

Unbiased χ^2 Estimator for Linear Function Fit Involving Correlated Data^{*}

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Abstract An unbiased factorized chi-square estimator is constructed to deal with the correlated data for linear function fit. The difference between the biased and unbiased chi-square fitting is expounded. In addition, the simplified R -value measurement is quoted to test the conclusion quantitatively.

Key words χ^2 estimator, linear function, biasness, unbiasedness, correlated data

1 Introduction

There are two frequently used methods, the covariance matrix and the scale factor method, to deal with the correlated data, and the equivalence between them was discussed in Ref. [1] for two measurements and constant fit. After that, the equivalent conclusion has been extended to multi-measurements for constant fit^[2, 3], then for linear function fit^[4].

In previous researches^[3], two points are worthy of notice: first, it is comparatively easy to acquire analytical results by using the factorized χ^2 form, which avoids complex calculations of inverse matrix; second, the estimates of parameters interested from both the matrix and the factor approach deviate from the expected average value, and the deviation may be considerably striking, if the measurement points are quite many, or the uncertainty of the scale factor is rather large.

This article is devoted to the factorized χ^2 estimators. An unbiased χ^2 estimator is constructed based on the study of Ref. [5]; the minimization estimates for both the biased and unbiased estimators are worked out explicitly and the differences between them are discussed. Furthermore, some simplified experimental results are adopted to confirm the theo-

retical conclusions.

2 Minimization of two χ^2 estimators

2.1 Minimization of biased chisquare

As presented in Ref. [4], the biased χ^2 estimator is constructed as follows

$$\chi_b^2 = \sum_{i=1}^n \frac{[fy_i - (\alpha x_i + \beta)]^2}{\sigma_i^2} + \frac{(f-1)^2}{\sigma_f^2}, \quad (1)$$

which is equivalent to matrix χ^2 estimator in the sense that both minimizers for the corresponding fitting parameters are exactly the same. According to Ref. [4],

$$\begin{cases} \hat{\alpha} = \sum_{ij} \frac{x_i y_i - x_i y_j}{\sigma_i^2 \sigma_j^2} / (\sigma_f^2 \cdot D_\Sigma), \\ \hat{\beta} = \sum_{ij} \frac{x_i^2 y_j - x_i x_j y_j}{\sigma_i^2 \sigma_j^2} / (\sigma_f^2 \cdot D_\Sigma), \\ \hat{f} = \sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2} / (\sigma_f^2 \cdot D_\Sigma); \end{cases} \quad (2)$$

and their covariances

$$\begin{cases} \sigma_\alpha^2 = \left(\sum_i \frac{1}{\sigma_i^2} + \sigma_f^2 \cdot \sum_{ij} \frac{y_i^2 - y_i y_j}{\sigma_i^2 \sigma_j^2} \right) / (\sigma_f^2 \cdot D_\Sigma), \\ \sigma_\beta^2 = \left(\sum_i \frac{x_i^2}{\sigma_i^2} + \sigma_f^2 \cdot \sum_{ij} \frac{x_i^2 y_j^2 - x_i y_i x_j y_j}{\sigma_i^2 \sigma_j^2} \right) / (\sigma_f^2 \cdot D_\Sigma), \\ \sigma_f^2 = \sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2} / D_\Sigma; \end{cases} \quad (3)$$

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with

$$D_{\Sigma} = \frac{1}{\sigma_f^2} \cdot \left[\sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2} + \sigma_f^2 \cdot \sum_{ijk} \frac{(x_i^2 - x_i x_j) y_k^2 - x_i^2 y_j y_k - x_i y_i x_j y_j + 2x_i y_i x_j y_k}{\sigma_i^2 \sigma_j^2 \sigma_k^2} \right]. \quad (4)$$

If we denote $f_i(\mathbf{r})$ as the function at i -th point of variables $\mathbf{r} = (x, y, z, \dots)$ with experimental uncertainty σ_i , the weighted average of $f_i(\mathbf{r})$ can be defined as

$$\bar{f}(\mathbf{r}) = \sigma_s^2 \cdot \sum_i \frac{f_i(\mathbf{r})}{\sigma_i^2},$$

with

$$\frac{1}{\sigma_s^2} \equiv \sum_{i=1}^n \frac{1}{\sigma_i^2} \quad \text{or} \quad \sigma_s^2 \equiv 1 / \left(\sum_{i=1}^n \frac{1}{\sigma_i^2} \right).$$

Using the above definition, together with Eqs. (2) and (3) we get the following expressions

$$\hat{f} = \frac{\sigma_s^2 + \sigma_f^2 \cdot (\hat{\alpha} \bar{x} y + \hat{\beta} \bar{y})}{\sigma_s^2 + \sigma_f^2 \cdot \bar{y}^2}, \quad (5)$$

and

$$\sigma_{\hat{f}}^2 = \hat{f} \cdot \sigma_f^2. \quad (6)$$

2.2 Minimization of unbiased chisquare

As enlightened by Ref. [5], we construct the following χ^2 form¹⁾

$$\chi_u^2 = \sum_i \frac{[y_i - g(\lambda x_i + \rho)]^2}{\sigma_i^2} + \frac{(g-1)^2}{\sigma_g^2}, \quad (7)$$

then

$$\frac{\partial \chi_u^2}{\partial \lambda} = -2g \cdot \sum_i \frac{[y_i - g(\lambda x_i + \rho)] x_i}{\sigma_i^2}, \quad (8)$$

$$\frac{\partial \chi_u^2}{\partial \rho} = -2g \cdot \sum_i \frac{[y_i - g(\lambda x_i + \rho)]}{\sigma_i^2}, \quad (9)$$

$$\frac{\partial \chi_u^2}{\partial g} = \frac{\lambda}{g} \cdot \frac{\partial \chi_u^2}{\partial \lambda} + \frac{\rho}{g} \cdot \frac{\partial \chi_u^2}{\partial \rho} + \frac{2(g-1)}{\sigma_g^2}. \quad (10)$$

The minimization condition requires all these derivatives to be zero, i.e.

$$\frac{\partial \chi_u^2}{\partial \lambda} = \frac{\partial \chi_u^2}{\partial \rho} = \frac{\partial \chi_u^2}{\partial g} = 0.$$

From Eq. (10), we immediately obtain $\hat{g} = 1$ (for $g \neq 0$). Then replacing g with 1 in Eqs. (8) and (9), we have

$$T \begin{pmatrix} \hat{\lambda} \\ \hat{\rho} \end{pmatrix} = \begin{pmatrix} \sum_i \frac{x_i y_i}{\sigma_i^2} \\ \sum_i \frac{y_i}{\sigma_i^2} \end{pmatrix},$$

with

$$T = \begin{pmatrix} \sum_i \frac{x_i^2}{\sigma_i^2} & \sum_i \frac{x_i}{\sigma_i^2} \\ \sum_i \frac{x_i}{\sigma_i^2} & \sum_i \frac{1}{\sigma_i^2} \end{pmatrix}.$$

It is easy to figure out

$$\begin{cases} \hat{\lambda} = \sum_{ij} \frac{x_i y_i - x_i x_j}{\sigma_i^2 \sigma_j^2} / \sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2}, \\ \hat{\rho} = \sum_{ij} \frac{x_i^2 y_j - x_i x_j y_j}{\sigma_i^2 \sigma_j^2} / \sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2}, \\ \hat{g} = 1. \end{cases} \quad (11)$$

With further derivation, we acquire

$$\mathbf{A} = \frac{1}{2} \begin{pmatrix} \frac{\partial^2 \chi_u^2}{\partial \lambda \partial \lambda} & \frac{\partial^2 \chi_u^2}{\partial \lambda \partial \rho} & \frac{\partial^2 \chi_u^2}{\partial \lambda \partial g} \\ \frac{\partial^2 \chi_u^2}{\partial \rho \partial \lambda} & \frac{\partial^2 \chi_u^2}{\partial \rho \partial \rho} & \frac{\partial^2 \chi_u^2}{\partial \rho \partial g} \\ \frac{\partial^2 \chi_u^2}{\partial g \partial \lambda} & \frac{\partial^2 \chi_u^2}{\partial g \partial \rho} & \frac{\partial^2 \chi_u^2}{\partial g \partial g} \end{pmatrix} \equiv \begin{pmatrix} \mathcal{A} & \mathcal{D} & \mathcal{E} \\ \mathcal{D} & \mathcal{B} & \mathcal{F} \\ \mathcal{E} & \mathcal{F} & \mathcal{C} \end{pmatrix},$$

where we have defined

$$\begin{aligned} \mathcal{A} &= \sum_i \frac{x_i^2}{\sigma_i^2}, & \mathcal{B} &= \sum_i \frac{1}{\sigma_i^2}, \\ \mathcal{E} &= \sum_i \frac{[2(\hat{\lambda} x_i + \hat{\rho}) - y_i] x_i}{\sigma_i^2}, \\ \mathcal{D} &= \sum_i \frac{x_i}{\sigma_i^2}, & \mathcal{C} &= \frac{1}{\sigma_g^2} + \sum_i \frac{(\hat{\lambda} x_i + \hat{\rho})^2}{\sigma_i^2}, \\ \mathcal{F} &= \sum_i \frac{2(\hat{\lambda} x_i + \hat{\rho}) - y_i}{\sigma_i^2}. \end{aligned} \quad (12)$$

Here \mathbf{A} is the inverse of covariance matrix, according to which we obtain the corresponding covariance for $\hat{\lambda}$, $\hat{\rho}$, and \hat{g} as follows

$$\begin{cases} \sigma_{\hat{\lambda}}^2 = \left(\sum_i \frac{1}{\sigma_i^2} + \sigma_g^2 \cdot \sum_{ij} \frac{z_i^2 - y_i y_j + 4z_i (y_j - z_j)}{\sigma_i^2 \sigma_j^2} \right) / (\sigma_g^2 \cdot D_{\mathcal{A}}), \\ \sigma_{\hat{\rho}}^2 = \left(\sum_i \frac{x_i^2}{\sigma_i^2} + \sigma_g^2 \cdot \sum_{ij} \frac{x_i^2 z_j^2 - x_i y_i x_j y_j + 4x_i z_i x_j (y_j - z_j)}{\sigma_i^2 \sigma_j^2} \right) / (\sigma_g^2 \cdot D_{\mathcal{A}}), \\ \sigma_{\hat{g}}^2 = \sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2} / D_{\mathcal{A}}; \end{cases} \quad (13)$$

where

1) Here for distinction, we adopt symbols λ , ρ , g for χ_u^2 , which are equivalent to α , β , f of χ_{α}^2 . In addition, the χ_u^2 is the extension of the unbiased estimator χ_{α}^2 in Ref. [5], herein χ_u^2 is for linear function fit while χ_{α}^2 is merely for constant fit.

$$D_A = \frac{1}{\sigma_g^2} \cdot \left[\sum_{ij} \frac{x_i^2 - x_i x_j}{\sigma_i^2 \sigma_j^2} + \sigma_g^2 \cdot \sum_{ijk} \frac{(x_i^2 - x_i x_j) z_k^2 - x_i^2 y_j y_k - x_i y_i x_j y_j + 2x_i y_i x_j y_k}{\sigma_i^2 \sigma_j^2 \sigma_k^2} + 4\sigma_g^2 \cdot \sum_{ijk} \frac{(x_i^2 z_j + x_i z_i x_k - 2x_i z_i x_j)(y_k - z_k)}{\sigma_i^2 \sigma_j^2 \sigma_k^2} \right]. \quad (14)$$

In the above expressions, we utilize the definition $z_i = (\hat{\lambda}x_i + \hat{\rho})$, which is the minimization expectation of y_i .

2.3 Discussion

Comparing Eqs. (2) and (11), we find

$$\hat{\lambda} = \hat{\alpha}/\hat{f}, \quad \hat{\rho} = \hat{\beta}/\hat{f}.$$

As mentioned in Ref. [4], the minimizers $\hat{\alpha}$ and $\hat{\beta}$ are biased, which need correcting by factor \hat{f} in order to give the reasonable fit for correlated experiment data. From this point of view, we draw a conclusion that the χ_u^2 provides an unbiased minimization estimates. So far as covariance is concerned, we first consider the case $z_i \approx y_i$, under which the term containing residual, $(z_i - y_i)$ or $(y_i - z_i)$ can be neglected, then comparing Eq. (3) with Eq. (13), we have

$$\sigma_{\hat{\lambda}}^2 \approx \sigma_{\hat{\alpha}}^2, \quad \sigma_{\hat{\rho}}^2 \approx \sigma_{\hat{\beta}}^2, \quad \sigma_{\hat{g}}^2 \approx \sigma_{\hat{f}}^2, \quad (15)$$

with $D_A \approx D_{\Sigma}$. When z_i 's differ from y_i 's prominently, the difference between two kinds of covariance enlarges accordingly. It is obvious that the parameters' uncertainties due to χ_u^2 minimization contain more information than those due to χ_b^2 . In this sense, χ_b^2 is apt to mis-estimate the minimization error.

At first sight, it seems a little puzzling, Eq. (1) and Eq. (7) have a similar form but lead to so distinct results. However, scrutinizing the expressions, we find the minimization of two equations is rather distinctive. For Eq. (1), the first summation term is minimized at $f = \alpha = \beta = 0$, while the second term is minimized at $f = 1$. Therefore, as the number of data points increases, minimizing χ_b^2 has the effect of decreasing the first term by decreasing f at the expense of making the second term large. In another word, χ_b^2 improves the agreement between data points by simply rescaling all fitted quantities (say f, α, β of χ_b^2 in Eq. (1)) to zero! On the contrary, for Eq. (7),

the last term constrains g to 1, under such case, the first summation of χ_u^2 is equivalent to the usual χ^2 minimization, which only depends on the experimental measurements. Therefore, we deem that χ_u^2 gives an unbiased estimation, the effect of scale factor g is only on the corresponding uncertainty determination. This character has been displayed in minimization derivation of χ_u^2 .

3 Experiment testing

R , the ratio of the hadron production cross section via single photon annihilation to the lowest order point-like QED $\mu^+\mu^-$ cross section $\sigma_{\text{pt}} = 4\pi\alpha^2/3s$, is a fundamental quantity in e^+e^- interaction. It is calculated in the naive quark-parton model as $R = 3\sum_q Q_q^2$, where Q_q is the quark electric charge, and the summation runs over all the produced flavors. Taking the lowest order QCD correction and the electro-weak effect into consideration, R value would be larger than the naive value (10/3), and the corrected term is a slowly varying smooth function of center-of-mass (C.M.) energy, in the region without any resonances, therefore, R could reasonably be described as a linear function in a good approximation.

In experiment, many factors should be considered in R value calculation¹⁾. As a pedagogical example, a comparatively concise R expression^[6] is given here

$$R = \frac{(N - N_{\text{bg}})}{L\epsilon(1 + \delta) \cdot \sigma_{\text{pt}}},$$

where N is the number of multi-hadronic events detected, N_{bg} is the estimated number of background events, L is the integrated luminosity, $\epsilon(1 + \delta)$ is the acceptance for the multi-hadronic events with radiative effect included and $(1 + \delta)$ is the radiative correction factor due to higher order QED processes up to order α^3 . Table 1 lists thirty eight experiment R -values^[9]. From a study of data taken at different times at the same C.M. energy, the estimated systematic point-to-point errors are given as $\pm 3\%$. For the R value used here, the systematic uncertainty in the detection efficiency ($\pm 8\%$), the luminosity measurement ($\pm 6\%$), the event selection procedure ($\pm 2\%$),

1) The R value measurement at BESII has been described in Refs. [7,8], where the detailed calculation about experiment R value could be found.

and the background subtraction ($\pm 3\%$) yielded an common systematic error of $\pm 10\%$, which should be considered as normalization error. Now these thirty eight R -values will be used to test foregoing conclusions. For minimization, the MINUIT package, one of useful CERN packages in high energy physics^[10], is utilized.

Table 1. Values for $R^{[9]}$. The errors quoted are point-to-point systematic errors.

E_{cm}/GeV	R value	error ΔR	E_{cm}/GeV	R value	error ΔR
5.60	4.08	0.32	6.60	4.50	0.17
5.70	4.09	0.16	6.65	4.25	0.16
5.75	4.12	0.20	6.70	4.63	0.15
5.80	4.13	0.16	6.75	4.38	0.15
5.85	4.13	0.19	6.80	4.44	0.16
5.90	4.09	0.14	6.85	4.50	0.13
5.95	4.17	0.16	6.90	4.41	0.15
6.00	4.17	0.09	6.95	4.23	0.17
6.05	4.16	0.18	7.00	4.10	0.12
6.10	4.04	0.15	7.05	4.31	0.09
6.15	4.34	0.16	7.10	4.32	0.14
6.20	4.05	0.08	7.15	4.29	0.11
6.25	3.96	0.14	7.20	4.27	0.11
6.30	4.27	0.14	7.25	4.39	0.11
6.35	4.47	0.17	7.30	4.29	0.11
6.40	4.31	0.13	7.35	4.33	0.09
6.45	4.23	0.14	7.40	4.46	0.08
6.50	4.40	0.15	7.45	4.51	0.14
6.55	4.66	0.16	7.50	4.18	0.59

In the χ^2 construction, the following substitutes are adopted

$$x_i \rightarrow E_{\text{cm}}^i, \quad y_i \rightarrow R_{\text{exp.}}^i, \quad \sigma_i \rightarrow \Delta R_{\text{exp.}}^i,$$

$$\beta, \rho \rightarrow R_0, \quad \text{and} \quad \alpha, \lambda \rightarrow \eta,$$

then Eqs. (1) and (7) become

$$\chi_{\text{b}}^2 = \sum_i \frac{[fR_{\text{exp.}}^i - (\eta E_{\text{cm}}^i + R_0)]^2}{(\Delta R_{\text{exp.}}^i)^2} + \frac{(f-1)^2}{\sigma_f^2},$$

$$\chi_{\text{u}}^2 = \sum_i \frac{[R_{\text{exp.}}^i - g(\eta E_{\text{cm}}^i + R_0)]^2}{(\Delta R_{\text{exp.}}^i)^2} + \frac{(g-1)^2}{\sigma_g^2},$$

where $\sigma_f(\sigma_g)$ is the overall error of normalization factor $f(g)$, which equals to 10%.

Fig. 1 shows the fitting result, where the solid line is drawn according to the best fitted linear function

$$F(E_{\text{cm}}^i) = a \cdot E_{\text{cm}}^i + b.$$

Here $a = \hat{\eta}$, $b = \hat{R}_0$ for χ_{u}^2 fit, or $a = \hat{\eta}/\hat{f}$, $b = \hat{R}_0/\hat{f}$ for χ_{b}^2 fit. The dashed line is drawn according to χ_{b}^2 fit without re-scaling by factor f . For constant fit, this biasness due to χ_{b}^2 scaling scheme has been noticed in previous papers^[1, 3, 5], herein we encounter the same biasness for linear function fit.

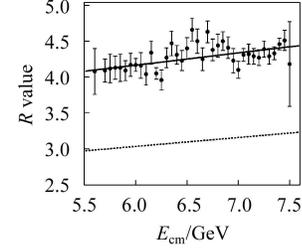


Fig. 1. The R value, error bars indicate point-to-point systematic errors. The data points taken from Ref. [6]. The solid line represents the best fitted from χ_{u}^2 or the re-scaled result from χ_{b}^2 , while the dashed line from χ_{b}^2 .

The fitting results are summarized in Table 2. At the same time, using Eqs. (2), (3), (11) and (13) we can compute the corresponding values theoretically, which are also listed in Table 2. We can see the fit results consist with the theoretical ones fairly well. As to the difference between two χ^2 estimators, besides the larger deviation for the central values, the relative errors from χ_{b}^2 fit are quit larger than those from χ_{u}^2 . If we rescale the central values from χ_{b}^2 by factor f , we have

$$\hat{R}_0/\hat{f} = 3.1442 \pm 0.5219 [16.60\%],$$

$$\hat{\eta}/\hat{f} = 0.1704 \pm 0.0543 [31.85\%],$$

here the correlation coefficients from fit program have been taken into consideration for error calculation¹⁾. Comparing with χ_{u}^2 results, it is noticeable that although the central values of χ_{b}^2 can be re-scaled to give a reasonable results, the relative errors are still larger than those from χ_{u}^2 estimation.

1) The correlation coefficient matrices for χ_{b}^2 and χ_{u}^2 are presented as follows

$$\begin{array}{ccc} & R_0 & \eta & f \\ R_0 & \left(\begin{array}{ccc} 1.000 & -0.412 & 0.711 \\ -0.412 & 1.000 & 0.345 \\ 0.711 & 0.345 & 1.000 \end{array} \right), & & \\ \eta & & & \\ f & & & \end{array} \quad \begin{array}{ccc} & R_0 & \eta & g \\ R_0 & \left(\begin{array}{ccc} 1.000 & -0.277 & -0.768 \\ -0.277 & 1.000 & -0.400 \\ -0.768 & -0.400 & 1.000 \end{array} \right). & & \\ \eta & & & \\ g & & & \end{array}$$

The stem of bias due to χ_b^2 fit can be explained quantitatively by the chisquare-value provided in Table 2. The theoretical calculation indicates that the chisquare-value contribution owing to the last term of χ_b^2 accounts for 20%. Just as we mentioned before, the scale factor f tends to diminish the scaled

values to improve the agreement between data points and simultaneously amplify the proportion from the factor itself in the total chisquare-value.

Last, note Eq. (6), we can calculate $\sigma_{\hat{f}}$ with formula $\sqrt{\hat{f} \cdot \sigma_f^2}$ to get value 0.0853, which is exactly the same as the corresponding value listed in Table 2.

Table 2. The experimentally fitted and theoretically calculated values of parameters and relevant information.

parameter	biased fit	theoretical calculation	unbiased fit	theoretical calculation
$\hat{R}_0 \pm \Delta \hat{R}_0$	2.2895 ± 0.3772	2.2895 ± 0.3772	3.1442 ± 0.4143	3.1442 ± 0.4113
$[\Delta \hat{R}_0 / \hat{R}_0]$	[16.48%]		[13.18%]	
$\hat{\eta} \pm \Delta \hat{\eta}$	0.1241 ± 0.0421	0.1241 ± 0.0421	0.1704 ± 0.0431	0.1704 ± 0.0430
$[\Delta \hat{\eta} / \hat{\eta}]$	[33.93%]		[25.30%]	
$(\hat{f}, \hat{g}) \pm \Delta(\hat{f}, \hat{g})$	0.7282 ± 0.0853	0.7282 ± 0.0853	1.0000 ± 0.1012	$\dagger(1 \pm 0.1000)$
$[\Delta(\hat{f}, \hat{g}) / (\hat{f}, \hat{g})]$	[11.72%]	$\ddagger(0.7275 \pm 0.0853)$	[10.12%]	
$\chi^2/\text{d.o.f}$	27.18/35	$*(19.79 + 7.39)/35$	37.33/35	$*(37.33 + 0)/35$

\dagger : The \hat{g} is set to be 1 in theoretical calculation. \ddagger : The \hat{f} and σ_f^2 are calculated by Eqs. (5) and (6).

*: The chisquare-value is calculated according to Eqs. (1) and (7), respectively. The first number indicates the contribution due to the summation term while the second the contribution due to the last term only.

4 Summary

For linear function fitting, the minimization estimates due to the biased and the unbiased χ^2 estimators have been compared. From our study it follows that the unbiased χ^2 estimator is more robust than the biased one about the correlated data fitting whatever for the best estimates or the corresponding variances. Our conclusions are based on the

strictly mathematical calculation and tested quantitatively by a typical simplified R value measurement experiment.

Pay attention to the equivalent conclusion in Ref. [4]. The matrix χ^2 estimator also leads to biased estimates, which is also unfavorable compared with the unbiased χ^2 estimator recommended in this paper.

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关联实验数据线性函数拟合情况下无偏 χ^2 估计量的构造*

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摘要 针对线性函数拟合的情况构造了一种无偏的因子化形式的 χ^2 估计量, 用以处理关联数据的极小化. 详细比较并说明了有偏性与无偏性 χ^2 拟合的区别. 利用简化的 R 值测量数据对相关的结论进行了定量的检验.

关键词 χ^2 估计量 线性函数 有偏性 无偏性 关联数据

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