SAVE: A METHOD FOR DIMENSION REDUCTION AND GRAPHICS IN REGRESSION

R. Dennis Cook
Department of Applied Statistics
University of Minnesota
St. Paul, MN 55108

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ABSTRACT

Sliced average variance estimation (SAVE) is a method for constructing sufficient summary plots in regressions with many predictors. The summary plots are designed to capture all the information about the response that is available from the predictors, and do not require a model for their construction. They can be particularly helpful for guiding the choice of a first model. Methodological aspects of SAVE are studied in this article.

1. INTRODUCTION

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

Graphical displays can be quite useful for investigating $Y|X$, 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 $X$ without losing information on $Y|X$, and without requiring a model for $Y|X$. Borrowing terminology from classical statistics, we call this sufficient dimension reduction. Sufficient dimension reduction leads to the
pursuit of sufficient summary plots which contain all of the information on the regression that is available from the sample.

There are a variety of approaches to the graphical exploration of regression data and the pursuit of “interesting” low-dimensional projections. The approach based on sufficient dimension reduction differs from others because it rests on views that contain all the regression information.

2. BANK NOTES

To illustrate these basic ideas, consider a regression involving counterfeit Swiss bank notes (Flury and Riedwyl 1988, p. 5). The binary response indicates a note’s authenticity: $Y = 0$ for genuine notes and $Y = 1$ for counterfeit notes. There are $p = 6$ predictors in $X$, each giving a different aspect of the size of a note: length at the top, bottom, left and right edges, and along the diagonal and center. There are many ways to start an analysis of these data. For example, we might inspect a scatterplot matrix of the predictors with the points marked to indicate counterfeit and authentic notes. Or we might begin with a logistic model, adding or deleting terms in the model as necessary in response to numerical or graphical diagnostics.

However, the idea of sufficient dimension reduction took us down a rather different data-analytic path, leading to the inference that only two linear combinations of $X$, say $\eta_1^T X$ and $\eta_2^T X$, are needed to characterize $Y \mid X$ fully. In effect, we reduced the dimension of $X$, passing from the original six predictors to $(\eta_1^T X, \eta_2^T X)$, without any notable evidence in the data that this reduction would result in loss of information on $Y \mid X$, and without assuming a model. Letting $\eta = (\eta_1, \eta_2)$, this reduction is based on the inference that $Y$ is independent of $X$ given $\eta^T X$, so that the conditional distributions of $Y \mid X$ and $Y \mid \eta^T X$ are the same. Since all the information about $Y$ that is available from $X$ is contained in the two linear combinations $\eta^T X$, a 3D plot of $Y$ versus $(\eta_1^T X, \eta_2^T X)$ is a sufficient summary plot for the regression. With a binary $Y$,
this is equivalent to a 2D binary response plot (Cook 1996) with $(\eta_1^T X, \eta_2^T X)$ on the axes, and points marked to indicate the states of $Y$.

The coefficient vectors $\eta_1$ and $\eta_2$ are unknown in the previous inference. Estimating them we obtained the estimated linear combinations $h_1^T X$ and $h_2^T X$, and thus the estimated sufficient summary plot for the regression shown in Figure 1. We thus inferred that all the information about $Y$ that is available from $X$ is contained in this one plot. The bimodal distribution within the counterfeit notes could indicate a change in the manufacturing process, or two different counterfeiting operations. Also, there appears to be an outlying authentic note, which could be a mislabeled counterfeit note or an indication of a second low-frequency mode among the authentic notes. It seems unlikely that we would have found this summary plot without using the graphical methods discussed in this article.

<table>
<thead>
<tr>
<th>Predictor</th>
<th>$h_1$ Raw</th>
<th>$h_1$ Std.</th>
<th>$h_2$ Raw</th>
<th>$h_2$ Std.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bottom</td>
<td>0.594</td>
<td>0.768</td>
<td>0.505</td>
<td>0.636</td>
</tr>
<tr>
<td>Diagonal</td>
<td>-0.466</td>
<td>-0.480</td>
<td>0.725</td>
<td>0.727</td>
</tr>
<tr>
<td>Left</td>
<td>-0.200</td>
<td>-0.064</td>
<td>-0.055</td>
<td>-0.017</td>
</tr>
<tr>
<td>Length</td>
<td>-0.033</td>
<td>-0.011</td>
<td>-0.284</td>
<td>-0.093</td>
</tr>
<tr>
<td>Right</td>
<td>0.250</td>
<td>0.090</td>
<td>-0.158</td>
<td>-0.055</td>
</tr>
<tr>
<td>Top</td>
<td>0.571</td>
<td>0.410</td>
<td>0.333</td>
<td>0.233</td>
</tr>
</tbody>
</table>

The coefficient vectors $h_1$ and $h_2$ are shown in Table I for the original predictors ($h_j$ Raw) and the predictors marginally standardized ($h_j$ Std.) to have a sample standard deviation of one. The summary plot in Figure 1 would look the same with the marginally standardized predictors. As in linear regression, relative contributions of the predictors may be easier to understand.
when they are measured in the units of their standard deviations. We see from
Table I that the measurements along the bottom, diagonal and top of a note
may be most useful for distinguishing between authentic and counterfeit types.

How we proceed with the analysis depends on the application context. In
some cases a summary plot like that in Figure 1 may be enough to conclude
the analysis. In other cases, we may wish to go further and formulate a first
model for \(Y \mid X\) based on the summary plot.

To illustrate how a first model might be developed, let \(f_j(x)\) denote the
conditional density of \(X \mid (Y = j)\), \(j = 0, 1\). So far no assumptions have been
placed on the conditional distribution of \(Y \mid X\). Our first assumption, which
seems consistent with the plot in Figure 1, is that for authentic notes \(f_0(x)\)
is multivariate normal with mean \(\mu_0\) and covariance matrix \(\Sigma\). Following the
indications in Figure 1 we assume further that for counterfeit notes \(f_1(x)\) is a
mixture of two normal densities,

\[
 f_1(x) = \alpha f_{11}(x) + (1 - \alpha)f_{12}(x)
\]

where \(f_{1k}(x)\) is the multivariate normal density with mean \(\mu_{1k}\) and covariance
matrix \(\Sigma\), \(k = 1, 2\). After a little algebra, the regression odds ratio can be
expressed as (Cook and Lee 1999)

\[
 \frac{\Pr(Y = 0 \mid X = x)}{\Pr(Y = 1 \mid X = x)} = \frac{\exp\{(\mu_0 - \mu_{11})^T \Sigma^{-1} x\}}{\omega_0 + \omega_1 \exp\{(\mu_{12} - \mu_{11})^T \Sigma^{-1} x\}}
\]

where \(\omega_0\) and \(\omega_1\) are unknown constants not depending on \(x\). This odds ratio
can be re-expressed in terms of the logit

\[
 \log \frac{\Pr(Y = 0 \mid X = x)}{\Pr(Y = 1 \mid X = x)} = \gamma_{01} + \gamma_1^T x - \log(1 + \exp(\gamma_{02} + \gamma_2^T x))
\]  \hspace{1cm} (1)

where the \(\gamma\)'s are unknown coefficient vectors. This provides a first (nonlinear)
logistic model for the regression. We could now proceed using standard fitting
and diagnostic methods to study the adequacy of the model based on this or
future data sets. It may have been difficult to arrive at a model of this form without the guidance available from the summary plot in Figure 1.

Our analysis of the bank note data was based on Sliced Average Variance Estimation (SAVE), a model-free method for constructing summary plots. The idea for SAVE was introduced by Cook and Weisberg (1991) and theoretical underpinnings were developed by Cook and Lee (1999). The goal of this article is to describe SAVE as methodology, after giving a description of its population foundations in Section 3 and 4.

Informally, SAVE provides a sample basis \( \{h_1 \ldots h_p\} \) for \( \mathbb{R}^p \) and corresponding SAVE predictors \( \{h_1^T X \ldots h_p^T X\} \). Both sets are ordered on their likely importance to the regression. Thus, the first SAVE predictor \( h_1^T X \) is likely more important than the second SAVE predictor \( h_2^T X \), and so on. Plots of \( Y \) versus various combinations of the SAVE predictors can provide useful information on the regression, the 3D plot of \( Y \) versus the first two SAVE predictors often being the most informative. The plot in Figure 1 is a 2D binary response plot of the first two SAVE predictors.

### 3. CENTRAL SUBSPACES AND SUFFICIENT VIEWS

Sufficient dimension reduction in a regression with response \( Y \) and random \( p \times 1 \) predictor vector \( X = (X_j) \) centers on finding a subspace \( S \) of \( \mathbb{R}^p \) so that

\[
Y \perp X | P_S X
\]

where the notation \( \perp \) (Dawid 1979) indicates independence and \( P_S \) is the orthogonal projection operator on \( S \) with respect to the standard inner product. The statement is equivalent to requiring that \( Y|X \) and \( Y|P_S X \) have the same distribution. When (2) holds we follow Li (1991, 1992) and call \( S \) a dimension reduction subspace for the regression of \( Y \) on \( X \).

The usual objective of a dimension reduction analysis is to infer about a smallest dimension reduction subspace, because this leads to pursuit of the
sufficient summary plot with minimal dimension. We might define a smallest subspace as simply a dimension reduction subspace with the minimal dimension. This subspace always exists, but it is not necessarily unique and thus it can be difficult to use in theory and practice (Cook 1998a, p. 104-105). In this article we rely instead on the central (dimension reduction) subspace, denoted by $\mathcal{S}_{Y|X}$, which was introduced by Cook (1994b, 1996). $\mathcal{S}_{Y|X}$ is defined to be the intersection of all dimension reduction subspaces for the regression. It is trivially a subspace but it is not necessarily a dimension reduction subspace. When it is a dimension reduction subspace it is unique by construction and is called the central subspace. The existence of central subspaces can be assured under quite weak restrictions (Cook 1996, 1998a). We assume that the central subspace exists throughout this article.

The central subspace $\mathcal{S}_{Y|X}$ is in effect a meta-parameter for $Y$ given $X$. Letting the columns of the matrix $\eta$ be a basis for $\mathcal{S}_{Y|X}$, a plot of $Y$ versus the coordinates $\eta^T X$ is then a minimal sufficient summary plot (Cook 1998a) for the regression of $Y$ on $X$. Cook and Weisberg (1999a) gave an introductory account of regression graphics based on central subspaces. A detailed account of central subspaces, including issues of existence and uniqueness, was given by Cook (1998a). The view shown in Figure 1 is based on an estimate $\hat{\mathcal{S}}_{Y|X}$ that can be described as $\hat{\mathcal{S}}_{Y|X} = \text{Span}(h_1, h_2)$, where $h_2$ and $h_2$ are the coefficient vectors given in Table I.

4. PROPERTIES OF THE CENTRAL SUBSPACE

Two properties of central subspaces are particularly useful in practice. Let $A$ be a $p \times p$ full rank matrix. Then the first property is that

$$\mathcal{S}_{Y|AX} = A^{-1} \mathcal{S}_{Y|X}$$

Consequently, there is no loss of information on the central subspace under full rank transformations of $X$. In particular, summary plots based on $X$ and $AX$
will contain the same information since one can be obtained from the other by
a full rank transformation of the plotting coordinates.

As an instance, consider standardization of the predictors: If \( \Sigma_X = \text{Var}(X) \)
is positive definite, taking \( Z = \Sigma_X^{-1/2}(X - E(X)) \) we have \( \mathcal{S}_{Y|Z} = \Sigma_X^{-1/2} \mathcal{S}_{Y|X} \). We work mostly in terms of the standardized predictors \( Z \) throughout the rest of this article, constructing the sample version by replacing \( \Sigma_X \) and \( E(X) \) with their usual estimates. Let the columns \( \beta_j \) of the \( p \times d \) matrix \( \beta \) be a basis for the central subspace \( \mathcal{S}_{Y|Z} \) in the \( Z \) scale.

For the second property, consider any function \( g(Y) \) of the response. Then

\[
\mathcal{S}_{g(Y)|X} \subseteq \mathcal{S}_{Y|X} \tag{4}
\]

In particular, if \( g \) is strictly monotonic then \( Y \perp\!\!\!\perp X|\eta^T X \) if and only if
\( g(Y) \perp\!\!\!\perp X|\eta^T X \) which implies that \( \mathcal{S}_{g(Y)|X} = \mathcal{S}_{Y|X} \). Consequently, to improve the appearance of plots, we can replace the response with a strictly monotonic transformation of it without altering \( \mathcal{S}_{Y|X} \). See Cook (1998a, p. 115–117) for further discussion of these remarks.

As another instance of useful response transforms, consider a binary version of the response obtained by setting \( \tilde{Y} = 1 \) if \( Y > c \) and \( \tilde{Y} = 0 \) otherwise, for some constant \( c \). Then from (4), \( \mathcal{S}_{Y|X} \subseteq \mathcal{S}_{Y|X} \), and thus we may be able to gain information on \( \mathcal{S}_{Y|X} \) by investigating \( \mathcal{S}_{Y|X} \). The advantage is that \( \mathcal{S}_{Y|X} \) can be investigated graphically when \( p = 3 \) by using 3D binary response plots (Cook 1996; 1998a, Chapter 5). Extensions of this idea are immediate: We can partition the range of \( Y \) into \( H \) slices, \( L_s, s = 1 \ldots H \) and define the sliced response \( \tilde{Y} = s \) if \( Y \in L_s \). Again, \( \mathcal{S}_{Y|X} \subseteq \mathcal{S}_{Y|X} \).

5. SAVE

In this section we discuss SAVE, and how it can be used to construct summary plots in practice. Like other dimension reduction methods in regression, SAVE requires conditions on the marginal distribution of \( X \). We consider the conditions first, before turning to the details of the method.
SAVE requires that $E(Z|\beta^T Z)$ be linear in $\beta^T Z$, where $\beta$ is still a basis matrix for $S_{Y|Z}$. This is equivalent to requiring that $E(Z|\beta^T Z) = P_{S_{Y|Z}} Z$ (Cook 1998a, p. 57). We will refer to this restriction as the linearity condition which involves only the marginal distribution of $Z$, and is required to hold only for the basis matrix $\beta$. Since $\beta$ is unknown, in practice we may require that it hold for all possible $\beta$. This expanded condition is equivalent to elliptical symmetry of the distribution of $Z$ (Eaton 1986), which includes the normal.

By construction, $Y \perp Z|\beta^T Z$ and thus $E(Z|\beta^T Z) = E(Z|\beta^T Z, Y)$. For this reason the linearity condition will be satisfied if it is satisfied within each subpopulation determined by a value of $Y$. This may not be of much use in practice when $Y$ is continuous, but it can be of use when $Y$ is discrete. To assess the linearity condition in the bank note data, we constructed a scatterplot matrix of the predictors with the points marked to indicate the states of $Y$. Failing to find any notable curvature in the predictors conditional on $Y$, we concluded that the linearity condition is satisfied to a reasonable degree. Failure to find curvature in the cells of a scatterplot matrix does not by itself guarantee that the linearity condition holds. Nevertheless, it often seems to be a good indicator.

While minor deviations from the linearity condition may not matter much, substantial deviations can produce misleading results. When curvature is present in the predictors, it can often be reduced sufficiently by using simultaneously estimated power transformations so that the joint predictor distribution might be approximately normal on the transformed scale. This involves no loss of generality because the distribution of $Y$ given the original predictors is the same as the distribution of $Y$ given the transformed predictors. Additional background on the linearity condition and an introduction to relevant literature was given by Cook (1998a, Ch. 8).

In addition to the linearity condition, SAVE also requires a constant 
\textit{covariance condition}: $\text{Var}(Z|\beta^T Z)$ must be constant, where $\beta$ is still a basis
matrix for $S_{Y|Z}$. Experience has shown that this condition, which is equivalent to requiring that $\text{Var}(Z|\beta^T Z) = Q_{S_{Y|Z} Z}$, is less important than the linearity condition. Like the linearity condition, it holds when $Z$ is normally distributed and can also be checked from the cells of a scatterplot matrix. It may be called into question if some of the cells show clear heteroscedasticity. Homoscedasticity may provide some reassurance that the condition is reasonable.

Under the linearity and constant covariance conditions,

$$\text{Span}\{\text{E}(I - \text{Var}(Z|Y))^2\} \subseteq S_{Y|Z}$$

(5)

which is the basis for SAVE (Cook and Weisberg 1991, Cook and Lee 1999). Let $\lambda_j$ and $\beta_j$ denote the eigenvalues and eigenvectors of $\text{E}(I - \text{Var}(Z|Y))^2$, $j = 1 \ldots p$, and let $k$ denote the number of nonzero eigenvalues. The population SAVE predictors are then defined as $\beta_j^T Z$. According to (5), the eigenvectors corresponding to the $k$ positive eigenvalues are in the central subspace, and the population summary plot would be a $k + 1$ dimensional plot of $Y$ versus the first $k$ SAVE predictors.

For use in applications it is necessary to estimate the conditional covariance matrices $\text{Var}(Z|Y)$. This might be done straightforwardly when $Y$ is discrete, as in the bank note data. When $Y$ is continuous or many-valued, there may not be enough data to allow for straightforward estimation of $\text{Var}(Z|Y)$. In such cases, we replace the response with a discrete sliced response $\tilde{Y}$ as defined at the end of Section 4. The conditional covariance matrices are then based on the sliced response leading to a corresponding version of (5):

$$\text{Span}\{\text{E}(I - \text{Var}(Z|\tilde{Y}))^2\} \subseteq S_{Y|\tilde{Z}} \subseteq S_{Y|Z}$$

(6)

Slicing was not necessary in the bank note data because there are only two values of $Y$ with 100 counterfeit and 100 authentic notes. Thus 100 observations were available for estimating each $6 \times 6$ conditional covariance matrix. We are now in a position to describe how to implement SAVE.
SAVE Algorithm:

1. Construct the sample mean \( \hat{E}(X) \) and covariance matrix \( \hat{\Sigma}_X \) and then form the sample standardized predictors \( \hat{Z}_i = \hat{\Sigma}_X^{-1/2}(X_i - \hat{E}(X)), \ i = 1 \ldots n. \)

2. Assuming that \( Y \) is many-valued, divide its observed range into \( H \) slices and construct the sample covariance matrix \( \hat{V}_s \) of the \( \hat{Z} \)'s using the data within slice \( s = 1 \ldots H. \) \( \hat{V}_s \) is then an estimate of \( \text{Var}(Z|\hat{Y}) \) for slice \( s. \) Slicing may not be necessary to estimate \( \text{Var}(Z|Y) \) if \( Y \) is discrete, as in the bank note data.

3. Letting \( f_s \) denote the fraction of observations in slice \( s, \) construct

\[
M = \sum_{s=1}^{H} f_s(I - \hat{V}_s)^2
\]

4. The \( j \)-th sample SAVE predictor can now be constructed as

\[
S_j = b_j^T \hat{Z}_i, \ j = 1 \ldots p; \ i = 1 \ldots n
\]

where \( b_j \) is the \( j \)-th eigenvector of \( M \) corresponding to its ordered sample eigenvalues \( \hat{\lambda}_1 \geq \ldots \geq \hat{\lambda}_p. \)

5. Finally, the eigenvectors \( b_j \) in the \( Z \) scale can be transformed to vectors in the original scale as \( h_j = \hat{\Sigma}_X^{-1/2} b_j. \) These are the same as the raw coefficients in Table I. They can now be marginally standardized to aid interpretation.

Two and three dimensional plots of the response versus selected SAVE predictors \( S_j \) are useful for studying the regression graphically. Often, plots involving the first three SAVE predictors will be enough to guide the remaining analysis, as in the bank note data. Occasionally, there may be an issue of how many SAVE predictors contain relevant information on the regression.
There are several ways to address this issue. Cook and Lee (1999) studied asymptotic tests to determine the eigenvalues $\hat{\lambda}_j$ that are estimating 0 in the population. These tests can be helpful but, as with many asymptotic tests, accuracy issues can arise in applications. Another option is to consider the relative magnitudes of the $\hat{\lambda}_j$ along with visual assessment, with relatively large eigenvalues indicating a probable significant contribution to the regression. In clear cases, a relatively large $\hat{\lambda}_j$ will be accompanied by visual recognition of the importance of $\mathbf{b}_j^T \mathbf{Z}$ in plots with the response. The spirit here is much like that adopted by Gnanadesikan (1977, p. 86) in his use of CRIMCORDS for classification and clustering.

For example, the six eigenvalues $\hat{\lambda}_j$ for the bank note data are 0.872, 0.431, 0.131, 0.039, 0.017 and 0.001, suggesting that the first two SAVE predictors are likely important, that the last three are likely unimportant and that the third is questionable. These indications are supported by the tests of Cook and Lee (1999) and can also be confirmed by graphical analyses. The plot shown in Figure 1 sustains the importance of the first two SAVE predictors, as discussed previously. A 3D binary response plot of the last three $S_j$ (not shown) has uniform relative density of note types throughout the plot, indicating that these predictors carry little if any information about the regression. More precisely, the indication is that $Y \perp (S_4, S_5, S_6)|1(S_1, S_2, S_3)$. This latter statement and the theory behind it is an instance of graphical regression (Cook 1994a; Cook 1998a, Chapter 7), which works well in concert with a SAVE analysis. Remembering that the goal of this analysis it to gain intuition about the regression and useful information on how to form a first model, rigorous inference about the eigenvalues may not be necessary as long as the lion's share of the information is contained in the first few SAVE predictors.

The number $H$ of slices is a tuning parameter, much like those encountered in smoothing. Experience indicates that $H$ should be chosen so that the number of observations per slice is large enough to allow reasonable estimation
of the intra-slice covariance matrices $\text{Var} (Z|\hat{Y})$. With too much variability in $\hat{V}_2$, the SAVE predictors may be too far from the central subspace to be useful. Comparing the results from different choices for $H$ can be informative in practice. The number of observations per slice could be too small if, as $H$ is varied, any systematic trends are unstable in summary plots of the first two or three SAVE predictors.

6. DISCUSSION

There are a variety of approaches to the graphical exploration of regression data, and the pursuit of “interesting” low-dimensional views. The usefulness of modern graphics might be increased if we could recognize situations in which low-dimensional views provide exhaustive information on the regression. SAVE is one method for pursuing that goal via the central subspace and sufficient summary plots. Other methods like SIR (Li 1991) and pHd (Li 1992, Cook 1998b) can also be used to construct summary plots, but SAVE seems to be the most comprehensive. In the bank note data, neither SIR nor pHd is as successful as SAVE in capturing the structure of the regression.

Extreme nonlinearity among the predictors should be avoided, perhaps by using power transformations. The constant covariance condition is less important and might be neglected unless it is quite extreme.

SAVE can be used as a diagnostic by replacing the response with residuals $r$ from the fit of a model. All of the ideas described in this article apply in this case, except interest focuses on detecting deviations from the hypothesis $S_{r|x} = \{0\}$.

SAVE is available in Arc (Cook and Weisberg 1999b), a comprehensive regression program that integrates many standard regression techniques with the dimension reduction methods discussed here. Information about the program is available at the Internet site http://www.stat.umn.edu/arc/.
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BIBLIOGRAPHY


FIG. 1: Summary plot for the bank note data. Open circles denote authentic notes; filled circles denote counterfeit notes.