An evaluation of KL-optimum designs to discriminate between rival copula models

Una valutazione della capacità del disegno KL-ottimo di discriminare tra modelli copula rivali

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Abstract The problem of model discrimination has prompted a great amount of research over last years. According to the specific characteristics of the rival models (nested, non-nested, linear or not) different optimum criteria have been proposed to select design points with the aim to discriminate between rival models. Ds-, T- and KL-criteria are the most known. Up to our knowledge, in the literature there is not any study to evaluate the performance of these discrimination criteria. In this work, via a simulation study and focusing on rival copula models, we analyze the performance of the KL-optimum design applying the likelihood ratio test for non-nested models.

Abstract *Nel corso degli ultimi anni il problema di discriminare tra modelli rivali ha prodotto una grande quantità di ricerche. A seconda della tipologia di modelli rivali (annidati, non annidati, lineari o non lineari), diversi criteri sono stati proposti con l'obiettivo di selezionare il disegno ottimo per la discriminazione. Tra i più noti ricordiamo i criteri Ds-, T- e KL-. Per quanto ci consta, in letteratura non esistono studi relativi alla valutazione della loro effettiva capacità discriminatoria. In questo lavoro, attraverso uno studio di simulazione in cui abbiamo applicato il test del rapporto di verosimiglianza per modelli non annidati, abbiamo analizzato le prestazioni del disegno KL-ottimo per discriminare tra modelli bivariati la cui struttura di dipendenza è descritta attraverso una funzione copula.*

Key words: Copula model, Cox's test, Optimal experimental design

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1 Introduction

A major limitation associated with the design of an experiment is that the optimality of a design depends on a priori true model that is not known in advance. Actually, very often, the experimenter has not just one but several possible models for describing a phenomenon. Thus, his/her first goal is to collect data in order to discriminate among rival models. The problem of model discrimination has prompted a great amount of research over last years. To discriminate between nested models (linear or not) [1] propose the D_s-criterion where the models are embedded in a more general one and the design aims at estimating the additional parameters as precisely as possible. A criterion to obtain optimal designs for discriminating between two homoscedastic models for normally distributed observations is T-optimality, which was introduced by [2]. A criterion based on the popular Kullback-Leibler (KL) distance is proposed by [6] for any non-normal assumption.

About discrimination between copula models, [9] apply the D_s-criterion which can be used only for nested models; for this reason, they need to introduce the mixture copula model (which includes the rival copulae as special cases). In this paper, instead, we consider the KL-optimality criterion proposed by [6] which compares directly the competing models without using any other auxiliary reference model. Specifically, we consider a bivariate model with two possible dependence structures: Clayton and Gumbel copulae (the competing models). Since, up to our knowledge, there are no studies to evaluate the performance of a discrimination criterion, in this work we analyze the performance of the KL-optimum design through a simulation study where we apply a version of Cox's test. For comparison purposes, we also describe the performance of the Uniform design, which is very often adopted in real case studies.

The paper is organized as follows. In Section 2 the bivariate copula model is introduced and the main definitions are given. The KL-optimality criterion is introduced in Section 3. Section 4 concerns the simulation study to evaluate the performance of the KL-optimum design.

2 Bivariate Copula-Based Model

Let (Y_1, Y_2) be a bivariate response variable with marginal distributions $F_{Y_1}(y_1; \alpha)$ and $F_{Y_2}(y_2; \beta)$, which depend on the unknown parameter vectors α and β, respectively. If there is an association between Y_1 and Y_2, it is necessary to define a joint model for (Y_1, Y_2).

A bivariate copula is a function $C: I^2 \rightarrow I$, with $I^2 = [0,1] \times [0,1]$ and $I = [0,1]$, that, with an appropriate extension of the domain in R^2, satisfies all the properties of a cumulative distribution function (cdf). In particular, it is the cdf of a bivariate random variable (U_1, U_2), with uniform marginal distributions in $[0,1]$:

$$C(u_1, u_2; \theta_C) = P(U_1 \leq u_1, U_2 \leq u_2; \theta_C), \quad 0 \leq u_1 \leq 1 \quad 0 \leq u_2 \leq 1, \qquad (1)$$

where $\theta_C \in \Theta_C$ is a parameter measuring the dependence between U_1 and U_2.

The importance of copulae in statistical modelling stems from Sklar's theorem [7], which states that a joint distribution can be expressed in terms of marginal distributions and a function $C(\cdot, \cdot; \theta_C)$ that binds them together. In more detail, according to Sklar's theorem, if $F_{Y_1, Y_2}(y_1, y_2; \delta, \theta_C)$ is the joint cdf of (Y_1, Y_2), where $\delta = (\alpha, \beta)$, then there exists a copula function $C: I^2 \to I$ such that

$$F_{Y_1, Y_2}(y_1, y_2; \delta, \theta_C) = C\{F_{Y_1}(y_1; \alpha), F_{Y_2}(y_2; \beta); \theta_C\}, \quad y_1, y_2 \in \mathbb{R}. \qquad (2)$$

If $F_{Y_1}(y_1; \alpha)$ and $F_{Y_2}(y_2; \beta)$ are continuous functions then the copula $C(\cdot, \cdot; \theta_C)$ is unique. Conversely, if $C(\cdot, \cdot; \theta_C)$ is a copula function and $F_{Y_1}(y_1; \alpha)$ and $F_{Y_2}(y_2; \beta)$ are marginal cdfs, then $F_{Y_1, Y_2}(y_1, y_2; \delta, \theta_C)$ given in (2) is a joint cdf.

From (2) we have that a copula captures the dependence structure between the marginal probabilities. This idea allows researchers to consider marginal distributions and the dependence between them as two separate but related issues. For each copula there exists a relationship between the parameter θ_C and Kendall's τ coefficient (see [7] pp. 158-170) and between θ_C and the lower and upper tail dependence parameters λ_l and λ_u (which measure the association in the tails of the joint distribution; see [7] pp. 214-216). Several bivariate copulae have been proposed in the literature (see for instance [7]). In this paper we consider only Clayton and Gumbel copulae, which are recalled in Table 1. Both these copulae allow only for positive association between variables ($\tau \geq 0$) but they exhibit strong *left* and strong *right* tail dependence, respectively.

3 KL-Optimality Criterion

An approximate design ξ is a discrete probability measure on a compact experimental domain $\mathscr{X}$; $\xi(x)$ represents (at least approximatively) the proportion of observations to be taken at the experimental condition x. An optimal design maximizes a concave functional of ξ, which is called optimality criterion and reflects an inferential goal.

Let (Cl, G) denote Clayton and Gumbel copulae, respectively and let (θ_{Cl}, θ_G) be the corresponding dependence parameters. From now on, we assume that nominal values for δ, θ_{Cl} and θ_G are available; hence, we compute locally optimum designs. In order to discriminate between the two rival copulae, we propose to use

Table 1 Copula functions and related association parameters

Copula	$C(u_1, u_2; \theta)$	$\theta \in \Theta$	$\tau = \tau(\theta)$
Clayton	$(u_1^{-\theta} + u_2^{-\theta} - 1)^{-1/\theta}$	$\theta \in (0, \infty)$	$\tau = \theta/(\theta + 2)$
Gumbel	$\exp\left(-\left[\{-\ln(u_1)\}^\theta + \{-\ln(u_2)\}^\theta\right]^{1/\theta}\right)$	$\theta \in [1, \infty)$	$\tau = 1 - 1/\theta$

the following geometric mean of KL-efficiencies:

$$\Phi_{KL}(\xi;\delta,\theta_{Cl},\theta_G) = \left\{\mathrm{Eff}_{G,Cl}(\xi;\theta_{Cl})\right\}^{\gamma} \cdot \left\{\mathrm{Eff}_{Cl,G}(\xi;\theta_G)\right\}^{1-\gamma} \quad 0 \le \gamma \le 1,$$

where γ is a suitably chosen weight which balances the belief in the two competing copulae;

$$\mathrm{Eff}_{i,j}(\xi;\theta_j) = \frac{I_{i,j}(\xi;\theta_j)}{I_{i,j}(\xi_{i,j}^*;\theta_j)}, \quad \xi_{ij}^* = \arg\max_{\xi} I_{i,j}(\xi;\theta_j), \quad i,j = Cl,G \qquad (3)$$

and

$$I_{i,j}(\xi;\theta_j) = \inf_{\theta_i} \sum_{x \in \mathscr{X}} \mathscr{I}\left\{f_{y_1 y_2}^j(x;\delta,\theta_j), f_{y_1 y_2}^i(x;\delta,\theta_i)\right\} \xi(x), \qquad (4)$$

is the KL-criterion proposed by [6]. Here $\mathscr{I}\left\{f_{y_1 y_2}^j(x;\delta,\theta_j), f_{y_1 y_2}^i(x;\delta,\theta_i)\right\}$ denotes the Kullback-Leibler divergence between the true density function $f_{y_1 y_2}^j(x;\delta,\theta_j)$ and the rival one $f_{y_1 y_2}^i(x;\delta,\theta_i)$, with $i,j = Cl,G$.

4 Evaluation of the performance of the KL-optimum design: an example with bivariate binary logistic model

In order to assess the ability of the KL-optimum design to discriminate between two competing copula models we employ a version of Cox's test (see [3] and [4]).

Given δ, τ and a design ξ, let (y_{1i}, y_{2i}) for $i = 1,2,...n$ be a sample of outcomes from one of the two rival models. For a specific Scenario δ and for a specific value of Kendall's τ coefficient, we generate M samples of size n, at a design ξ. Then, we check how many times the likelihood ratio test provides an evidence in favour of each model. Following [8] we have to test both the following systems of hypotheses:

$$A) \begin{cases} H_{Cl} : \mathscr{F}_{Cl} = \{f_{y_1 y_2}^{Cl}(x;\delta,\theta_{Cl}), \ \theta_{Cl} \in \Theta_{Cl}\} \\ H_G : \ \mathscr{F}_G = \{f_{y_1 y_2}^{G}(x;\delta,\theta_G), \ \theta_G \in \Theta_G\} \end{cases}$$

$$B) \begin{cases} H_G : \ \mathscr{F}_G = \{f_{y_1 y_2}^{G}(x;\delta,\theta_G), \ \theta_G \in \Theta_G\} \\ H_{Cl} : \mathscr{F}_{Cl} = \{f_{y_1 y_2}^{Cl}(x;\delta,\theta_{Cl}), \ \theta_{Cl} \in \Theta_{Cl}\} \end{cases}$$

From now on, we omit the argument x and δ for ease of notation. As test statistics, we consider the log-likelihood ratios:

$$T_{ClG} = L_{Cl}(\widehat{\theta}_{Cl}) - L_G(\widehat{\theta}_G) \quad \text{and} \quad T_{GCl} = L_G(\widehat{\theta}_G) - L_{Cl}(\widehat{\theta}_{Cl}), \qquad (5)$$

where $L_{Cl}(\theta_{Cl})$ and $L_G(\theta_G)$ are the log-likelihood functions under H_{Cl} and H_G, respectively, and $\widehat{\theta}_{Cl}$ and $\widehat{\theta}_G$ are the corresponding maximum likelihood estimators.

Let p_{ClG} and p_{GCl} be the p-values of T_{ClG} and T_{GCl}, respectively. Whenever $p_{ClG} > p_{GCl}$ (or $p_{GCl} > p_{ClG}$) we accept Clayton (or Gumbel) model.

In the case of non-nested models the log-likelihood ratio is not (asymptotically) distributed as a Chi-squared random variable (see for instance [4, 8]). Hence, we implement a Monte Carlo procedure to approximate the sample distribution of T_{ClG} and T_{GCl} and to compute the corresponding p-values, $\hat{p}_{ClG}$ and $\hat{p}_{GCl}$ under H_{Cl} and H_G, respectively. Differently, [3, 4] proposed the asymptotic distribution of the log-likelihood ratio suitably standardized.

Consider now an example in dose finding study. Let (Y_1, Y_2) be a binary response variable where both Y_1 and Y_2 take values in $\{0, 1\}$ (1 denotes occurrence and 0 denotes no occurrence). We consider (see [5]) the following logistic models for the marginal success probabilities of efficacy and toxicity:

$$\pi_1(x; \alpha) = P(Y_1 = 1 | x; \alpha) = \frac{e^{\alpha_0 + \alpha_1 x + \alpha_2 x^2}}{1 + e^{\alpha_0 + \alpha_1 x + \alpha_2 x^2}}, \quad \alpha = (\alpha_0, \alpha_1, \alpha_2),$$

$$\pi_2(x; \beta) = P(Y_2 = 1 | x; \beta) = \frac{e^{\beta_0 + \beta_1 x}}{1 + e^{\beta_0 + \beta_1 x}}, \quad \beta = (\beta_0, \beta_1),$$

where $x \in \mathscr{X} = [-1, 1]$ denotes the standardized dose of a drug.

If $C(\cdot, \cdot; \theta_C)$ is a copula function which models the dependence between $\pi_1(x; \alpha)$ and $\pi_2(x; \beta)$, then the joint probability of (Y_1, Y_2) at the dose x is

$$p_{11}^C(x; \delta, \theta_C) = P(Y_1 = 1, Y_2 = 1 | x; \delta, \theta_C) = C\{\pi_1(x; \alpha), \pi_2(x; \beta); \theta_C\}. \quad (6)$$

Given $\delta = (1, 1.5, -3, 2.5, 5)$ and $\tau = 0.8$, we perform two Monte Carlo simulations, based on the generation of $M = 5000$ samples of size n from model (6) using (in the data generating model) the Clayton copula with $\theta_{Cl} = 8$ and the Gumbel copula with $\theta_G = 5$, respectively ($\theta_{Cl} = 8$ and $\theta_G = 5$ correspond to the same value of the association parameter $\tau = 0.8$). The doses and the proportions of observations to be taken at each dose are given by the KL-optimum design, which is reported in the first column of Table 2.

Table 2 KL-optimal design ξ_{KL} for $(\theta_{Cl}; \theta_G) = (8; 5)$ and Uniform design ξ_{Unif}

ξ_{KL}	ξ_{Unif}
$\left\{\begin{array}{cc} -0.793 & -0.050 \\ 0.470 & 0.530 \end{array}\right\}$	$\left\{\begin{array}{ccccc} -1 & -0.5 & 0 & 0.5 & 1 \\ 0.2 & 0.2 & 0.2 & 0.2 & 0.2 \end{array}\right\}$

We apply the likelihood test and compute the Monte Carlo p-values of T_{GCl} and T_{ClG}: p_{ClG}^m and p_{GCl}^m for $m = 1, \ldots, M$. We calculate the percentages of correct selection of the true model, i.e. the percentage of times that $p_{ClG}^m > p_{GCl}^m$ for $m = 1, \ldots, M$, when the data are generated from the Clayton copula, and the percentage of times that $p_{GCl}^m > p_{ClG}^m$ for $m = 1, \ldots, M$, when the data are generated from the Gumbel copula. The results are reported in the third and the fourth columns of Table 3.

We can observe that using the KL-optimum design the percentage of correct decision is around 72% from $n = 100$ and it exceed 90% from $n = 500$. Furthermore, the percentage of wrong decision decreases substantially as n increases. Taking into

Table 3 Monte Carlo simulation of the likelihood ratio test ($M = 5000$): data generated from Clayton and Gumbel copulae for $\tau = 0.8$ at the KL-optimum design ξ_{KL} (columns 3-4) and at the Uniform design ξ_{Unif} (columns 5-6)

n	Test decision	ξ_{KL} True copula model (%)		ξ_{Unif} True copula model (%)	
		Clayton	Gumbel	Clayton	Gumbel
100	Correct decision	72	71.88	60.54	32.64
	Wrong decision	28	28.12	39.46	67.36
200	Correct decision	82.28	84.04	67.50	43.12
	Wrong decision	17.72	15.96	32.50	56.88
500	Correct decision	95.56	95.4	81.20	63.38
	Wrong decision	4.44	4.6	18.80	36.62
1000	Correct decision	99.5	99.2	92.84	81.14
	Wrong decision	0.5	0.8	7.16	18.86

account that the competing models differ only for the tail dependence, the obtained results are excellent. Finally, for comparison purposes, we analyze the performance of the Uniform design defined in the second column of Table 2. The corresponding percentages of correct decision and wrong decision are listed in the fifth and sixth columns of Table 3. We can observe that the percentage of correct selections obtained with the KL-optimum design is substantially better than those corresponding to the uniform design, especially for $n < 500$.

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