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Visualizing 1D Regression

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Visualizing 1D Regression

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Abstract. Regression is the study of the conditional distribution of the response $y$ given the predictors $x$. In a 1D regression, $y$ is independent of $x$ given a single linear combination $\beta^T x$ of the predictors. Special cases of 1D regression include multiple linear regression, binary regression and generalized linear models. If a good estimate $\hat{b}$ of some non-zero multiple $c\beta$ of $\beta$ can be constructed, then the 1D regression can be visualized with a scatterplot of $\hat{b}^T x$ versus $y$. A resistant method for estimating $c\beta$ is presented along with applications.

1. INTRODUCTION

Regression is the study of the conditional distribution of the response $y$ given the $(p-1) \times 1$ vector of nontrivial predictors $x$. In a 1D regression (or regression with 1-dimensional structure), $y$ is conditionally independent of $x$ given a single linear combination $\beta^T x$ of the predictors, written

$$ y \perp x | \beta^T x. $$

A 1D regression model has the form

$$ y = g(\alpha + \beta^T x, e) $$

where $g$ is a bivariate (inverse link) function and $e$ is a zero mean error that is independent of $x$. See [20] and [14, p. 414].

The above class of models is very rich. A single index model uses

$$ y = g(\alpha + \beta^T x, e) \equiv m(\alpha + \beta^T x) + e, $$

and the multiple linear regression model is an important special case where $m$ is the identity function: $m(\alpha + \beta^T x) = \alpha + \beta^T x$. Another important special case of 1D regression is the response transformation model where

$$ g(\alpha + \beta^T x, e) = t^{-1}(\alpha + \beta^T x + e) $$

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and $t^{-1}$ is a one to one (typically monotone) function so that $t(y) = \alpha + \beta^T x + e$. Generalized linear models (GLM’s) are also a special case of 1D regression.

Some notation from the regression graphics literature will be useful. *Dimension reduction* can greatly simplify our understanding of the conditional distribution $y|x$. If a 1D regression model is appropriate, then the $(p - 1)$-dimensional vector $x$ can be replaced by the 1-dimensional scalar $\beta^T x$ with no loss of information. A *sufficient summary plot* (SSP) is a plot that contains all the sample regression information about the conditional distribution of $y|x$.

If a 1D regression model is appropriate, then the $(p - 1)$-dimensional vector $x$ can be replaced by the 1-dimensional scalar $\beta^T x$ with no loss of information. A *sufficient summary plot* (SSP) is a plot that contains all the sample regression information about the conditional distribution of $y|x$. If a consistent estimator $\hat{\beta}$ can be found for some nonzero $c$, then an *estimated sufficient predictor* (ESP) $\hat{\beta}^T x$ versus $y$.

Additional notation is needed before giving theoretical results. Let $x$, $a$, $t$, and $\beta$ be $(p - 1) \times 1$ vectors where only $x$ is random. The predictors $x$ satisfy the condition of *linearly related predictors* with 1D structure ([14, p. 431]) if

$$E[x|\beta^T x] = a + t^\beta^T x.$$  

Notice that $\beta$ is a fixed $(p - 1) \times 1$ vector. If $x$ is elliptically contoured (EC) with 1st moments, then the assumption of linearly related predictors holds. See [6, p. 130].

Following [6, pp. 143-144], assume that there is an objective function

$$L_n(a, b) = \frac{1}{n} \sum_{i=1}^{n} L(a + b^T x_i, y_i)$$

where $L(u, v)$ is a bivariate function that is a convex function of the first argument $u$. Assume that the estimate $(\hat{a}, \hat{b})$ of $(a, b)$ satisfies

$$\hat{a}, \hat{b} = \arg\min_{a, b} L_n(a, b).$$

For example, the ordinary least squares (OLS) estimator uses

$$L(a + b^T x, y) = (y - a - b^T x)^2.$$  

Maximum likelihood type estimators such as those used to compute GLM’s and Huber’s M-estimator also work, as does the Wilcoxon rank estimator. Assume that the population analog $(\alpha, \eta)$ is the unique minimizer of $E[L(a + b^T x, y)]$ where the expectation exists and is with respect to the joint distribution of $(y, x^T)$.

For example, $(\alpha, \eta)$ is unique if $L(u, v)$ is strictly convex in its first argument. The following result is a useful extension of [2, 3].

**Theorem 1.** ([20, p. 1016]): Assume that the $x$ are linearly related predictors, that $(y_i, x^T_i)$ are iid observations from some joint distribution and that Cov$(x_i)$ exists and is positive definite. Assume $L(u, v)$ is convex in its first argument and that $\eta$ is unique. Assume that $y \perp x|\beta^T x$. Then $\eta = c\beta$ for some scalar $c$.  


Remark 1. If $\hat{b}$ is a consistent estimator of $\eta = \beta_b$, then certainly
\[ \beta_b = c\beta + u_g \]
where $u_g = \beta_b - c\beta$ is the bias vector. If the conditions of Theorem 1 hold, then $u_g = 0$. Under additional conditions, $(\hat{a}, \hat{b}^T)^T$ is asymptotically normal (see [20, p. 1031]). In particular, the OLS estimator frequently has a $\sqrt{n}$ convergence rate. Often if no strong nonlinearities are present among the predictors, the bias vector is small enough so that $\hat{b} \approx c\beta$. See [14, pp. 431-441] for checking whether the predictors are linearly related and whether a 1D regression model is appropriate.

A very useful result is that if $y = m(x)$ for some function $m$, then $m$ can be visualized with both a plot of $x$ versus $y$ and a plot of $c x$ versus $y$ if $c \neq 0$. In fact, there are only three possibilities: if $c > 0$, then the two plots are nearly identical. If $c < 0$, then the plot appears to be flipped about the vertical axis. If $c = 0$, then the plot is a dot plot. Similarly, if $y_i = g(\alpha + \beta^T x_i, e_i)$, then the plot of $\beta^T x$ versus $y$ and the plot of $c\beta^T x$ versus $y$ will be nearly identical in overall shape if $c > 0$.

Example 1. Suppose that $x_i \sim N_3(0, I_3)$ where $I_3$ is the $3 \times 3$ identity matrix, and
\[ y = m(\beta^T x) + e = (x_1 + 2x_2 + 3x_3)^3 + e \quad \text{with} \quad n = 100. \]
Then a 1D regression model holds with $\beta = (1, 2, 3)^T$. Figure 1 shows the sufficient summary plot of $\beta^T x_i$ versus $y_i$, and Figure 2 shows the sufficient summary plot
The SSP using -SP.

Figure 2. Another SSP for \( m(u) = u^3 \)

of \(-\beta^T x_i\) versus \( y_i\). Notice that the functional form \( m \) appears to be cubic in both plots and that both plots can be smoothed by eye or with a scatterplot smoother.

Remark 2. The OLS estimator \((\hat{a}_o, \hat{b}_o)\) is obtained from the usual multiple linear regression of \( y_i \) on \( x_i \), but we are not assuming that the multiple linear regression model holds; however, we are hoping that the 1D regression model \( y \perp x | \beta^T x \) is a useful approximation to the data and that \( \hat{b}_o \approx c\beta \) for some nonzero constant \( c \). Theorem 1 provides some conditions for the above approximation to hold. Notice that if the multiple linear regression model does hold and if the errors \( e_i \) are such that OLS is a consistent estimator, then \( c = 1 \), and \( u_g = 0 \).

The following result, perhaps first noted by [2, 3], is called the 1D Estimation Result by [14, p. 432]; let \((\hat{a}_o, \hat{b}_o)\) denote the OLS estimate obtained from the OLS multiple linear regression of \( y \) on \( x \). The OLS view is a plot of \( \hat{b}_o^T x \) versus \( y \). If the 1D regression model is appropriate and if no strong nonlinearities are present among the predictors, then the OLS view will frequently be a useful estimated sufficient summary plot. Hence the OLS predictor \( \hat{b}_o^T x \) is a useful ESP.

Three additional methods considered in this paper that have proven useful for estimating the ESP are sliced inverse regression (SIR), principal Hessian directions (PHD), and sliced average variance estimation (SAVE). See [10] for a discussion of when these methods can fail. These methods frequently perform well if there are no strong nonlinearities present in the predictors. All of these methods fail if \( c = 0 \).
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or if the bias vector $u_g$ is “large” compared to $c\beta$. For example, the OLS view can fail if the sufficient summary plot of $\beta^T x$ versus $y$ is approximately symmetric, and all of these methods can perform poorly if outliers are present ([17] shows that a single outlier can cause SIR to fail). Some useful references for SIR and related methods include [6, 7, 8], [14, 15], [16], [19] and [24].

Ellipsoidal trimming is a method for estimating the ESP that can reduce the bias $u_g$. See [11] and [6, p. 152]. To perform ellipsoidal trimming, an estimator $(T, C)$ is computed where $T$ is a $(p-1) \times 1$ multivariate location estimator and $C$ is a $(p-1) \times (p-1)$ symmetric positive definite dispersion estimator. Then the $i$th squared Mahalanobis distance is the scalar

$$D_i^2 = (x_i - T)^T C^{-1} (x_i - T)$$

for each vector of observed predictors $x_i$. If the ordered distance $D_{(j)}$ is unique, then $j$ of the $x_i$’s are in the ellipsoid

$$\{ x : (x - T)^T C^{-1} (x - T) \leq D_{(j)}^2 \}.$$  

The $i$th case $(y_i, x_i^T)^T$ is trimmed if $D_i > D_{(j)}$. Then an estimator of $c\beta$ is computed from the untrimmed cases. For example, if $j \approx 0.9n$, then about 10% of the cases are trimmed, and OLS could be used on the remaining cases.

The following procedure was suggested by [21]. First compute $(T, C)$ using the Splus function cov.md (see [23]). Trim the $K\%$ of the cases with the largest Mahalanobis distances, and then compute the OLS estimator $(\hat{\alpha}, \hat{\beta}_K)$ from the untrimmed cases. Use $K = 0, 10, 20, 30, 40, 50, 60, 70, 80, 90$ to generate ten plots of $\hat{\beta}_K^T x$ versus $y$ using all $n$ cases. These plots will be called “OLS trimmed views.” Notice that $K = 0$ corresponds to the OLS view. The best OLS trimmed view is the trimmed view with a smooth mean function and the smallest variance function and is the estimated sufficient summary plot. If $K^* = E$ is the percentage of cases trimmed that corresponds to the best trimmed view, then $\hat{\beta}_E^T x$ is the estimated sufficient predictor.

Example 2. For the data in Example 1, the OLS view is similar to Figure 1 except the plot is not quite as smooth and the horizontal scale is multiplied by $c \approx 42$. The best trimmed view appears to be identical to Figure 1 except that the horizontal scale is multiplied by $c \approx 12.5$. The OLS view used $\hat{\beta}_0 = (41.68, 87.40, 120.83)^T \approx 42\beta$ while the best trimmed view used $\hat{\beta}_{50} = (12.61, 25.07, 37.26)^T \approx 12.5\beta$.

This section has reviewed the existing literature on 1D regression. Section 2 shows that 1D regression can provide useful diagnostics when $g$ is known. Section 3 considers estimating $g$ when $g = g_\lambda$ and $\lambda \in \{\lambda_1, \ldots, \lambda_k\}$ where $k$ is a small integer. Section 4 suggests using ellipsoidal trimming with methods other than OLS. This technique gives a resistant version of SIR and shows that the Splus function lmsreg can be very useful for finding certain types of curvature.
2. 1D REGRESSION DIAGNOSTICS

In this section, we suggest that when \( g \) is known, an estimated sufficient summary plot should be used in addition to the usual diagnostics for checking the model. Assume that the 1D regression model is \( y_i = g(\alpha + \beta^T x_i, e_i) \) for \( i = 1, ..., n \) where the \( e_i \) are iid with zero mean and variance \( V(e_i) = \sigma^2 \).

**Remark 3.** If \( y \perp x \mid \beta^T x \) then \( y \perp x \mid a + c\beta^T x \) for any constants \( a \) and \( c \neq 0 \). Hence if \( \hat{b}^T x \) is an ESP, so is \( a + \hat{b}^T x \).

A good example is the multiple linear regression (MLR) model \( y_i = \alpha + \beta^T x_i + e_i \). Let \((\hat{a}, \hat{b})\) be a MLR estimator of \((\alpha, \beta)\). Then the fitted values are \( \hat{y}_i = \hat{a} + \hat{b}^T x_i \), and the residuals are \( r_i = y_i - \hat{y}_i \). The most used residual plot is a plot of \( \hat{y}_i \) versus \( r_i \), and the *forward response plot* is a plot of the fitted values \( \hat{y}_i \) versus the response \( y_i \).

Remark 3 shows that the forward response plot is an ESSP. Let the scalars \( w_i = \alpha + \beta^T x_i \). Ignoring the errors gives \( y_i = w_i \) which is the equation of the *identity line* that has unit slope and zero intercept. Hence if the MLR model is appropriate and if \((\hat{a}, \hat{b})\) is a good estimator of \((\alpha, \beta)\), then the plotted points in the forward response plot should scatter about the identity line. The vertical deviations from the identity line are the residuals \( r_i \) since these deviations are \( y_i - \hat{y}_i \). When the OLS estimator is used, the coefficient of determination \( R^2 \) is equal to the squared correlation of \( y_i \) and \( \hat{y}_i \). See [4, p. 280].
High leverage outliers challenge conventional numerical MLR diagnostics such as Cook’s distance ([5]), but, as shown in Example 3 below, can often be detected using the forward response and residual plots. Using trimmed views (see § 4) is also effective for detecting outliers and other departures from the MLR model.

**Example 3.** In the well known artificial HBK data set ([18]), the first 10 cases are outliers while cases 11-14 are good leverage points. This data set has \( n = 75 \) cases and \( p - 1 = 3 \) nontrivial predictors. Figure 3 shows the residual and forward response plots based on the OLS estimator. The highlighted cases have Cook’s distance > \( \min(0.5, 2p/n) \), and the identity line is shown in the ESSP.

Now suppose that model (1.2) holds where \( g \) is known. If the estimator \((\hat{a}, \hat{b})\) satisfies \( \hat{b} \approx c\beta \), then the plot of \( \hat{a} + \hat{b}^T x \) or \( \hat{b}^T x \) versus \( y \) can be used to visualize \( g \) provided that \( c \neq 0 \). Since \( g \) is known, the classical (e.g. maximum likelihood) estimator for \( \beta \) should be used since then \( c = 1 \) and the bias vector should be small for large sample size \( n \). Often adding a parametric fit and a lowess smooth to the plot will be useful.

Plots are also useful for additive error models

\[
y_i = m(x_{i,1}, ..., x_{i,p-1}) + e_i = m(x_i^T) + e_i = m_i + e_i.
\]

Many anova, categorical, nonlinear regression, nonparametric regression, and multivariate models have this form. For these models \( \hat{y}_i = \hat{m}_i \) and the residuals \( r_i = \)
In the fit–response plot (FY plot) of \( \hat{y}_i \) versus \( y_i \), the plotted points should scatter about the identity line, and the vertical deviations from the identity line are equal to the residuals.

### 3. 1D REGRESSION MODEL SELECTION

In this section, we assume that a 1D regression model holds with \( g = g_{\lambda_0} \) where \( \lambda_0 \in \Lambda = \{\lambda_1, ..., \lambda_k\} \) and \( k > 1 \) is a small integer. To estimate \( \lambda_0 \), make an ESSP for each of the \( k \) possible models. Examples include choosing a frequentist or a Bayesian model; a proportional hazards model or one of several competing 1D survival models; a logistic, probit or complementary log–log model in binary regression; a full or sub model in variable selection.

A good example for illustration is the response transformation model

\[
(3.1) \quad t_{\lambda_0}(y_i) \equiv y_i^{(\lambda_0)} = \alpha_0 + \beta_0^T x_i + e_i
\]

where the response variable \( y_i > 0 \) and the power transformation family

\[
(3.2) \quad t_{\lambda}(y) \equiv y^{(\lambda)} = \frac{y^\lambda - 1}{\lambda}
\]

for \( \lambda \neq 0 \) and \( y^{(0)} = \log(y) \). Assume \( \lambda_0 \in \Lambda = \{0, \pm 1/4, \pm 1/3, \pm 1/2, \pm 2/3, \pm 1\} \).

The literature for estimating \( \lambda_0 \) is enormous, and at least two papers using results from 1D regression have appeared. Let the OLS estimator \( (\hat{a}_0, \hat{b}_0) \) be computed from the multiple linear regression of \( y_i \) on \( x_i \). Then [13] suggests that the inverse response plot of \( y \) versus \( \hat{y}_{OLS} \) will often show \( t_{\lambda_0} \). Hence the forward response plot of \( \hat{y}_{OLS} \) versus \( y \) will show \( t_{\lambda_0}^{-1} \). If \( t_{\lambda} \) is the appropriate transformation, [12] suggests that a plot of \( \hat{y}_{OLS} \) versus \( t_{\lambda}(y) \) will follow the identity line.

These ideas suggest a graphical method for selecting response transformations that can be used with any good MLR estimator. Let \( w_i = t_{\lambda}(y_i) \) for \( \lambda \neq 1 \), and let \( w_i = y_i \) if \( \lambda = 1 \). Next, perform the multiple linear regression of \( w_i \) on \( x_i \) and make the forward response plot of \( \hat{w}_i \) versus \( w_i \). If the plotted points follow the identity line, then take \( \lambda_0 = \lambda \). One plot is made for each of the eleven values of \( \lambda \in \Lambda \), and if more than one value of \( \lambda \) works, contact subject matter experts and use the simplest or most reasonable transformation. (Note that this procedure can be modified to create a graphical diagnostic for a numerical estimator by adding the estimate \( \hat{\lambda} \) of \( \lambda_0 \) to \( \Lambda \).

**Example 4.** A textile data set is given in [1] where samples of worsted yarn with different levels of the three factors were given a cyclic load until the sample failed. The goal was to understand how \( y = \text{the number of cycles to failure} \) was related to the predictor variables length, amplitude and load. Figure 4 shows the forward response plots for two MLR estimators: OLS and the \textit{Splus} function \texttt{lmsreg}. Figures 4a and 4b show that a response transformation is needed while 4c and 4d both suggest that \( \log(y) \) is the appropriate response transformation. Using OLS and a resistant estimator as in Figure 4 may be very useful if outliers are present.
4. IMPROVING 1D ESTIMATORS

Assume that the 1D regression model (1.2) holds but both $g$ and $\beta$ are unknown. If a good estimator $\hat{b} \approx c\beta$ can be found where $c \neq 0$, then the ESSP can be used to visualize $g$. The next step might be to fit a tentative parametric or nonparametric model in the ESP.

Since methods for estimating the sufficient predictor such as OLS, PHD, SAVE and SIR can fail if strong nonlinearities such as outliers are present in the predictors or if $\hat{b} \approx 0$, techniques for improving these methods are needed. The basic tool will be to use $(\hat{b}, T, C)$ trimmed views where $\hat{b}$ is an estimator of $c\beta$ and $(T, C)$ is an estimator of multivariate location and dispersion. Two good choices for $(T, C)$ are the classical estimator ([6, p. 152]) or a robust estimator such as cov.mcd. Then, for example, SIR trimmed views generalize the SIR ESSP in the same way that OLS trimmed views generalize the OLS view: use ellipsoidal trimming to delete the $K\%$ of the cases with the largest Mahalanobis distances.

Next, plot $\hat{b}_K^T \mathbf{x}_i$ versus $y_i$, where $\hat{b}_K$ is the first SIR direction computed from the untrimmed cases. Again use 10 values of $K$ where $K = 0$ corresponds to the usual SIR ESSP, and the best SIR trimmed view is the trimmed view with a smooth mean function and the smallest variance function.

Using trimmed views seems to work for several reasons. The ellipsoidal trimming divides the data into two groups: the trimmed cases and the untrimmed cases. Trimming often removes strong nonlinearities from the predictors, and the
untrimmed predictor distribution is often more nearly elliptical contoured than the predictor distribution of the entire data set (recall Winsor’s principle: “data are roughly Gaussian in the middle”). Secondly, under heavy trimming, the mean function of the untrimmed cases may be more linear than the mean function of the entire data set. Thirdly, if \(|c|\) is very large, then the bias vector \(u_g\) may be small relative to \(c\beta\).

From Remarks 1 and 2, any of these three reasons could produce a better estimated sufficient predictor. Also notice that trimmed views are resistant to \(y\)-outliers since the \(y\) values are plotted, and trimmed views are resistant to \(x\)-outliers if \((T, C)\) is a resistant estimator.

**Example 5.** To illustrate the above discussion, an artificial data set with 200 trivariate vectors \(x_i\) was generated. The marginal distributions of \(x_{i,j}\) are iid lognormal for \(j = 1, 2,\) and 3. Since the response \(y_i = \sin(\beta^T x_i)/\beta^T x_i\) where \(\beta = (1, 2, 3)^T\), the random vector \(x_i\) is not elliptically contoured and the function \(g\) is strongly nonlinear. The \texttt{cov.mcd} estimator was used for trimming, and Figure 5 shows the estimated sufficient summary plots for SIR, PHD, SAVE (using 8 slices), and the OLS 90% trimmed view. The OLS trimmed view is the best, while SAVE completely fails. Figure 6 shows that for this data, the \texttt{lmsreg} trimmed view is very useful for visualizing \(g\). The \texttt{lmsreg} estimator attempts to make the median squared MLR residual small and implements the PROGRESS algorithm described in [22, pp. 197-204]. Table 1 shows the estimated sufficient predictor coefficients \(\hat{b}\) when the sufficient predictor coefficients are \(c(1, 2, 3)^T\). Only the OLS and \texttt{lmsreg}
Table 1. Estimated Sufficient Predictors Estimating $c(1,2,3)^T$

<table>
<thead>
<tr>
<th>method</th>
<th>$\hat{b}_1$</th>
<th>$\hat{b}_2$</th>
<th>$\hat{b}_3$</th>
</tr>
</thead>
<tbody>
<tr>
<td>OLS View</td>
<td>0.0032</td>
<td>0.0011</td>
<td>0.0047</td>
</tr>
<tr>
<td>SIR</td>
<td>-0.394</td>
<td>-0.361</td>
<td>-0.845</td>
</tr>
<tr>
<td>PHD</td>
<td>-0.072</td>
<td>-0.029</td>
<td>-0.0097</td>
</tr>
<tr>
<td>SAVE</td>
<td>-1.09</td>
<td>0.870</td>
<td>-0.480</td>
</tr>
<tr>
<td>OLS 90% Trimmed View</td>
<td>0.086</td>
<td>0.182</td>
<td>0.338</td>
</tr>
<tr>
<td>LMSREG 70% Trimmed View</td>
<td>0.143</td>
<td>0.287</td>
<td>0.428</td>
</tr>
</tbody>
</table>

trimmed views produce estimated sufficient predictors that are highly correlated with the sufficient predictor. (The SAVE 40% trimmed view was also very good.)

Figure 6 helps illustrate why the best lmsreg trimmed view worked. This view used 70% trimming, and the open circles denote cases that were trimmed while the highlighted squares are the untrimmed cases. Note that the highlighted cases are far more linear than the data set as a whole. Also lmsreg will give about half of the highlighted cases zero weight, further linearizing the function. In Figure 6 the weighted lmsreg constant $\hat{\alpha}_{70}$ is included, and the plot is simply the forward response plot of the weighted lmsreg fitted values versus $y$. The vertical deviations from the identity line are the “MLR residuals” $y_i - \hat{\alpha}_{70} - \hat{\beta}_{70}^T \mathbf{x}_i$ and at least half of the highlighted cases have small MLR residuals. There exist data sets where OLS is better than lmsreg for showing curvature (see [9]), but, as illustrated by Example 5, lmsreg often performed better for single index models when $m$ was smooth.

A great deal of work remains to be done in the area of resistant dimension reduction. When a 1D regression model holds, the trimmed views work at least as well as the untrimmed view since the untrimmed view corresponds to 0% trimming. The webpage (http://www.math.siu.edu/olive/) contains programs and a good introduction to 1D regression models.

References


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