# METHODS OF REGULARIZATION AND THEIR JUSTIFICATIONS 

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We turn to the question of both understanding and justifying various methods for regularizing statistical models. While many of these methods were introduced in the context of linear models, they are now effectively used in a wide range of contexts beyond simple linear modeling, and serve as a cornerstone for doing inference or learning in high-dimensional contexts.

## 1. Motivations for Regularization

Let us start our discussion by considering the model matrix

$$
X \equiv\left(\begin{array}{cccc}
X_{11} & X_{12} & \cdots & X_{1 p} \\
X_{21} & X_{22} & \cdots & X_{2 p} \\
\vdots & \vdots & \ddots & \vdots \\
X_{n 1} & X_{n 2} & \cdots & X_{n p}
\end{array}\right)
$$

of size $n \times p$, where we have $n$ observations of dimension $p$.
As our sensors and metrics become more precise, versatile, and omnipresent i.e., what has been dubbed the age of "big data" - there is a growing trend not only of larger $n$ (larger sample sizes are available for our datasets) but also of larger $p$. In other words, our datasets increasingly contain more varied covariates, rivaling $n$. This runs counter to the typical assumption in statistics and data science, namely $p \ll n$, the regime under which most inferential methods operate.

There are a number of issues that arise as a result of such considerations. First, from a mathematical standpoint, a larger value of $p$, on the order of $n$, makes objects such as $X^{T} X$ (also called the Gram matrix, which is crucial for many applications, in particular for linear estimators) very ill-behaved. Intuitively, one can imagine that each observation gives us a "piece of information" about the model, and if the degrees of freedom of the model (in an informal sense) are as large as the number of observations, it is hard to make precise statements about the model. This is primarily due to the following proposition.

Proposition 1.1. The least-squares estimator $\hat{\beta}$ has

$$
\operatorname{var}(\hat{\beta})=\sigma^{2}\left(X^{T} X\right)^{-1}
$$

Proof. Note that the least-squares estimator is given by

$$
\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} Y
$$

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Thus, the variance can be computed as

$$
\operatorname{var}(\hat{\beta})=\left(X^{T} X\right)^{-1} X^{T} \operatorname{var}(Y)\left[\left(X^{T} X\right)^{-1} X^{T}\right]^{T}=\sigma^{2}\left(X^{T} X\right)^{-1}
$$

as desired, noting that $\operatorname{var}(Y)=\sigma^{2} I$.
Thus, an unstable $\left(X^{T} X\right)^{-1}$ implies the instability of the variance of our estimator. In other words, small changes in our data can yield large changes for the variability of the estimator, which is problematic.

Second, from scientist's point of view, it is an extremely unsatisfying situation for a statistical analysis to yield a conclusion such as

$$
Y=\alpha_{1} X_{1}+\alpha_{2} X_{2}+\cdots+\alpha_{5000} X_{5000}
$$

Regardless of how complicated the system or experiment may be, it is impossible for the human mind to be able to interpret the effect of thousands of predictors. Indeed, psychologists have found that human beings can typically only hold seven items in memory at once (though later studies argue for even fewer). Consequently, it is desirable to be able to derive a smaller model despite the existence of many predictors - a task that is related to regularization but is known as variable selection. In general, model parsimony is a goal often sought after in statistical methodology, as it helps shed light on the relationship between the predictors and response variables.

Third, from a statistician's or machine learner's viewpoint, it is troubling to have as many predictors as there are observations, which is related to the mathematical problem named above. For example, suppose that $n=p$, and we are considering a linear model

$$
Y=X \beta+\epsilon
$$

Then, if $X$ is full-rank, we can simply invert the matrix to obtain $\beta=X^{-1} Y$, which will yield perfect results on the linear regression task. However, the model has learned nothing, so has dramatically failed at the implicit task at hand. This can be seen by the fact that such a model, which is said to be overfit, will typically have no generalization properties; that is, on unseen data, it will generally perform very poorly. This is evidently an undesirable scenario.

Thus, we are drawn to methods of regularization, which combat such tendencies by (usually) putting constraints on the magnitude of the coefficients $\beta$. This prevents the scenario from the above paragraph; if we constrain $\beta$ sufficiently, it will not be able to take the perfect precision value $\beta=X^{-1} Y$, and thus will (hopefully) be led to a value in which learning happens.

## 2. Deriving the Ridge Estimator

The ridge estimator was proposed as an $a d$ hoc fix to the above instability issues by Hoerl and Kennard (1970). ${ }^{1}$ From this point onward, we will generally assume that the model matrix is standardized, with column means set to zero and sample variances set to one. One of the signs that the matrix $\left(X^{T} X\right)^{-1}$ may be unstable (or super-collinear) is if the eigenvalues of the $X^{T} X$ are close to zero. This is because by the spectral decomposition,

$$
X^{T} X=Q \Lambda Q^{-1}
$$

[^0]and so the inverse is
$$
\left(X^{T} X\right)^{-1}=Q \Lambda^{-1} Q^{-1}
$$
where $\Lambda^{-1}$ is simply the diagonal matrix of eigenvalues $k_{j}^{-1}$ for $j=1, \ldots, p$. Thus, if some $\kappa_{j} \approx 0$, then $\left(X^{T} X\right)^{-1}$ becomes very unstable.

The fix proposed by the ridge regression method is to simply replace $X^{T} X$ by

$$
X^{T} X+\lambda I_{p}
$$

for $\lambda>0$ and $I_{p}$ being the $p$-dimensional identity matrix. This artificially inflates the eigenvalues of $X^{T} X$ by $\lambda$, making it less susceptible to the instability problem above.

Note that the resulting estimator, which we will denote as $\hat{\beta}_{r}$, is defined by

$$
\begin{equation*}
\hat{\beta}_{R}=\left(X^{T} X+\lambda I_{p}\right)^{-1} X^{T} Y=\left(I_{p}+\lambda\left(X^{T} X\right)^{-1}\right)^{-1} \hat{\beta} \tag{2.1}
\end{equation*}
$$

where the $\hat{\beta}$ on the right is the regular least-squares estimator.
Example 2.2. To get some feel for how the $\hat{\beta}_{R}$ behaves, let us consider the simple one-dimensional case; then

$$
X=\left(x_{1}, \ldots, x_{n}\right)
$$

is simply a column vector of observations. Let us suppose we have normalized the covariates, so that $\|X\|_{2}^{2}=1$. Then the ridge estimator is

$$
\hat{\beta}_{R}=\frac{\hat{\beta}}{1+\lambda}
$$

Thus, we can see how increasing values of $\lambda$ shrink the least-squares estimate further and further. Interestingly, we can also see that no matter what the value of $\lambda$ is, $\hat{\beta}_{R} \neq 0$ as long as $\hat{\beta} \neq 0$. This explains why the ridge regression method does not perform variable selection; it does not make any coefficient go to zero, but rather shrinks them uniformly.

After the fact, statisticians realized that this ad hoc method is equivalent to regularizing the least-squares problem using an $L_{2}$ norm. That is, we can solve the ridge regression problem

$$
\begin{equation*}
\min _{\beta \in \mathbb{R}^{p}}\|Y-X \beta\|_{2}^{2}+\lambda\|\beta\|_{2}^{2} \tag{2.3}
\end{equation*}
$$

In other words, we want to minimize the least-squares problem as before (the first term) while also ensuring that the $L_{2}$ norm of the coefficients $\|\beta\|_{2}$ remains small as well. Thus, the optimization must tradeoff the least-squares minimization with the minimization of the $L_{2}$ norm.

Theorem 2.4. The solution of the ridge regression problem (2.3) is precisely the ridge estimator (2.1).

Proof. As in the least-squares problem, we can write the above in matrix form as

$$
(Y-X \beta)^{T}(Y-X \beta)+\lambda \beta^{T} \beta=Y^{T} Y-2 Y^{T} X \beta+\beta^{T}\left(X^{T} X\right) \beta+\lambda \beta^{T} \beta
$$

Taking matrix derivatives, we find that the first-order condition is

$$
2\left(X^{T} X\right) \beta-2 X^{T} Y+2 \lambda \beta=0 \Rightarrow\left(X^{T} X+\lambda I_{p}\right) \hat{\beta}_{R}=X^{T} Y
$$

which yields the desired estimator.

Thus, we have arrived at the regularized regression problem in (2.3) by considering an $a d h o c$ method of inflating eigenvalues. From an optimization perspective, the problem in (2.3) is also equivalent to the constrained optimization problem

$$
\begin{equation*}
\min _{\|\beta\|_{2} \leq \kappa}\|Y-X \beta\|_{2}^{2} \tag{2.5}
\end{equation*}
$$

for some $\kappa>0$. Thus, from this perspective, we are simply doing least-squares optimization, except under the constraint that the magnitude of the coefficients $\|\beta\|_{2}$ be smaller than a maximum value $\kappa$ that we are willing to allow. Of course, there is an inverse relationship between $\lambda$ and $\kappa$; constraining smaller values of $\|\beta\|_{2}$ (decreasing $\kappa$ ) is equivalent to more harshly regularizing the least-squares problem (increasing $\lambda$ ).

Finally, it is interesting to note that there is always a value of $\lambda$ for which the ridge regression problem (2.3) yields an estimator (2.1) that has strictly lower meansquared error than the least-squares estimator, which we state here without proof. The proof is given in Hoerl and Kennard (1970).

Theorem 2.6. There always exists $\lambda>0$ such that

$$
E\left[\left\|\hat{\beta}_{R}-\beta\right\|_{2}^{2}\right]<E\left[\|\hat{\beta}-\beta\|_{2}^{2}\right]
$$

That is, regardless of $Y$ and $X$, there exists a value of $\lambda$ for which the ridge regression estimator performs strictly better than the least-squares estimator in terms of mean-squared error.

Note that this result and the following discussion concerns the mean-squared error in estimating the coefficients (that is, inference), not performance in terms of prediction. This theorem is interesting since the least-squares estimator is unbiased:

$$
E[\hat{\beta}-\beta]=0
$$

This can easily be derived, noting that

$$
E[\hat{\beta}]=\left(X^{T} X\right)^{-1} X^{T} E[Y]=\left(X^{T} X\right)^{-1} X^{T} X \beta=\beta
$$

Recalling the linear model $Y=X \beta+\epsilon$ and assuming that $\epsilon$ has mean zero, which is generally the case. On the other hand, the ridge estimator is biased. Using (2.1), we find that

$$
E\left[\hat{\beta}_{R}\right]=\left(I_{p}+\lambda\left(X^{T} X\right)^{-1}\right)^{-1} \beta \neq \beta
$$

Thus, the fact that the mean-squared error of the ridge estimator is lower than that of the least-squares estimator implies that the variance of the ridge estimator must more than make up for the increase in bias. This is a tradeoff that is increasingly the case in statistics and machine learning; by relinquishing an unbiased estimator, we can try to obtain biased estimators that have sufficiently low variance to keep the mean-squared error low. This has become known as the bias-variance tradeoff in statistics and machine learning.

## 3. Deriving the LASSO Estimator

Allowing for biased estimators opens up a whole variety of different estimators and procedures for generating them. This also formally allows for the use of regularization techniques, which generally introduce some bias in the estimation, with
the benefit of reducing variance. An obvious relative to ridge regression is to replace the $L_{2}$ norm by the $L_{1}$ norm as follows:

$$
\min _{\beta \in \mathbb{R}^{p}}\|Y-X \beta\|_{2}^{2}+\lambda\|\beta\|_{1}
$$

where $\|\beta\|_{1}=\sum_{j=1}^{p}\left|\beta_{j}\right|$ is the $L_{1}$ norm of the coefficients. ${ }^{2}$ Again, from an optimization view, this is equivalent to the constrained optimization problem,

$$
\min _{\|\beta\|_{1} \leq \kappa}\|Y-X \beta\|_{2}^{2}
$$

Indeed, this latter formulation was how the LASSO estimator was first proposed in Tibshirani (1996). ${ }^{3}$

Example 3.1. Let us again consider a simpler example to gain some intuition about the properties of the LASSO estimator. A slightly more complex but similar example to the one-dimensional case above is when the model matrix is orthonormal; that is,

$$
X^{T} X=I_{p}
$$

In this case, we have that

$$
\hat{\beta}=\left(X^{T} X\right)^{-1} X^{T} Y=X^{T} Y
$$

and we can derive the exact solution to the LASSO to be

$$
\hat{\beta}_{L, j}=\operatorname{sign}\left(\hat{\beta}_{j}\right)\left[\left|\hat{\beta}_{j}\right|-\lambda\right]^{+}
$$

where $[x]^{+}=x$ if $x>0$ and is 0 otherwise, and $\hat{\beta}_{L}$ denotes the LASSO estimator. In this case, the ridge estimator is

$$
\hat{\beta}_{R, j}=\frac{\hat{\beta}_{j}}{1+\lambda}
$$

as in the one-dimensional case.
Proof. For the ridge estimator, note that we have

$$
\hat{\beta}_{R}=\left(I_{p}+\lambda\left(X^{T} X\right)^{-1}\right)^{-1} \hat{\beta}=\left[(1+\lambda) I_{p}\right]^{-1} \hat{\beta}=(1+\lambda)^{-1} \hat{\beta}
$$

which yields the estimator above.
For the LASSO estimator, we can again take the same matrix derivatives to find that the first-order condition is

$$
X^{T} Y=\left(X^{T} X\right) \hat{\beta}_{L}+\lambda \operatorname{sign}\left(\hat{\beta}_{L}\right)
$$

By multiplying both sides by $\left(X^{T} X\right)^{-1}=I_{p}$, we find that

$$
\hat{\beta}=\hat{\beta}_{L}+\lambda \operatorname{sign}\left(\hat{\beta}_{L}\right)
$$

which, in terms of the components, are the equations

$$
\hat{\beta}_{L, j}=\hat{\beta}_{j}-\lambda \operatorname{sign}\left(\hat{\beta}_{L, j}\right)
$$

Now we solve this by considering the sign of $\hat{\beta}_{L, j}$. If it is positive, then we have $\hat{\beta}_{L, j}=\hat{\beta}_{j}-\lambda>0$; if it is negative, we have $\hat{\beta}_{L, j}=\hat{\beta}_{j}+\lambda<0$. In either case, we

[^1]

Figure 1. A comparison of the estimators from LASSO (left) and ridge (right) regression. Figure from Tibshirani (1996).
must have that the sign of $\hat{\beta}_{j}$ must be the same as the sign of $\hat{\beta}_{L, j}$, since $\lambda>0$. Moreover, we can express $x=|x| \operatorname{sign}(x)$. Thus, we have

$$
\hat{\beta}_{L, j}=\hat{\beta}_{j}-\lambda \operatorname{sign}\left(\hat{\beta}_{j}\right)=\operatorname{sign}\left(\hat{\beta}_{j}\right)\left[\mid \hat{\beta}_{j}-\lambda\right]^{+}
$$

as desired.
Note that the form of the estimators reveals much about their properties. As we discussed above, the ridge estimator components $\hat{\beta}_{R, j}$ are shrunk versions of $\hat{\beta}_{j}$, but are strictly nonzero. On the other hand, the LASSO estimator components can very much be zero, if $\hat{\beta}_{j} \leq \lambda$. That is, if we choose $\lambda$ large enough such that certain components of the least-squares estimator $\hat{\beta}$ are smaller than $\lambda$, then we will be setting those components to zero (in the case of an orthonormal model matrix).

## 4. Geometry of Estimators and Their Properties

Note that the above example was given in the case of an orthonormal model matrix, for which $X^{T} X=I_{p}$. This begs the question of whether the properties discussed above hold in more general settings. In particular, we noted that such regularization techniques are often desirable in the case of unstable $X^{T} X$, where the eigenvalues become nearly zero. This is clearly a large departure from the unit matrix situation when $X$ is orthonormal.

The above properties do in fact hold in general. Namely, the ridge estimator shrinks but does not generally zero out any of the coefficients, whereas the LASSO estimator does for appropriate values of $\lambda$, the regularization parameter. One intuition follows from Figure 1. The figure considers a two-dimensional case ( $p=$ $2)$, in which each of the axes represent $\beta_{1}, \beta_{2}$; that is, the plane represents the parameter space. The shaded portion depicts the part of the parameter space that satisfies the constraints $\|\beta\| \leq \kappa$, for the norm being $L_{1}$ or $L_{2}$ respectively, known as the feasible region. The ellipses depict typical level curves of the error term $\|Y-X \beta\|_{2}^{2}$. The dot at the center of the ellipses represents the true parameter $\beta$.

Intuitively, note that the error is zero at $\beta$, and increases quadratically outward as $\hat{\beta}$ moves farther away from $\beta$. However, we are indifferent to where exactly on the level curve we are; the optimization cost (or error) is exactly the same at any point on the same level curve. Thus, our goal is to find the point that is within the shaded area (satisfying the norm constraint) that is on the level curve with the smallest error.

It should be clear from the geometry that this will happen at the point where one of the level curves is precisely tangent to the edge of the feasible region. In the case of LASSO, this tends to occur at one of the axes, as shown in the figure (though it is possible that it does not). This implies that some of the coefficients are zero; in the example shown in the figure, $\hat{\beta}_{L, 1}=0$ whereas $\hat{\beta}_{L, 2}=\kappa$.

On the other hand, the ridge regression estimates will generally happen within the quadrant of the true value (rather than on the axes). This explains why the coefficients of the ridge estimator are generally nonzero, though they may be small in magnitude. For example, we see that in the figure, $\hat{\beta}_{R, 1}$ is quite small relative to $\hat{\beta}_{R, 2}$, but not strictly zero.

## 5. Bayesian Interpretations of Ridge Regression and LASSO

In addition to the regularization and constrained optimization perspectives, it turns out that both ridge and LASSO regression have a very natural interpretation from a Bayesian viewpoint. While we emphasize that the estimators were not derived in this manner originally, the Bayesian interpretation, developed later, provides good intuition for the two regularization methods.

Recall that the linear regression problem models the responses $Y$ as a function of the model matrix $X$ via the linear predictor $X \beta$, with noise $\epsilon$. Typically, we assume Normal errors, namely $\epsilon \sim \mathcal{N}\left(0, \sigma^{2} I_{n}\right)$. That is, each error term is independently distributed according to a Normal distribution. Thus, instead of the typical $Y=$ $X \beta+\epsilon$ formulation, we can instead view this as putting a distribution on $Y$ as

$$
\begin{equation*}
Y \mid \beta \sim \mathcal{N}\left(X \beta, \sigma^{2} I_{n}\right) \tag{5.1}
\end{equation*}
$$

That is, if we knew the parameters or coefficients $\beta$, then the distribution of $Y$ is Normal with the linear predictor $X \beta$ as the mean. ${ }^{4}$

From a Bayesian perspective, it is natural to consider distributions over $\beta$, both before and after conditioning on the data. These are the prior and posterior distributions of $\beta$, respectively. The prior is generally left to the statistician's discretion, and it turns out that there are two priors for the coefficients that lead to the ridge and LASSO estimators as the maximum a posteriori (MAP) estimators.

Theorem 5.2. Consider the linear regression model above (5.1), and the MAP estimator

$$
\hat{\beta}_{M} \equiv \arg \max _{\beta} p(\beta \mid Y)
$$

where $p(\beta \mid Y)$ denotes the posterior distribution of $\beta$ given the data $Y$.
(a) If the prior is

$$
\beta \sim \mathcal{N}\left(0, \sigma^{2} / \lambda\right)
$$

then $\hat{\beta}_{M}=\hat{\beta}_{R}$.

[^2](b) If the prior is
$$
\beta \sim \mathcal{L}\left(0,2 \sigma^{2} / \lambda\right)
$$
where $\mathcal{L}(a, b)$ denotes the Laplace distribution with location a and scale b, then $\hat{\beta}_{M}=\hat{\beta}_{L}$.

Proof. We first note that by Bayes' rule, we can write

$$
p(\beta \mid Y)=\frac{p(Y \mid \beta) p(\beta)}{p(Y)} \propto p(Y \mid \beta) p(\beta)
$$

where $p(Y)$ is the marginal distribution of $Y$, which does not involve $\beta$, and $p(\beta)$ is the prior distribution. Thus, by the monotonicity of the logarithm,

$$
\arg \max _{\beta} p(\beta \mid Y)=\arg \max _{\beta} p(Y \mid \beta) p(\beta)=\arg \max _{\beta}[\log p(Y \mid \beta)+\log p(\beta)]
$$

Since we are assuming the model (5.1), we have

$$
\log p(Y \mid \beta) \propto-\left(2 \sigma^{2}\right)^{-1}\|Y-X \beta\|_{2}^{2}
$$

again dropping any constants that do not involve $\beta$. Multiplying the entire optimization problem by -1 , we turn a maximization into a minimization, and obtain

$$
\arg \max _{\beta} p(\beta \mid Y)=\arg \min _{\beta}\left[\left(2 \sigma^{2}\right)^{-1}\|Y-X \beta\|_{2}^{2}-\log p(\beta)\right]
$$

Thus, if $\beta \sim \mathcal{N}\left(0, \tau^{2}\right)$, then we have

$$
\arg \min _{\beta}\left[\left(2 \sigma^{2}\right)^{-1}\|Y-X \beta\|_{2}^{2}+\left(2 \tau^{2}\right)^{-1}\|\beta\|_{2}^{2}\right]
$$

and setting $\tau^{2}=\sigma^{2} / \lambda$ yields the result. Similarly, for $\beta \sim \mathcal{L}(0, b)$, we obtain

$$
\arg \min _{\beta}\left[\left(2 \sigma^{2}\right)^{-1}\|Y-X \beta\|_{2}^{2}+b^{-1}\|\beta\|_{1}\right]
$$

and again setting $b=2 \sigma^{2} / \lambda$ completes the proof.
Just as the consideration of biased estimators opened up the possibility of using various regularization techniques, the Bayesian perspective also inspires a wide variety of regression models, some of which are not immediate from the regularization perspective. For example, while both of the Normal and Laplace distributions are symmetric about their means, this need not be the case. We can consider asymmetric Laplace (or other) distributions if we have prior evidence to suggest that, for example, $\beta_{1}$ should be positive. In this case, we may want to have a small scale parameter for $\beta_{1}<0$, but a larger one for $\beta_{1}>0$. In general, while the Normal and Laplace distributions have found most common use for Bayesian linear regression, any other prior distribution can be used in principle, depending on the problem at hand.

Moreover, the regularized regression models correspond only to the MAP estimators under the Normal or Laplace priors, as discussed above. As we will discuss later, Bayesian analysis generally goes beyond simple point estimators, such as the MAP estimator, and instead involves computation and analysis of the entire posterior distribution of $\beta$. Thus, "regularizing" using a Bayesian prior yields more precise statements and information about the parameter of interest, compared with least-squares estimation using a regularized model.

## 6. Combining Ridge and LASSO: Elastic Net Regularization

Unfortunately, both of the $L_{1}$ and $L_{2}$ regularizations discussed above are not without problems. ${ }^{5}$ First, we have already discussed the main problem of ridge regression. Though it can effectively tradeoff bias with variance to yield an estimator with lower mean-squared error, it always keeps all of the predictors in the model, and thus never yields a parsimonious model.

On the other hand, though the LASSO estimator does often yield a sparse representation, it has a number of limitations. When $p>n$, which is the case we are interested in most when considering regularization methods, it has been shown that LASSO can only select at most $n$ predictors. That is, given a sample size of $n$ and a large number of predictors $p>n$, LASSO will only yield up to $n$ predictors with nonzero coefficients, even if there were more in the true model.

In addition, both empirical evidence and theoretical analysis (Efron et al., 2004) show that when there are a number of highly-correlated predictors, then the LASSO estimator indifferently selects one among them and discards the rest. This can be highly problematic in practice; for example, if a group of clustered genes jointly predict for a disease but are correlated, it would be scientifically invalid to randomly select one of these genes and ignore the rest.

As a result of these considerations, Zou and Hastie (2005) developed the elastic net estimator, which combines both the LASSO $\left(L_{1}\right)$ and ridge $\left(L_{2}\right)$ penalties. The elastic net problem can be formulated as

$$
\begin{equation*}
\min _{\beta \in \mathbb{R}^{p}}\|Y-X \beta\|_{2}^{2}+\lambda_{1}\|\beta\|_{1}+\lambda_{2}\|\beta\|_{2}^{2} \tag{6.1}
\end{equation*}
$$

or, equivalently, as

$$
\min _{\beta \in \mathbb{R}^{p}}\|Y-X \beta\|_{2}^{2}+\lambda\left[\alpha\|\beta\|_{1}+(1-\alpha)\|\beta\|_{2}^{2}\right]
$$

where we define $\lambda=\lambda_{1}+\lambda_{2}$ and $\alpha=\frac{\lambda_{1}}{\lambda_{1}+\lambda_{2}}$. Thus, elastic net evidently combines both the $L_{1}$ and $L_{2}$ penalties into one regularization term, which is a convex combination of the two.

As in the case of ridge regression and LASSO, this is equivalent to a constrained optimization problem, which can be written as

$$
\begin{equation*}
\min _{\alpha\|\beta\|_{1}+(1-\alpha)\|\beta\|_{2}^{2} \leq t}\|Y-X \beta\|_{2}^{2} \tag{6.2}
\end{equation*}
$$

where $\alpha \in[0,1]$ is a fixed hyperparameter. In particular, note that ridge regression and LASSO are special cases of the elastic net, with $\alpha=0$ or $\alpha=1$, respectively.

What makes the elastic net both interesting and effective is that it combines not just the penalties, but also the benefits of each regularization method as well. The elastic net generally yields an estimator $\hat{\beta}_{E}$ that is both sparse as in the LASSO estimator and shrunk as in the ridge estimator. This is made clear in the following theorem.
Theorem 6.3. Let $\hat{\beta}_{E}$ be the elastic net estimator that solves (6.1) for given $Y$ and $X$, and hyperparameters $\lambda_{1}, \lambda_{2}$. Construct the augmented problem

$$
Y^{*} \equiv\binom{Y}{0} \in \mathbb{R}^{n+p}
$$

[^3]$$
X^{*}=\left(1+\lambda_{2}\right)^{-1 / 2}\binom{X}{\lambda_{2}^{1 / 2} I} \in \mathbb{R}^{(n+p) \times p}
$$
and define $\gamma \equiv \lambda_{1} /\left(1+\lambda_{2}\right)^{1 / 2}$ and the augmented $\beta^{*}=\left(1+\lambda_{2}\right)^{1 / 2} \beta$. Then, the elastic net problem can be written as
\[

$$
\begin{equation*}
\hat{\beta}^{*}=\arg \min _{\beta^{*} \in \mathbb{R}^{p}}\left\|Y^{*}-X^{*} \beta^{*}\right\|_{2}^{2}+\gamma\left\|\beta^{*}\right\|_{1} \tag{6.4}
\end{equation*}
$$

\]

and the elastic net estimator satisfies

$$
\begin{equation*}
\hat{\beta}_{E}=\left(1+\lambda_{2}\right)^{-1 / 2} \hat{\beta}^{*} \tag{6.5}
\end{equation*}
$$

Proof. Some matrix calculations can show that the problems are equivalent. Note that

$$
\left\|Y^{*}-X^{*} \beta^{*}\right\|_{2}^{2}=\|Y-X \beta\|_{2}^{2}+\lambda_{2}\|\beta\|_{2}^{2}
$$

and similarly $\gamma\left\|\beta^{*}\right\|_{1}=\lambda_{1}\|\beta\|_{1}$. Thus, the problem is in fact identical to the elastic net problem in (6.1).

In other words, the theorem states that the elastic net problem can be reformulated as a LASSO problem on augmented data. This augmented formulation, while seemingly trivial, does provide a number of insights into the behavior and possibilities of the elastic net estimator. First, note that since the sample size of $X^{*}$ is $n+p>p$, the elastic net estimator can actually select all $p$ predictors, unlike the LASSO estimator. On the other hand, the fact that $\hat{\beta}_{E}$ is simply a shrunk version of $\hat{\beta}^{*}$ indicates that the elastic net estimator does perform variable selection in the sense of LASSO, yielding a sparse representation. Thus, the elastic net estimator overcomes the primary difficulties faced by the LASSO and ridge estimators separately.


[^0]:    ${ }^{1}$ Hoerl, A. E., and R. W. Kennard (1970). "Ridge Regression: Biased Estimation for Nonorthogonal Problems." Technometrics 12 (1): 55-67.

[^1]:    ${ }^{2}$ Note that the error in the estimation is still given in $L_{2}$; that is, we still minimize the squared error. Minimizing the absolute error (using the $L_{1}$ norm for the error term as well) is known as least absolute deviation regression.
    ${ }^{3}$ Tibshirani, R. "Regression Shrinkage and Selection via the Lasso." JRSS B 58 (1): 267-288.

[^2]:    ${ }^{4}$ In all regression contexts, we assume that the model matrix $X$ is fixed and known, so we do not explicitly condition on it.

[^3]:    ${ }^{5}$ Zou, H., and T. Hastie (2005). "Regularization and Variable Selection via the Elastic Net." JRSSB 67 (2): 301-320.

