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Extending Sliced Inverse Regression: the Weighted Chi-Squared Test

Efstathia BURA and R. Dennis COOK

Sliced inverse regression (SIR) and an associated chi-squared test for dimension have been introduced as a method for reducing the dimension of regression problems whose predictor variables are normal. In this article the assumptions on the predictor distribution, under which the chi-squared test was proved to apply, are relaxed, and the result is extended. A general weighted chi-squared test that does not require normal regressors for the dimension of a regression is given. Simulations show that the weighted chi-squared test is more reliable than the chi-squared test when the regressor distribution digresses from normality significantly, and that it compares well with the chi-squared test when the regressors are normal.

KEY WORDS: Dimension estimation; Dimension reduction.

1. INTRODUCTION

The overarching goal of a regression analysis is to understand how the conditional distribution of the univariate response Y given a vector \mathbf{X} of p predictors depends on the value assumed by \mathbf{X} . Although attention is often restricted to the mean function $E(Y|\mathbf{X})$ and perhaps the variance function $\text{var}(Y|\mathbf{X})$, in full generality the object of interest is the conditional distribution of $Y|\mathbf{X}$.

Graphical displays can be quite useful for investigating $Y|\mathbf{X}$, especially when an adequate parsimoniously parameterized model is not available and when looking for patterns in residuals. *Dimension reduction without loss of information* is a dominant theme of regression graphics: We try to reduce the dimension of \mathbf{X} without losing information on $Y|\mathbf{X}$ and without requiring a model for $Y|\mathbf{X}$. Borrowing terminology from classical statistics, we call this *sufficient dimension reduction*, which leads to the pursuit of *sufficient summary plots* containing all of the information on $Y|\mathbf{X}$ available from the sample.

Sliced inverse regression (SIR) is an innovative method for constructing summary plots developed by Li (1991). Informally, SIR provides a basis $\{\mathbf{b}_1, \dots, \mathbf{b}_p\}$ for \mathbb{R}^p , and corresponding *SIR predictors* $\{\mathbf{b}_1^T \mathbf{X}, \dots, \mathbf{b}_p^T \mathbf{X}\}$ that are ordered according to their likely importance to the regression. Thus the first SIR predictor, $\mathbf{b}_1^T \mathbf{X}$, is likely more important than the second, $\mathbf{b}_2^T \mathbf{X}$, and so on. Plots of Y versus various combinations of the SIR predictors can provide useful information on the regression, with the three-dimensional plot of Y versus the first two SIR predictors often being the most informative.

It can be helpful to know whether we need to inspect plots involving all p SIR predictors, or whether we can concentrate on the first few without losing important information. Li (1991) provided a testing procedure to help determine the number of "significant SIR predictors." The procedure requires that \mathbf{X} be normally distributed, which results in a chi-squared reference distribution. This requirement can be worrisome in practice, because deviations from normality can influence the outcome.

In this article we discuss an alternative testing procedure that is based on the test statistic suggested by Li (1991), but does not require normally distributed predictors. Relaxing the

normal requirement results in a reference distribution that is a weighted sum of chi-squares rather than a chi-square. The weights are unknown in general and thus must be estimated from the sample. This alternative procedure can be helpful in practice for two reasons: (a) it can confirm the indications of Li's chi-squared test, increasing confidence in the results, and (b) it can help decide ambiguous situations.

In Section 2 the regression context is set out, and SIR and the associated chi-squared test are reviewed. The weighted chi-squared test is developed in Section 3.1, and a description of how it can be implemented in practice is given in Section 3.2. Special cases resulting from the imposition of additional distributional assumptions are explored in Section 3.3. There it is also shown that for the chi-squared test to apply, joint normality of the predictors is not required, but rather constant second moments of the conditionals of the predictors suffices. The mussel data are analyzed in Section 4. A simulation comparison of the two tests is given in Section 5. We conclude from those simulation results that estimation of the weights does not compromise the advantages that the weighted chi-squared test has over the chi-squared test in cases with nonnormal predictors. The article concludes with a brief discussion in Section 6.

2. REGRESSION CONTEXT AND SLICED INVERSE REGRESSION

Sufficient dimension reduction in regression focuses on finding $k \leq p$ linear combinations $\boldsymbol{\eta}_1^T \mathbf{X}, \dots, \boldsymbol{\eta}_k^T \mathbf{X}$ that can replace \mathbf{X} without loss of information and without requiring restrictive conditions on $Y|\mathbf{X}$. Letting $\boldsymbol{\eta}$ denote the $p \times k$ matrix with columns $\boldsymbol{\eta}_j$, we require that

$$Y \perp\!\!\!\perp \mathbf{X} | \boldsymbol{\eta}^T \mathbf{X}, \quad (1)$$

where the notation $\perp\!\!\!\perp$ indicates independence. The statement is thus that Y is independent of \mathbf{X} given any value for $\boldsymbol{\eta}^T \mathbf{X}$.

For any vector or matrix $\boldsymbol{\alpha}$, let $S(\boldsymbol{\alpha})$ denote its range space with dimension $\dim(S(\boldsymbol{\alpha}))$. If (1) holds, then it also holds with $\boldsymbol{\eta}$ replaced by any basis for $S(\boldsymbol{\eta})$. In this sense, (1) can be regarded as a statement about $S(\boldsymbol{\eta})$ rather than a statement about a basis $\boldsymbol{\eta}$ per se. Thus when (1) holds, we follow Li

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(1991, 1992) and call $S(\boldsymbol{\eta})$ a *dimension-reduction subspace* for the regression of Y on \mathbf{X} .

The usual objective of a dimension-reduction analysis is to infer about a *smallest* dimension-reduction subspace. Although there is more than one way to define such a subspace, here we rely on the *central (dimension-reduction) subspace*, denoted by $S_{Y|\mathbf{X}}$, which was introduced by Cook (1994b, 1996). $S_{Y|\mathbf{X}}$ is the intersection of all dimension-reduction subspaces for the regression. It is trivially a subspace, but it is not necessarily a dimension-reduction subspace. The existence of central subspaces can be ensured by placing fairly weak restrictions on aspects of the joint distribution of Y and \mathbf{X} (Cook 1994a, 1996, 1998a,b). We assume throughout that the central subspace exists.

The central subspace $S_{Y|\mathbf{X}}$ is in effect a meta-parameter used to index the conditional distribution of Y given \mathbf{X} . We use the columns of the $p \times k$ matrix $\boldsymbol{\eta}$ to represent a basis for the central space $S_{Y|\mathbf{X}}$. The plot of Y versus $\boldsymbol{\eta}^T \mathbf{X}$ is a *minimal sufficient summary plot* (Cook 1998a) for the regression of Y on \mathbf{X} .

Several methods can be used to estimate $S_{Y|\mathbf{X}}$, or portions thereof. In this article we are concerned only with SIR, which we have found to be a useful first method in any dimension-reduction inquiry.

In this article we work mostly in terms of the standardized predictor

$$\mathbf{Z} = \boldsymbol{\Sigma}_x^{-1/2}(\mathbf{X} - E(\mathbf{X})),$$

where $\boldsymbol{\Sigma}_x = \text{var}(\mathbf{X}) > 0$. This facilitates development and involves no loss of generality, because we can always back-transform to the original scale because $S_{Y|\mathbf{X}} = \boldsymbol{\Sigma}_x^{-1/2} S_{Y|\mathbf{Z}}$. Moreover, the SIR predictors reviewed in this section are invariant under full rank linear transformations of \mathbf{X} . Consequently, summary plots will look the same whether we work in the scale of \mathbf{X} or \mathbf{Z} .

Let the columns $\boldsymbol{\beta}_j$ of the $p \times k$ matrix $\boldsymbol{\beta}$ be a basis for the central subspace $S_{Y|\mathbf{Z}}$. In practice, \mathbf{Z} is constructed by replacing $\boldsymbol{\Sigma}_x$ and $E(\mathbf{X})$ with the usual moment estimates. SIR requires that the conditional expectation $E(\mathbf{Z}|\boldsymbol{\beta}^T \mathbf{Z})$ be linear. This is equivalent to requiring that $E(\mathbf{Z}|\boldsymbol{\beta}^T \mathbf{Z}) = \mathbf{P}_\beta \mathbf{Z}$, where \mathbf{P}_β is the orthogonal projection operator for $S(\boldsymbol{\beta}) = S_{Y|\mathbf{Z}}$ with respect to the usual inner product (Cook 1998b, p. 57). We call this restriction the *linearity condition*. The linearity condition involves only the marginal distribution of \mathbf{Z} , and is required to hold only for the basis $\boldsymbol{\beta}$. Although minor deviations from the linearity condition may not matter much, substantial deviations can produce misleading results.

SIR makes use of the *inverse regression subspace* $S_{E(\mathbf{Z}|Y)}$, defined as the span of $E(\mathbf{Z}|Y)$ as Y varies in its marginal sample space. Under the linearity condition,

$$S_{E(\mathbf{Z}|Y)} \subseteq S_{Y|\mathbf{Z}}. \quad (2)$$

If Y is discrete, then this result can be used to justify using conditional sample means $\widehat{E}(\mathbf{Z}|Y)$ as estimates of vectors in the central subspace. When Y is continuous, Li (1991) suggested replacing Y with a discrete version \tilde{Y} based on partitioning the observed range of Y into H fixed, nonoverlapping slices. By (1), $\tilde{Y} \perp \mathbf{Z}|\boldsymbol{\beta}^T \mathbf{Z}$ and thus $S_{\tilde{Y}|\mathbf{Z}} \subseteq S_{Y|\mathbf{Z}}$. In addition, provided that H is sufficiently large, $S_{\tilde{Y}|\mathbf{Z}} = S_{Y|\mathbf{Z}}$, and there is no loss of

information when Y is replaced by \tilde{Y} . Using (2), SIR can be justified on the following line of reasoning:

$$S\{\text{cov}[E(\mathbf{Z}|\tilde{Y})]\} = S_{E(\mathbf{Z}|\tilde{Y})} \subseteq S_{\tilde{Y}|\mathbf{Z}} \subseteq S_{Y|\mathbf{Z}}, \quad (3)$$

where the first equality follows from proposition 2.7 of Eaton (1983, p. 75). (See also Cook 1998b, prop. 11.1.)

Thus $S_{E(\mathbf{Z}|\tilde{Y})}$ is spanned by the eigenvectors corresponding to the nonzero eigenvalues of $\mathbf{V} = \text{cov}[E(\mathbf{Z}|\tilde{Y})]$. Consequently, an estimate of $S_{E(\mathbf{Z}|\tilde{Y})}$ can be constructed from the estimated covariance matrix $\widehat{\mathbf{V}}$ by using its eigenvectors corresponding to its eigenvalues, which are inferred to be nonzero in the population.

2.1 Sliced Inverse Regression Algorithm

Given a random sample $\{(Y_i, \mathbf{X}_i^T)\}_{i=1}^n$ from (Y, \mathbf{X}^T) , begin by constructing a discrete version \tilde{Y} of Y . The number of slices H is chosen much like a tuning parameter in smoothing (see Li 1991 for further discussion). Next, form the intraslice means $\bar{\mathbf{Z}}_s$, $s = 1, \dots, H$, of the sample version of the standardized predictor vector. Finally, form the sample version $\widehat{\mathbf{V}}$ of $\mathbf{V} = \text{cov}[E(\mathbf{Z}|\tilde{Y})]$,

$$\widehat{\mathbf{V}} = \sum_{s=1}^H f_s \bar{\mathbf{Z}}_s \bar{\mathbf{Z}}_s^T = \widehat{\mathbf{Z}}_n \widehat{\mathbf{Z}}_n^T,$$

where $f_s = n_s/n$ is the fraction of observations falling in slice s and

$$\widehat{\mathbf{Z}}_n = (\bar{\mathbf{Z}}_1 \sqrt{f_1}, \dots, \bar{\mathbf{Z}}_H \sqrt{f_H}) \quad (4)$$

is the $p \times H$ matrix of weighted intraslice sample means of the standardized predictors. Letting $\hat{\boldsymbol{\beta}}_j$ denote the j th eigenvector of $\widehat{\mathbf{V}}$, the j th SIR predictor is constructed as $\hat{\boldsymbol{\beta}}_j^T \mathbf{Z}$, $j = 1, \dots, p$.

Let $d = \dim(S_{E(\mathbf{Z}|\tilde{Y})})$. The span of the d eigenvectors $\hat{\boldsymbol{\beta}}_j$, $j = 1, \dots, d$, of $\widehat{\mathbf{V}}$ that correspond to its first d eigenvalues $\lambda_1 \geq \dots \geq \lambda_d > \dots \geq \lambda_p$ is an estimate of $S_{E(\mathbf{Z}|\tilde{Y})} \subseteq S_{Y|\mathbf{Z}}$. Under the assumption of normal predictors, Li (1991) proved that the test statistic

$$\widehat{\Lambda}_d = n \sum_{j=d+1}^p \hat{\lambda}_j \quad (5)$$

has an asymptotic chi-squared distribution with $(p-d)(H-d-1)$ degrees of freedom. Consequently, the number d of nonzero eigenvalues of \mathbf{V} , which is also the dimension of the subspace $S_{E(\mathbf{Z}|\tilde{Y})}$, can be estimated as follows: The null hypothesis that $d = j$ is rejected in favor of the alternative that $d \geq j+1$ when $\widehat{\Lambda}_j$ is larger than the percentage points of a chi-squared distribution with $(p-j)(H-j-1)$ degrees of freedom.

Other testing techniques that use the same simple nonparametric estimation method as Li (1991) have been developed. Schott (1994) proposed a test that requires elliptically symmetric regressors and for which the tuning constant is the number of observations c per slice, as opposed to the number of slices H of Li (1991). To obtain the asymptotic distribution of his test statistic, Schott lets c go to infinity. Velilla (1998) introduced testing method that does not impose restrictions

on the regressor distribution, where c is fixed and the number of slices H varies. Ferré (1998) took a model selection approach to the estimation of dimension by studying the quality of estimation through a measure of closeness between $S_{E(\mathbf{X}|\tilde{Y})}$ and its estimates.

Our method extends SIR's applicability by lifting the normality assumption on the regressors and replacing it by the minimal requirement of finite second moments. The tuning parameter is the number of slices and is assumed to be fixed, as in SIR. The only comparable method among the ones listed earlier is Velilla's, because it does not restrict the regressor distribution. Nevertheless, Velilla uses the number of points per slice as a tuning parameter and imposes several regularity conditions on both the regressor distribution and the regression curve $E(Y|\mathbf{X})$.

3. WEIGHTED CHI-SQUARED TEST

Various results on the distribution of $\hat{\Lambda}_d$ are presented in this section. The development of the general weighted chi-squared test in Section 3.1 requires only that the data be iid with finite first two moments. The general logic behind this development is similar to that used by Cook (1998a) to derive the asymptotic distribution of statistics used in the method of principal Hessian directions (Li 1992). But the details here are different, because the methods and statistics are different. Subsequent results given in Section 3.3 require various additional conditions.

3.1 Development

Letting p_s denote the probability that Y is in slice s , the matrix of weighted intraslice means $\hat{\mathbf{Z}}_n$ converges almost surely to

$$\mathbf{B} = (E(\mathbf{Z}|\tilde{Y}=1)\sqrt{p_1}, \dots, E(\mathbf{Z}|\tilde{Y}=H)\sqrt{p_H}) \quad (6)$$

with singular value decomposition

$$\mathbf{B} = \mathbf{\Gamma}_1 \begin{bmatrix} \mathbf{D} & 0 \\ 0 & 0 \end{bmatrix} \mathbf{\Gamma}_2^T,$$

where $\mathbf{\Gamma}_1$ is an orthonormal $p \times p$ matrix, $\mathbf{\Gamma}_2$ is an orthonormal $H \times H$ matrix, and \mathbf{D} is a $d \times d$ diagonal matrix with the positive singular values of \mathbf{B} along its diagonal. Recalling that $d = \dim(S_{E(\mathbf{Z}|\tilde{Y})})$, partition $\mathbf{\Gamma}_1 = (\mathbf{\Gamma}_{11}, \mathbf{\Gamma}_{12})$, where $\mathbf{\Gamma}_{11}: p \times d$, $\mathbf{\Gamma}_{12}: p \times (p-d)$, and partition

$$\mathbf{\Gamma}_2^T = \begin{bmatrix} \mathbf{\Gamma}_{21}^T \\ \mathbf{\Gamma}_{22}^T \end{bmatrix}, \quad (7)$$

where $\mathbf{\Gamma}_{21}^T: d \times H$, $\mathbf{\Gamma}_{22}^T: (H-d) \times H$. The columns of $\mathbf{\Gamma}_{11}$ form a basis for $S_{E(\mathbf{Z}|\tilde{Y})} = S(\mathbf{V})$.

Given a $r \times c$ matrix $\mathbf{A} = (a_1, \dots, a_c)$, let $\text{vec}(\mathbf{A})$ denote the $rc \times 1$ vector constructed by stacking the columns of \mathbf{A} one after another, that is, $\text{vec}(\mathbf{A})^T = (a_1^T, \dots, a_c^T)$.

Let $\tilde{\mathbf{Z}}_n = \sqrt{n}(\hat{\mathbf{Z}}_n - \mathbf{B})$, where $\hat{\mathbf{Z}}_n$ and \mathbf{B} are defined in (4) and (6). By the multivariate central limit theorem and the multivariate version of Slutsky's theorem, the $pH \times 1$ vector $\text{vec}(\tilde{\mathbf{Z}}_n)$

converges to a multivariate normal distribution with mean 0 and covariance matrix Δ ,

$$\text{vec}(\tilde{\mathbf{Z}}_n) \xrightarrow{D} N_{pH}(0, \Delta) \quad \text{as } n \rightarrow \infty. \quad (8)$$

It follows from Eaton and Tyler (1994) that the limiting distribution of the smallest $\min(p-d, H-d)$ singular values of $\tilde{\mathbf{Z}}_n$ is the same as the limiting distribution of the corresponding singular values of the $(p-d) \times (H-d)$ matrix

$$\sqrt{n} \mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22}. \quad (9)$$

The operation applied to $\hat{\mathbf{Z}}_n$ in (9) selects the space spanned by the eigenvectors corresponding to the $p-d$ smallest eigenvalues of \mathbf{V} . This space coincides with the space spanned by the eigenvectors corresponding to the largest $p-d$ eigenvalues of $E(\text{cov}(\mathbf{Z}|\tilde{Y}))$ (see Li 1991, remarks 3.1 and 5.3). Hsing and Carroll (1992) obtained the asymptotic normality of their estimate of $E(\text{cov}(\mathbf{Z}|\tilde{Y}))$, which they constructed using two observations per slice, by imposing restrictions on both the regressor and the conditional distribution of $\mathbf{X}|Y$. Zhu and Ng (1995) generalized their results to more than two observations per slice.

The asymptotic distribution of $\hat{\Lambda}_d$ is the same as that of the sum of the squares of the singular values of (9), which can be expressed as $n \times \text{trace}[\mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22} (\mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22})^T]$. Therefore, the asymptotic distribution of $\hat{\Lambda}_d$ is the same as the asymptotic distribution of $n \text{vec}(\mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22})^T \text{vec}(\mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22})$. By (8), the limiting distribution of the vector version of (9) is

$$\sqrt{n} \text{vec}(\mathbf{\Gamma}_{12}^T \hat{\mathbf{Z}}_n \mathbf{\Gamma}_{22}) \xrightarrow{D} N_{(H-d)(p-d)}(0, (\mathbf{\Gamma}_{22}^T \otimes \mathbf{\Gamma}_{12}^T) \Delta (\mathbf{\Gamma}_{22} \otimes \mathbf{\Gamma}_{12})), \quad (10)$$

where \otimes denotes the Kronecker product. Finally, the asymptotic distribution of $\hat{\Lambda}_d$ is given in the following theorem.

Theorem 1. Assume that $H > d+1$ and $p > d$. Then the limiting distribution of $\hat{\Lambda}_d$ is the same as that of

$$C = \sum_{k=1}^{(p-d)(H-d)} \omega_k C_k$$

where the C_k 's are independent chi-squared random variables each with 1 degree of freedom, $\omega_1 \geq \omega_2 \geq \dots \geq \omega_{(p-d)(H-d)}$ are the ordered eigenvalues of

$$\Delta_C = (\mathbf{\Gamma}_{22}^T \otimes \mathbf{\Gamma}_{12}^T) \Delta (\mathbf{\Gamma}_{22} \otimes \mathbf{\Gamma}_{12}), \quad (11)$$

and \otimes denotes the Kronecker product.

Theorem 1 allows for a general test of dimension provided that we can obtain a consistent estimate of Δ_C from which to construct estimates of the eigenvalues ω_k . To this end, it is useful to investigate the form of Δ .

Δ can be represented as an $H \times H$ array of $p \times p$ matrices Δ_{ts} by partitioning according to the intraslice averages $\bar{\mathbf{Z}}_j$. Letting $\Sigma_{u|s} = \text{cov}(\mathbf{U}|\tilde{Y}=s)$ denote the conditional covariance matrix of a random vector \mathbf{U} in slice s , the various sub-matrices Δ_{ts} can be computed as follows. For $t = s$,

$$\Delta_{ss} = np_s \Sigma_x^{-1/2} \text{cov}(\bar{\mathbf{X}}_s - \bar{\mathbf{X}}) \Sigma_x^{-1/2}$$

But

$$\begin{aligned}\text{cov}(\bar{\mathbf{X}}_s - \bar{\mathbf{X}}) &= \text{cov}(\bar{\mathbf{X}}_s) - 2\text{cov}(\bar{\mathbf{X}}_s, \bar{\mathbf{X}}) + \text{cov}(\bar{\mathbf{X}}) \\ &= \frac{\boldsymbol{\Sigma}_{x|s}}{n_s} - 2\text{cov}\left(\bar{\mathbf{X}}_s, \sum_{s=1}^H p_s \bar{\mathbf{X}}_s\right) + \frac{\boldsymbol{\Sigma}_x}{n} \\ &= \frac{1}{n} \left(\boldsymbol{\Sigma}_x + \frac{1-2p_s}{n_s} \boldsymbol{\Sigma}_{x|s} \right).\end{aligned}$$

Thus

$$\boldsymbol{\Delta}_{ss} = \mathbf{I}_p p_s + (1-2p_s) \boldsymbol{\Sigma}_{z|s}, \quad (12)$$

where

$$\boldsymbol{\Sigma}_{z|s} = \boldsymbol{\Sigma}_x^{-1/2} \boldsymbol{\Sigma}_{x|s} \boldsymbol{\Sigma}_x^{-1/2}.$$

For $t \neq s$,

$$\begin{aligned}\boldsymbol{\Delta}_{ts} &= n\sqrt{p_t p_s} \boldsymbol{\Sigma}_x^{-1/2} \text{cov}(\bar{\mathbf{X}}_t - \bar{\mathbf{X}}, \bar{\mathbf{X}}_s - \bar{\mathbf{X}}) \boldsymbol{\Sigma}_x^{-1/2} \\ &= \sqrt{p_t p_s} (\mathbf{I}_p - \boldsymbol{\Sigma}_{z|t} - \boldsymbol{\Sigma}_{z|s})\end{aligned} \quad (13)$$

because

$$\text{cov}(\bar{\mathbf{X}}_t - \bar{\mathbf{X}}, \bar{\mathbf{X}}_s - \bar{\mathbf{X}}) = \frac{1}{n} (\boldsymbol{\Sigma}_x - \boldsymbol{\Sigma}_{x|t} - \boldsymbol{\Sigma}_{x|s})$$

Clearly, $\boldsymbol{\Delta}$ can be estimated consistently by substituting sample versions of p_s , $\boldsymbol{\Sigma}_{x|s}$, $s = 1, \dots, H$, and $\boldsymbol{\Sigma}_x$. Additionally, under a hypothesized value of d , $\boldsymbol{\Gamma}_{22}$ and $\boldsymbol{\Gamma}_{12}$ can be estimated consistently using the sample versions computed from $\hat{\mathbf{Z}}_n$. Let $\hat{\boldsymbol{\Delta}}_C$ denote the resulting estimated version of $\boldsymbol{\Delta}_C$, and let $\hat{\omega}_k$ denote the eigenvalues of $\hat{\boldsymbol{\Delta}}_C$. The limiting distribution of $\hat{\Lambda}_d$ is then consistently estimated to be the same as that of

$$\hat{C} = \sum_{k=1}^{(p-d)(H-d)} \hat{\omega}_k C_k \quad (14)$$

These results can be used to estimate $d = \dim(S_{E(\mathbf{Z}|Y)})$ just as described for Li's chi-squared test procedure.

3.2 Test Algorithm

In this section we give a methodological version of the test of $d = j$ implied by the developments in the previous section:

1. From the singular value decomposition of $\hat{\mathbf{Z}}_n$, let $\hat{\boldsymbol{\Gamma}}_1$ denote the orthonormal $p \times p$ matrix of left singular vectors, and let $\hat{\boldsymbol{\Gamma}}_2$ denote the orthonormal $H \times H$ matrix of right singular vectors. This step is the same for all values of j .
2. Construct $\hat{\boldsymbol{\Gamma}}_{22}$ as the matrix of the last $H-j$ columns of $\hat{\boldsymbol{\Gamma}}_2$, and construct $\hat{\boldsymbol{\Gamma}}_{12}$ as the last the last $p-j$ columns of $\hat{\boldsymbol{\Gamma}}_1$.
3. Construct $\hat{\boldsymbol{\Delta}}$ by using estimates $\hat{\boldsymbol{\Delta}}_{st}$ of its submatrices from (12) for $s = t$ and (13) for $s \neq t$.
4. Use the results from steps 2 and 3 to construct $\hat{\boldsymbol{\Delta}}_C$, and find its eigenvalues $\hat{\omega}_k$.
5. Construct the p value for the weighted chi-squared test as

$$p \text{ value} = \Pr(\hat{C} > \text{observed } \hat{\Lambda}_j),$$

where the distribution of \hat{C} is given by (14). There is a substantial literature to assist in computing the tail probabilities of linear combinations of chi-squared random variables (see Field 1993 for an introduction).

The linearity condition, an essential part of the justification for SIR, is not required for Theorem 1, which provides a general method for inferring about $\dim(S_{E(\mathbf{Z}|\tilde{Y})})$. But the linearity condition is required for (3), which establishes the necessary relation between the inverse regression subspace and the central subspace.

When the number of observations per slice is small, the variation in the estimated weights $\hat{\omega}$ might mitigate the usefulness of the estimated distribution of $\hat{\Lambda}_d$. For this reason, it may be useful to know whether there are special cases in which the limiting distribution simplifies. We address such cases in the next section. These cases may help us gain a better feeling for the relative merits of the two test procedures under consideration.

3.3 Special Cases

The following lemma is used later in this section.

Lemma 1. Let \mathbf{g} denote the $H \times 1$ vector with elements $\sqrt{p_s}$, $s = 1, \dots, H$. Then $\|\mathbf{g}\| = 1$ and $\mathbf{g} \in S(\boldsymbol{\Gamma}_{22})$, where $\boldsymbol{\Gamma}_{22}$ is as defined in (7).

This lemma follows from the singular value decomposition of \mathbf{B} near (6) and the fact that $\mathbf{B}\mathbf{g} = \mathbf{E}(\mathbf{Z}) = \mathbf{0}$. The next result, stated as a corollary to Theorem 1, gives the first simplified result on the distribution of $\hat{\Lambda}_d$.

Corollary 1. Assume that the conditional covariance matrices $\boldsymbol{\Sigma}_{z|s}$ are constant across slices. Then the limiting distribution of $\hat{\Lambda}_d$ is chi-squared with $(p-d)(H-d-1)$ degrees of freedom.

Justification. Because the conditional covariance matrices are constant, $\boldsymbol{\Sigma}_{z|s} = \mathbf{I}_p$ for $s = 1, \dots, H$. Substituting this into the form for $\boldsymbol{\Delta}$ given previously yields $\boldsymbol{\Delta} = \mathbf{I}_{pH} - \mathbf{g}\mathbf{g}^T \otimes \mathbf{I}_p$, and thus

$$\boldsymbol{\Delta}_C = \mathbf{I}_{(p-d)(H-d)} - \boldsymbol{\Gamma}_{22}^T \mathbf{g}\mathbf{g}^T \boldsymbol{\Gamma}_{22} \otimes \mathbf{I}_{p-d},$$

which, from Lemma 1, is a symmetric idempotent matrix. The conclusion follows because $\text{trace}(\boldsymbol{\Delta}_C) = (p-d)(H-d-1)$.

We next develop another set of conditions under which $\hat{\Lambda}_d$ is asymptotically chi-squared. Let \mathbf{P}_{11} be the orthogonal projection operator onto $S(\boldsymbol{\Gamma}_{11})$, where $\boldsymbol{\Gamma}_{11}$ is the basis for $S_{E(\mathbf{Z}|\tilde{Y})}$ defined near (7). The linearity condition of Theorem 1 is equivalent to $\mathbf{E}(\mathbf{Z}|\boldsymbol{\Gamma}_{11}^T \mathbf{Z}) = \mathbf{P}_{11} \mathbf{Z}$. Also assume that

$$\text{cov}(\mathbf{Z}|\boldsymbol{\Gamma}_{11}^T \mathbf{Z}) = \mathbf{I}_p - \mathbf{P}_{11}. \quad (15)$$

Let $\boldsymbol{\Gamma}_{22} = (\gamma_{ts})$, $t = 1, \dots, H$, $s = 1, \dots, H-d$, denote the elements of $\boldsymbol{\Gamma}_{22}$. Then the (s, k) th block of $\boldsymbol{\Delta}_C$ in (11) is found by taking the product of the s th row block of $\boldsymbol{\Gamma}_{22}^T \otimes \boldsymbol{\Gamma}_{12}^T$ with $\boldsymbol{\Delta}$ and the k th column block of $\boldsymbol{\Gamma}_{22} \otimes \boldsymbol{\Gamma}_{12}$:

$$[\boldsymbol{\Delta}_C]_{sk} = \sum_l \sum_t \gamma_{ts} \gamma_{lk} \boldsymbol{\Gamma}_{12}^T \boldsymbol{\Delta}_{tl} \boldsymbol{\Gamma}_{12}.$$

For $t = l$,

$$\boldsymbol{\Gamma}_{12}^T \boldsymbol{\Delta}_{tt} \boldsymbol{\Gamma}_{12} = \boldsymbol{\Gamma}_{12}^T \boldsymbol{\Gamma}_{12} p_t + (1-2p_t) \boldsymbol{\Gamma}_{12}^T \boldsymbol{\Sigma}_{z|t} \boldsymbol{\Gamma}_{12}. \quad (16)$$

Next,

$$\begin{aligned}\Sigma_{z|t} &= E_{z|t}[\text{cov}(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z}, \tilde{Y} = t)] + \text{cov}_{z|t}[E(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z}, \tilde{Y} = t)] \\ &= E_{z|t}[\text{cov}(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z})] + \text{cov}_{z|t}[E(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z})],\end{aligned}$$

where the second equality follows because $Y \perp\!\!\!\perp \mathbf{Z}|\Gamma_{11}^T \mathbf{Z}$. By the linearity condition and (15), we have

$$\Gamma_{12}^T \text{cov}_{z|t}(E(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z}))\Gamma_{12} = \text{cov}_{z|t}(\Gamma_{12}^T \mathbf{P}_{11} \mathbf{Z}) = 0$$

and

$$\Gamma_{12}^T \text{cov}_{z|t}(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z})\Gamma_{12} = \Gamma_{12}^T (\mathbf{I}_p - \mathbf{P}_{11})\Gamma_{12} = \mathbf{I}_{p-d}.$$

Thus

$$\Gamma_{12}^T \Delta_{tt} \Gamma_{12} = (1 - p_t) \mathbf{I}_{p-d}.$$

Similarly, $\Gamma_{12}^T \Delta_{tt} \Gamma_{12} = -\sqrt{p_t p_l} \mathbf{I}_{p-d}$. Using Lemma 1 and $\Gamma_{22}^T \Gamma_{22} = \mathbf{I}_{H-d}$, we obtain the following.

Theorem 2. Let \mathbf{P}_{11} be the orthogonal projection operator onto $S(\Gamma_{11})$, where Γ_{11} is the basis for $S_{E(\mathbf{Z}|\tilde{Y})}$ defined near (7). Assume that the following conditions hold:

1. $Y \perp\!\!\!\perp \mathbf{Z}|\Gamma_{11}^T \mathbf{Z}$.
2. $E(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z}) = \mathbf{P}_{11} \mathbf{Z}$.
3. $\text{cov}(\mathbf{Z}|\Gamma_{11}^T \mathbf{Z}) = \mathbf{I}_p - \mathbf{P}_{11}$.
4. $H > d + 1$ and $p > d$.

Then $\hat{\Lambda}_d$ has an asymptotic chi-squared distribution with $(p - d)(H - d - 1)$ degrees of freedom.

Condition 1 of Theorem 2 ensures that the inverse mean function depends on \tilde{Y} only via $\Gamma_{11}^T \mathbf{Z}$. It implies that SIR will not miss any part of the central dimension-reduction subspace. Condition 2 is the linearity assumption, expressed in terms of the projection onto $S_{E(\mathbf{Z}|\tilde{Y})}$. Condition 4 is imposed to avoid trivial cases. Condition 3 is necessary to obtain an asymptotic chi-squared distribution. It is always satisfied when the original predictors are independent and $\Gamma_{11} = (\mathbf{I}_d, 0)$, regardless of the distribution of \mathbf{X} .

Conditions 1–3 are obviously satisfied when Y is stochastically independent of \mathbf{X} , so that $d = 0$. This means that SIR can be used as a diagnostic test for goodness of fit of a postulated model by using residuals in place of the response.

Li (1991) computed the asymptotic distribution of $\hat{\Lambda}_d$ for only the case in which the vector of predictors \mathbf{X} has a p -variate normal distribution, and then conditions 2 and 3 are obviously satisfied. Further, if condition 3 holds and \mathbf{X} is elliptically contoured, as might be required to ensure condition 2 for all possible Γ_{11} , then \mathbf{X} must be multivariate normal (Cambanis, Huang, and Simons 1981; Kelker 1970).

If, as required for Corollary 1, $\Sigma_{z|s}$ is constant across slices and conditions 1, 2, and 4 hold, then it can be shown that condition 3 is again satisfied. This is an important observation. Li (1991) said that constant conditional variance across slices is not required for his result to hold. But in his proof he assumed normal regressors, and nonconstant variance is not an issue.

In effect, Corollary 1 and Theorem 2 state that the defining condition that must be met for the chi-squared test to apply is constant covariance of the conditional distribution of $\mathbf{Z}|Y$, or of the conditionals of the regressor distribution, and not normality

of the regressors. In practice, both conditions can be checked by visually inspecting the scatterplot matrix of the regressors and the response.

It is also worth pointing out that if $S_{E(\mathbf{Z}|Y)}$ is a proper subspace of $S_{Y|\mathbf{Z}}$, then $\hat{\Lambda}_d$ may no longer have a chi-squared distribution. Of course, even in this case, if the covariance structure of \mathbf{X} is constant across slices, then Corollary 1 implies that $\hat{\Lambda}_d$ has an asymptotic chi-squared distribution with $(p - d)(H - d - 1)$ degrees of freedom.

4. AN ILLUSTRATIVE EXAMPLE: THE MUSSEL DATA

Consider a regression that arose as part of an ecological study of New Zealand mussels. The response is a mussel's muscle mass M (measured in grams), the edible part of the mussel. The $p = 4$ predictors are the shell length L , height Ht , and width W , each in mm, and the shell mass S in g. There are $n = 172$ observations. Portions of these data were used for illustration by Cook and Weisberg (1994) and Cook (1998b).

We noted substantial curvature in the cells of a scatterplot matrix of the predictors, particularly cells involving shell mass S . We compensated for this nonlinearity by simultaneously estimating power transformations of the predictors so that their joint distribution might be approximately normal on the transformed scale. This resulted in the logarithmic transformation of S and W . Of course, there is no guarantee that the transformed predictors are jointly normal. With the linearity condition reasonably satisfied, we proceeded with the SIR analysis.

The chi-squared p values are shown for $j = 0, 1, 2$ in the fourth column of Table 1. The results indicate that $d = 2$ and thus that the first two SIR predictors are required to characterize the regression. But we were unable to visually confirm the need for two SIR predictors by using the corresponding visualization tools described by Cook and Weisberg (1994, chap. 6) and Cook (1998b, chap. 4), which indicated instead that only the first SIR predictor is needed. One possible explanation could involve the assumption of normally distributed predictors that Li (1991) used in the derivation of his chi-squared test procedure. We resolved the conflict by using the weighted chi-squared test described in this article.

The p values from the weighted chi-squared test applied to the mussel regression are shown in the fifth column of Table 1. The resulting inference, which agrees with our visual assessment, is that $d = 1$, suggesting that the chi-squared test may have responded to nonnormality in the predictors. The estimated limiting distribution of $\hat{\Lambda}_d$ that we used for this inference should be useful when the number of observations per slice is large enough to allow reasonable estimation of the intraslice

Table 1. Test Results From Application of SIR With $H = 8$ to the Mussel Regression

j	$\hat{\Lambda}_j$	df	Chi-squared p value	Weighted Chi-squared p value
0	164.9	28	0	0
1	29.0	18	.048	.183
2	11.9	10	.292	.290

covariance matrices $\Sigma_{z|s}$. We used $H = 8$ slices, leaving about 22 observations per slice to estimate the 4×4 intraslice covariance matrices.

5. SIMULATION RESULTS

We compared the power of the chi-squared test and the weighted chi-squared test via a simulation study. For all regression models considered in this section, we used three sample sizes: $n = 100, 200, 300$. For each sample size and each distribution of the regressor vector \mathbf{X} , the p values corresponding to the test statistics for selected dimensions for both tests were collected over 1,000 replications.

Two two-dimensional models are considered. First, the response Y is generated according to the model

$$Y = (4 + X_1)(2 + X_2 + X_3) + .5\epsilon, \quad (17)$$

where ϵ is a standard normal variate and

$$\begin{aligned} X_1 &= W_1, \\ X_2 &= V_1 + \frac{W_2}{2}, \\ X_3 &= -V_1 + \frac{W_2}{2}, \\ X_4 &= V_2 + V_3, \end{aligned} \quad (18)$$

and

$$X_5 = V_2 - V_3.$$

The only restriction placed on \mathbf{V} and \mathbf{W} is that they be independent. The variables V_1, V_2, V_4 are iid, and $t_{(4)}, V_3 \sim t_{(3)}, V_5 \sim t_{(5)}$, and W_1 and W_2 are iid gamma(.25) random variables.

The second model is

$$Y = \frac{X_1}{.5 + (X_2 + 1.5)^2} + .5\epsilon, \quad (19)$$

where ϵ is a standard normal variate and

$$\begin{aligned} X_1 &= V_3 + V_4 + \frac{W}{6}, \\ X_2 &= -V_3 + V_4 + \frac{W}{6}, \\ X_3 &= -V_4 + \frac{W}{3}, \\ X_4 &= V_1 + V_2, \end{aligned} \quad (20)$$

and

$$X_5 = -V_1 + V_2,$$

where V_1, V_2, V_3 , and V_4 are iid $U(-4, 4)$ random variables and W is a standard normal random variable.

Model (17) is model (24) of Velilla (1998), and model (19) is model (6.3) of Li (1991). The central subspace for both (17) and (19) is two-dimensional. The joint regressor distributions (18) and (20) satisfy the linearity condition by construction (Velilla 1998, pp. 1092–1093), even though \mathbf{X} does not have an elliptically contoured distribution in either case.

The numerical entries of the rows of Tables 2, 3, and 4 corresponding to the test statistics indexed by 0 and 1 are empirical estimates of the power of the corresponding test. They represent the proportion of times the corresponding null hypothesis $d = 0$ and $d = 1$ is rejected, when the nominal significance level is .05 and .01 indicated parenthetically. The entries for the test statistics indexed by 2 are empirical estimates of the size of the test. The row entries of the tables throughout this section are to be interpreted in the same or in an analogous way. Computations were carried out in Arc (Cook and Weisberg 1999). The p values for the weighted chi-squared test were calculated with an algorithm of Field (1993).

Figure 1 gives scatterplots of 100 data points generated according to (17) and (19). The scatterplots reveal the presence

Table 2. Empirical Power and Size for the Chi-Squared and Weighted Chi-Squared Tests Applied to (17)

\mathbf{X} distributed as in (18)						
Chi-squared test				Weighted Chi-squared test		
$n = 100$						
H	5	10	15	5	10	15
$\widehat{\Lambda}_0$	1 (1)	1 (1)	1 (1)	1 (.998)	1 (.996)	1 (.967)
$\widehat{\Lambda}_1$.052 (.014)	.07 (.03)	.134 (.05)	.159 (.034)	.225 (.064)	.367 (.12)
$\widehat{\Lambda}_2$.004 (0)	.005 (.001)	.007 (0)	.018 (.005)	.041 (.005)	.078 (.01)
$n = 200$						
H	10	15	20	10	15	20
$\widehat{\Lambda}_0$	1 (1)	1 (1)	1 (1)	1 (1)	1 (1)	1 (1)
$\widehat{\Lambda}_1$.114 (.052)	.171 (.068)	.167 (.081)	.258 (.103)	.357 (.152)	.410 (.164)
$\widehat{\Lambda}_2$.038 (.004)	.01 (0)	.003 (0)	.038 (.005)	.077 (.013)	.095 (.015)
$n = 300$						
H	15	20	30	15	20	30
$\widehat{\Lambda}_0$	1 (1)	1 (1)	1 (1)	1 (1)	1 (1)	1 (1)
$\widehat{\Lambda}_1$.176 (.091)	.202 (.1)	.199 (.102)	.41 (.172)	.479 (.205)	.549 (.257)
$\widehat{\Lambda}_2$.008 (0)	.007 (.001)	.005 (0)	.061 (.007)	.088 (.011)	.15 (.033)

Table 3. Empirical Power and Size for the Chi-Squared and the Weighted Chi-Squared Tests Applied to (19)

X distributed as in (20)						
Chi-square			Weighted Chi-square			
n = 100						
H	5	10	15	5	10	15
$\hat{\Lambda}_0$	1 (1)	1 (.999)	.998 (.974)	1 (1)	1 (1)	.999 (.996)
$\hat{\Lambda}_1$.182 (.054)	.145 (.033)	.113 (.032)	.255 (.079)	.29 (.085)	.384 (.143)
$\hat{\Lambda}_2$.006 (0)	.009 (.001)	.007 (0)	.017 (.001)	.035 (.005)	.09 (.013)
n = 200						
H	10	15	20	10	15	20
$\hat{\Lambda}_0$	1 (1)	1 (1)	1 (1)	1 (1)	1 (1)	1(1)
$\hat{\Lambda}_1$.301 (.099)	.238 (.077)	.196 (.055)	.457 (.183)	.472 (.202)	.519 (.24)
$\hat{\Lambda}_2$.008 (0)	.019 (.005)	.014 (.001)	.021 (.006)	.064 (.016)	.099 (.022)
n = 300						
H	15	20	30	15	20	30
$\hat{\Lambda}_0$	1 (1)	1 (1)	1 (1)	.999 (.999)	1 (1)	1(1)
$\hat{\Lambda}_1$.379 (.163)	.353 (.133)	.261 (.085)	.604 (.342)	.619 (.356)	.704 (.413)
$\hat{\Lambda}_2$.013 (.001)	.016 (.002)	.008 (0)	.052 (.01)	.096 (.025)	.173 (.049)

of significant heteroscedasticity in the conditionals of the regressor distribution and the conditional distribution of $\mathbf{X}|Y$. Thus the main conditions of both Corollary 1 and Theorem 2 appear to be violated. In consequence, the asymptotic distribution of the test statistic $\hat{\Lambda}_d$ is not expected to be chi-squared, but rather weighted chi-squared.

Tables 2 and 3 indicate that the chi-squared test has consistently smaller power than the weighted chi-squared test across sample sizes and choice of number of slices. From Table 3, it seems that the power of the chi-squared test can decrease as the number of slices increases, whereas the power of the weighted chi-squared test increases.

The level of the chi-squared test is too small in all cases of Tables 2 and 3, suggesting that it may be conservative when the predictors are not normal. This may partially account for the relatively low power of the chi-squared test. The level of the weighted chi-squared test increases with the number of slices. This observation supports the idea that the weighted chi-squared test is expected to be adversely affected by a small number of observations per slice, because of the variation in the estimated weights \hat{w} in (14).

In addition to the results reported here, a number of other distributions and models were investigated. One conclusion from

these studies is that the chi-squared test is robust when the predictor distribution deviates from normality *provided that there is no significant nonconstant variance in the X conditionals* and that the linearity condition holds. The weighted chi squared test also performed very well even in cases where the chi squared test has a clear advantage—namely, when the regressor is a normal vector, as shown in Table 4, where Y is generated according to (19), $n = 100$, and the five predictors are independent standard normal random variables. The results of Table 4 suggest that the chi-squared test is conservative even when the predictors are normal. In addition, the results of Tables 2, 3, and 4 and other results not reported here suggest that the number of slices for the weighted chi-squared test should not be more that 5%–7% of the sample size to keep test levels from being much larger than the nominal level.

6. DISCUSSION

SIR is a simple and useful first method for dimension reduction in regression analysis. As such, it seems important to have a well-grounded inference tool for studying the dimension of the inverse regression subspace.

Table 4. Empirical Power and Size for the Chi-Squared and the Weighted Chi-Squared Tests Applied to (19)

X ~ N ₅ (0, I ₅); n = 100						
	Chi-squared test			Weighted chi-squared test		
H	5	10	15	5	10	15
$\hat{\Lambda}_0$.996 (.975)	.988 (.933)	.976 (.881)	.997 (.977)	.993 (.952)	.992(.944)
$\hat{\Lambda}_1$.435 (.203)	.414 (.174)	.295 (.091)	.52 (.259)	.585 (.293)	.631 (.285)
$\hat{\Lambda}_2$.016 (.001)	.013 (.003)	.016 (.002)	.032 (.003)	.056 (.009)	.123 (.025)

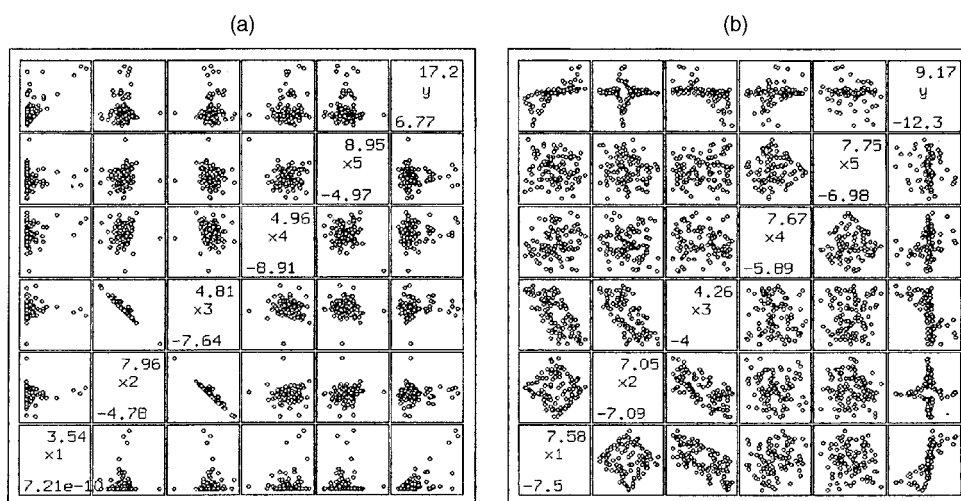


Figure 1. Scatterplots of the Simulated Data. (a) Model (17) with X following (18); (b) model (19) with X following (20).

Li (1991) proposed the chi-squared test procedure for situations when X is normal. In this article we have shown that normality of the predictors is not necessary for the asymptotic result to hold, but rather that restrictions should be placed on the conditional covariance structure of the predictors instead. These restrictions are trivially satisfied if X has a multivariate normal distribution, but they also contradict Li's claim that the asymptotic distribution of $\hat{\Lambda}_d$ does not depend on the constant variance assumption of the conditional distribution of X given Y .

Theorem 1 is the basis for the weighted chi-squared test, which applies regardless of the predictor distribution. SIR would now seem to be a more widely applicable dimension-reduction technique, requiring only the linearity condition.

The general applicability of the weighted chi-squared test does not seem to be overwhelmed by the variability induced by estimating the weights required for its computation, provided that the number of slices does not exceed 5%–7% of the sample size. As shown in the simulation study, the weighted chi-squared test performs noticeably better than the chi-squared test when the regressors are far from normal. In addition, it also compares well to the chi-squared test in cases where the regressors are normal.

The testing procedure for dimension can be viewed as a sequence of at most p (the number of predictors) tests. How this multiple testing affects the overall size of the testing procedure has not been investigated. Approaches similar to those in multiple testing might be appropriate. Additionally, it should be mentioned that detection of a direction by a testing procedure does not guarantee that it will be close enough to the central subspace to be useful. Directions detected by the weighted chi-squared test with a marginal p value may be farther from the central subspace than directions with a relatively small p value. Because the chi-squared test is conservative, the directions that it does detect might be relatively close to the central subspace.

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