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A Hybrid Modeling Approach for Optimizing Detection Timing Based on Male Fetal Y Chromosome Concentration and Individual Variability

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Abstract: This study focuses on the correlation analysis and model construction of factors influencing male fetal Y chromosome concentration. First, prenatal data from female fetuses underwent preprocessing, including excluding samples outside the 10–25 week gestational range, handling samples with special gestational patterns, and converting gestational age to a uniform "week" unit. The Lilliefors test confirmed that variables such as age, gestational age, Y chromosome concentration, and BMI did not satisfy the assumption of normal distribution. At the population level, Spearman's rank correlation analysis revealed a weak positive correlation between Y chromosome concentration and gestational age, and a weak negative correlation with BMI, though neither reached statistical significance. Subsequently, a Support Vector Machine (SVM) model was constructed and trained to capture potential nonlinear relationships among variables, achieving 92.31% accuracy on the test set. Finally, individual-level analysis via binary linear fitting of randomly selected representative samples revealed that gestational age showed a significant positive correlation with Y chromosome concentration, while BMI effects varied among individuals. This confirms that population-level statistical patterns often fail to fully account for individual-specific characteristics. These findings underscore the critical importance of individual heterogeneity, challenging the conventional one-size-fits-all paradigm. This study provides a robust methodological foundation for advancing personalized NIPT strategies, moving beyond population averages towards precision prenatal care.

Keywords: Non-Invasive Prenatal Testing, Y Chromosome Concentration, Individual Variation, Support Vector Machine, Spearman's Rank Correlation.

1. Introduction

Non-invasive prenatal testing (NIPT) employs next-generation sequencing technology to perform bioinformatics analysis on fetal cell-free DNA fragments in maternal peripheral blood, effectively screening for three major chromosomal disorders: trisomy 21, trisomy 13, and trisomy 18. NIPT accuracy is highly dependent on fetal sex chromosome concentration. Results are generally considered reliable when male fetuses exhibit Y chromosome concentrations ≥4% and female fetuses show no abnormalities in X chromosome concentration. Testing is recommended between 10 and 25 weeks of gestation, as earlier detection of fetal abnormalities reduces risks associated with therapeutic windows. Y-chromosome concentration in male fetuses correlates closely with gestational age and maternal BMI[1-2]. However, traditional BMI-based grouping for determining NIPT timing is susceptible to individual variations, compromising accuracy. This study proposes a systematic approach to address critical issues in optimizing NIPT detection for male fetuses and identifying abnormalities in female fetuses. Previous research indicates that NIPT timing determination primarily relies on BMI grouping, lacking comprehensive consideration of multiple factors (such as age, height, weight) and detailed capture of individual variations. The innovation of this paper lies in combining machine learning with statistical modeling to propose a precision solution based on multifactorial influences. Specifically, this study employs Support Vector Machines (SVM) and Gradient Boosting Decision Trees (GBDT) to capture nonlinear relationships, utilizes k-means clustering and hierarchical clustering to segment pregnant women populations, and constructs a risk quantification optimization model incorporating age bias and pass rate constraints[3]. This model is solved using particle swarm optimization and an elite retention genetic algorithm. The main research approach includes: First, conducting correlation analysis and model construction for factors influencing fetal Y chromosome concentration, exploring correlations between Y concentration and gestational age/BMI. Second, determining the optimal timing for non-invasive prenatal testing (NIPT) based on BMI-based grouping to minimize risk. Third, incorporating factors such as maternal age, height, and weight to comprehensively determine the optimal timing and analyze compliance rates. Finally, a classification model is constructed to establish a specific method for identifying female fetal abnormalities[4-5].

2. Data Preprocessing

2.1. Data cleaning

Before conducting data modeling and analysis, data cleaning is a crucial step to ensure the reliability and accuracy of subsequent research results. Its core goal is to eliminate invalid information, correct data deviations, and provide a high-quality dataset for model construction[6-7].

2.1.1. Handling samples with special pregnancy methods

To ensure the representativeness and homogeneity of the samples, targeted handling of samples with special pregnancy

methods is necessary. In this dataset, there are samples of two special pregnancy methods: in vitro fertilization (IVF) and artificial insemination (Column G). Statistical analysis shows that IVF samples account for 0.7% of the total sample size, and artificial insemination samples account for 0.8%. The combined proportion of the two types of samples is only 1.5%, which is too small to support separate subgroup analysis. If they are included in the overall dataset, it is likely to introduce abnormal fluctuations, thereby interfering with the model's accurate capture of the overall population's patterns. Therefore, considering the above factors, to ensure data homogeneity and improve the stability and reliability of the analysis results, it is decided to exclude the samples of IVF and artificial insemination[8].

2.1.2. Outlier analysis

It can be observed from Figure 1 that there are some outliers in the pregnant women's BMI. The BMI is mainly concentrated in the range around 30. The distribution of the box and scatter points shows that its value range is larger than that of the detected gestational age, and the degree of dispersion is also more obvious, indicating that the BMI difference among pregnant women is relatively significant.

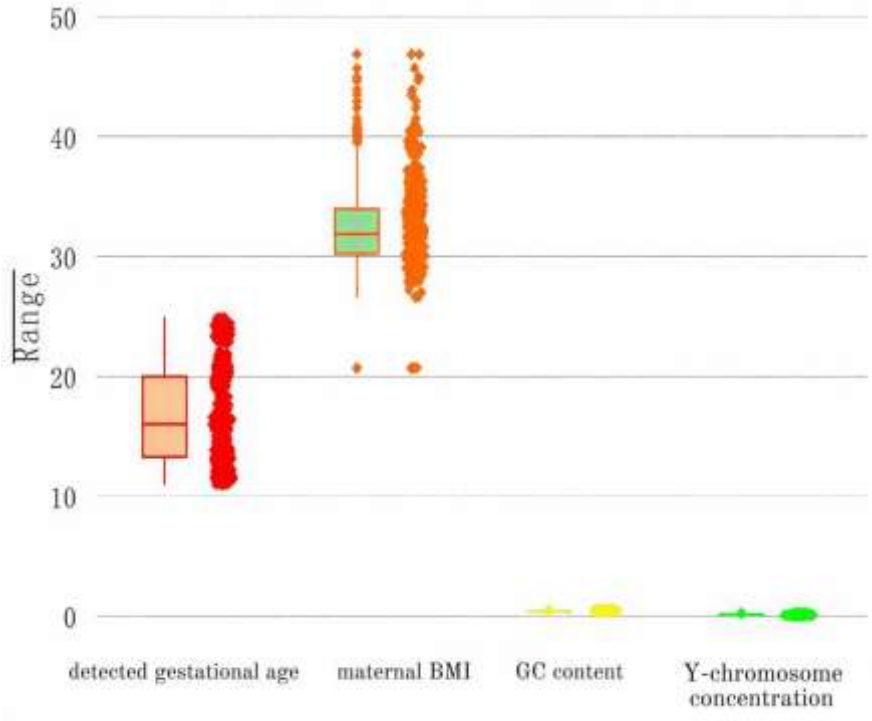

Figure 1. Box plot of data distribution of fetal-related indicators

The mean BMI1 is 32.32, the median is 31.90, and the overall weight is relatively high with a certain degree of dispersion. There are 24 outliers. Considering that special weight conditions are allowed, these outliers are not excluded for the time being. In subsequent steps, the impact of these outliers on fetal-related tests needs to be analyzed in combination with other indicators[9-10].

2.2. Data Transformation

Data is transformed into a format acceptable to the model or to eliminate the influence of dimensions.

For the "detected gestational age (weeks + days)" (Column J), the original data is presented in a composite format of "weeks + days", which cannot be directly used for quantitative analysis and model calculations. To uniformly convert it into a continuous value in the unit of "weeks", the following calculation formula is adopted:

$$t + \frac{b}{7} \tag{1}$$

where t is the number of weeks of the detected gestational age, and b is the number of days of the detected gestational age. After conversion using this formula, the gestational age data is standardized into a continuous variable in the unit of weeks (e.g., "11w + 6" is converted to 11.857 weeks). This conversion not only eliminates the dimensional difference of the original format, enabling the gestational age data to directly participate in subsequent quantitative research processes such as correlation analysis and regression modeling, but also retains the detailed information of the gestational age, improves the resolution of the data, and helps to more accurately capture the subtle patterns of fetal chromosome concentration changes with gestational age.

3. Data analysis

3.1. Normality analysis of variables

Whether the distribution of variables involved in this study, such as age, gestational age, Y-chromosome concentration, and BMI, conforms to normality will directly affect the rationality of subsequent analysis. The Lilliefors test is suitable for testing whether a sample follows a normal distribution when the overall distribution is unknown, and can well meet the needs of exploring the distribution of these variables. Based on this, the Lilliefors test is used to conduct normality analysis on the variables included in the analysis. The results are shown in the following table 1:

Table 1. Normality test results

Variable Name	Lilliefors_p Value	Normally Distributed?
Age	0.001	false
Gestational Age	0.001	false
Y1	0.001	false
BMI1	0.001	false

The test results show that the p-values of the variables included in the analysis, such as age, gestational age, Y-chromosome concentration, and BMI, are all less than 0.05, and none of them meet the normal distribution assumption. The non-normal distribution of Y-chromosome concentration and BMI is consistent with the characteristic that "the Y-chromosome concentration of male fetuses is closely related to the pregnant woman's gestational age and BMI, and individual differences are significant".

Since these variables do not follow a normal distribution, the traditional Pearson correlation coefficient is no longer applicable. Therefore, Spearman's rank correlation coefficient is used for correlation analysis to capture the possible monotonic correlations between variables.

3.2. Calculation and analysis of spearman's rank correlation coefficient

Multiple test data from the same pregnant woman may not be completely independent because they are affected by the relatively stable physiological characteristics of the pregnant woman herself (such as genetic factors and basic health status). If these data are directly used for analysis, it may violate the independence assumption and lead to deviations in the results of statistical tests. Therefore, the average value method is adopted. Assume that the number of blood draws for testing of the pregnant woman with serial number i is u. Thus, the average values of BMI, gestational age, and Y-chromosome concentration of the pregnant women are obtained for correlation analysis. SPSS is used to conduct Spearman's correlation coefficient analysis on the three indicators of "Y-chromosome concentration", "pregnant woman's BMI", and "detected gestational age", and the visualization heat map of the specific results is as figure 2:

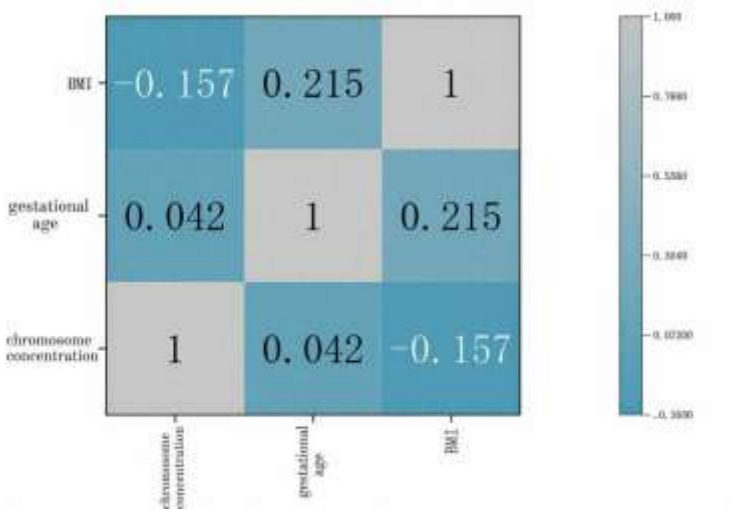

Figure 2. Heat map of spearman's correlation coefficient analysis

Y-chromosome concentration and gestational age: The correlation coefficient is 0.042 ($p = 0.678$), showing almost no correlation, and the p-value is much greater than 0.05, which is not statistically significant.

BMI and gestational age: The correlation coefficient is 0.215 ($p = 0.032$), showing a weak positive correlation, and it is significant at the 5% significance level ($p < 0.05$), indicating that pregnant women with higher BMI may have a slightly larger gestational age at the time of testing.

Y-chromosome concentration and BMI: The correlation coefficient is -0.157 ($p = 0.118$), showing a weak negative correlation, and it does not reach the 10% significance level ($p > 0.05$), indicating that the linear correlation between the two is not statistically significant.

3.3. Analysis of multiple linear regression model

$$y = 0.056 - 0.002 \cdot \mathrm{BMI} + 0.004 \cdot t \quad (2)$$

Table 2. Multicollinearity and regression model fitting statistics

	VIF	R^2	Adjusted R^2	F
Constant	-	0.062	0.042	$F = 3.178,\ P = 0.046$
BMI	1.013	-	-	-
Gestational Age	1.013	-	-	-

Multicollinearity and Regression Model Fitting Statistics is shown in table 2. Among them, the constant term is 0.056, the coefficient of BMI is -0.002, and the coefficient of gestational age is 0.004. Model fitting effect: The coefficient of determination $R^2 = 0.062$, and the adjusted $R^2 = 0.042$, indicating that the model can only explain 4.2% of the

variation in Y-chromosome concentration, and the fitting degree is low. The variance inflation factor (VIF = 1.013) is close to 1, indicating that there is no multicollinearity between the independent variables BMI and gestational age.

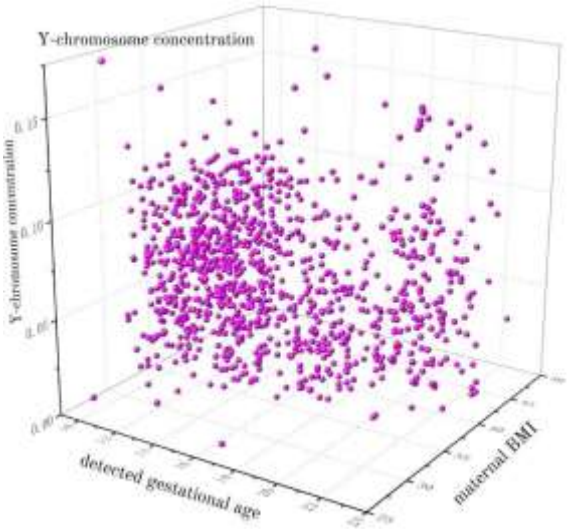

Figure 3(a) 3D Diagram of BMI and Gestational Age

3.4. Visual analysis of "chromosome concentration", "pregnant woman's BMI", and "Detected gestational age"

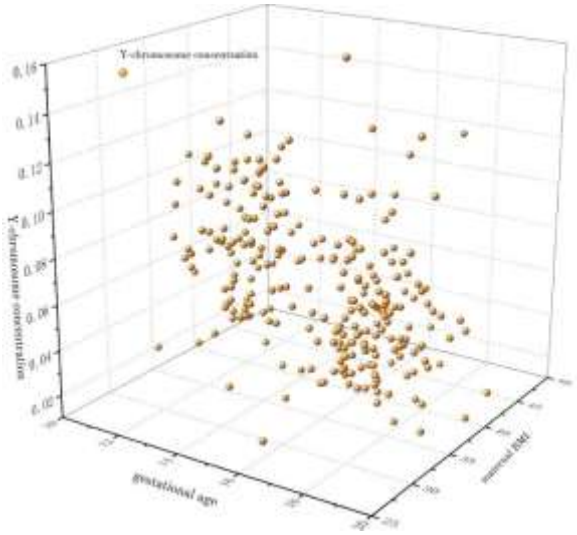

Figure 3(b) Y-Chromosome Concentration Distribution (Before and After Averaging)

Figure 3(a) and Figure 3(b) is conducted on "Y-chromosome concentration", "pregnant woman's BMI", and "detected gestational age". The 3D diagram of BMI and gestational age vs. Y-chromosome concentration distribution (before and after averaging) further verifies that there is no significant correlation among these three variables.

3.5. Analysis and solution of support vector machine model

Given that the multiple linear regression model has limited explanatory power for Y-chromosome concentration (the adjusted R^2 is only 0.042), and there are non-normal distributions and potential non-linear correlations between variables, this study further adopts the Support Vector Machine (SVM) model for analysis. As a powerful non-linear modeling tool, SVM is especially suitable for dealing with small-sample, non-normal data, and complex feature interaction problems. It can map low-dimensional features to a high-dimensional space through kernel functions, thereby capturing the implicit correlations between variables.

3.5.1. Data Preparation and Preprocessing

In this study, a Support Vector Machine (SVM) classification model is constructed based on 263 sample data points. Among them, the independent variables are the gestational age (unit: weeks) in the first column and the BMI (unit: kg/m^2) in the second column, and the dependent variable is the Y-chromosome concentration in the third column.

To implement the classification task, the Y-chromosome concentration is first discretized and divided into 4 levels according to the preset threshold:

Table 3. Correspondence table of value ranges

Effect Level	Extremely Poor Effect	Poor Effect	Partially Successful	Basically Successful
Value Range	(0, 0.02]	(0.02, 0.03]	(0.03, 0.04]	(0.04, 0.20)

Correspondence Table of Value Ranges are shown in table 3. The dataset is divided into three subsets using the stratified sampling method: 70% of the samples (184 samples) are used as the training set for model parameter learning; 20% of the samples (53 samples) are used as the validation set for parameter optimization and overfitting control; the remaining 10% of the samples (26 samples) are used as the test set for evaluating the generalization ability of the model. Stratified sampling can ensure that the class distribution of each subset is consistent with that of the original dataset, avoiding the impact of sample division deviation on model performance. All independent variables are standardized (with a mean of 0 and a standard deviation of 1) to eliminate the interference of dimensional differences on the SVM kernel function distance calculation. The standardization formula is as follows:

$$x' = \frac{x - \mu}{\sigma} \quad (3)$$

where μ is the variable mean and σ is the variable standard deviation. The support vector machine classifier in the MATLAB machine learning toolbox is used to build the model. The linear kernel (linear), radial basis function kernel (RBF), and polynomial kernel (poly) (Formulas 3-5) are selected as kernel functions, and the one with the best effect is selected as the final result.

$$K(x_i, x_j) = x_i \cdot x_j \quad (4)$$

This formula represents the dot product operation of vectors x_i and x_j. Under the action of the linear kernel function, the Support Vector Machine (SVM) attempts to find a linear classification hyperplane in the original low-dimensional feature space to separate samples of different classes. Its calculation process is only a simple dot product, so the computational complexity is low, and the interpretability of the model is also strong. It can intuitively

reflect the linear correlation between features and the target variable, and is suitable for scenarios where the features and the target variable show an obvious linear relationship.

$$K(x_i, x_j) = \exp\left(-\gamma \|x_i - x_j\|^2\right) \quad (5)$$

where $\|x_i - x_j\|^2$ is the square of the Euclidean distance between vectors x_i and x_j. From the perspective of the function form, the closer the two vectors x_i and x_j are, the smaller the Euclidean distance is, the smaller the value of $\|x_i - x_j\|^2$ is, the closer $-\gamma\|x_i - x_j\|^2$ is to 0, and the closer the value of $\exp\left(-\gamma\|x_i - x_j\|^2\right)$ is to 1. This indicates that these two vectors have a high degree of similarity in the high-dimensional space mapped by the RBF kernel function; on the contrary, when the distance between the two vectors is large, the kernel function value tends to 0, and the similarity is very low.

$$K(x_i, x_j) = (\gamma x_i \cdot x_j + r)^d \quad (6)$$

where r is used to adjust the scaling degree of the dot product, r is an offset parameter, and d is the order of the polynomial. Through this polynomial operation, the polynomial kernel function can map the original feature space to a finite-dimensional high-dimensional polynomial space. Different orders d can capture non-linear relationships of different degrees. The higher the order, the higher the dimension of the mapped space, and the more complex the non-linearity that can be captured.

3.5.2. Evaluation of model prediction accuracy

The accuracy of the test set reaches 92.31%. This relatively high value indicates that the Support Vector Machine model performs well in this prediction task and has strong prediction ability. From a practical application perspective, such a high accuracy means that the model can accurately judge the category of Y-chromosome concentration based on the input features (such as gestational age and BMI) in most cases, providing a relatively reliable reference for relevant testing and analysis.

3.5.3. Correlation analysis between features and prediction results

Impact of gestational age on prediction results:

Analysis shows that there is no obvious direct correlation between gestational age and prediction accuracy. Although gestational age reflects the fetal development stage and may theoretically affect the Y-chromosome concentration, the data does not show a simple linear relationship. It is speculated that its individual effect is masked by the comprehensive effect of other multiple factors.

Impact of BMI on prediction results:

There is also no intuitive and simple correlation between the level of BMI and prediction accuracy. As an important indicator reflecting the physical condition of pregnant women, BMI may indirectly affect the Y-chromosome concentration through various physiological mechanisms, but it needs to work together with other features. A single BMI cannot determine the prediction result, indicating that the prediction of Y-chromosome concentration requires comprehensive multi-factor analysis.

3.5.4. Advantages and limitations of the model

Advantages: The Support Vector Machine model shows significant advantages. The accuracy of 92.31% confirms its ability to capture complex data patterns. By mapping the high-dimensional space through kernel functions, it can effectively explore the non-linear correlations between gestational age, BMI, and Y-chromosome concentration, providing reliable support for relevant research.

Limitations: The model still has room for improvement: some feature information is not fully explored, which may miss key influencing factors; parameter optimization has not reached the optimal state; there may be noise in the data or important features not included, all of which may affect the prediction accuracy.

3.6. Correlation analysis and solution at the individual level

At the population level, the gestational age is weakly positively correlated with the Y-chromosome concentration, and BMI is weakly negatively correlated with it, but the significance is insufficient, which may be masked by individual differences. To further explore the correlation characteristics between the fetal Y-chromosome concentration and the pregnant woman's gestational age and BMI at the individual level, 12 groups of pregnant woman samples are randomly selected for visual analysis:

At the individual level, the Y-chromosome concentration of pregnant women carrying male fetuses will increase during pregnancy, which is consistent with the conclusions in the literature; while the third figure shows that the impact of BMI on it is relatively small. Therefore, for these 12 samples, the overall upward trend of Y-chromosome concentration is valid.

At the same time, it is observed that in some samples, the Y-chromosome concentration does not change significantly or even decreases slightly with the change of BMI or gestational age. Due to time and space limitations, further discussion is not conducted for the time being.

Among the upward curves, representative samples A018, A056, A209, and A230 are selected for binary linear fitting, and then F-test and t-test are respectively performed on the fitting results.

3.6.1. Group 1 (A018)

Data regression analysis regression equation:

$$Y = -0.1961 + 0.0050 \cdot t + 0.0057 \cdot \text{BMI} \quad (7)$$

Coefficient of determination $R^2 = 0.9310$ (the model can explain 93.10% of the variation in Y-chromosome concentration)

F-test (model overall significance): $F = 33.7376$, $p = 0.0013 < 0.05$, the null hypothesis is rejected, and the model is overall significantly effective.

t-test (coefficient significance): Intercept term: $t = -555.9373$, $p = 0.00001 < 0.05$, significantly not zero. Gestational age coefficient: $t = 678.3883$, $p = 0.00002 < 0.05$, showing a significant positive correlation with Y-chromosome concentration. BMI coefficient: $t = 496.9699$, $p = 0.00004 < 0.05$, showing a significant positive correlation with Y-chromosome concentration.

Table 4: Individual Regression Analysis Results Table

Group	Regression Equation	Coefficient of Determination R^2	F-test
Group 2 (A056)	$Y = -0.0958 + 0.0010 \cdot t + 0.0044 \cdot BMI$	0.9964	$F = 700.4168,\ p = 0.00001 < 0.05$
Group 3 (A209)	$Y = -0.0052 + 0.0059 \cdot t - 0.0006 \cdot BMI$	0.9746	$F = 95.9902,\ p = 0.0001 < 0.05$
Group 4 (A230)	$Y = -0.0602 + 0.0032 \cdot t + 0.0024 \cdot BMI$	0.9976	$F = 1042.7848,\ p = 0.00001 < 0.05$

It can be seen from the table 4 that $p < 0.05$, so the model is overall significantly effective

3.6.2. Conclusions of individual analysis: differences between Individuals and overall patterns

The overall analysis results show that the linear correlation between Y-chromosome concentration and gestational age and BMI is weak (adjusted $R^2 = 0.042$), indicating that from the population level, the overall explanatory power of these two factors on Y-chromosome concentration is limited. However, at the individual level, the regression models of the 4 groups of samples have extremely high fitting degrees ($R^2 > 0.93$), indicating that there are significant heterogeneities among individuals, and the general laws at the population level cannot fully cover the specific characteristics of individuals.

In the 4 groups of samples, gestational age is significantly positively correlated with Y-chromosome concentration, which is consistent with the clinical logic that "the increase of gestational age may promote the increase of Y-chromosome concentration". However, the direction of the impact of BMI varies among individuals: in 3 groups of samples, BMI is significantly positively correlated with Y-chromosome concentration, while in 1 group of samples, it is significantly negatively correlated. This suggests that the effect of BMI on Y-chromosome concentration may be regulated by other individual-specific factors.

3.6.3. Individual characteristics of model significance

The F-test and t-test of the 4 groups of individual models all reach the significant level ($p < 0.05$), indicating that at the individual level, the combination of gestational age and BMI has a strong explanatory power for Y-chromosome concentration, which provides strong data support for the evaluation of personalized NIPT testing time points.

4. Conclusions

Through multi-model integration and in-depth data analysis, this study successfully established strategies for optimizing NIPT detection and identifying female fetal abnormalities. We first identified the correlation patterns between male fetal Y chromosome concentration and gestational age/BMI, utilizing a support vector machine model to achieve effective prediction of Y chromosome concentration. Subsequently, we grouped pregnant women by BMI using k-means clustering and developed a risk-quantified optimization model incorporating detection failure risk and intervention delay risk. Through traversal algorithms and stochastic inertial weight particle swarm optimization, we determined the optimal NIPT timing based on BMI groups, revealing that higher BMI delays the optimal testing window. After further incorporating multiple factors including age, height, and weight, hierarchical clustering and an elite retention genetic algorithm identified optimal timing for more refined subgroups, achieving compliance rates exceeding 80%. For female fetuses, we constructed models based on linear discriminant analysis, binary GLM logistic regression, and quadratic discriminant analysis for anomaly detection, with the linear discriminant model achieving the highest accuracy of 90.8%. Overall, this study provides scientific evidence and operational recommendations for the precise clinical implementation of NIPT. However, limitations remain. For instance, in the optimized model, risk coefficients were primarily set based on clinical experience and data feature inference, lacking statistical support from large-scale clinical data. Additionally, complex algorithms like GBDT and genetic algorithms involve intricate computational processes, demanding substantial computational resources and time, while offering less intuitive interpretability regarding factor influences. Looking ahead, the model framework established in this paper can be extended for application in prenatal screening across more healthcare institutions. By incorporating physiological indicator variations among pregnant women from different regions and ethnicities, model parameters can be fine-tuned to provide personalized and precise recommendations for optimal screening timing and fetal anomaly detection. Furthermore, this modeling approach can be explored for application in other physiological indicator-based screening programs, thereby broadening the model's scope and validating its applicability in a wider range of medical diagnostic workflows.

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