Solving the NIPT optimal timing problem based on NSGA-II

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Abstract: This study addresses the optimal timing of noninvasive prenatal testing (NIPT) testing. A multi-objective optimization model centered on minimizing testing error and maternal and fetal risk was established and solved using the NSGA-II algorithm. Results demonstrated that the model effectively reflects the optimal gestational age distribution across populations with varying BMIs (BMIs). The optimal timing for NIPT testing was 18.63 weeks for those with a BMI ⩾ 38.3, 23.74 weeks for those with a BMI 28.6–34.5, and 24.72 weeks for those with a BMI 20.0-28.6. With increasing iterations, the uniformity and diversity of the Pareto front significantly improved, and the HV index continued to rise. Monte Carlo perturbation and sensitivity analyses validated the model's stability and robustness, with BMI having the greatest impact on the results. Overall, the NSGA-II-based model effectively addresses the optimal timing of NIPT testing, providing accurate and reliable results and providing an effective quantitative basis for stratified and personalized testing.

Keywords: Non-invasive prenatal testing; Multi-objective optimization; NSGA-II algorithm; Optimal testing time; body mass index

1 INTRODUCTION

Non-invasive prenatal testing (NIPT) is widely used due to its safety and accuracy. However, the timing of testing is significantly affected by the week of pregnancy, the proportion of maternal cfDNA, and individual differences. Improper selection will result in repeated sampling or uncertain results. At the national level, birth defect prevention and control and maternal and child health improvement have been incorporated into long-term planning. Local governments have successively improved the technical specifications and quality control requirements for prenatal screening and diagnostic services and encouraged the implementation of standardized NIPT services under the premise of ensuring safety and accessibility [1]. In this context, this paper takes the fetal Y chromosome concentration that meets the standard as the core representation, integrates factors such as BMI, age, height, weight, and test error, and establishes a dual-objective model of "test error-pregnancy risk". Through constraints such as feasible gestational age, standard probability, error threshold, and risk upper limit, the solution is made to meet clinical feasibility [2]. In order to balance accursampling andlity, the non-dominated sorting, elite retention and crowding distance strategies of NSGA-II were used to search the Pareto frontier, and the uniformity, diversity and frontier quality of the solution were evaluated with indicators such as Spacing, Spread and HV,

in order to provide the individualized optimal time point for different BMI stratifications, improve the success rate of one-time sampling, and reduce unnecessary clinical and psychological burdens [3].

2 RESEARCH FRAMEWORK AND BASIC ASSUMPTIONS

This paper constructs a systematic research framework around the problem of determining the optimal time point for NIPT, which mainly includes the following three parts: First, a dual-objective optimization model with "Minimizing detection error" and "Minimizing pregnancy and childbirth risks" as the core is established. The model comprehensively considers detection accuracy and clinical risk in the objective function, and sets multiple constraints such as the feasible domain of gestational age (10-16 weeks), the probability of Y chromosome concentration reaching the standard ($\geqslant$80%), and the detection error threshold ($\leqslant$0.5%) to ensure that the model output results meet the requirements of clinical practice [4]. Second, the non-dominated sorting genetic algorithm with elite retention strategy (NSGA-II) is used to solve the model. The algorithm stratifies the solution set through non-dominated sorting and combines crowding distance calculation to maintain population diversity, thereby gradually approaching and constructing a uniformly distributed Pareto optimal frontier during the iteration process. Finally, the quality of the Pareto solution set is quantitatively evaluated by multi-objective performance indicators such as Spacing, Spread, and Hypervolume (HV). To further validate the robustness of the model, this study introduced a Monte Carlo random perturbation method to simulate the impact of testing errors and conducted sensitivity analyses on key parameters such as BMI and age. Ultimately, based on this, recommendations for personalized NIPT testing timing were proposed for different BMI strata.

To ensure the rationality and feasibility of the model construction and solution process, this study proposed the following basic assumptions:

Hypothesis 1: The relationship between fetal Y chromosome concentration and gestational age can be characterized by a parameterized function, whose random error term follows a Gaussian distribution with mean zero.

Hypothesis 2: A fetal Y chromosome concentration threshold of 4% can effectively identify test compliance, and this threshold has clinically recognized reliability.

Hypothesis 3: Individual maternal characteristics (Such as BMI and age) have a significant impact on the time it takes for Y chromosome concentration to reach the standard, and this impact can be expressed in the model using linear or nonlinear coefficients.

Hypothesis 4: The NSGA-II algorithm can converge stably under the multi-objective and multi-constraint conditions set in this paper. The quality of its output Pareto frontier improves with increasing iterations, as evidenced by a continuous increase in the HV index.

Hypothesis 5: By setting reasonable constraints such as the gestational age range, the lower limit of the probability of reaching the concentration standard, and the upper limit of the error, the feasibility and applicability of the model output results in clinical practice can be effectively guaranteed.

3 MODEL ESTABLISHMENT AND SOLUTION

3.1 Construction of multi-objective optimization model

This problem considers the impact of multiple factors on achieving acceptable concentrations and minimizes potential risks to pregnant women. This model involves multiple decision variables, such as height, weight, and age, and sets two primary objectives to provide an optimal solution while accounting for detection errors.

To explore the factors that affect the time when the Y chromosome concentration of male fetuses reaches the standard, this paper sets the relationship between the fetal Y chromosome concentration and variables such as maternal BMI and gestational age. The model can be expressed as:

$$Y = f(BMI, Pregnancy_{Week}, \epsilon) \tag{1}$$

Where Y is the fetal Y chromosome concentration, $Pregnancy_{Week}$ is the gestational age, and ϵ is the error term, which conforms to a Gaussian distribution $\mathcal{N}(0, \sigma^2)$ [5]. By optimizing this relationship to determine the optimal NIPT timing, the goal is to minimize the potential error and risk of NIPT timing within different maternal BMI ranges [6].

The potential risk function is defined as:

$$R = \sum_{i=1}^{n} w_i \cdot \left(t_{\text{optimal},i} - t_{\text{actual},i}\right)^2 \tag{2}$$

Where R is the total risk, w_i is the weight of the pregnant woman in group i, $t_{\text{optimal},i}$ is the ideal optimal NIPT time, and $t_{\text{actual},i}$ is the actual test time in the simulation. The goal of optimization is to minimize this risk function.

3.1.1 Decision variables

In this model, the decision variables mainly include:

Pregnant women's BMI grouping variable: reasonably grouping pregnant women's BMI values and discretizing them according to the BMI interval.

NIPT detection time: setting the optimal detection time, in units of gestational weeks, that is, each BMI group corresponds to one or more optimal detection time points [7].

Y chromosome concentration reaching the standard ratio: that is, whether the Y chromosome concentration of male fetuses in each BMI group reaches or exceeds 4%. This ratio can be regarded as a control variable, affecting the final detection time point selection [8].

The coefficients of influencing factors such as age, height, and weight: these factors will affect the time when the Y chromosome concentration reaches the standard and needs to be considered through parameterization in the model.

3.1.2 Objective function

The two objective functions in this multi-objective optimization model are:

Minimize detection error: This aims to minimize the model's prediction error, allowing a given NIPT time point to accurately predict the time when male fetal Y chromosome concentration reaches the target.

$$Objective\ Function1 = \sum_{i=1}^{n} w_1 \cdot (\hat{C_i} - C_i)^2 \tag{3}$$

Where $\hat{C}_i$ is the predicted time point when the Y chromosome concentration reaches 4%; C_i is the actual time point when the standard is reached; w_1 is the error weight; and n is the sample size.

Minimize potential risks to pregnant women: Aims to minimize potential risks to pregnant women and fetuses and select a reasonable NIPT timing to reduce these risks.

$$Objective\ Function2 = \sum_{i=1}^{n} w_2 \cdot Risk_i \tag{4}$$

Where $Risk_i$ is the potential risk of the i-th pregnant woman; w_2 is the risk weight. The potential risk can be calculated based on BMI, age, weight, and genetic factors [9].

3.1.3 Constraints

In the optimization model, multiple constraints need to be set to ensure the feasibility and rationality of the model. Common constraints include:

（1）BMI grouping constraints

Each pregnant woman's BMI should be assigned to a reasonable group, such as:

$$BMI_i \in [20,25), [25,30), [30,35), [35,40) \tag{5}$$

This constraint ensures that the BMI grouping conforms to the actual clinical distribution and avoids extreme values.

（2）Feasibility constraint of NIPT timing

The NIPT testing time should be within the effective gestational age range, that is:

$$10 \leq PregnancyWeek_i \leq 16 \tag{6}$$

This constraint ensures the practical feasibility of the detection time point and avoids selecting a time point that does not meet clinical standards.

（3）Probabilistic constraint on Y chromosome concentration reaching the target

The probability of each pregnant woman's Y chromosome concentration meeting the standard should meet certain minimum requirements, such as:

$$P\left(\hat{C}_i \geq 4\%\right) \geq 0.80 \tag{7}$$

This constraint ensures that the test can effectively identify male fetuses with a Y chromosome concentration of 4% z at the predetermined time point.

（4）Detection error constraints

The measurement error should be kept within a preset range to ensure that the time point output by the model does not deviate too much from the actual time point. This can be expressed by setting an error threshold:

$$\left|\hat{C}_i - C_i\right| \leq \epsilon \tag{8}$$

Here, ϵ is the error threshold, which is usually set to 0.5%.

（5）Risk minimization constraints

The risk level for pregnant women needs to be within a clinically acceptable range. An upper limit for risk can be set:

$$Risk_i \leq Risk_{max} \tag{9}$$

This constraint ensures that the potential risk to pregnant women remains within acceptable limits.

By constructing the above decision variables, objective functions, and constraints, we can solve the multi-objective optimization model, thereby providing the best NIPT testing time for pregnant women in different BMI groups, ensuring that the Y chromosome concentration meets the standard requirements, and minimizing the potential risks of pregnant women [10].

3.2 Model solution based on NSGA-II

NSGA-II is a popular multi-objective optimization algorithm. It is based on the genetic algorithm (GA) but uses a unique strategy to handle multi-objective problems, resulting in

higher efficiency than traditional GAs in multi-objective optimization. In this problem, it comprehensively considers factors such as BMI, height, weight, and age, while optimizing multiple conflicting objectives, including the time to reach target Y chromosome concentration, the risk of test failure, and the impact of errors. Through non-dominated sorting, elitist strategies, and crowding comparison, it finds multiple equilibrium solutions, demonstrating strong adaptability and robustness.

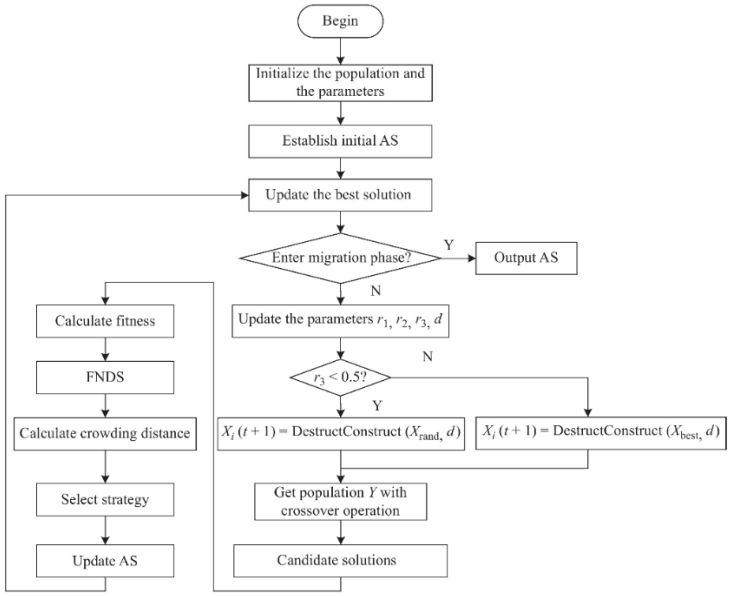

Fig. 1 Principle of the NSGA-II model.

3.2.1 Non—dominatedSorting

The key to NSGA-II is non-dominated sorting. For two solutions x_1 and x_2, if x_1 is not worse than x_2 in all objectives and is better in at least one objective, then x_1 is said to dominate x_2.

Dominance relationship:

The objective function is $f(x) = [f_1(x), f_2(x), \ldots, f_m(x)]$, where $f_i(x)$ is the target value of solution x at the i-th target, and m is the number of targets. The condition for solution x_1 to dominate solution x_2 is:

$$\forall i \in \{1,2,\ldots,m\}, f_i(x_1) \le f_i(x_2), \exists j \in \{1,2,\ldots,m\} \text{such that} f_j(x_1) < f_j(x_2) \quad (10)$$

Non-dominated sorting:

The goal of non-dominated sorting is to divide the entire population into different "Levels" or "fronts" based on dominance relationships. The first front contains all individuals that cannot be dominated by any other individual, the second front contains individuals that are dominated only by individuals in the first front, and so on.

3.2.2 Crowding Distance

In multi-objective optimization, we hope to distribute solutions as evenly as possible. To avoid crowding of solutions, NSGA-II introduces the crowding distance to evaluate the relative position of individuals in their frontier.

For an individual i in a certain frontier, its crowding distance can be calculated by the following formula:

$$CD_i = \sum_{k=1}^{m} \left(\frac{f_{k,i+1} - f_{k,i-1}}{f_{\max}^k - f_{\min}^k} \right) \tag{11}$$

Where: $f_{k,i+1}$ and $f_{k,i-1}$ are the target values of the $i+1$th and $i-1$th individuals on target k after sorting; $f_{\max}^k$ and $f_{\min}^k$ are the maximum and minimum values of target k respectively.

3.2.3 Selection

The selection operation of NSGA-II consists of two steps:

(1) Non-dominated sorting: The population is divided into different levels according to the non-dominated sorting.

(2) Crowding degree comparison: Within the same level, individuals with smaller crowding degrees are compared based on the crowding degree distance. The selection operation formula is:

$$P_i = \begin{cases} \mathrm{x}_i \text{ if } \mathrm{x}_i \text{ belongs to the frontier } F_1 \\ \mathrm{x}_i \text{selected according to the congestion, if it is the } k \text{ frontier } F_k, \mathrm{k} > 1 \end{cases} \tag{12}$$

3.2.4 GeneticOperators

NSGA-II uses traditional genetic operations, including crossover, mutation, and elite selection. For crossover and mutation, NSGA-II typically uses the following operators:

（1）Crossover

The crossover operation is used to exchange genetic information between two parent individuals to generate offspring individuals. Commonly used crossover operators are binary crossover and simulated binary crossover (SBX). The generation process of the SBX operator can be expressed as:

$$\begin{aligned} \mathrm{x}_i' &= \mathrm{x}_i + \lambda \cdot (\mathrm{x}_i - \mathrm{x}_j) \\ \mathrm{x}_j' &= \mathrm{x}_j + \lambda \cdot (\mathrm{x}_j - \mathrm{x}_i) \end{aligned} \tag{13}$$

Where λ is a random number that controls the degree of crossover.

（2）Mutation

The mutation operation is used to make small random modifications to individuals to explore the solution space. The commonly used mutation operator is polynomial mutation, which is formulated as follows:

$$x_i' = x_i + \delta \cdot (x_{\max} - x_{\min}) \tag{14}$$

Where δ is a random variable that controls the degree of variation, and x_{max} and x_{min} are the maximum and minimum values in the solution space. Figure 2 shows the distribution of solutions in the objective space during multi-objective optimization, using non-dominated sorting and congestion calculation.

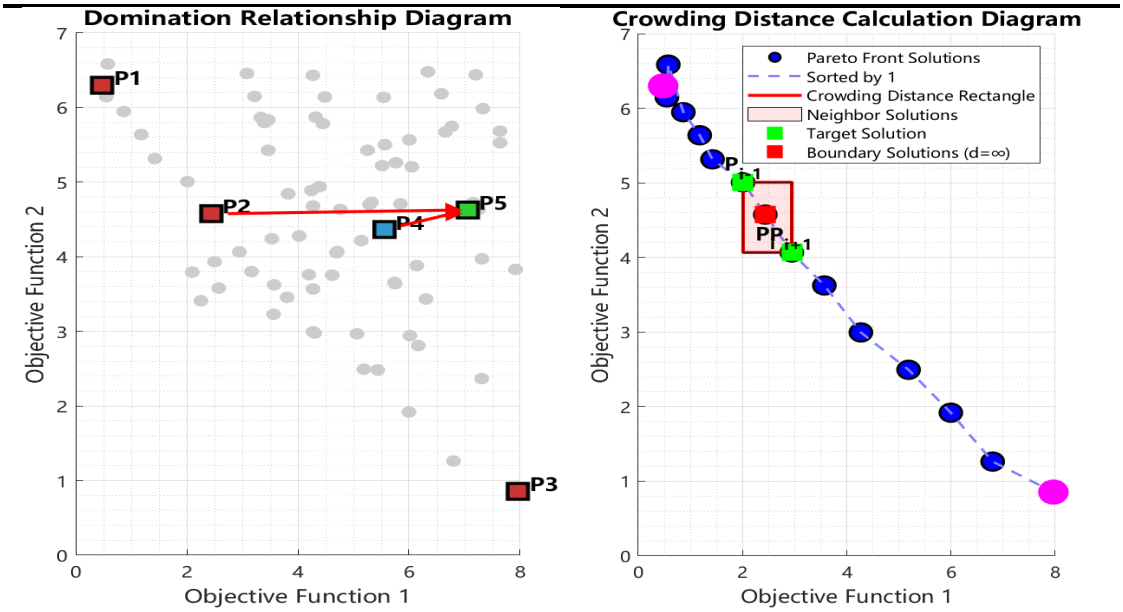

Fig. 2 Non-dominated sorting and congestion calculation in multi-objective optimization.

The left side of Figure 2 shows a schematic diagram of the dominance relationship, and the right side shows a schematic diagram of the congestion calculation. In the left figure, the red square (P1), green square (P2), blue square (P4), and other solutions (Gray dots) illustrate the distribution of solutions in the objective function space. P1 is the initial solution, P2 is the target solution, and P3, P4, and P5 are solutions obtained through the optimization process. The red arrow indicates the transition from P2 to P5, demonstrating that the optimization algorithm gradually approaches the ideal solution by continuously adjusting the weights of the solutions.

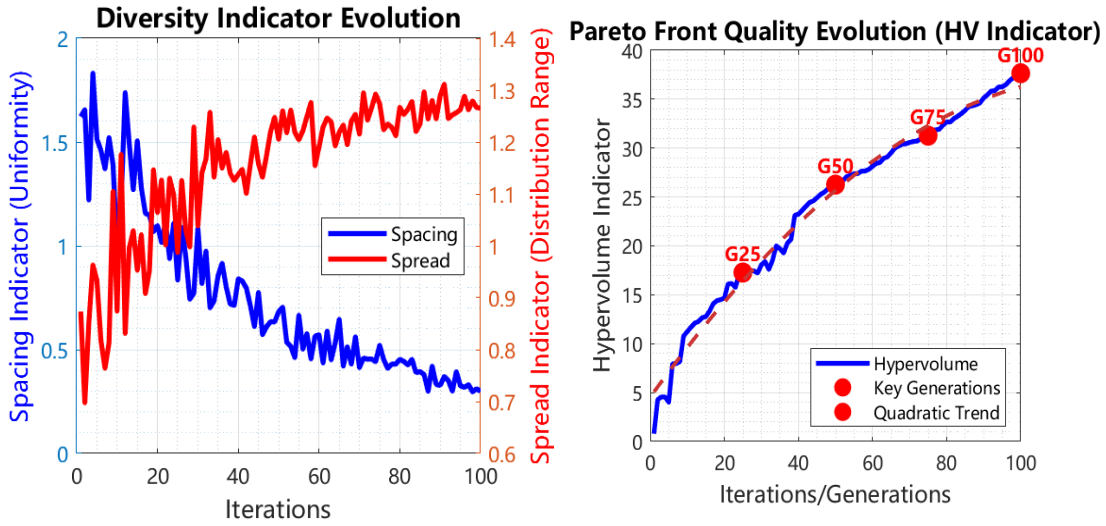

Fig. 3 Iteration curve and Pareto front analysis.

The left panel of Figure 3 shows the curves of the Spacing and Spread metrics as they change with the number of iterations. The Spacing metric (Blue line) indicates the uniformity of solutions; closer to 1, the more uniform the distribution of solutions. The Spread metric (Red line) measures the range of solutions in the target space; larger values indicate greater diversity. As shown in Figure 3, the Spacing metric decreases with increasing iterations, indicating that the distances between solutions are becoming more uniform. Meanwhile, the Spread metric fluctuates, but the overall trend is a gradual increase, indicating that the range of solutions is

increasing. The NSGA-II algorithm effectively expands the distribution of solutions for this problem, improving diversity.

The right panel shows the Pareto frontier quality (HV metric) as the number of iterations changes. The red dots in the figure represent solutions at different iteration numbers, and the blue curve shows the changing trend of the frontier quality. As the number of iterations increases, the quality of the frontier gradually improves. From the marking points of G25, G50 to G100, the HV index continues to increase, indicating that with the increase of generations, the quality of the solution set gradually approaches the ideal solution, and the optimization process gradually approaches the optimal frontier.

3.3 Model solution results

As can be seen from Table 1, there are significant differences in the optimal detection time points corresponding to different BMI groups.

Table. 1 Model solution results.

BMI range	Number of samples	Detection time
[20.0,28.6)	58	24.72215
[28.6,34.5)	806	23.74262
[34.5,35.6)	76	24.93422
[35.4,38.2)	105	22.162364
[38.3,Inf)	44	18.626646

Specifically, the optimal testing time for pregnant women with a BMI $\geqslant$ 38.3 was the earliest, at 18.63 weeks, while the optimal time for women with a BMI between 20.0 and 28.6 was the latest, at 24.72 weeks. This result indicates that as BMI increases, the time at which fetal Y chromosome concentration reaches the standard tends to shift earlier, suggesting that pregnant women with a high BMI may need to schedule NIPT testing earlier to reduce the risk of test failure due to insufficient fetal DNA concentration.

3.4 Error Analysis Based on Monte Carlo Perturbation Experiment

In NIPT, the impact of testing error on test results is a critical issue. Testing error arises from various processes, including sample collection, DNA extraction, and sequencing. Such as these errors can affect the accurate measurement of fetal Y chromosome concentration, thereby impacting the selection of the optimal NIPT timing and the reliability of test results. Here, to quantitatively analyze the impact of error on NIPT timing, a Monte Carlo simulation experiment was conducted. By introducing error through multiple random sampling attempts, we simulated the optimal NIPT timing under varying error conditions and evaluated the impact of error on timing shifts.

3.4.1 Impact of detection error on the optimal NIPT timing

In NIPT, a 4% concentration threshold is set. When the fetal Y chromosome concentration reaches or exceeds this threshold, the fetus is considered to have met the standard. Therefore, the optimal NIPT timing refers to the time in pregnancy when the fetal Y chromosome concentration reaches this threshold.

Ideally, the fetal Y chromosome concentration will gradually increase as the pregnancy progresses, and when it reaches 4%, it should be considered as the target point. The relationship between the fetal Y chromosome concentration and the gestational period is set as:

$$Y_{\text{true}}(t) = f(t) \tag{15}$$

Where t is the gestational time and $Y_{\text{true}}(t)$ is the true Y chromosome concentration of the fetus.

According to the testing criteria, the optimal NIPT time point t_{optimal} is reached when $Y_{\text{true}}(t) \geq 4\%$. However, due to testing errors, the actual measured value $Y_{measured}(t)$ may deviate from the true value $Y_{\text{true}}(t)$, resulting in a shift in the optimal NIPT time point t_{measured}.

3.4.2 Simulation steps

(1) Define input parameters: including the true value of the fetal Y chromosome concentration Y_{true}, the standard deviation of the error σ, and the threshold for the concentration to reach the standard.

(2) Generate random error: For each simulated sample, generate a random error term $\varepsilon \sim \mathcal{N}(0, \sigma^2)$.

(3) Calculate the measured value: Calculate the measured Y chromosome concentration $Y_{\text{measured}} = Y_{\text{true}} + \varepsilon$.

(4) Calculate the time point of reaching the standard: Based on the measured value, calculate the time point t_{measured} when the fetal concentration reaches 4%.

(5) Repeat the simulation: Through multiple simulations, record the time point offset caused by the measurement error in each simulation.

3.4.3 Deviation Analysis

For each simulation result, the deviation $\Delta t = t_{\text{measured}} - t_{\text{optimal}}$ between the measured time point and the true time point is calculated, and the distribution of the deviation is obtained through statistical analysis.

3.4.4 Robustness analysis

Robustness analysis assesses the stability of a model under varying error conditions. By varying the error standard deviation, σ, we can observe how the optimal NIPT time point shifts as the error increases. Larger shifts indicate that the model is sensitive to error and lacks robustness.

$$\text{Var}(\Delta t) = \frac{1}{N}\sum_{i=1}^{N} \left(\Delta t_i - \overline{\Delta t}\right)^2 \tag{16}$$

If the deviation variance is large, it means that the error has a greater impact on the results, and the model is less robust.

3.4.5 Sensitivity analysis

Sensitivity analysis is used to identify factors that significantly influence the optimal NIPT timing. In this experiment, we analyzed the impact of parameters such as the standard deviation of the error, the Y chromosome concentration threshold, and the mother's height, weight, and age on the time to reach the target, assessing the sensitivity of these factors to the results.

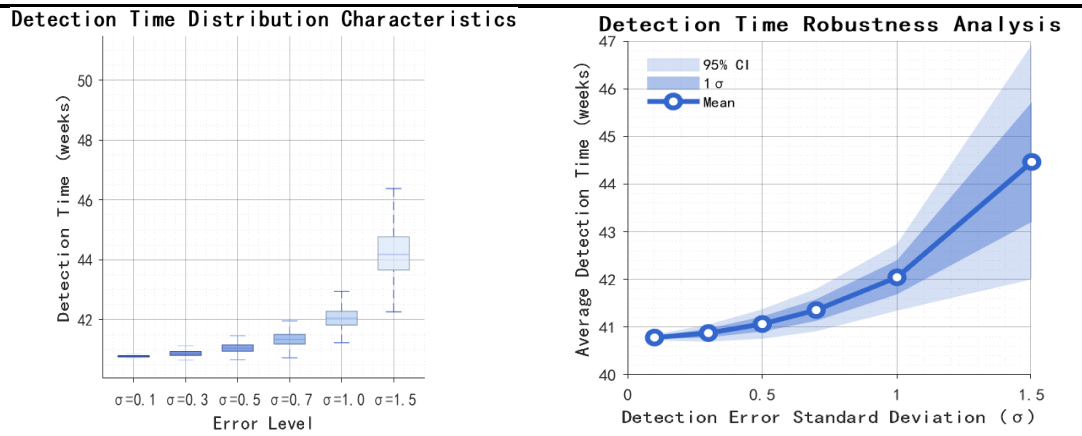

Fig. 4 Detection performance robustness analysis.

The sensitivity index of each parameter was calculated to assess its influence on the optimal NIPT timing. Table 2 shows the results of sensitivity analysis of the impact of various factors on the optimal detection time point.

Table. 2 Sensitivity analysis.

Index name	BMI	Age	Height	Weight
Sensitivity coefficient	0.1049	0.0462	0.0022	0.0007

As can be seen, BMI has the highest sensitivity coefficient (0.1049), far exceeding that of other factors, indicating that BMI is the most critical variable influencing the optimal timing of NIPT testing. Age, with a sensitivity coefficient of 0.0462, while having some influence, is significantly lower than BMI. The sensitivity coefficients of height and weight are both close to zero, indicating that their influence on testing timing is negligible. This analysis further validates the rationale for using BMI as a stratification factor and provides quantitative support for prioritizing pregnant women with higher BMIs in clinical practice.

4 CONCLUSION

The NSGA-II-based optimal NIPT testing time model proposed in this paper comprehensively considers individual differences among pregnant women and testing errors, achieving a coordinated optimization of testing errors and maternal and childbirth risks. Experimental results demonstrate good convergence of the model solution process, continuous improvement in the quality of the Pareto frontier, and high accuracy and robustness of the output results across multiple BMI strata. Sensitivity analysis further confirmed BMI as a key influencing factor. Overall, the model can effectively solve complex multi-objective optimization problems and provide scientific recommendations for NIPT testing time in clinical practice. Future research could introduce more risk variables and adaptive optimization mechanisms to further enhance the model's clinical applicability and promotional value.

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