行政院國家科學委員會補助專題研究計

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※ 留間隔的機率計算在 ※

※ Kolmogorov-Smirnov 統計量的應用 ※

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計畫主持人：林千代

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本成果報告包括以下應繳交之附件：

□赴國外出差或研習心得報告一份

□赴大陸地區出差或研習心得報告一份

☒出席國際學術會議心得報告及發表之論文各一份

□國際合作研究計畫國外研究報告書一份

執行單位：淡江大學數學系

中 華 民 國 89 年 10 月 30 日

行政院國家科學委員會專題研究計畫成果報告

留間隔的機率計算在 Kolmogorov-Smirnov 統計量的應用

計畫編號:NSC 89 - 2118- M- 032- 008

執行期限:88年8月1日至89年10月31日

主持人: 林千代　　執行機構及單位名稱: 淡江大學數學系

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中文摘要

我們利用一個能夠計算一般化留間隔或指數隨機變數 的線性組合的機率分配之演算法來取得 Kolmogorov-Smirnov 統計量的機率分配之 真實值.

關鍵詞:Kolmogorov-Smirnov 統計量, 符號計算.

Abstract

We use an algorithm which is capable of computing exact expressions for the distribution of the maximum or minimum of an arbitrary finite collection of linear combinations of spacings or exponential random variables with rational coefficients to obtain the distributions of the Kolmogorov-Smirnov statistic.

Keywords: Kolmogorov-Smirnov statistic, symbolic computations.

1 Introduction

Let $S^{(n)}$ denote the vector of spacings between n random points on the interval $(0,1)$. More precisely, suppose that $X_1, X_2, \ldots, X_n$ are i.i.d. from a uniform distribution on the interval (0, 1), and let $X_{(1)} \leq X_{(2)} \leq \cdots \leq X_{(n)}$ be the corresponding order statistics. We define the spacings $S_1, S_2, \ldots, S_{n+1}$ to be the successive differences between the order statistics $S_i = X_{(i)} - X_{(i-1)}$, where we take $X_{(0)} = 0$ and $X_{(n+1)} = 1$. Finally, we define $\boldsymbol{S}^{(n)} = (S_1, S_2, \ldots, S_{n+1})'$. This report is concerned with the application of the evaluation of probabilities involving linear combinations of spacings with arbitrary rational coefficients. We use an algorithm which is able to evaluate

$$P(\boldsymbol{A}\boldsymbol{S}^{(n)} > t\boldsymbol{b}) \tag{1}$$

where $\boldsymbol{A}$ is any matrix of rational values, $\boldsymbol{b}$ is any vector of rational values, and $t > 0$ is a real-valued scalar. (Note that, for vectors $\boldsymbol{x} = (x_i)$ and $\boldsymbol{y} = (y_i)$, we define $\boldsymbol{x} > \boldsymbol{y}$ to mean that $x_i > y_i$ for all i.) The algorithm produces an exact expression for the probability in (1) which is a piecewise polynomial in the argument t. With the derived expression, we can use symbolic math packages such as MAPLE to evaluate (1) to any required degree of precision.

2 Example

Before proceeding, we establish one notational convention. It is convenient to regard the probability in (1) as being defined even when the number of columns in $\boldsymbol{A}$ is less than $n+1$, the number of entries in $\boldsymbol{S}^{(n)}$. Let k be the number of columns in $\boldsymbol{A}$. If $k < n+1$, then in computing $\boldsymbol{A}\boldsymbol{S}^{(n)}$ we simply discard the extra entries of $\boldsymbol{S}^{(n)}$, or equivalently, we pad the matrix $\boldsymbol{A}$ with extra columns of zeros and define

$$\boldsymbol{A}\boldsymbol{S}^{(n)} = (\boldsymbol{A} \,|\, 0)\boldsymbol{S}^{(n)}. \tag{2}$$

Our expressions for (1) are written in terms of a function $R(j,\lambda)$ defined for integers $j \geq 0$ and real values $\lambda \geq 0$ by

$$R(j,\lambda) = \begin{cases} \binom{n}{j} t^j (1-\lambda t)^{n-j} & \text{for } \lambda t < 1, \\ 0 & \text{for } \lambda t \geq 1. \end{cases} \tag{3}$$

The dependence of R on n and t can be left implicit because these values are fixed in any given application of our methods. If we replace $\boldsymbol{S}^{(n)}$ in (1) by a vector $\boldsymbol{Z}$ of i.i.d. exponential random variables with mean 1, then our expressions remain valid so long as we redefine R to be

$$R(j,\lambda) = \frac{t^j}{j!} e^{-\lambda t}. \tag{4}$$

We use the algorithm to compute the distribution of the Kolmogorov-Smirnov (K-S) statistic $D_n = \sup_x |F_n(x) - F(x)|$ where F_n is the empirical cdf of n i.i.d. observations from a continuous distribution F. The distribution of D_n does not depend on F, so we can assume that F is the uniform distribution on $(0,1)$.

We may express D_n in terms of the spacings as $D_n = \max(D_n^+, D_n^-)$ where

$$\begin{aligned} D_n^+ &= \sup_x (F_n(x) - x) \qquad (5) \\ &= 0 \vee \max_{1\leq k\leq n} \left(\frac{k}{n} - (S_1 + \cdots + S_k) \right) \end{aligned}$$

and

$$\begin{aligned} D_n^- &= \sup_x (x - F_n(x)) \\ &= 0 \vee \max_{1\leq k\leq n} \left((S_1 + \cdots + S_k) - \frac{k-1}{n} \right). \end{aligned}$$

Thus, for any integer i from 1 to $n-1$, we have

$$\{D_n < i/n\} = \{D_n^+ < i/n\} \cap \{D_n^- < i/n\}$$

where

$$\{D_n^+ < i/n\} = \bigcap_{i+1\leq k\leq n} \{S_1 + \cdots + S_k > (k-i)/n\} \tag{6}$$

and

$$\{D_n^- < i/n\} = \bigcap_{1\leq k\leq n-i} \{S_1 + \cdots + S_k < (k+i-1)/n\}.$$

Now, we obtain a problem in the form (1) which can be solved by the algorithm. Note that for this problem we do not need the variable t in equation (1), that is, we set $t = 1$.

Here are some numerical results obtained using the algorithm.

$$\begin{aligned} P(D_{14} < 3/14) &= \frac{14831925552873}{28346956187648} \\ &\approx .52322815383388 \\ P(D_{14} < 5/14) &= \frac{2661531270146463}{2778001706389504} \\ &\approx .95807402278582 \end{aligned} \tag{7}$$

In this example, these expressions have no useful interpretations as functions of t, so we have simply evaluated them at $t = 1$.

It is, of course, well known how to compute the exact distribution of D_n, at least when n is not too large. For instance, the original approach of Kolmogorov (see Birnbaum (1952)) can also be used to obtain the results in (7). The algorithm has no advantage over Kolmogorov's approach in this particular problem. The advantage of our method is its flexibility. For example, a popular variant of the K-S statistic uses $k/(n+1)$ in place of k/n and $(k-1)/n$ in (6). Our method can handle this statistic by making the obvious minor changes to the setup above. As another example, if the larger values of X_i are censored, then one may wish to define a K-S type statistic based only on the lower order statistics $X_{(1)}, \ldots, X_{(m)}$ where $m < n$. Such statistics are also easily handled by our approach.

3 References

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行政院國家科學委員會補助國內專家學者出席國際學術會議報告

89 年 10 月 30 日

附件三

報告人姓名	林千代	服務機構及職稱	淡江大學數學系 副教授
會議 時間 地點	8/13/00-8/17/00 Indianapolis, USA	本會核定補助文號	
會議名稱	(中文)2000 年美國統計年會 (英文)2000 Joint Statistical Meetings		
發表論文題目	(中文)臨床試驗調適和隨機配置的模擬研究 (英文)A simulation study on the adaptive assignment versus randomization in clinical trials		

報告內容應包括下列各項：

一、參加會議經過

我抵達 Indianapolis 之後就遇上數位相熟國內外的學者.常常利用休息時間互相交換研究心得. 8/16/00 當天我發表論文，並獲得熱烈迴響，有多位國外學者對我的論文表示興趣，向我索取論文回去. 此外，多位國外學者也邀請我多參與他們的研究領域或會議.

二、與會心得

此次會議在大會的精心安排下頗為成功. Data Mining, Missing Data and Multiple Imputation, Longitudinal Data, Survival Analysis, Genetic Applications, Spatial Statistic, Semiparametric Latent Structures, Introductory Overview Lectures, Box's talk about Prof. Demings 都是我此行參與的部分. 其中, Bayesian Computation in Win Bugs 是最吸引我的內容. 我希望能將此流行的軟體帶回系裡與研究生分享.

三、考察參觀活動(無是項活動者省略)

無

四、建議

會議內容很多，可以吸收目前流行的研究與新知. 大會安排下之 Introductory Overview Lectures 更可以幫助我在演講中瞭解更多學識. 大家應該多參與國際會議.

五、攜回資料名稱及內容

大會議程，會議論文大綱，論文數篇.

六、其他

A Simulation Study on the Adaptive Assignment versus Randomization in Clinical Trials

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Abstract

Consider a clinical trial to compare two treatments where response is dichotomous and patients enter the trial sequentially. We investigate the conduct of such a trial where four adaptive procedures and three randomizations are used to assign patients to the different therapies. Our goal of this study is to find a suitable policy that we can cure at least certain percent of patients with high probability.

Key words: Play-the-winner/switch-from-a-loser; Robust Bayes.

1 Introduction

Suppose that two treatments are available for use in a clinical trial. Further suppose that the response to treatment is either positive (a success) or negative (a failure) and that the patients arrive sequentially, with each patient's response available before the next patient is to be treated. The number of patients in the trial is fixed at n. Our goal is to maximize the probability of getting at least k successes out of n patients (treatments). Is there any satisfactory procedure to achieve this goal?

To answer this question, one may first consider to use the randomized designs. Randomization is usually used to provide insurance against the possibility of systematic differences between the units, which might affect inferences about the treatments under investigation. Other compatible methods that have received considerable recent attention are adaptive procedures. The aim of these methods is to treat patients in the trial effectively, which is accomplished by allowing treatment allocation to depend on accumulating information. See Thompson (1933), Feldman (1962), Zelen (1969), Sobel and Weiss (1971), Berry (1978), Bather (1981), and Berry and Fristedt (1985) for more details on the application of the adaptive methods in clinical trials.

More recently, Berry and Eick (1995) have given some discussion and comparison among randomization and the adaptive allocation of patients to treatments by maximizing the expected number of successes over all present and future patients. In this work we extend their study on a different aspect which may provide a substantial information on medical practice.

We now give a formal statement of the optimization problem. Suppose that each of n patients is to be treated with one of two treatments, A and B. Treatment allocation is sequential and the responses are dichotomous and immediate. The probability of a success with treatment A is α, and with treatment B is β (we can assume (α, β) uniformly distributed over $(0,1) \times (0,1)$). We are interested in searching an appropriate procedure that maximizes the probability of getting at least k successes out of n patients (treatments). It is not difficult to study the asympotic behavior of this problem. Now the main objective to this research is to study the case with finite n.

In order to formulate it, we need some notation. Let $Z_j, j = 1, 2, ..., n$, denote the response of patient j. The value of Z_j is 1 or 0 if the response is positive or negative respectively. Let $\mathcal{D}$ be the class of all treatment allocation procedures. Given any n and k $(1 \leq k \leq n)$, the conditional probability of reaching the goal (given α and β) of procedure $\tau \in \mathcal{D}$ is

$$P_\tau(k, n|\alpha, \beta) = P_\tau(\sum_{i=1}^{n} Z_i \geq k|\alpha, \beta), \tag{1}$$

where the distribution of the Z_i's is determined by τ. It is easy to see that the probability in (1) can not be greater than

$$P(k, n|\alpha, \beta) = \sum_{i=k}^{n} \binom{n}{i} \gamma^i (1-\gamma)^{n-i},$$

where $\gamma = \max(\alpha, \beta)$. Let

$$L_\tau(k, n|\alpha, \beta) = P(k, n|\alpha, \beta) - P_\tau(k, n|\alpha, \beta)$$

be the conditional probability lost (CPL) under the procedure τ. From these numerical results we can then find our suitable procedure.

2 Procedures

There are 7 possible procedures used in this kind of bandit problems. For convenience we shall assume that n is an even positive integer. A complete account of these procedures can be found in the paper of Berry and Eick (1995) and the references contained therein.

• Procedure **ER** (Equal Randomized): Half of the n patients are randomly assigned to treatment A and the other half to B.

• Procedure **RR** (Repeatedly Randomized): Randomized every time, but with equal probability.

• Procedure **SR** (Single Randomized): Randomized only the first time, then use that treatment all the time.

• Procedure **JB**: Randomized each time with the following adaptive procedure. Treatments A and B are randomly assigned to first two patients so that each patient receives a different therapy. Suppose that during the trial t $(2 \leq t < n)$ patients have been treated, and successes and failures on the treatments A and B, s_x, f_x, s_y, and f_y have been observed respectively ($s_x + f_x + s_y + f_y = t$). Define

$$\lambda(k) = \frac{4+\sqrt{k}}{15k} .$$

Let

$$\lambda_x = \lambda(s_x + f_x),\ \lambda_y = \lambda(s_y + f_y),$$

and

$$q = \frac{s_x}{s_x + f_x} - \frac{s_y}{s_y + f_y} + 2(\lambda_x - \lambda_y).$$

Under this procedure the next patient (patient $t+1$) receives treatment A with probability

$$\begin{cases} \dfrac{\lambda_x}{\lambda_x + \lambda_y} \exp(q/\lambda_x) & \text{for } q \leq 0, \\ 1 - \dfrac{\lambda_y}{\lambda_x + \lambda_y} \exp(q/\lambda_y) & \text{for } q \geq 0. \end{cases}$$

- Procedure **PW** (Play–the–winner/Switch–from–a–loser): The first patient will either receive treatment A or B, each with probability 0.5. For patients 2 to n the treatment given to the previous patient is used again if it was successful; otherwise the other treatment is used.
- Procedure **RB** (Robust Bayes): The randomization of this policy is based on a uniform prior density

$$\pi(\alpha, \beta) = 1 \text{ on } (0,1) \times (0,1).$$

Because of the symmetry property of the uniform prior distribution, the treatments for the first patient are initially equivalent and hence can be chosen at random. If the first patient has a success, then the second patient receives the same treatment. On the contrary, if the first patient has a failure, then the second patient receives the other treatment. That is, procedure RB imitates procedure PW for the first two treatment assignments. The same treatment is used as long as it is successful. However, after a failure, switching to the other treatment may or may not be optimal. If the data sufficiently strongly favor the treatment that has just failed, then that treatment will be used again. In other words, if the current probability of success of treatment A (which is the current posterior expected value of α, $(s_A + 1)/(s_A + f_A + 2)$, is greater than that of treatment B, then treatment A is used. Also, if both treatments are judged equally effective at any stage, then the next treatment assignment will be randomized.

- Procedure **PR** (Posterior Probability Ratio): A new proposed procedure which uses the posterior probability to select treatment A or B. Like procedure JB, for patients 1 to n this procedure randomizes between treatment A and B. Randomization is based on the current expected values of α and β assuming a uniform prior density on (α, β). The next patient receives treatment A with probability equal to

$$\frac{E(\alpha)}{E(\alpha) + E(\beta)} = \frac{(s_A + 1)/(s_A + f_A + 2)}{(s_A + 1)/(s_A + f_A + 2) + (s_B + 1)/(s_B + f_B + 2)}.$$

3 Probabilities

For the procedures ER, SR, RR and PW we can derive the necessary formula for computing the probabilities of gettig at least k successes out of n trials , $P_\tau(k, n|\alpha, \beta)$, for various α and β. Since n is even, we let $n = 2m$.

For procedures ER, SR, and RR we can easily write the explicit formula as the followings:

$$\begin{aligned} P_{ER}(k, 2m|\alpha, \beta) &= \sum_{j=0}^{m} \binom{m}{j} \alpha^j (1-\alpha)^{m-j} \left[\sum_{\ell=k-j}^{m} \binom{m}{\ell} \beta^\ell (1-\beta)^{m-\ell} \right], \\ P_{SR}(k, 2m|\alpha, \beta) &= \frac{1}{2} \sum_{j=k}^{2m} \binom{2m}{j} \left\{ \alpha^j (1-\alpha)^{2m-j} + \beta^j (1-\beta)^{2m-j} \right\}, \\ P_{RR}(k, 2m|\alpha, \beta) &= \sum_{j=k}^{2m} \binom{2m}{j} \left(\frac{\alpha+\beta}{2} \right)^j \left(1 - \frac{\alpha+\beta}{2} \right)^{2m-j}. \end{aligned}$$

For procedure PW and the number of successes k in $2m$ trials is even, we may terminate with a success on treatment A and an equal number of failures, $(2m-k)/2$ on both treatments if we start with treatment A (probability 1/2). If we start with treatment B (probability 1/2) and make a success termination with treatment A, then k is odd and the number of failures for treatment A, B is $(2m-k-1)/2$, $(2m-k+1)/2$, repectively. The same argument implies to the case if the process terminates with a success on treatment B. Then, for k is even,

$$\begin{aligned} & P_{PW}\left(\sum_{i=1}^{2m} Z_i = k|\alpha, \beta \right) \\ = \; & \frac{1}{2} \sum_{\ell=1}^{k} \binom{\frac{2m-k}{2} + \ell - 1}{\frac{2m-k}{2}} \alpha^\ell (1-\alpha)^{\frac{2m-k}{2}} \binom{\frac{2m-k}{2} + k - \ell - 1}{k-\ell} \beta^{k-\ell} (1-\beta)^{\frac{2m-k}{2}} \\ + \; & \frac{1}{2} \sum_{\ell=1}^{k} \binom{\frac{2m-k}{2} + \ell - 1}{\frac{2m-k}{2}} \beta^\ell (1-\beta)^{\frac{2m-k}{2}} \binom{\frac{2m-k}{2} + k - \ell - 1}{k-\ell} \alpha^{k-\ell} (1-\alpha)^{\frac{2m-k}{2}}, \end{aligned}$$

and, for k is odd,

$$\begin{aligned} & P_{PW}\left(\sum_{i=1}^{2m} Z_i = k|\alpha, \beta \right) \\ = \; & \frac{1}{2} \sum_{\ell=1}^{k} \binom{\frac{2m-k-1}{2} + \ell - 1}{\frac{2m-k-1}{2}} \alpha^\ell (1-\alpha)^{\frac{2m-k-1}{2}} \binom{\frac{2m-k-1}{2} + k - \ell}{k-\ell} \beta^{k-\ell} (1-\beta)^{\frac{2m-k+1}{2}} \\ + \; & \frac{1}{2} \sum_{\ell=1}^{k} \binom{\frac{2m-k-1}{2} + \ell - 1}{\frac{2m-k-1}{2}} \beta^\ell (1-\beta)^{\frac{2m-k-1}{2}} \binom{\frac{2m-k-1}{2} + k - \ell}{k-\ell} \alpha^{k-\ell} (1-\alpha)^{\frac{2m-k+1}{2}}. \end{aligned}$$

Thus,

$$\begin{aligned} & P_{PW}(k, 2m|\alpha, \beta) \\ = \; & \sum_{j=k}^{2m} \left[P_{PW}\left(\sum_{i=1}^{2m} Z_i = j \text{ and } j \text{ is even } |\alpha, \beta \right) + P_{PW}\left(\sum_{i=1}^{2m} Z_i = j \text{ and } j \text{ is odd } |\alpha, \beta \right) \right] \end{aligned}$$

Remark. The fundamental dynamic program equations for this problem under the procedures RB, JB, and PR have not been developed.

4 Numerical Studies

The recursive formula to calculate the probability that of gettig at least k successes out of n trials for these procedures can be developed, however, the formula can be very difficult to compute. Therefore, we conduct a simulation study to estimate these probabilities obtained from 10000 iterations. For selected values of k, α, β, and $n = 100$, we evaluate these procedures on the basis of the conditional probability lost (CPL) discussed in Section 2.

Among three randomizations procedures ER and RR perform most likely to each other and

- for $\alpha = 0.25$ and $k = 40, 50, 60, 70, 80$, procedure SR does better than procedures ER and RR when $\beta \leq k/n + 0.1$. However, SR is the worse if $\beta > 0.55$ with $k = 40$, and $\beta > 0.75$ with $k = 50$.
- for $\alpha = 0.5$, procedure SR is the best when $k = 80$. It also does better in the cases in which $\beta \leq 0.3$ with $k = 40$, $\beta \leq 0.5$ with $k = 50$, $\beta \leq 0.7$ with $k = 60$, $\beta \leq 0.85$ with $k = 70$, however, it performs badly for other values of β in each k.
- for $\alpha = 0.75$, procedure SR is the worse when $k = 40$. It does better again in the cases in which $\beta < 0.3$ with $k = 50$, $\beta < 0.45$ with $k = 60$, $\beta < 0.7$ with $k = 70$, $\beta < 0.8$ with $k = 80$, but performs poorly for other values of β in each k.

Among four adaptive procedures, procedures PW and PR are very compatible, but not as good as procedures JB and RB. Procedure PW does better than PR when $k = 40$ and 50, and procedure PR performs better than PW when $k = 60, 70, 80$. Also, the best procedure among three randomizations only performs better than PW or PR in some particular cases.

The comparison of procedures JB and RB can be summarized as follows:

- For $\alpha = 0.25$, procedure RB is the best if $\beta < k/n + 0.1$ and procedure JB is the best in other values of β with $k = 40, 50, 60$, and 70. Procedure RB is the best with $k = 80$.
- When $\alpha = 0.5$, procedure RB is the best in the cases in which $\beta < 0.2$ with $k = 40$, $\beta < k/n$ with $k = 50, 60, 70$, $\beta < 0.85$ with $k = 80$, and procedure JB performs better in other values of β in each k.
- When $\alpha = 0.75$, procedure JB is as good as other procedures or the best with $k = 40, 50, 60$. Also, procedure RB is the best whenever $\beta < 0.5$ with $k = 70$, and $\beta < 0.75$ with $k = 80$, and procedure JB is the best for the rest values of β for $k = 70, 80$.

On the whole, three randomizations are not doing as good as four adaptive procedures. Procedure RB is superior when $\alpha = 0.25, 0.5$ with $\beta < k/n + 0.1$, and JB is as good or better than any other procedures when $\alpha = 0.75$. To conclude the current study, I would like to make some recommendation for using these procedures in maximizing the proportion of the successes in the trial. For small or intermediate value of α with $\beta < k/n + 0.1$ I recommend using RB, and using JB for other values of β. For large value of α I recommend using JB for $\beta \leq k/n$.

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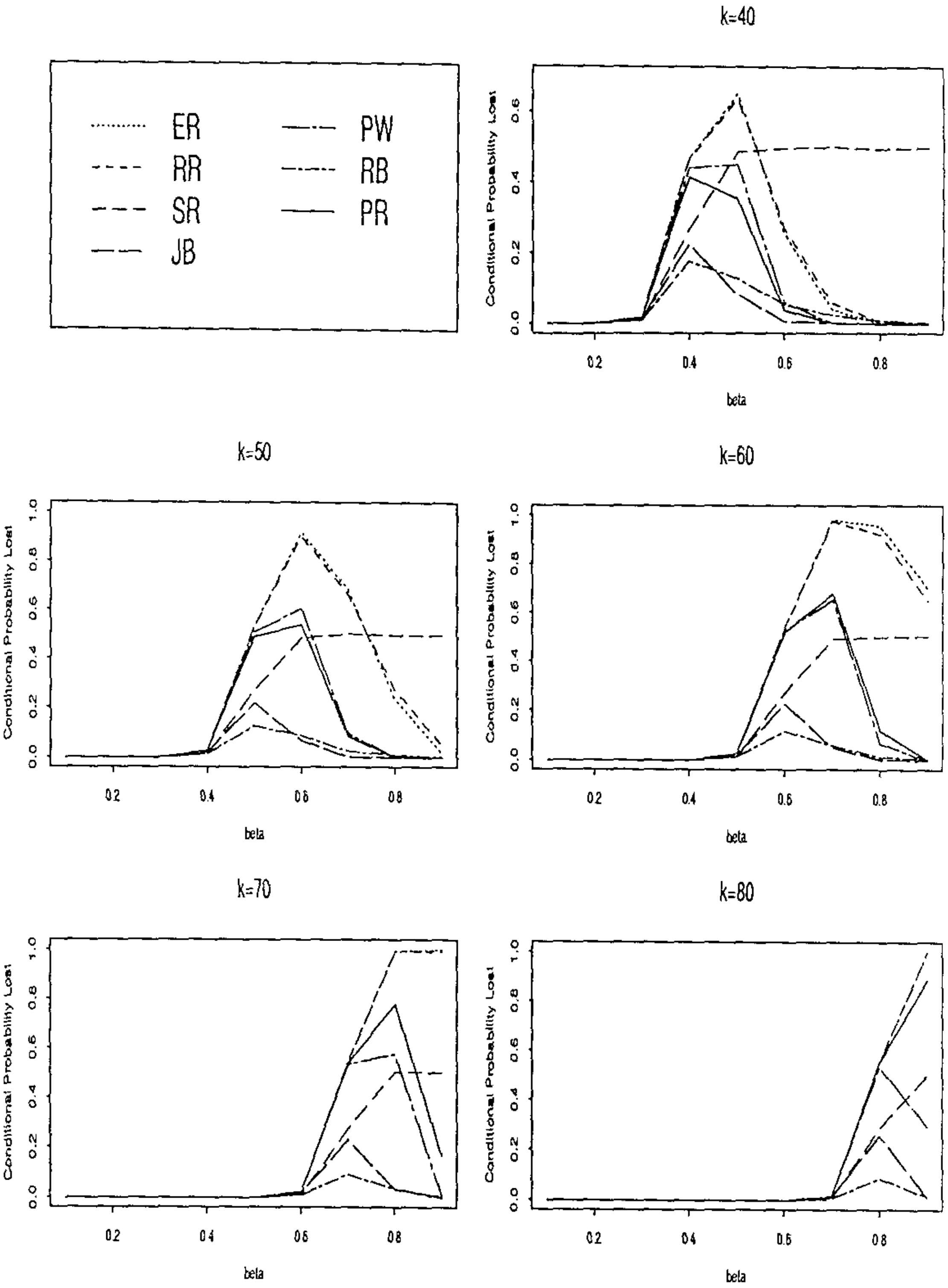

Figure 1: These lines show the conditional probability lost for the indicated procedures with $\alpha = 0.25$ and $n = 100$.

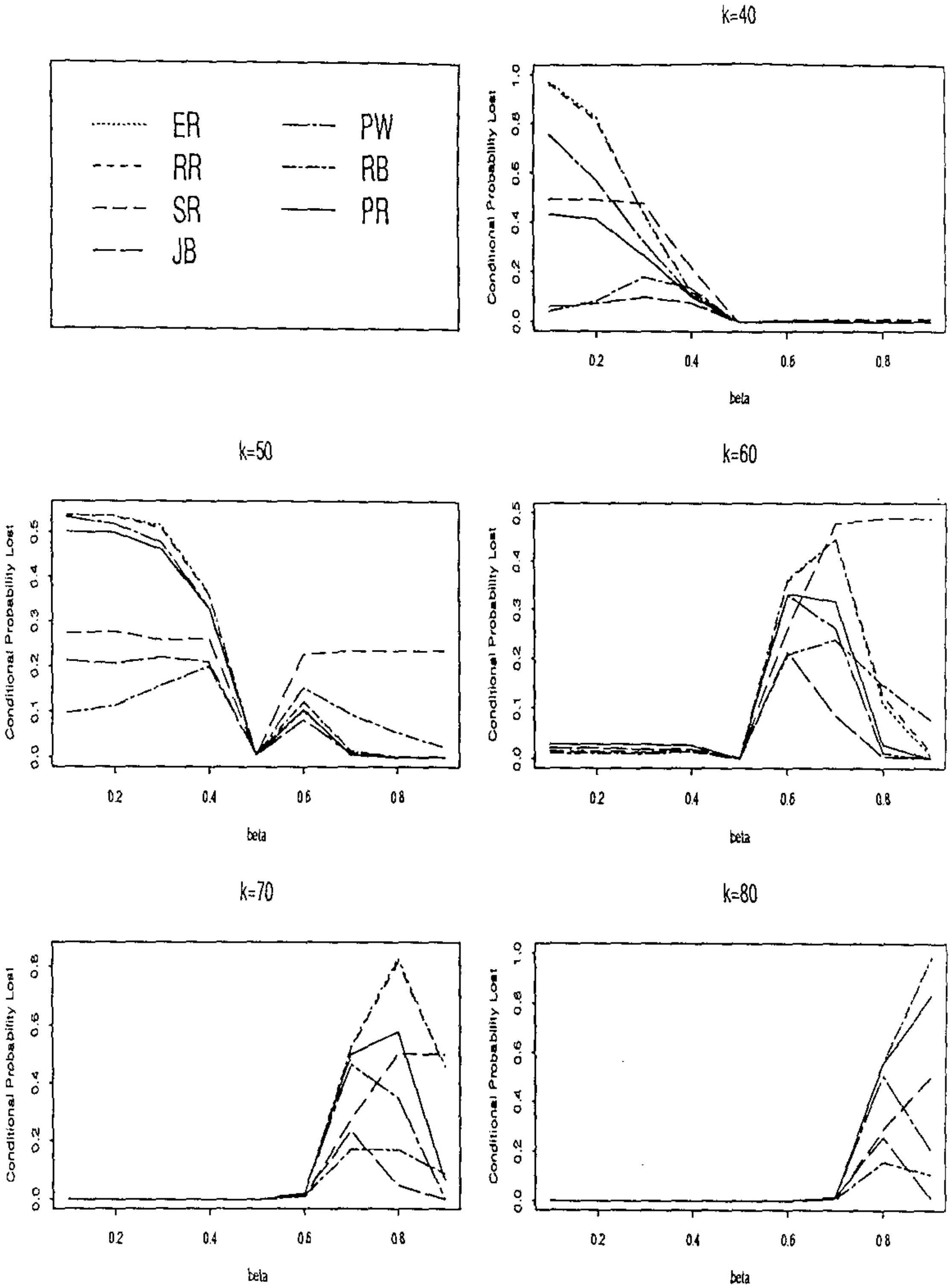

Figure 2: These lines show the conditional probability lost for the indicated procedures with $\alpha = 0.50$ and $n = 100$.

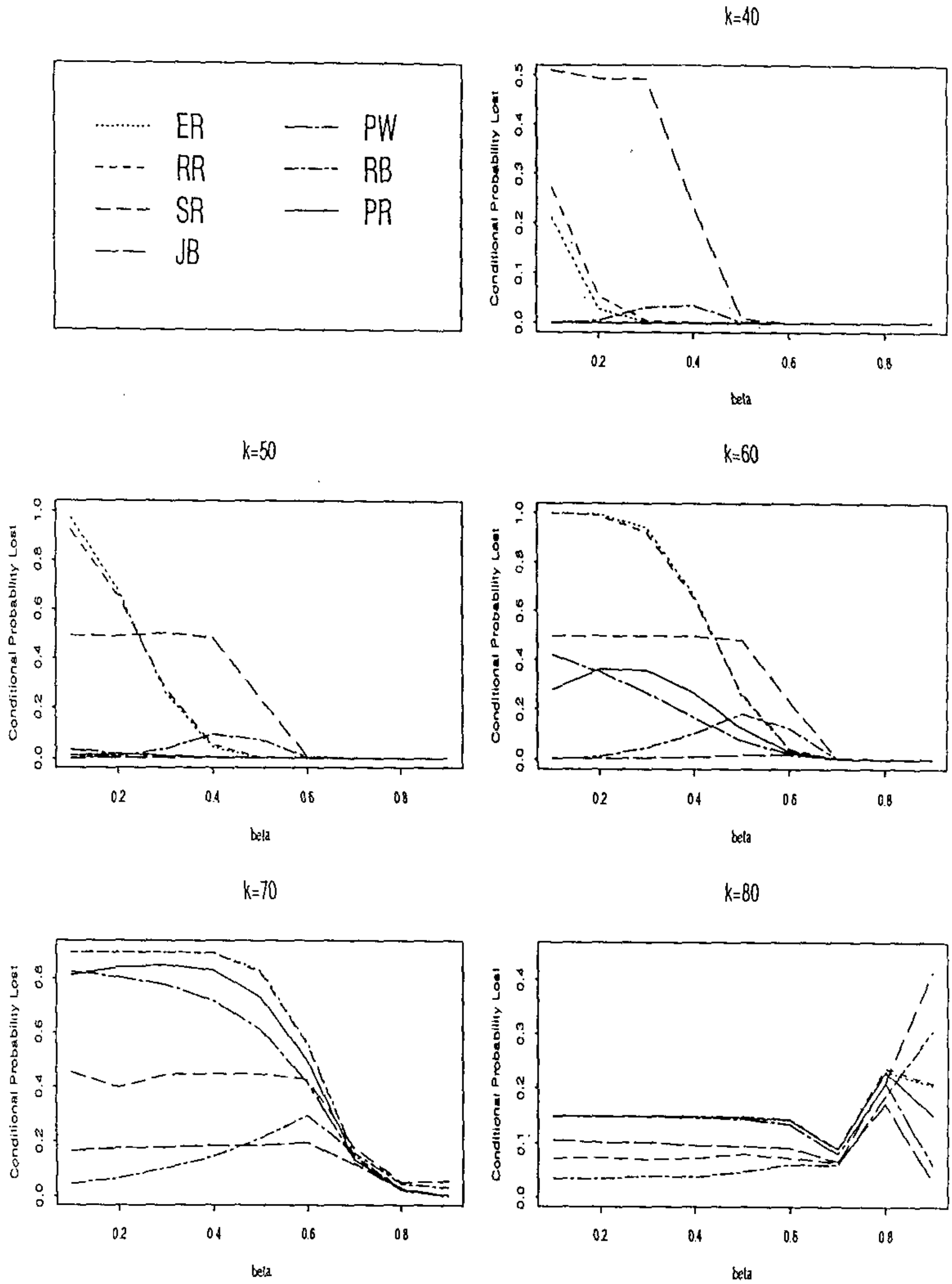

Figure 3: These lines show the conditional probability lost for the indicated procedures with $\alpha = 0.75$ and $n = 100$.