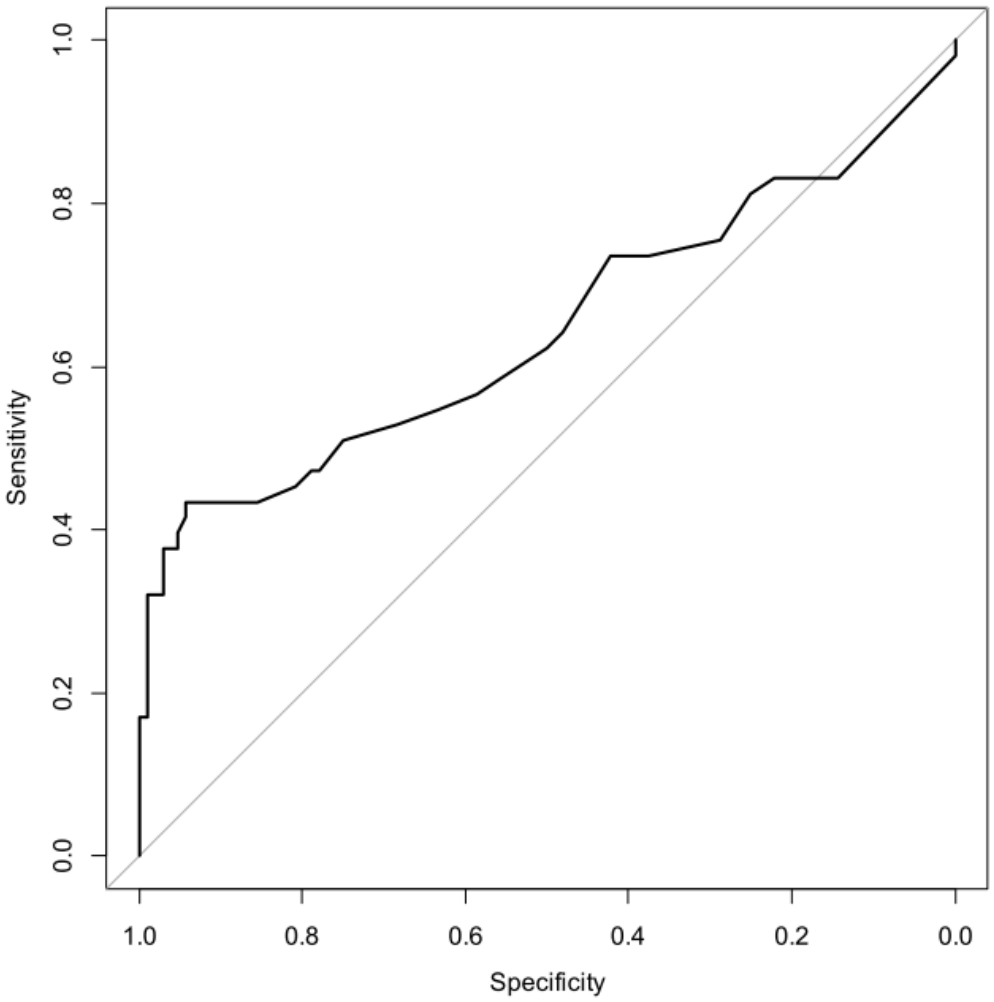
Figure legend

Supplementary Figure 1. Receiver-operating characteristics curve for predicting the presence of HCC presence based on single tumor markers. (a) AFP: area under the curve for HCC prediction, 0.766. (b) DCP:-area under the curve for HCC prediction, 0.644. (c) AFP-L3: area under the curve for HCC prediction was 0.683.

Supplementary Figure 1a



Supplementary Figure 1b



Supplementary Figure 1c