



# 行政院國家科學委員會補助專題研究計畫成果報告

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※ 樣本半偏差和樣本共變異量的比較 ※

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計畫類別： 個別型計畫     整合型計畫

計畫編號：NSC 89-2118-M-034-003-

執行期間：89 年 8 月 1 日至 90 年 7 月 31 日

計畫主持人：呂小娟

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執行單位：私立中國文化大學應用數學系

# 行政院國家科學委員會專題研究計畫成果報告

## 樣本半偏差和樣本共變異量的比較

計畫編號：NSC 89-2118-M-034-003-

中華民國 90 年 10 月

執行期間：89 年 8 月 1 日至 90 年 7 月 31 日

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### 中文摘要

半偏差和共變異數皆可用以量度一隨機場的二階相依性。在時間數列上，資料分析者較常使用共變異數，而在地理統計學上，則幾乎皆使用半偏差。主要是半偏差存在於較被廣泛應用的內部穩定隨機場，但共變異數則常侷限於二階穩定的隨機場上討論。在實際應用上，資料的二階相依性通常是未知的，須經由資料作估計，因此本研究主要針對樣本半偏差和樣本共變數的極限性質做比較，由研究結果發現樣本半偏差經過自然對數變換後，只須中等大小的樣本數，其極限分佈便已非常趨近於常態，因此應用於方向的對稱性質之檢定上，其檢定力通常都大於其他估計量，此結果更進一步肯定半偏差在地理統計應用上的重要性，統計學者在資料二階相依性的探討上應多使用半偏差。

**關鍵詞：**樣本半偏差、樣本共變異數、地理統計學、極限分佈

### Abstract

For a second-order stationary process, the semivariogram and the covariogram are two measures of the second-order dependence. In time series, the covariogram is used more often, while in geostatistics, the

semivariogram is preferred. The main reason is because the semivariogram can be discussed in more general processes. However, the covariogram can only be used when the underlying process satisfies second-order stationarity which is more restrictive than intrinsic stationarity. In practical application, these measures of second-order dependence are usually unknown and have to be estimated from the data. Hence, the main object of this study is to compare the asymptotic properties of the sample semivariogram and the sample covariogram. In this research, I found that a logarithmic transformation of the sample semivariogram shows good normality approximation for moderately large sample size. Thus, we can usually have higher power in testing some directional symmetry properties with the logarithm of the sample semivariogram. This result shows the importance of the semivariogram in the application of geostatistics further. Data analysts ought to use the smivariogram more often.

**Keywords:** sample semivariogram, sample covariogram, geostatistics, asymptotic distribution

## The Cause and the Object

The problem considered in this study arises that the variogram is widely used in geostatistics, while the covariogram is used much more often in time series. The main reason why variograms are more popular in geostatistics is because of its extra generality. Essentially, the variogram and covariogram are two equivalent tools in characterizing the second-order dependence of the data when the underlying process is second-order stationary. However, if the process only satisfies intrinsic stationarity, then only the smivariogram can be used. Thus, it is common to work with the estimator of the variogram in geostatistical analysis. In this study, it is shown that beyond the greater generality, estimation of the variogram has more important advantages over estimation of the covariogram.

### Results and Discussion.

Let  $\{Z(S); S \in D\}$  denote a random field defined over a domain  $D$ . The population semivariogram at lag  $h$  is defined by

$$\gamma(h) = \frac{1}{2} \text{Var}[Z(x+h) - Z(x)],$$

for all  $x, x+h \in D$ .

The covariogram is

$$C(h) = \text{Cov}[Z(x+h), Z(x)].$$

A second-order stationary random field is intrinsically stationary, with the semivariogram  $\gamma(h) = C(0) - C(h)$ .

Now suppose that  $\{Z(x)\}$  is observed at distinct sites,  $x_1, x_2, \dots, x_n \in D$  yielding observations,  $Z(x_1), \dots, Z(x_n)$ . The Classical

estimator of  $\gamma(h)$  is

$$\hat{\gamma}(h) = \frac{1}{2N} \sum_x \{Z(x+h) - Z(x)\}^2,$$

where  $N$  denotes the number of pairs  $\{Z(x_i), Z(x_j)\}$  such that  $x_i = x_j + h$  and the summation is over the  $N$  available pairs. This estimator is called the sample semivariogram. Similarly, the covariogram is estimated by the sample covariogram

$$\hat{C}(h) = \frac{1}{N} \sum_x \left\{ \left( Z(x+h) - \bar{Z} \right) \left( Z(x) - \bar{Z} \right) \right\}$$

where  $\bar{Z} = \frac{1}{n} \sum_{i=1}^n Z(x_i)$ .

The correlogram  $\rho(h)$  can be estimated by the sample correlogram

$$\hat{\rho}(h) = \hat{C}(h) / \hat{C}(0).$$

Since in most geostatistical applications two dimensional processes are observed much more often, the study focuses the comparisons on the two dimensional cases. Specifically, the semivariogram is denoted as  $\gamma(h, k)$ , where  $h$  is the lag in the  $x$ -direction and  $k$  is the lag in the  $y$ -direction. Results of the comparisons of the sample covariogram and the sample semivariogram are stated in the following.

#### (1) Asymptotic Bias

**Theorem 1** Let  $\{Z(S); S \in D\}$  be a second-order stationary random field which is observed on a regular rectangular  $r \times c$  lattice. Assume that the sequence of covariances,  $\{C(i, j)\}$  is absolutely summable, i.e.  $\sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} |C(i, j)| < \infty$ . Then for any fixed  $h, k$

$$\lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc E \left[ \hat{C}(h, k) - C(h, k) \right] = - \sum_{i=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} C(i, j).$$

Several interesting aspects of the asymptotic bias are given by Theorem 1. First, this bias is the same for every lag regardless of the latter's size or direction. Second, under the assumption of a nonnegative covariance function, an increased correlation in any one direction worsens the bias in every direction.

Third, let us compare the bias of  $N\hat{C}(h, 0)$  with that of  $N\hat{C}(h)$  since  $\hat{C}(h, 0)$  can be

regarded as an estimator of  $\hat{C}(h)$  in the  $x$ -direction. Assuming again that the covariogram is nonnegative, the asymptotic bias of  $N\hat{C}(h, 0)$  is larger in magnitude than

that of  $N\hat{C}(h)$  if there is any dependence whatsoever in the  $y$ -direction. None of these features apply to the sample semivariogram, of course, because it is unbiased.

## (2) Asymptotic Covariance Structures

By investigating the asymptotic covariance structures of the sample semivariogram and the sample covariogram, I conclude that if the process is reflection symmetric then so are the asymptotic covariance structures of the sample covariogram and the sample semivariogram. Furthermore, if the process is isotropic then the asymptotic covariance of the sample covariogram and the sample semivariogram at any two lags may be equal to that corresponding to those lags obtained by interchanging the  $x$  and  $y$  coordinates of the original lags.

**Theorem 2** Let all the assumptions of Theorem 1 hold. If, in addition, the process is reflection symmetric, then for any fixed

$(h_x, h_y)$  and  $(g_x, g_y)$ ,

$$\lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{C}(h_x, h_y), \hat{C}(g_x, g_y) \right]$$

$$= \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{C}(-h_x, h_y), \hat{C}(-g_x, g_y) \right].$$

$$\lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{\gamma}(h_x, h_y), \hat{\gamma}(g_x, g_y) \right]$$

$$= \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{\gamma}(-h_x, h_y), \hat{\gamma}(-g_x, g_y) \right].$$

Furthermore, if the process is isotropic and the internodal spacing is the same in the  $x$  and  $y$  directions, then

$$\lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{C}(h_x, h_y), \hat{C}(g_x, g_y) \right]$$

$$= \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{C}(h_y, h_x), \hat{C}(g_y, g_x) \right]$$

$$= \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{C}(-h_y, h_x), \hat{C}(-g_y, g_x) \right]$$

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$$\lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{\gamma}(h_x, h_y), \hat{\gamma}(g_x, g_y) \right]$$

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$$= \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left[ \hat{\gamma}(-h_x, h_y), \hat{\gamma}(-g_x, g_y) \right]$$

It is noted that  $\gamma(h_x, h_y) = C(0, 0) - C(h_x, h_y)$

under second order stationarity. However, the sample semivariogram and sample covariogram do not satisfy the same relation in general i.e.  $\hat{\gamma}(h_x, h_y) \neq \hat{C}(0,0) - \hat{C}(h_x, h_y)$ .

To investigate whether the sample covariogram or the sample semivariogram is most suitable for testing the goodness of fit of any proposed second-order property, the sampling variations of the sample covariogram and semivariogram are compared. Now, define

$$\sigma_{(h_x, h_y)(g_x, g_y)}^c \equiv \lim_{r \rightarrow \infty} r c \operatorname{Cov} \left[ \hat{C}(h_x, h_y), \hat{C}(g_x, g_y) \right]$$

$$c \rightarrow \infty$$

$$\sigma_{(h_x, h_y)(g_x, g_y)}^r \equiv \lim_{r \rightarrow \infty} r c \operatorname{Cov} \left[ \hat{\gamma}(h_x, h_y), \hat{\gamma}(g_x, g_y) \right]$$

$$c \rightarrow \infty$$

Theorem 3 Assume that  $\{Z(\mathcal{S})\}$  is a second-order stationary Gaussian process. For any fixed lags  $(h_x, h_y)$  and  $(g_x, g_y)$ ,

$$\sigma_{(h_x, h_y)(g_x, g_y)}^r > \sigma_{(h_x, h_y)(g_x, g_y)}^c \quad \text{if and only}$$

$$\text{if. } \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} C(p, q) \left[ C(p, q) - C(p - h_x, q - h_y) - C(p + g_x, q + g_y) \right] > 0$$

An important special case of Theorem 3 is that the asymptotic variance of  $\sqrt{rc} \hat{\gamma}(h_x, h_y)$  is larger than the asymptotic variance of  $\sqrt{rc} \hat{C}(h_x, h_y)$  if and only if

$$\sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} C(p, q) \left[ C(p, q) - C(p - h_x, q - h_y) - C(p + h_x, q + h_y) \right] > 0$$

Corollary 3.1 Assume that  $\{Z(\mathcal{S})\}$  is an

$(m_x, m_y)$ -dependent, second-order stationary Gaussian process. For any two lags  $(h_x, h_y)$  and  $(g_x, g_y)$ ,

(i) If  $\max(|h_x|, |g_x|) > 2m_x$  or  $\max(h_y, g_y) > 2m_y$ ,

then  $\sigma_{(h_x, h_y)(g_x, g_y)}^r \geq \sigma_{(h_x, h_y)(g_x, g_y)}^c$ ;

(ii) If  $(|h_x| > 2m_x \text{ or } h_y > 2m_y)$  and

$(|g_x| > 2m_x \text{ or } g_y > 2m_y)$  then

$$\sigma_{(h_x, h_y)(g_x, g_y)}^r - \sigma_{(h_x, h_y)(g_x, g_y)}^c = 2 \sum_{p=-\infty}^{\infty} \sum_{q=-\infty}^{\infty} C^2(q, p);$$

(iii) If  $(|h_x| > m_x \text{ or } h_y > m_y)$  and

$(|g_x| > m_x \text{ or } g_y > m_y)$  then

$$\sigma_{(h_x, h_y)(g_x, g_y)}^r > \sigma_{(h_x, h_y)(g_x, g_y)}^c.$$

Since the differences among elements of the sample covariogram or sample emivariogram are used in testing for some directional properties, it is important to investigate the asymptotic covariance matrix of those differences further. It is interesting that although the asymptotic covariance matrices are different, the asymptotic covariance matrices of vectors of within-estimator differences are the same.

Theorem 4. Assume that  $\{Z(\mathcal{S})\}$  is a second-order stationary Gaussian process. For any fixed lags  $(h_x, h_y)$ ,  $(g_x, g_y)$ ,  $(u_x, u_y)$  and  $(v_x, v_y)$

$$\lim_{r \rightarrow \infty} r c \operatorname{Cov} \left\{ \left[ \hat{C}(h_x, h_y) - \hat{C}(g_x, g_y) \right], \right.$$

$$c \rightarrow \infty$$

$$\begin{aligned} & \left[ \hat{C}(u_x, u_y) - \hat{C}(v_x, v_y) \right] \\ = & \lim_{\substack{r \rightarrow \infty \\ c \rightarrow \infty}} rc \text{Cov} \left\{ \left[ \hat{\gamma}(h_x, h_y) - \hat{\gamma}(g_x, g_y) \right], \right. \\ & \left. \left[ \hat{\gamma}(u_x, u_y) - \hat{\gamma}(v_x, v_y) \right] \right\}. \end{aligned}$$

### (3) Asymptotic Normality

Lu (1994), (1997) showed that under the same assumptions, the sample covariogram and sample semivariogram have asymptotic normal distributions. Moreover, by the classical variance stabilization transformation,  $\log\{\hat{\gamma}(h)\}$  and  $\hat{\rho}(h)$  also have asymptotic normal distributions. In practice, the variance stabilization transformation may lead to normality faster for moderately small sample sizes. To support this evidence, the Anderson-Darling normality test was used. Realizations of zero mean, second-order stationary Gaussian random fields with the semivariogram given by

$$\gamma(r; \theta) = \begin{cases} \theta_1 \left( \frac{3r}{2\theta_2} - \frac{r^3}{2\theta_2^3} \right) & \text{if } 0 \leq r \leq \theta_2 \\ \theta_1 & \text{o.w.} \end{cases}$$

were generated on a 10x10 square grid with unit spacing,  $\theta_1 = 1$  and  $\theta_2 = .$  From the results, it's evident that  $\log\{\hat{\gamma}(h)\}$  has converged to normal distribution very well for moderately large sample sizes,  $n=100$ . However, the convergence of  $\hat{\gamma}(h)$  and  $\hat{C}(h)$  is not good. Especially,  $\hat{C}(h)$  shows very strong abnormality. According to the simulation, it needs about 400 samples or

more for  $\hat{C}(h)$  having good normal approximation. It is interesting that the results show that the rate of convergence of  $\hat{\rho}(h)$  is faster than that of  $\hat{\gamma}(h)$ . Thus, using  $\hat{\rho}(h)$  in testing for directional symmetry properties is better than using  $\hat{\gamma}(h)$ . This also implies that  $\hat{\rho}(h)$  would be the best choice for testing for separability.

### (4) Tests for Reflection Symmetry and Isotropy

Lu (1994) established a  $\chi^2$ -test for reflection symmetry and isotropy with the sample semivariogram and the sample covariogram. Since  $\log\{\hat{\gamma}(h)\}$  and  $\hat{\rho}(h)$  converge faster than  $\hat{\gamma}(h)$  and  $\hat{C}(h)$ , their tests for reflection symmetry and isotropy perform better, too. So here I focus the comparisons of test performance on  $\log\{\hat{\gamma}(h)\}$  and  $\hat{\rho}(h)$ . Specifically, I report the isotropy test results here.

Gaussian random fields exhibiting isotropy or geometric anisotropy of different strengths and orientations were generated on a  $c \times c$  square grid with unit spacing. Each random field had a covariance structure determined by an isotropic or geometrically anisotropic spherical semivariogram given by

$$\gamma(r; \theta) = \begin{cases} \theta_1 \left( \frac{3r}{2\theta_2} - \frac{r^3}{2\theta_2^3} \right) & \text{if } 0 \leq r \leq \theta_2 \\ \theta_1 & \text{o.w.} \end{cases}$$

where  $\gamma = (h' B h)^{1/2}$  and  $B$  is a  $2 \times 2$  positive definite matrix. Parameter  $\theta_1$  was equal to 1

throughout the study and  $\theta_2$  corresponding to different strength of spatial dependence was taken to equal to 1, 5 and 8 respectively. Five  $B$ -matrices were used:

$$B_0 = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}, \quad B_1 = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix}, \quad B_2 = \begin{bmatrix} 1 & 0 \\ 0 & 16 \end{bmatrix},$$

$$B_3 = \begin{bmatrix} 5/2 & -3/2 \\ -3/2 & 5/2 \end{bmatrix}, \quad B_4 = \begin{bmatrix} 17/2 & -15/2 \\ -15/2 & 17/2 \end{bmatrix}.$$

One thousand realizations of  $n=c^2$  observations were obtained for each choice of  $B$ -matrix and two choices of  $n$ ,  $n=100$  and  $n=400$ . We took  $\ell_x = \ell_y \equiv \ell$  with  $\ell=1$  and  $\ell=2$  and  $m_x = m_y \equiv m_0$ . Basically, when  $\ell=1$ , tests based on  $\log\{\hat{\gamma}(h)\}$  and  $\hat{\rho}(h)$  almost perform equivalently well. Especially, the Type I error rates of tests based on  $\hat{\rho}(h)$  are always less than nominal levels and the power is often high. However, when  $\ell=2$ , the power of tests based on  $\hat{\rho}(h)$  seems less than that of  $\log\{\hat{\gamma}(h)\}$ . Hence, it is suggested to use  $\log\{\hat{\gamma}(h)\}$  in testing reflection symmetry and isotropy and  $\hat{\rho}(h)$  may be used in testing for separability.

#### 4 Comments on the results of the study.

For a second-order stationary process, the covariogram and the semivariogram are two functions which can be used to characterize the spatial dependence. Each has its merits, but the semivariogram has been given priority in spatial statistics mainly because use of the

semivariogram allows more general processes to be considered. In this study, I compare the two estimators in terms of their asymptotic bias, covariance structures, rate of convergence, and capability of testing for directional symmetry properties. Through the simulation study, I conclude that  $\log\{\hat{\gamma}(h)\}$  is most suitable for testing the goodness of fit of any proposed second-order property. However, some theoretical works still need to be done about the rate of convergence of these estimators and the reasons which may affect the test performance. Finally, I would like to emphasize further that practitioners of geostatistics ought to make more use of variogram in analyzing geostatistical data.

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Table 1 Number of rejections for the 20 data sets using the Anderson-Darling test of normality.

$lag\ h$	$\hat{\gamma}(h)$	$\log\{\hat{\gamma}(h)\}$	$\hat{C}(h)$	$\hat{\rho}(h)$
(1,0)	11	1	19	7
(0,1)	11	3	20	5
(1,1)	15	1	20	3
(-1,1)	11	1	20	3

Table 2(a) Isotropy Tests based on  $\log(\hat{\gamma}(h))$ . ( the empirical proportion of times that isotropy was rejected )

$n$	$\theta_2$	$l$	$m_0$	$B_0$	$B_1$	$B_2$	$B_3$	$B_4$
100	2	1	1	0.071	0.525	0.500	0.153	0.143
			2	0.034	0.400	0.381	0.083	0.081
		2	1	0.194	0.355	0.355	0.213	0.227
			2	0.126	0.290	0.290	0.140	0.139
	5	1	1	0.070	0.822	0.993	0.595	0.919
			2	0.042	0.674	0.988	0.498	0.878
			3	0.026	0.449	0.937	0.264	0.787
			5	0.000	0.049	0.458	0.026	0.186
		2	1	0.133	0.396	0.625	0.286	0.490
			2	0.104	0.338	0.609	0.276	0.485
			3	0.059	0.210	0.530	0.187	0.317
			5	0.007	0.053	0.171	0.048	0.073
	8	1	1	0.086	0.816	0.997	0.546	0.931
			2	0.040	0.647	0.989	0.448	0.919
			4	0.019	0.170	0.802	0.112	0.587
			8	0.000	0.000	0.000	0.000	0.000
		2	1	0.156	0.391	0.656	0.280	0.537
			2	0.084	0.300	0.655	0.213	0.438
			4	0.035	0.088	0.347	0.081	0.216
			8	0.000	0.000	0.000	0.000	0.000
400	2	1	1	0.056	0.986	0.990	0.283	0.325
			2	0.050	0.984	0.984	0.249	0.295
		2	1	0.057	0.920	0.920	0.131	0.127
			2	0.044	0.892	0.892	0.100	0.100
	5	1	1	0.075	1.000	1.000	0.997	1.000
			2	0.038	1.000	1.000	0.991	1.000
			3	0.034	1.000	1.000	0.994	1.000
		2	5	0.011	1.000	1.000	0.988	1.000
			1	0.206	0.923	0.926	0.883	0.908



8	1	2	0.180	0.970	0.999	0.948	0.993
		3	0.101	0.988	1.000	0.960	0.995
		5	0.054	0.974	0.998	0.890	0.993
		1	0.081	1.000	1.000	0.995	0.994
		2	0.048	1.000	1.000	0.991	1.000
		4	0.032	0.999	1.000	0.983	1.000
	2	8	0.002	0.941	1.000	0.841	1.000
		1	0.184	0.881	0.931	0.774	0.925
		2	0.150	0.910	0.949	0.824	0.909
		4	0.100	0.940	0.965	0.877	0.955
		8	0.029	0.597	0.988	0.462	0.963

Table 2(b) Isotropy Tests based on  $\hat{\rho}(h)$

$n$	$\theta_2$	$\ell$	$m_0$	$B_0$	$B_0$	$B_0$	$B_0$	$B_0$
100	2	1	1	0.104	0.613	0.589	0.174	0.193
			2	0.068	0.532	0.506	0.123	0.128
		2	1	0.117	0.529	0.489	0.204	0.212
			2	0.216	0.534	0.496	0.287	0.296
	5	1	1	0.007	0.551	0.719	0.478	0.814
			2	0.016	0.621	0.592	0.576	0.795
			3	0.009	0.484	0.569	0.460	0.762
			5	0.006	0.202	0.511	0.214	0.599
		2	1	0.008	0.290	0.512	0.294	0.656
			2	0.069	0.404	0.273	0.429	0.521
			3	0.074	0.302	0.236	0.287	0.480
			5	0.039	0.148	0.174	0.127	0.322
	8	1	1	0.000	0.210	0.884	0.177	0.807
			2	0.001	0.279	0.648	0.339	0.695
			4	0.005	0.180	0.488	0.234	0.513
			8	0.000	0.000	0.000	0.000	0.000
		2	1	0.004	0.088	0.614	0.121	0.589
			2	0.021	0.229	0.326	0.243	0.344
			4	0.028	0.143	0.161	0.153	0.236
			8	0.000	0.000	0.000	0.000	0.000
400	2	1	1	0.061	0.985	0.990	0.315	0.341
			2	0.053	0.985	0.988	0.288	0.326
		2	1	0.033	0.933	0.936	0.123	0.157
			2	0.055	0.930	0.937	0.141	0.161
	5	1	1	0.000	0.989	0.938	0.956	0.991
			2	0.003	0.999	0.816	0.996	0.983
			3	0.011	0.997	0.793	0.994	0.974
		5	1	0.011	0.990	0.799	0.983	0.967

	2	1	0.002	0.784	0.829	0.630	0.982
		2	0.004	0.973	0.514	0.977	0.914
5	2	3	0.008	0.960	0.359	0.950	0.912
		5	0.012	0.865	0.363	0.872	0.906
8	1	1	0.000	0.514	1.000	0.557	0.994
		2	0.000	0.701	0.907	0.865	0.871
		4	0.001	0.890	0.565	0.964	0.567
		8	0.000	0.551	0.681	0.794	0.624
	2	1	0.000	0.138	0.994	0.193	0.974
		2	0.000	0.383	0.698	0.463	0.586
		4	0.000	0.708	0.250	0.758	0.342
		8	0.003	0.326	0.300	0.385	0.367