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Selection for linear structure models with different variances

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abstract

This paper is concerned with selection of some linear structure models with different variances. The models are based on the study of relationships between two fracture toughness testing methods of dental luting cemments. The measurements are made by using several kinds of materials. They are assumed to have different variances depending on the materials, but they have the same variance between two testing methods. For such data, we consider three types of structures between two methods: (1) proportionality, (2) linearity, and (3) no structure. We give Akaike information criterion, AIC, to evaluate these models. Then, we derive corrected AIC (CAIC) which is useful for small samples. By simulation experiments, we find that CAIC is more effective than AIC in the case of small samples. Our results are applied to a real data of dental luting cements.

1 Introduction

This paper is concerned with selection of linear structure models with different variances. The models are based on the study of relationships between two fracture toughness testing methods of dental luting cemments, by using several kinds of materials. Such an example is given in Section 5.

Suppose that two testing methods are examined by using m materials. Let

$$X_{ijk},\ i=1,2;\ j=1,\ldots,m;\ k=1,\ldots,n_{ij}, \tag{1.1}$$

be the kth measurement of the jth material by the ith testing method. It is assumed that $X_{ij1},\ldots,$ $X_{ijn_{ij}}$ are independently and identically distributed as $N(\mu_{ij},\sigma_j^2)$, i.e., for $i=1,2$ and $j=1,\ldots,m$,

$$X_{ijk}\sim N(\mu_{ij},\sigma_j^2),\ k=1,\ldots,n_{ij}. \tag{1.2}$$

The data are expressed as in Table 1 below.

Table 1. The data on toughness testing methods by using diffent dental luting cements

method i	material j	sample			mean	variance
1	1	x_{111}	$\cdots$	$x_{11n_{11}}$	μ_{11}	σ_1^2
	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$
	m	x_{1m1}	$\cdots$	$x_{1mn_{1j}}$	μ_{1m}	σ_m^2
2	1	x_{211}	$\cdots$	$x_{21n_{21}}$	μ_{21}	σ_1^2
	$\vdots$	$\vdots$		$\vdots$	$\vdots$	$\vdots$
	m	x_{2m1}	$\cdots$	$x_{2mn_{2j}}$	μ_{2m}	σ_m^2

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Now we are intersting wheter there is a linear structure between $(\mu_{11},\ldots,\mu_{1m})$ and $(\mu_{21},\ldots,\mu_{2m})$ or not. For that purpose we consider three types of structure models:

$$\begin{aligned} &M_1: \ \mu_{2j}=\gamma\mu_{1j},\ \gamma\neq 0,\quad j=1,\cdots,m,\\ &M_2: \ \mu_{2j}=\beta\mu_{1j}+\alpha,\ \beta\neq 0,\quad j=1,\cdots,m,\\ &M_3: \ \text{otherwise}, \end{aligned} \tag{1.3}$$

where γ, α and β are unknown. The models M_1 and M_2 show that two methods are essentially the same, though their relationships are different. We apply Akaike information criterion (AIC, Akaike (1973)) to evaluate these models. Various linear functional relationships have been considered, see e.g. Anderson (1984), Fuller (1987). However, it may be noted that the linear functional relationship as in M_1 and M_2 has not been discussed.

The AIC is given in Section 2. In Section 3 we study the risk and the bias of AIC, and propose a corrected AIC, i.e., CAIC. In Section 4, two criteria AIC and CAIC are compared by simulation experiments. It is shown that CAIC is more effective than AIC in the case of small samples. In Section 5, we give an example of two fracture toughness testing methods by using six dental luting cemments.

2 Derivation of AIC

In general, AIC was proposed as a criterion of evaluating a model by Akaike (1973). Let $\boldsymbol{x}$ and $\boldsymbol{\theta}$ be the column vectors of all the observations x_{ijk} and the parameters μ_{ij} and σ_j^2, respectively. Let the log-likelihood be denoted by $\ell(\boldsymbol{\theta}|\boldsymbol{x})$. Then, AIC is given by

$$AIC=-2\ell(\hat{\boldsymbol{\theta}}|\boldsymbol{x})+2d, \tag{2.1}$$

where $\hat{\boldsymbol{\theta}}$ is the maximum likelihood estimator (MLE) of $\boldsymbol{\theta}$, and d is the dimension of a model, or the number of independent parameters involved in a model.

Let d_1, d_2 and d_3 be the dimension d for models M_1, M_2 and M_3 given in (1.3), respectively. Then, the dimensions are as follows:

$$d_1=2m+1\ ,\ d_2=2m+2\ ,\ d_3=3m. \tag{2.2}$$

The density function of X_{ijk} is

$$f(x_{ijk}|\mu_{ij},\sigma_j^2)=\frac{1}{\sqrt{2\pi\sigma_j^2}}\exp\left\{-\frac{1}{2}\frac{(x_{ijk}-\mu_{ij})^2}{\sigma_j^2}\right\},$$

since X_{ijk} is distributed as $N(\mu_{ij},\sigma_j^2)$. Then, the log-likelihood function of $\boldsymbol{\theta}$ is

$$\begin{aligned} \ell(\boldsymbol{\theta}|\boldsymbol{x}) &= \log\prod_{i=1}^{2}\prod_{j=1}^{m}\prod_{k=1}^{n} f(x_{ijk}|\mu_{ij},\sigma_j^2)\\ &= -\frac{1}{2}\sum_{j=1}^{m}\left\{n_j\log 2\pi+n_j\log\sigma_j^2\right\}\\ &\quad -\frac{1}{2}\sum_{i=1}^{2}\sum_{j=1}^{m}\frac{1}{\sigma_j^2}\sum_{k=1}^{n_{ij}}(x_{ijk}-\mu_{ij})^2, \end{aligned} \tag{2.3}$$

where $n_j = n_{1j} + n_{2j},\ j = 1, \ldots, m$. Let $\hat{\sigma}^2_{j;a}$ be the MLE of σ_j^2 under the model M_a. Then, the AIC for M_a is expressed as

$$AIC_a = \sum_{j=1}^{m} n_j \log \hat{\sigma}^2_{j;a} + n\{\log(2\pi) + 1\} + 2d_a,\ a = 1, 2, 3, \tag{2.4}$$

where $n = n_1 + \cdots + n_m$. In the following, we give the MLE's of the unknown parameters as well as σ_j^2 under M_1, M_2 and M_3. Let

$$\bar{x}_{ij} = \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} x_{ijk},\quad s_{ij}^2 = \frac{1}{n_{ij}} \sum_{k=1}^{n_{ij}} (x_{ijk} - \bar{x}_{ij})^2.$$

For simplicity, first consider the case M_3. The independent unknown parameters are μ_{1j}, μ_{2j} and σ_j^2, and it is easy to see that their MLE's are given by

$$\hat{\mu}_{1j} = \bar{x}_{1j},\ \hat{\mu}_{2j} = \bar{x}_{2j},\ \hat{\sigma}_j^2 = \frac{1}{n_j}(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2). \tag{2.5}$$

Therefore, the $\hat{\sigma}^2_{j;3}$ in (2.4) is given by

$$\hat{\sigma}^2_{j;3} = \frac{1}{n_j}(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2),\ j = 1, \ldots, m. \tag{2.6}$$

Next consider the case M_1. The independent unknown parameters are μ_{1j}, γ and σ_j^2. It is shown that the MLE's are solutions of the following likelihood equations:

$$\frac{\partial}{\partial \mu_{ij}} \ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0,\ \frac{\partial}{\partial \sigma_j^2} \ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0,\ \frac{\partial}{\partial \gamma} \ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0.$$

Solving the likelihood equations $(\partial/\partial\mu_{1j})\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$,

$$\begin{aligned}
&-\frac{1}{2}\frac{1}{\sigma_j^2}\left\{-2\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j}) - 2\gamma\sum_{k=1}^{n_{2j}}(x_{2jk} - \gamma\mu_{1j})\right\} = 0,\\
&\Leftrightarrow (n_{1j}\bar{x}_{1j} + \gamma n_{2j}\bar{x}_{2j}) - (n_{1j} + \gamma^2 n_{2j})\mu_{1j} = 0,\\
&\Leftrightarrow \mu_{1j} = \frac{1}{n_{1j} + \gamma^2 n_{2j}}(n_{1j}\bar{x}_{1j} + \gamma n_{2j}\bar{x}_{2j}). \qquad (2.7)
\end{aligned}$$

Similarly, solving $(\partial/\partial\sigma_j^2)\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$,

$$\begin{aligned}
&-\frac{n_j}{2}\frac{1}{\sigma_j^2} + \frac{1}{2}\frac{1}{(\sigma_j^2)^2}\left\{\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j})^2 + \sum_{k=1}^{n_{2j}}(x_{2jk} - \gamma\mu_{1j})^2\right\} = 0,\\
&\Leftrightarrow \sigma_j^2 = \frac{1}{n_j}\left\{\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j})^2 + \sum_{k=1}^{n_{2j}}(x_{2jk} - \gamma\mu_{1j})^2\right\}. \qquad (2.8)
\end{aligned}$$

Sustituting (2.7) for (2.8), we have

$$\begin{aligned}
\sigma_j^2 = \frac{1}{n_j(n_{1j} + \gamma^2 n_{2j})}&\left\{(n_{1j} + \gamma^2 n_{2j})(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2)\right.\\
&\left.+ n_{1j}n_{2j}(\gamma\bar{x}_{1j} - \bar{x}_{2j})^2\right\}. \qquad (2.9)
\end{aligned}$$

Substituting (2.7) and (2.9) for the likelihood equation $(\partial/\partial\gamma)\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$, and simplfying the resultant equation, we find that the MLE $\hat{\gamma}$ of γ is a solution of

$$\sum_{j=1}^{m} \frac{(n_{1j}\bar{x}_{1j} + \gamma n_{2j}\bar{x}_{2j})(\gamma\bar{x}_{1j} - \bar{x}_{2j})}{(n_{1j} + \gamma^2 n_{2j})(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2) + n_{1j}n_{2j}(\gamma\bar{x}_{1j} - \bar{x}_{2j})^2} \times \frac{n_j n_{1j} n_{2j}}{n_{1j} + \gamma^2 n_{2j}} = 0. \tag{2.10}$$

Note that $\hat{\mu}_{1j}$ and $\hat{\sigma}_j^2 = \hat{\sigma}_{j;1}^2$ are given by (2.7) and (2.9) with $\gamma = \hat{\gamma}$, respectively.

Finally consider the case M_2. The independent unknown parameters are μ_{1j}, α, β and σ_j^2. The MLE's are solutions of the following likelihood equations:

$$\frac{\partial}{\partial\mu_{1j}}\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0,\ \frac{\partial}{\partial\sigma_j^2}\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0,\ \frac{\partial}{\partial\alpha}\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0,\ \frac{\partial}{\partial\beta}\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0.$$

Solving the likelihood equations $(\partial/\partial\mu_{1j})\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$,

$$\begin{aligned} & -\frac{1}{2}\frac{1}{\sigma_j^2}\left\{-2\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j}) - 2\beta\sum_{k=1}^{n_{2j}}(x_{2jk} - \alpha - \beta\mu_{1j})\right\} = 0, \\ & \Leftrightarrow (n_{1j}\bar{x}_{1j} + \beta n_{2j}\bar{x}_{2j} - \alpha\beta n_{2j}) - (n_{1j} + \beta^2 n_{2j})\mu_{1j} = 0, \\ & \Leftrightarrow \mu_{1j} = \frac{1}{n_{1j} + \beta^2 n_{2j}}(n_{1j}\bar{x}_{1j} + \beta n_{2j}\bar{x}_{2j} - \alpha\beta n_{2j}). \end{aligned} \tag{2.11}$$

Similarly, solving $(\partial/\partial\sigma_j^2)\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$,

$$\begin{aligned} & -\frac{n_j}{2}\frac{1}{\sigma_j^2} + \frac{1}{2}\frac{1}{(\sigma_j^2)^2}\left\{\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j})^2 + \sum_{k=1}^{n_{2j}}(x_{2jk} - \alpha - \beta\mu_{1j})^2\right\} = 0, \\ & \Leftrightarrow \sigma_j^2 = \frac{1}{n_j}\left\{\sum_{k=1}^{n_{1j}}(x_{1jk} - \mu_{1j})^2 + \sum_{k=1}^{n_{2j}}(x_{2jk} - \alpha - \beta\mu_{1j})^2\right\}. \end{aligned} \tag{2.12}$$

Sustituting (2.11) for (2.12), we have

$$\sigma_j^2 = \frac{1}{n_j(n_{1j} + \beta^2 n_{2j})}\left\{(n_{1j} + \beta^2 n_{2j})(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2) + n_{1j}n_{2j}(\bar{x}_2 - \alpha - \beta\bar{x}_{1j})^2\right\}. \tag{2.13}$$

Substituting (2.11) and (2.13) for the likelihood equations $(\partial/\partial\alpha)\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$ and $(\partial/\partial\beta)\ell(\boldsymbol{\theta}|\boldsymbol{x}) = 0$, and simplfying the resultant equations, we find that the MLE's $\hat{\alpha}$ and $\hat{\beta}$ of α and β are solutions of

$$\sum_{j=1}^{m} \frac{n_j n_{1j} n_{2j}(\bar{x}_{2j} - \alpha - \beta\bar{x}_{1j})}{(n_{1j} + \beta^2 n_{2j})(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2) + n_{1j}n_{2j}(\bar{x}_{2j} - \alpha - \beta\bar{x}_{1j})^3} = 0. \tag{2.14}$$

$$\sum_{j=1}^{m} \frac{(n_{1j}\bar{x}_{1j} + \beta n_{2j}\bar{x}_{2j} - \alpha\beta n_{2j})(\bar{x}_{2j} - \alpha - \beta\bar{x}_{1j})}{(n_{1j} + \beta^2 n_{2j})(n_{1j}s_{1j}^2 + n_{2j}s_{2j}^2) + n_{1j}n_{2j}(\bar{x}_{2j} - \alpha - \beta\bar{x}_{1j})^2} \times \frac{n_j n_{1j} n_{2j}}{n_{1j} + \beta^2 n_{2j}} = 0. \tag{2.15}$$

Note that $\hat{\mu}_{1j}$ and $\hat{\sigma}_j^2 = \hat{\sigma}_{j;2}^2$ are given by (2.11) and (2.13) with $\alpha = \hat{\alpha}$ and $\beta = \hat{\beta}$, respectively.

3 The bias of AIC and its correction

In general, AIC was introduced as an asymptotically unbiased estimator of the predictive risk function of a model. Let $\boldsymbol{X}$ be a random vector whose components consists of all the random variables X_{ijk}. In our model the risk function is expressed as

$$R_A = E^*_{\boldsymbol{Y}} E^*_{\boldsymbol{X}}[-2\ell(\hat{\boldsymbol{\theta}}|\boldsymbol{Y})] \tag{3.1}$$

where $\boldsymbol{Y}$ is a random vector whose componets consist of all the future variables Y_{ijk} corresponding to X_{ijk}. It is assumed that $\boldsymbol{Y}$ has the same distribution as $\boldsymbol{X}$ and is independent of $\boldsymbol{X}$. The expectation E^* denotes the one with respect to the true model. The bias when we estimate the risk function by $-2\ell(\hat{\boldsymbol{\theta}}|X)$ is written as

$$B_A = E^*_{\boldsymbol{Y}} E^*_{\boldsymbol{X}}[-2\ell(\hat{\boldsymbol{\theta}}|\boldsymbol{Y}) + 2\ell(\hat{\boldsymbol{\theta}}|\boldsymbol{X})]. \tag{3.2}$$

AIC uses $2d$ as an estimator of B_A. Sugiura (1978) obtained more precise expressions of B_A for some models, assuming that the true model is included in the model considered. The AIC with such biases is called CAIC. Further, Fujikoshi and Satoh (1997) proposed to estimate B_A, relaxing the assumption that the true model is included in the candidate model. The bias of AIC in our model is

$$\begin{aligned} B_A = &\sum_{j=1}^{m}(n_j\sigma_j^2)E\Big[\frac{1}{\hat{\sigma}_j^2}\Big] - n \\ &+E\Big[\frac{1}{\hat{\sigma}_j^2}\Big\{n_{1j}(\mu_{1j}-\hat{\mu}_{1j})^2 + n_{2j}(\mu_{2j}-\hat{\mu}_{2j})^2\Big\}\Big], \end{aligned} \tag{3.3}$$

where the $\hat{\mu}_{2j}$ in the cases M_1 and M_2 are $\hat{\gamma}\hat{\mu}_{1j}$ and $\hat{\alpha}+\hat{\beta}\hat{\mu}_{1j}$, respectively.

Let $B_{A;a}$ be the bias B_A for model M_a. Assume that $n_{ij} = n_0$ for all $i = 1, 2$ and $j = 1, \dots, m$. Then, it is shown that $B_{A;a}$ can be expanded as follows:

$$\begin{aligned} B_{A;1} &= d_1 + \frac{1}{n_0}c_1 + O(n_0^{-2}), \\ B_{A;2} &= d_2 + \frac{1}{n_0}c_2 + O(n_0^{-2}), \\ B_{A;2} &= d_3 + \frac{1}{n_0}c_3 + O(n_0^{-2}), \end{aligned} \tag{3.4}$$

where

$$\begin{aligned} c_1 &= 4(m+2) + \frac{4(m-1)}{1+\gamma^2}\frac{1}{t_{2,2}} - 2\frac{t_{4,4}}{t_{2,2}^2}, \\ c_2 &= 4(m+4) + \frac{4(m-2)}{1+\beta^2}\frac{t_{0,2}}{t_{0,2}t_{2,2}-t_{1,2}^2} - \frac{2R}{\left(t_{0,2}t_{2,2}-t_{1,2}^2\right)^2}, \\ c_3 &= 10m. \end{aligned}$$

and $t_{p,q} = \sum_{j=1}^{m}\mu_{1j}^p/\sigma_j^q$,

$$R = t_{4,4}t_{0,2}^2 + 2t_{2,2}t_{2,4}t_{0,2} - 4t_{1,2}t_{3,4}t_{0,2} + t_{0,4}t_{2,2}^2 - 4t_{1,2}t_{1,4}t_{2,2} + 4t_{1,2}^2t_{2,4}.$$

Using the above results, a corrected AIC is defined as

$$CAIC_a = AIC_a + \frac{1}{n_0}\hat{c}_a, \ \ a = 1, 2, 3, \tag{3.5}$$

where $\hat{c}_a$ is defined from c_a by substituting MLE's for the unknown parameters.

4 Simulation study

In order to investigate the actual behavior of AIC and CAIC, we examined their average biases and frequencies selected by simulation experiments. The simulations were made for the cases where the sample sizes n_{ij} are the same as n_0, and $n_0 = 6, 10, 30, 50, 100$. The parameters are defined as follows:

$$\begin{aligned}
&\gamma = 1.05, \quad \beta = 1.05, \quad \alpha = 0.05 \\
&\mu_{11} = 0.07, \quad \mu_{12} = 0.10, \quad \mu_{13} = 0.20, \\
&\mu_{14} = 0.70, \quad \mu_{15} = 1.00, \quad \mu_{16} = 2.00, \\
&\sigma_1^2 = 0.00007, \quad \sigma_2^2 = 0.00100, \quad \sigma_3^2 = 0.00400, \\
&\sigma_4^2 = 0.00600, \quad \sigma_5^2 = 0.01000, \quad \sigma_6^2 = 0.03000.
\end{aligned}$$

The numbers of iterations were set as 10,000. Tables 2 and 3 are frequencies of model selected by AIC and CAIC in the case that M_1 is true. Tables 4 and 5 show the ones in the case that M_2 is true. Figures 1 and 2 show the differences between the average of the true risk and the average of each of AIC and CAIC. Figure 1 shows the case that M_1 is true, and Figure 2 shows the case that M_2 is true. From these experiments, we can see that CAIC is more effective than AIC in the case of small samples.

Table 2. AIC when M_1 is true

	M1	M2	M3
n_0=6	7559	1271	1170
n_0=10	7883	1244	873
n_0=30	7820	1480	700
n_0=50	7935	1392	673
n_0=100	8018	1359	623

Table 3. CAIC when M_1 is true

M1(CAIC)	M1	M2	M3
n_0=6	9017	732	251
n_0=10	8838	847	315
n_0=30	8222	1319	459
n_0=50	8169	1301	530
n_0=100	8123	1312	565

Table 4. AIC when M_2 is true

	M1	M2	M3
n_0=6	0	8166	1834
n_0=10	0	8615	1385
n_0=30	0	8955	1045
n_0=50	0	9020	980
n_0=100	0	9034	966

Table 5. CAIC when M_2 is true

	M1	M2	M3
n_0=6	0	9425	575
n_0=10	0	9374	626
n_0=30	0	9195	805
n_0=50	0	9187	813
n_0=100	0	9121	879

Figure 1. Diferences between risks when M_1 is true

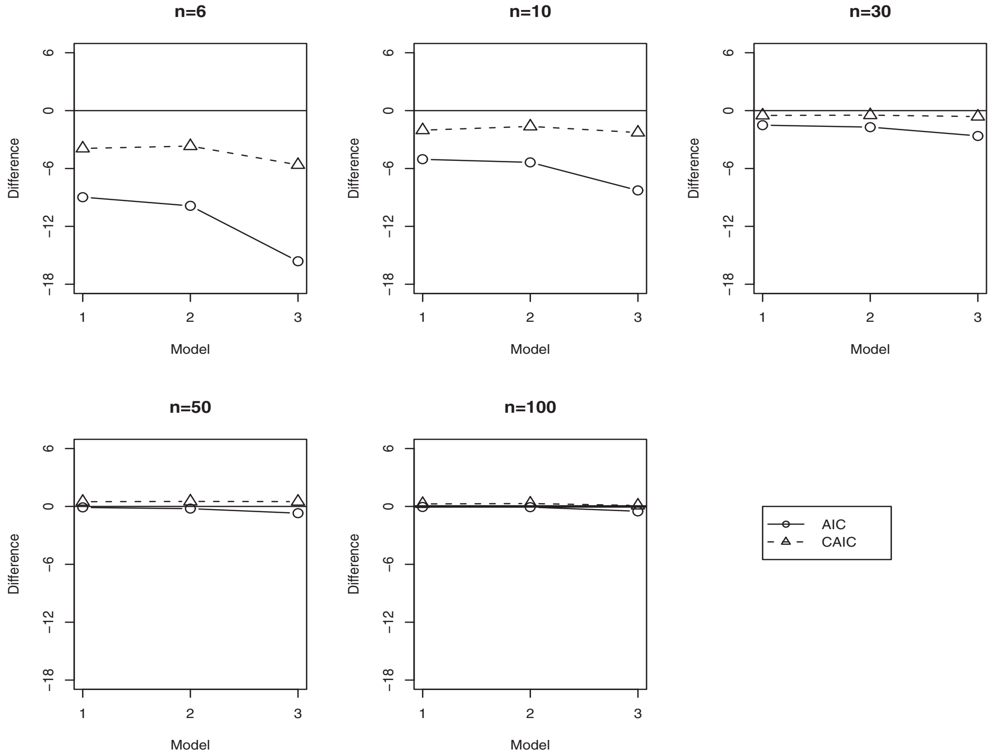
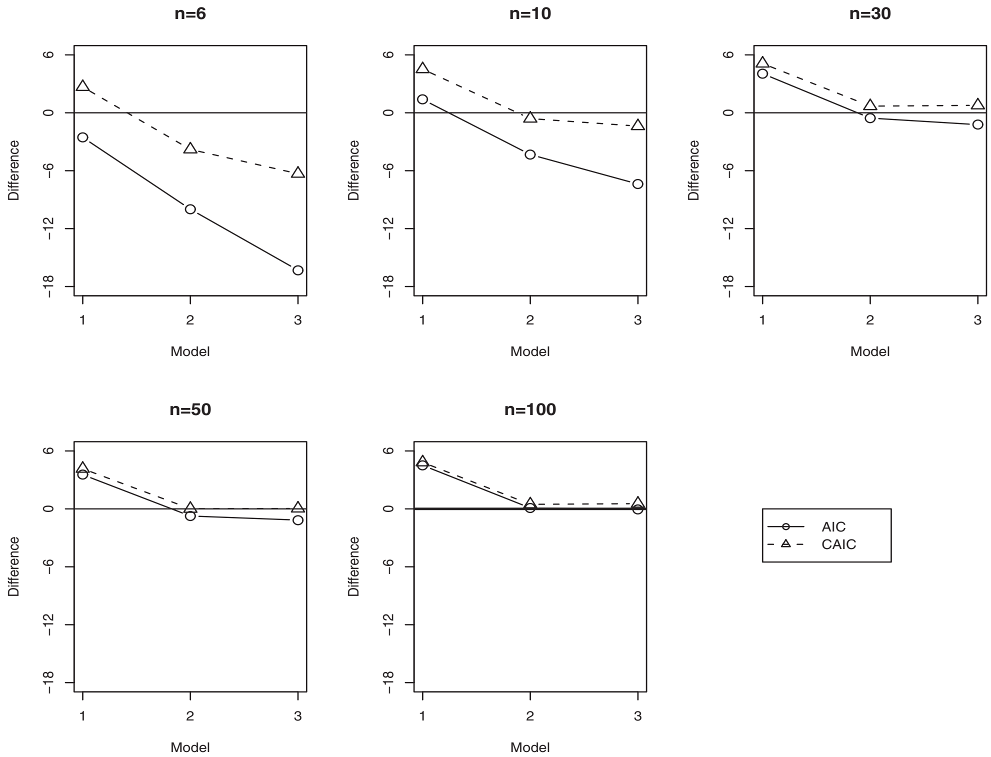


Figure 2. Diferences between risks when M_2 is true



5 An example

We consider the data (Kanai et al. (2007)) measured for different 6 materials by two fracture toughness testing methods. The sample sizes are all 6. The sample means and variances are given in Table 6. It may be noted that the variances are different between 6 materials, but are almost the same between testing methods. For the data, we examined three models M_1, M_2 and M_3. The results on MLE's, AIC and CAIC are given in Table 7. The sample sizes n_{ij} are all 6, and are relatively small. So, we use CAIC. As a result, it is concluded that M_2 is appropriate.

Table 6. Means and variances

i	j	n_0	mean	variance
1	1	6	0.07627	0.00007
	2	6	0.20938	0.00131
	3	6	0.21278	0.00428
	4	6	0.71098	0.02323
	5	6	1.92135	0.03125
	6	6	1.10768	0.03085
2	1	6	0.06138	0.00016
	2	6	0.15183	0.00146
	3	6	0.24127	0.00315
	4	6	0.77772	0.00428
	5	6	2.34835	0.11399
	6	6	1.17220	0.13070

Table 7. MLE, AIC and CAIC

	d	α	γ or β	AIC	CAIC
M_1	13		1.039820	-130.5692	-125.5097
M_2	14	-0.029578	1.161379	-140.6882	-134.4448
M_3	18			-140.9095	-130.9095

6 Conclusion

In this paper, we considered some linear structure models with different variances, based on the data (Kanai et al. (2007)) measured for different materials by two fracture toughness testing methods. More precisely, we considered three types of structures between two testing methods, which are denoted by M_1, M_2 and M_3. For selection of these models, we gave AIC, and further, we derived its corrected version, CAIC. It was pointed that CAIC is more effective than AIC in the case of small samples, based on simulation experiments. Based on our results, it was pointed that there is a linear structure between two fracture toughness testing methods.

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