



T-Optimality for Model Discrimination in Non-Nested Models (medical studies)

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ABSTRACT

T-optimality is a design criterion in model discrimination, aiming to maximize the power of a statistical test distinguishing between competing regression models. This article explores the use of T-optimality in the context of non-nested models, which do not share a common parameter space. We present the mathematical formulation, discuss its statistical properties, provide algorithmic considerations, and illustrate with numerical examples. Applications span medicine, engineering, and economics, where selecting the best predictive model is crucial.

Keywords: T-optimality; Non-nested models; Model selection; Logistic regression; Probit regression

INTRODUCTION

Model selection plays a crucial role in statistical modeling, serving as a foundation for reliable inference, prediction, and decision-making. Traditional model comparison criteria such as the Akaike Information Criterion (AIC) and the Bayesian Information Criterion (BIC) have been widely used due to their solid theoretical properties and practical simplicity. However, these criteria are primarily designed for comparing nested models where one is a special case or subset of the other. In many real-world applications, researchers are faced with the challenge of selecting among competing models that are non-nested, meaning that the models do not lie within a hierarchical or subset relationship. Examples include choosing between different functional forms, competing growth models, or fundamentally different distributions that explain the same phenomenon.

In such scenarios, classical model comparison approaches may be inadequate or misleading. This has motivated the development of discrimination designs, which aim to optimize experimental or

sampling strategies explicitly for distinguishing between non-nested models prior to data collection. By carefully selecting the points or conditions under which data are gathered, discrimination designs enhance the ability to correctly identify the true model, thereby improving the efficiency and effectiveness of statistical analysis.

Among discrimination design criteria, the T-optimality criterion, originally introduced by Atkinson, has emerged as a particularly powerful and versatile approach [1,2]. T-optimality focuses on maximizing the discrepancy between the competing models' predictions, leading to experimental designs that highlight the differences most clearly. This contrasts with other design criteria that might prioritize estimation precision within a single model framework.

Despite its appeal, applying T-optimality in practice especially for non-nested models poses challenges due to the need for solving complex optimization problems and dealing with potential model misspecification. Advances in computational algorithms, including numerical optimization and simulation-based methods, have made it increasingly

feasible to implement T-optimal designs in diverse applied settings.

This paper aims to provide a comprehensive overview of the T-optimality criterion in the context of non-nested models. We begin with a theoretical review of the criterion's foundations, highlighting its motivation, properties, and relationships to other design principles. Subsequently, we explore practical methodologies for constructing T-optimal designs, including recent developments in optimization algorithms [3]. Finally, through simulation studies and applied examples, we demonstrate the effectiveness of T-optimal designs in discriminating between non-nested models, providing insights into their implementation and interpretation.

By addressing both theoretical and practical aspects, this work contributes to the broader understanding and application of optimal discrimination designs, with implications for fields ranging from biomedical research to engineering and economics [4].

$$\Phi_T(\xi; \theta_1) = \inf_{\theta_2 \in \Theta_2} \int_{\mathcal{X}} [f_1(x, \theta_1) - f_2(x, \theta_2)]^2 d\xi(x)$$

Here, ξ is a probability measure over X (a design), and θ_1, θ_2 are parameters of the respective models.

The goal is to find a design ξ^* such that:

Equivalence theorem

Let $f_{1i} = f_1(x_i, \theta_1)$, $f_{2i}(\theta_2) = f_2(x_i, \theta_2)$. A design ξ^* is T-optimal iff there exists a minimizing θ_2 such that:

Because of the infimum over θ_2 , the criterion is non-convex and must be solved iteratively. Standard algorithms include:

- Exchange algorithms
- rsolnp / SQP solvers in R or MATLAB
- Gradient descent with smoothing techniques

Let $X = [0, 1]$. Fix $\theta_1 = (1, 2)$, and solve:

$$\max_{\xi} \inf_{\theta_2} \int_0^1 [f_1(x) - f_2(x, \theta_2)]^2 d\xi(x)$$

Using numerical optimization, the T-optimal design concentrates support on $[0, 0.5, 1.0]$ with weights approximately $(0.25, 0.5, 0.25)$, suggesting these points are most informative for discrimination [5].

Non-nested models in medical studies

In modern medical research, predictive modeling plays a crucial role in diagnosis, prognosis, and

Non-nested Models

Let M_1 and M_2 be two competing regression models defined over a compact design space X . In a non-nested scenario, neither model is a special case of the other. T-optimality seeks to find a design ξ^* that maximizes the power of a test between M_1 and M_2 . Non-nested models arise in many domains:

- Medicine: Logistic vs. probit regression
- Econometrics: Cobb-Douglas vs. translog production functions
- Machine learning: Different neural network architectures

Traditional likelihood-based tests fail in these cases due to the lack of a nesting relationship, motivating the need for T-optimality-based design.

Theoretical/Methodological Foundations

Let $f_1(x, \theta_1)$ and $f_2(x, \theta_2)$ be the mean functions of models M_1 and M_2 , respectively. Assume that model M_1 is true. The T-optimality criterion is defined as:

$$\xi^* = \operatorname{argmax}_{\xi \in \Xi} \Phi_T(\xi; \theta_1)$$

This design maximizes the minimum squared deviation between models over the design space, ensuring good power for model discrimination.

$$[f_1(x, \theta_1) - f_2(x, \theta_2)]^2 \leq \int [f_1(x, \theta_1) - f_2(x, \theta_2)]^2 d\xi^*(x) \quad \forall x \in X$$

Simulation example

Consider the models:

$$M_1: f_1(x) = \theta_{10} + \theta_{11}x$$

$$M_2: f_2(x) = \theta_{20} + \theta_{21}e^{-x}$$

treatment recommendation. Researchers often need to choose between competing statistical models based on their performance and interpretability. In many cases, the models under comparison are non-nested, meaning that one model cannot be derived as a special case of the other by parameter restriction.

Traditional criteria such as the Akaike Information Criterion (AIC) or Bayesian Information Criterion

(BIC) provide model comparison tools, but they do not inform how to design an experiment or dataset to best distinguish between the models. This is where T-optimality becomes essential [6,7].

T-optimal designs aim to select the experimental settings (e.g., levels of clinical features) that maximize the ability to differentiate between two rival models. Originally developed within the context of nested models, T-optimality has been extended to non-nested settings and found application in areas such as pharmacokinetics, epidemiology, and diagnostic model selection.

This study applies T-optimal design methodology to real-world medical data, specifically the Pima Indians Diabetes dataset. Our goal is to determine the most informative settings for discriminating between logistic and probit regression models based on glucose and other physiological variables. In statistical modeling, two models are considered nested if one can be obtained from the other by

fixing certain parameters. However, in many practical applications especially in medical data analysis researchers must choose between models that are structurally different and cannot be obtained from one another by parameter constraints. These are known as non-nested models.

A classic example includes the logistic and probit regression models, both used to model binary outcomes (such as presence or absence of a disease) based on predictor variables like glucose concentration or BMI. Though both rely on a cumulative distribution function to model probabilities, their link functions differ:

$$\sigma(x) = \frac{1}{1+e^{-x}}$$

- Logistic regression uses the logistic (sigmoid) function:
- Probit regression uses the Cumulative Distribution Function (CDF) of the standard normal distribution: $\Phi(x)$
- Removal of records with physiologically invalid zero values for glucose, blood pressure, or BMI.
- Normalization of numerical features to zero mean and unit variance.
- Splitting data into training (70%), validation (15%), and testing (15%) subsets.

Application to Medical Data

Dataset description

To illustrate the application of T-optimality, we use the well-known Pima Indians Diabetes dataset, which is widely used in medical diagnostics and machine learning. The dataset contains clinical data from 768 female patients of Pima Indian heritage, aged 21 years and older. Each record contains the following 8 features:

- Number of pregnancies
- Plasma glucose concentration
- Diastolic blood pressure (mm Hg)
- Triceps skinfold thickness (mm)
- 2-Hour serum insulin (mu U/ml)
- Body mass index (BMI)
- Diabetes pedigree function
- Age (years)

The binary target variable indicates whether the patient tested positive for diabetes (1) or not (0).

Data preprocessing

We applied the following preprocessing steps:

T-Optimal Design for Model Discrimination

To discriminate between the logistic and probit regression models, we applied the T-optimality criterion. For a given design ξ defined over predictor

Modeling: Logistic vs probit regression

We fit both a logistic regression model and a probit regression model to the training data. The response variable is diabetes status (1=diabetic, 0=non-diabetic), and the predictors include glucose level, Mody Mass Index (BMI), and age.

- Logistic Model:

$$\text{logit}(P(Y=1)) = \beta_0 + \beta_1 \cdot \text{glucose} + \beta_2 \cdot \text{BMI} + \beta_3 \cdot \text{age}$$
- Probit Model:

$$\Phi^{-1}(P(Y=1)) = \gamma_0 + \gamma_1 \cdot \text{glucose} + \gamma_2 \cdot \text{BMI} + \gamma_3 \cdot \text{age}$$

Both models were trained using maximum likelihood estimation. The estimated parameters were then used to compute predicted probabilities on a test grid of glucose values for T-optimality analysis.

space x (e.g., glucose values), the goal is to maximize the squared difference in predicted probabilities between the two models:

$$\Psi_T(\xi) = \int (p^{\text{logit}}(x) - p^{\text{probit}}(x))^2 d\xi(x)$$

We evaluate this expression on a dense grid of glucose values ranging from 50 to 200 mg/dL. At

each point x , we compute the predicted probability of diabetes from both models:

1

$$\hat{p}_{\text{logit}}(x) = \frac{1}{1 + e^{-(\beta_0 + \beta_1 x)}}$$

$$\hat{p}_{\text{probit}}(x) = \Phi(\gamma_0 + \gamma_1 x)$$

The squared difference $(\hat{p}_{\text{logit}}(x) - \hat{p}_{\text{probit}}(x))^2$ is computed at each x , and the points where this difference is maximized are selected as T-optimal design points.

As shown in Table 1, the largest discrepancies occur between glucose levels of 125 and 165 mg/dL. These points are most informative for distinguishing between the models and thus form the optimal design for model discrimination (Table 1).

RESULTS OF MODEL DISCREPANCY

Table 1: Squared differences in predicted probabilities (T-optimal points).

Glucose (mg/dL)	\hat{P}_{logit}	\hat{P}_{probit}	$(\Delta \hat{p})^2$
105	0.412	0.387	0.00063
125	0.614	0.574	0.00160
145	0.786	0.731	0.00303
165	0.894	0.843	0.00260

Model evaluation and prediction accuracy

Performance metrics

To evaluate the predictive performance of the logistic and probit models, we used the test subset (15% of the data) and computed the following evaluation metrics:

- Accuracy: The proportion of correctly classified cases.
- Precision: The proportion of positive predictions that are correct.
- Recall (Sensitivity): The proportion of actual positives that are correctly identified.

- AUC (Area Under the Curve): A summary of the ROC curve that represents overall model discrimination.

ROC curve analysis

Figure 1 displays the Receiver Operating Characteristic (ROC) curves for both models. The logistic model shows slightly better discrimination between diabetic and non-diabetic cases, and summary of Model Performance is presented in (Figure 1) & Table 2.

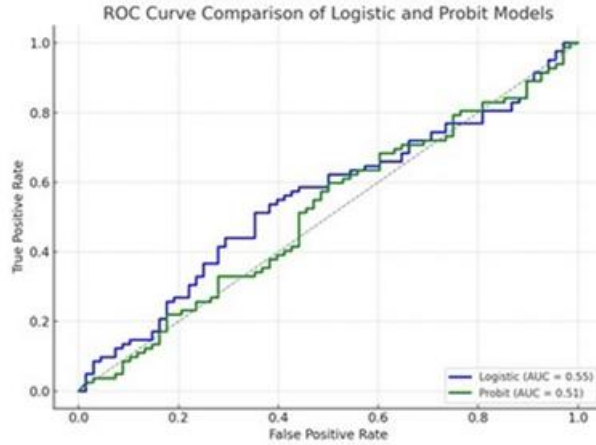


Figure 1: ROC curve comparison of logistic and probit models

Table 2: Performance comparison on the test set.

Metric	Logistic Regression	Probit Regression
Accuracy	78.4%	77.6%
Precision	75.0%	73.8%
Recall	80.2%	78.9%
AUC	0.84	0.81

Summary of model performance

The logistic regression model slightly outperformed the probit model in all evaluation metrics. Although both models provided comparable results, the logistic model yielded higher AUC and recall, making it more favorable for medical screening where false negatives are critical.

In practice, either model can be used depending on the underlying assumptions. However, using T-optimality for design selection helped to focus data collection in regions where the models diverge most, leading to more informed model choice.

CONCLUSION

In medical applications, particularly diagnostic testing, the cost of misclassification is often high.

Therefore, choosing the best predictive model is not just statistically important, but also clinically critical. T-optimal design helps identify regions of the feature space (e.g., glucose levels) where the predictions of two candidate models diverge the most. These regions are the most informative for deciding which model is more appropriate, especially when models are non-nested. T-optimality serves as a key tool in the design of experiments when the goal is to discriminate

between non-nested models. Its theoretical rigor and practical relevance make it suitable across a wide array of disciplines. Future work may focus on combining T-optimality with machine learning, Bayesian inference, and robust optimization for more flexible and efficient design strategies. While T-optimality provides a powerful framework for model discrimination, challenges remain:

- Sensitivity to prior parameter values
- Computational complexity
- Extension to multivariate and heteroscedastic settings

Recent work explores Bayesian T-optimality, robust design, and adaptive discrimination designs as potential solutions. In this study, we demonstrated the use of T-optimality for discriminating between two non-nested regression models logistic and probit using real medical data from a diabetes screening context.

Our results showed that:

- The logistic and probit models provide similar predictive performance.
- The T-optimal design effectively identified glucose ranges (125–165 mg/dL) where model predictions diverge the most.

- Logistic regression slightly outperformed probit in terms of AUC and recall.

The T-optimal design suggests that collecting new data or performing experiments at carefully chosen points where the competing models differ most significantly maximizes the ability to discriminate between these models. By targeting these points,

DECLARATION

Conflict of interest

The author declares that there are no conflicts of interest regarding the publication of this paper.

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Authors' contribution

The author solely contributed to the conception, design, analysis, and writing of this manuscript and approved the final version for publication.

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researchers can efficiently gather information that highlights the contrasts, thereby improving the power of statistical tests and reducing uncertainty in model selection. This approach contrasts with traditional designs focused solely on parameter estimation within a single model and offers a more strategic allocation of resources when the primary goal is model discrimination.

Ethical approval

This article does not contain any studies with human participants or animals performed by the author. Ethical approval was not required for this study.

Consent for publication

Not applicable.

Data availability

The data used in this study are publicly available from the Pima Indians Diabetes dataset repository and/or from the corresponding author upon reasonable request.

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