Ridge TRACE Diagnostics

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Abstract

We describe a new $p-$parameter generalized ridge-regression shrinkage-pattern recently implemented in the RXshrink CRAN R-package. The five distinct types of ridge TRACE displays discussed and illustrated here provide invaluable data-analytic insights and improved self-confidence to researchers and data scientists fitting linear models to ill-conditioned (confounded) data.

Keywords: linear models, generalized ridge regression, mean-squared-error risk, ridge diagnostic TRACE displays.

1 My Regularization Perspective

Let me start by recognizing the pioneering spirits of Arthur E. Hoerl (1921-1994) and Robert W. Kennard (1923-2011) in this 50$^{th}$ anniversary year of their landmark 1970 publications in Technometrics. Their ridge TRACE plot showed how the relative magnitudes of fitted regression coefficients can change as the coefficient-vector is forced to become shorter and shorter. In fact, under Normal distribution-theory, their “ordinary” ridge (1—parameter) path is well known to be the locus of shrunken $\hat{\beta}$—vectors with maximum-likelihood (ML) of being the unknown true $\beta$—coefficients of any specified reduced length.

I also harbor fond memories of helping Harry Smith, Jr. (1923-2012) with regression computations as a graduate assistant in the Department of Biostatistics in Chapel Hill, NC (1968-1969). Harry was the Editor of Technometrics who accepted the key Hoerl-Kennard papers, in spite of what some reviewers apparently thought.

My perspective on regularization focuses on how generalized ridge TRACE displays can enable researchers to literally “see” the effects of variance-bias trade-offs on measures of mean-squared-error (MSE) risk that accompany all changes in fitted coefficients. Normal-theory based maximum likelihood (ML) estimates are only available for linear-models using narrow-data. When the total number, $p$, of non-constant $x$—predictor variables included is strictly less than the number of observations, $n$, the ordinary least-squares (OLS) estimator
is uniquely determined. We also need to assume that at least one OLS fitted-residual is non-zero; this assures that the estimated error-variance, \( \hat{\sigma}^2 \), is strictly positive.

The generalized ridge estimator of \( \beta \)-coefficients that is most-likely to have minimum MSE risk under Normal-theory is known, but no 1- or 2-parameter path has been proposed that is guaranteed to pass through that “best” point-estimate when \( p > 2 \). We will explore a new unrestricted (UNR) \( p \)-parameter shrinkage-path that is fully efficient and does pass through this “best” point-estimate.

We focus on five distinct types of ridge TRACE display that, together, provide users with invaluable and highly “visual” linear-model diagnostics. Each plot displays estimates of \( p \geq 2 \) quantities that can change as shrinkage occurs. One TRACE displays \( p \) fitted linear-model coefficients (COEF), a second plots relative mean-squared-error (RMSE) estimates from the diagonal elements of the MSE-matrix divided by the OLS-estimate of \( \sigma^2 \), while the third displays direction-cosine estimates for any “inferior-direction” (INFD) in \( X \)-space where the shrunken coefficients have higher risk than OLS estimates. The two remaining types of TRACE diagnostics (SPAT and EXEV) refer to the \( p \) rotated axes defining the principal-coordinates of given (confounded) \( x \)-predictors. The ML estimates displayed in TRACES were introduced in Obenchain (1978) and are unbiased (or have correct-range) when \( p < (n - 3) \).

2 Shrinkage Estimation

Linear models and the OLS estimator, \( b^o \), of \( \beta \)-coefficients can be placed in a canonical form that is easy to generalize when defining the shrinkage-estimators of interest. We assume that the \( y \)-outcome vector has been both centered and re-scaled to have an observed mean of zero and variance 1, that each column of the \( X \)-matrix \( (n \times p) \) has been standardized in this same way, and that the resulting \( X \)-matrix has full (column) rank \( p \) that is \( \geq 2 \) and \( \leq (n - 1) \). Recalling that the OLS fit corresponds to an orthogonal projection in the \( n \)-dimensional space of individual observations onto the column-space of \( X \), we can write the following well-know matrix-expressions:

\[
\hat{y} = HH'y = Xb^o .
\]  

These results follow by writing the singular-value decomposition (SVD) of \( X \) as \( X = HA^{1/2}G' \). \( HH' \) then denotes an orthogonal projection; it is a \( n \times n \) symmetric and idempotent matrix of rank \( p \) known as the Hat-matrix for OLS. In particular, \( b^o = Gc \) where \( G \) is an orthogonal rotation within the column-space of \( X \), and \( c = \Lambda^{-1/2}H'y \) is the \( p \times 1 \) column vector containing the uncorrelated components of \( b^o \), Obenchain (1975).

The generalization of interest to us applies scalar-valued shrinkage-factors, each confined
to the range $0 \leq \delta_j \leq 1$, to the $p$ uncorrelated components of $b^\circ$. These $\beta-$coefficient estimators are of the form:

$$\text{shrinkage } \hat{\beta} = G\Delta c = \sum_{j=1}^{p} g_j \delta_j c_j ,$$

(2)

where $\Delta$ denotes the diagonal matrix containing all $p$ shrinkage $\delta-$factors and $g_j$ denotes the $j^{th}$ column of $G$.

While the above conventions have placed all $X-$information about the form and extent of any ill-conditioning into a convenient canonical-form, these conventions have done nothing to predetermine the relative importance of individual $x-$variables in predicting $y-$outcomes. That information, as well as information on the many effects of deliberate shrinkage, may well be best and most-clearly revealed via visual examination of TRACE diagnostic plots.

3 Quantifying Extent of Shrinkage

The multicollinearity allowance, $m$, measures the “extent” of shrinkage applied in equation (2):

$$m = p - \delta_1 - \cdots - \delta_p = \text{rank}(X) - \text{trace}(\Delta) ,$$

(3)

where $0 \leq m \leq p$, Obenchain (1977). Besides being the rank of $X$, $p$ is also the trace of the OLS Hat-matrix. Similarly, $\text{trace}(\Delta)$ is also the trace of the Hat-matrix ($n \times n$) for the shrinkage estimators in equation (2). Thus $m$ can be interpreted as a measure of inferred “rank deficiency” in the given $X-$matrix that is due to its ill-conditioning and is revealed via shrinkage.

Use of this $m-$scale for displaying TRACE diagnostics also suggests using the short-hand notation, $\hat{\beta}_m$, to denote individual $\hat{\beta}$ point-estimates in equation (2). The OLS solution is denoted by $\hat{\beta}_0 = b^\circ$ when $m = 0$ at the beginning of each shrinkage path. Similarly, $\hat{\beta}_p \equiv 0$ denotes the shrinkage terminus at $m = p$.

Since the range of the $m-$index of equation (3) is finite, this $m-$scale is ideal for use as the horizontal axis on all TRACE plots. Each TRACE then displays a full regularization path.

4 MSE Optimal Shrinkage

When the unknown true components of $\beta$ are denoted by $\gamma$, it follows that the $i^{th}$ uncorrelated component of the $c-$vector in equation (2) has mean $\gamma_i$ and variance $\sigma^2/\lambda_i$. 

The unknown true minimum MSE risk value for the $j^{th}$ shrinkage $\delta-$factor, Obenchain (1975), is then

$$
\delta_j^{MSE} = \frac{\gamma_j^2}{\gamma_j^2 + (\sigma^2/\lambda_j)} = \frac{\lambda_j}{\lambda_j + (\sigma^2/\gamma_j^2)} = \frac{\varphi_j^2}{\varphi_j^2 + 1},
$$

(4)

where $\varphi_j^2 = \gamma_j^2 \lambda_j/\sigma^2$.

The F-ratio for testing $\gamma_j = 0$ is $F_j = (n-p-1)\hat{\rho}_j^2/(1-R^2)$, where $\hat{\rho}_j$ denotes the observed principal correlation between the centered and rescaled $y-$vector and the $j^{th}$ column of the $H-$matrix in equation (1) and $R^2 = \hat{\rho}_1^2 + \hat{\rho}_2^2 + \cdots + \hat{\rho}_p^2$ is the familiar coefficient of determination. Since the unknown non-centrality of $F_j$ is $\varphi_j^2$, the ML estimator of $\varphi_j^2$ is $n \cdot \hat{F}_j/(n-p-1)$ under Normal-theory.

5  ML Estimation of Uncorrelated Components

When no restrictions are placed on the functional form of regularization, one is free to simply substitute ML estimates for the unknowns in equation (4) to identify the estimate most likely to have minimum MSE risk. This ML shrinkage estimate under Normal-theory is of the cubic (clearly nonlinear) form

$$
\hat{\gamma}_j^{ML} = \frac{n \cdot \hat{\rho}_j^3}{n \cdot \hat{\rho}_j^2 + (1-R^2)} \cdot \sqrt{y'y/\lambda_j}.
$$

(5)

Thompson(1968) studied this estimator using numerical integration and showed that it yields [i] reduced MSE risk when a true $|\gamma_j|$ is small relative to $\sigma$, [ii] increased risk when $|\gamma_j|$ is larger, but [iii] the same limiting risk as $|\gamma_j|$ approaches $+\infty$.

Under conditional distribution-theory for linear models, the $\hat{\gamma}_j^{ML}$ estimates of equation (5) are viewed as being given linear functions of $y$ multiplied by $\sqrt{y'y/\lambda_j}$. In other words, the Normal-theory conditional distributions of $\hat{\rho}_j-$estimates are not those of correlation coefficients where individual columns of the $H-$matrix would be considered random rather than given.

In the limit as the OLS estimate of $\sigma^2$ decreases to 0, $R^2$ naturally increases to 1 for a “correct” linear model. This causes equation (5) to simplify to $\hat{\gamma}_j^{ML} = \sqrt{y'y} \cdot \Lambda^{-1/2} \hat{\rho} = c_j$ when $R^2 = 1$. This is the special case of equation (2) where $\delta_j \equiv 1$, and the OLS fit becomes exact. In other words, OLS predictions, $Xb^o = \hat{y}$, from equation (1) are then identical to the observed $y-$outcomes.

6  Unrestricted ML Shrinkage

A new $p-$parameter shrinkage path satisfying equation (2) and passing through the unrestricted $\hat{\beta}^{ML} = G\hat{\gamma}^{ML}$ estimate defined by equation (5) is implemented by the unr.ridge()
function that was recently added to the RXshrink R-package, Obenchain (2020). TRACE plots for this new unrestricted ML path use $\delta^*_j$ shrinkage factors that, when $m > 0$, are of the form:

$$\delta^*_j(k^*) = \min(\delta_{max}, k^* \hat{\delta}_{j}^{MSE})$$  \(6\)

where $\delta_{max}$ is a fixed scalar, such as 0.999999, that as strictly less than 1; $k^*$ is a non-negative scalar parameter that must decrease to increase the extent of shrinkage, $m$; and the $\hat{\delta}_{j}^{MSE}$ parameters are the ML estimates of the unknown optimal shrinkage-factors in equation (4).

Since $\hat{\delta}_{j}^{MSE} \equiv 1$ can truly occur only when $\sigma^2 = 0$, the Normal-theory Likelihood of MSE optimal shrinkage could be computed to be 0 (i.e infinite negative log likelihood) when $\hat{\delta}^2 > 0$ if just one of the $\delta^*_j$ factors in equation (6) were exactly 1 for any $m > 0$. The $\delta_{max}$ upper limit on $\delta^*_j$ factors prevents this sort of misleading numerical result. Also note that the $k^*$ scalar and the $\hat{\delta}_{j}^{MSE}$ vector are multiplied together in equation (6). Thus this combination actually corresponds to a total of only $p$, rather than $(p+1)$, functionally independent path “parameters”.

The path defined by the $\delta^*_j$ factors of equation (6) corresponds to $p$ piece-wise linear spline functions that all have $p + 1$ knots at the $p$ values of $k^* = 1/\hat{\delta}_{j}^{MSE}$ and at $m = p$. This path starts at $k^* = 1/\min(\hat{\delta}_{j}^{MSE})$ where $m = 0$. As $m$ increases, $k^*$ decreases until the $p^{th}$ knot at $k^* = 1/\max(\hat{\delta}_{j}^{MSE})$, where $k^*$ remains strictly greater than 1. The more that $p$ exceeds 2, the more flexible is this initial portion of the unrestricted-path.

The final portion of the unrestricted-path, from the $p^{th}$ knot to the final knot at $m = p$, corresponds to straight-line (uniform) shrinkage until all lines intersect at $\delta^*_j \equiv 0$. This final portion always contains the point where $k^* = 1$, which is the overall estimate most likely, under Normal-theory, to be the shrinkage target values of equation (4). The $m$—extent of shrinkage corresponding to $k^* = 1$ is not predetermined because it does not usually coincide with a knot and also depends in other ways upon the observed $y$—vector.

Different functions within the RXshrink R-package implement different paths, but they all display a vertical gray dashed-line on all of their TRACE plots at the single $m$—extent most-likely under Normal-theory to be MSE risk optimal for their particular path. Different paths for the same linear model usually correspond to different $\approx$ optimal $m$—extents of shrinkage. The most-likely ($k^* = 1$) solution on the unrestricted-path cannot be less likely under Normal-theory than the “best” solution on any other path.

The shapes of traditional 1— or 2—parameter paths are predetermined almost exclusively by the eigenvalues of the $X$—matrix, a disadvantage pointed out in Hoerl and Kennard (1975).
7 $\textit{TRACE}$ Diagnostics

$\textit{TRACEs}$ are graphical aids that help users literally “see” most of the details needed to fully appreciate how and when shrinkage-estimators alleviate the effects of ill-conditioning on linear models. Here, we will use a well-known benchmark dataset that is quite favorable to shrinkage plus functions from the $\textit{RXshrink}$ R-package, Obenchain(2020), to perform calculations and plot $\textit{TRACES}$.

The Portland cement data of Woods, Steinour and Starke(1932) contain data on $n = 13$ cement mixtures, where the $y$–outcome variable is heat (cals/gm) evolved during hardening. The $p = 4$ predictor $x$–variables recorded are “ingredient percentages” that appear to have been “rounded down” to full integers. Due to the small size and limited number of digits reported, this dataset has served as both a benchmark for accuracy of manual OLS computations and as an example where the “sign” of a fitted OLS coefficient differs for that of the correlation between $y$ and the corresponding $x$–variable.

The $x$–predictors recorded in the Portland cement data are not numerically accurate; their sum varies from 95% to 99%. If these $x$–values had summed to exactly 100% for all 13 mixtures, the centered X-matrix would then be of rank $3$. In other words, this $p = 4$ regression model is rather clearly ill-conditioned in the sense of suffering an effective rank deficiency of at least $m = 1$. In fact, we will see that an $m$–extent of almost 2 is more appropriate and realistic.

The $\textit{TRACE}$ diagnostics displayed here in Figures 1 to 5 were generated using the plot() function for unr.ridge() objects in version 1.4 of the $\textit{RXshrink}$ package using $\texttt{steps} = 64$. Since calculations defining regularization paths are performed only on a lattice of $m$–extents from equation (3), each $m$–value is then a multiple of $1/64 = 0.015625$. The default setting for the unr.ridge() function uses only $\texttt{steps} = 8$ to produce a unit change in $m$. The extra “detail” that results from $\texttt{steps} = 64$ makes the curved portions of Figures 3, 4 and 5 appear to be more smooth.

The value of $m$ where shrunken coefficient estimates stabilize can be interpreted as the approximate “deficiency” in the rank of the centered $X'X$ matrix. For example, if there are only two relatively small $\delta^{MSE}$ estimates, the coefficient $\textit{TRACE}$ of unrestricted form typically consists essentially of $p$ straight lines starting near $m = 2$ that all converge to 0 at $m = p$.

For the Portland cement data, the unrestricted ML shrinkage-extent (i.e. $k^* = 1$) occurs at $m = 1.848$. Thus a gray vertical dashed line is plotted at this point on the $\textit{TRACES}$ displayed in Figures 1 to 5. In fact, the relative magnitudes of the $\hat{\beta}_m$ estimates in Figure 1 are perfectly stable between $m = 1.845$ and $m = 4$.

The four curves plotted in the unrestricted $\textit{Coefficient TRACE}$ of Figure 1 and corresponding $\textit{Shrinkage Pattern TRACE}$ of Figure 2 actually are $\text{Piece-wise Linear Spline}$
Figure 1: Unrestricted shrinkage coefficient estimates for the Portland cement data. This TRACE is a piece-wise linear spline with 5 knots. The vertical dashed-line marks the extent of shrinkage most likely to yield an optimal variance-bias trade-off under Normal distribution-theory.
Figure 2: Unrestricted shrinkage-pattern for the Portland cement data. This TRACE is also a piece-wise linear spline with the same 5 knots as in Figure 1. These $\delta$–factors are applied to the uncorrelated components vector, $c$, via equation (2) rather than directly to the OLS coefficients, $b^o$, of equation (1).
functions. This helps make them look more “simple” and easy to interpret. In sharp contrast, the three other types of TRACE plots need to contain “curved” lines to realistically depict the Non-Linear effects of shrinkage on measures of MSE Risk.

Note that Figure 1 features a “wrong sign” correction to the 3rd fitted coefficient (percentage of p4caf in the mix, green dotted-line). This 3rd coefficient becomes negative at $m = 1.250$ to agree in sign with the marginal correlation ($-0.5347$) of p4caf with the heat y—outcome.

Note that Figure 2 depicts the shrinkage $\delta^\star$—factors that apply to the 4 principal axes of centered $X$—variables. Since the $\delta^{MSE}$ estimates are (0.9986, 0.0743, 0.9266, 0.1528) here, the second shrinkage-factor, $\delta^\star_2$ (red dashed-line), starts decreasing first and is always smallest because it has the smallest $\delta^{MSE}$ factor. Next, $\delta^\star_4$ (blue dot-dashed line) also starts decreasing at $k^\star = 1/0.1528 = 6.545$ and $m = 0.5137$ because $\delta^{MSE}_4$ is the 2nd—smallest factor. Ultimately, $\delta^\star_3$ (green dotted-line) remains quite close to $\delta^\star_1$ (black solid-line) because their $\delta^{MSE}$—estimates are nearly equal and much larger than the other two.

The relative MSE TRACE of Figure 3, the excess eigenvalue TRACE of Figure 4 and the inferior direction TRACE of Figure 5 are all based upon risk-related ML estimators introduced in Obenchain(1978). In particular, relative-risk estimates are given by the diagonal elements of the $MSE/\hat{\sigma}^2$ matrix and are both particularly relevant and easy to interpret in Figure 3. While unbiased under Normal-theory, each estimated relative-risk is increased, if necessary, to assure it is at least as large as its relative-variance, $\hat{\delta}_j^2/\lambda_j$. Here, user interest rightly becomes focused upon the range $1.5 \leq m \leq 2.5$ where relative-risks are greatly reduced.

The eigenvalues and eigenvectors of the difference between risk matrices, $\{MSE(ols) - MSE(ridge)\}$, provide clear insights into key effects of ridge shrinkage. The good news is that at most one eigenvalue of this difference in MSE risks can be negative! While an “inferior direction” corresponding to a negative estimated excess-eigenvalue does suddenly appear in Figure 5 at $m \approx 1.8$, the largest positive excess eigenvalue in Figure 4 is relatively gigantic (+50) at this same $m$—extent. In fact, the only negative excess-eigenvalue indicates a MSE risk increase due to shrinkage of at most $|15.6|$ even at $m = 4$, while the concomitant decrease in MSE in a direction strictly orthogonal to the lone inferior direction exceeds +50. Thus, shrinkage along the path depicted in Figure 2 has clear potential for a net overall reduction in MSE risk.

Also note that the inferior-direction at the shrinkage terminus, $m = 4$, of Figure 5 ends up pointing almost directly “backwards” at the initial OLS $\hat{\beta}_0$ solution of Figure 1. The absolute value of the correlation between the two corresponding direction-cosine vectors is 0.988 here, and similar results would always be expected whenever the initial OLS solution is significantly different from the shrinkage terminus, $\hat{\beta}^\star_p \equiv 0$, at $m = p = 4$.

Finally, Figure 6 displays a type of plot not included within the RXshrink R-package. The
Figure 3: Unrestricted relative MSE risk for the Portland cement data. This TRACE looks flat initially, until it reaches the knot at $m = 0.514$. A numerically small but relatively precise effect is suppressed first. The relative risk TRACE then becomes quite flexible, revealing clearly non-linear effects of shrinkage both to and through the overall optimal $m$—extent of shrinkage at $m = 1.848$. 
Figure 4: Unrestricted Excess Eigenvalues for the Portland cement data. A positive Excess Eigenvalue emerges past $m = 0.514$ and grows rapidly until shrinkage exceeds the MSE risk optimal extent, $m = 1.848$. The bad-news is that the single possible negative Excess Eigenvalue appears at $m = 1.859$ and slowly becomes more and more negative as shrinkage progresses.
Figure 5: Unrestricted Inferior Direction-cosines for the Portland cement data. Note that there is no “Inferior Direction” to the left of $m = 1.859$. However, one does suddenly appear to the right of $m = 1.859$, and it then rotates slightly in 4–dimensional $x$–space until it reaches its final orientation at $m = 4$. 
Figure 6: Likelihood Ratio Plot for two different shrinkage-paths for the Portland cement data. The solid black line shows how the $-2 \log$ Likelihood-Ratio under Normal-theory drops all of the way to 0 at $m = 1.848$ for the new “unrestricted” 4-parameter path. The dashed blue line depicts the corresponding LR for the “best” 2-parameter path of $q - \text{Shape} = -5$. This LR reaches a minimum of $26.38$ at $m \approx 2.11$ For comparison, the upper 99%-point of a $\chi^2$-variate with 2 degrees-of-freedom is $9.21$. 


\(-2\log(\text{Likelihood Ratio})\) estimates for two rather different shrinkage paths are displayed here as functions of their shrinkage \(m\)–Extents for the Portland cement data. The unr.ridge() and qm.ridge() functions were each run with “steps=64” to generate the data needed to “focus in” on the range from \(m = 1.75\) to \(m = 2.5\) depicted in Figure 6. The solid curve shows how the Likelihood Ratio \(\chi^2\) for the unrestricted path of equation (6) plunges down from very large values all of the way to 0.0 at \(m = 1.848\), then starts increasing and approaches 43.2 at \(m = 2.5\). The blue dashed-line that enters the top of Figure 6 at \(m \approx 2\) shows the corresponding Likelihood Ratio \(\chi^2\) for the qm.ridge() function in the RXshrink R-package of most-likely \(q\)–Shape = \(-5\). This blue dashed-line approaches its minimum of 26.5 at \(m = 2.09\) (marked by the vertical red dot-dashed line), then increases to \(\approx 35\) at \(m = 2.5\). This graphic suggests that the unrestricted path is more “efficient” than the 2–parameter approach; it locates a more sharply defined optimum that uses a lesser \(m\)–extent of overall shrinkage.

Truly “favorable” cases for ridge shrinkage occur when an \(m\)-extent greater than 1.0 is favored in two senses: (a) no “inferior direction” has yet appeared, and (b) the relative MSE risk of all \(p\) coefficients is still decreasing. Both indicators are clearly present in the TRACE plots in Figures 4, 5 and 3 for the Portland cement benchmark.

8 Summary

When linear models are fit to ill-conditioned or confounded narrow-data, TRACE plots are useful in demonstrating and justifying deliberately biased estimation. This makes TRACE diagnostics powerful “visual” displays for use in training of advanced students and persuasion of people capable of basic statistical thinking.

All five types of ridge TRACE plots for a wide variety of ridge paths can be explored using functions from the RXshrink R-package. For example, TRACEs can be generated for the Least-Angle, Lasso and Forward Stagewise methods of Efron and Hastie(2005) when applied to narrow-data with \(p < (n - 3)\). These TRACE plots provide quick and deep insights into the MSE risk characteristics of shrinkage and selection methods.

Computers have shaped the theory as well as the practice of statistics ever since Efron(1979) helped initiate the emergence of Data Science. Software providing clear “visual insights” into the strengths and weaknesses of alternative estimation methods are indispensable components of standard Tool Bags.
9  Final Remarks

I wish to thank Vijay Nair for considerable feedback on how to make my writing more palatable to general audiences.

I am confident that my ridge shrinkage methods are valid, and my GRR software is both free and easy-to-use. I sincerely hope readers will consider applying shrinkage concepts using RXshrink tools on narrow data they have previously analyzed using a linear model. If nothing else, this “experience” should help you feel less blasé about making model predictions and extrapolations!

10  References

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