Lasso, Ridge, and Elastic Net: A Deeper Dive

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Contents

Repeated Features

A Very Simple Model

- Suppose we have one feature $x_1 \in \mathbf{R}$.
- Response variable $y \in \mathbf{R}$.
- Got some data and ran least squares linear regression.
- The ERM is
$$\hat{f}(x_1) = 4x_1.$$
- What happens if we get a new feature x_2,
    - but we always have $x_2 = x_1$?

Duplicate Features

- New feature x_2 gives no new information.
- ERM is still

$$\hat{f}(x_1, x_2) = 4x_1.$$

- Now there are some more ERMs:

$$\begin{aligned}\hat{f}(x_1, x_2) &= 2x_1 + 2x_2 \\ \hat{f}(x_1, x_2) &= x_1 + 3x_2 \\ \hat{f}(x_1, x_2) &= 4x_2\end{aligned}$$

- What if we introduce ℓ_1 or ℓ_2 regularization?

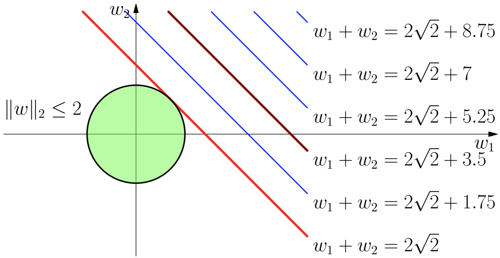
Duplicate Features: ℓ_1 and ℓ_2 norms

- $\hat{f}(x_1, x_2) = w_1 x_1 + w_2 x_2$ is an ERM iff $w_1 + w_2 = 4$.
- Consider the ℓ_1 and ℓ_2 norms of various solutions:

w_1	w_2	$\|w\|_1$	$\|w\|_2^2$
4	0	**4**	16
2	2	**4**	**8**
1	3	**4**	10
-1	5	6	26

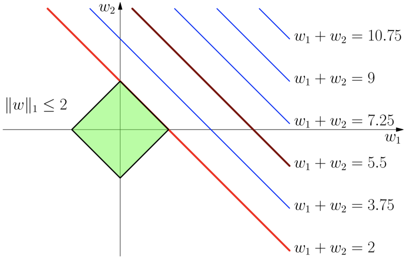
- $\|w\|_1$ doesn't discriminate, as long as all have same sign
- $\|w\|_2^2$ minimized when weight is spread equally
- Picture proof: Level sets of loss are lines of the form $w_1 + w_2 = 4$...

Equal Features, ℓ_2 Constraint



- Suppose the line $w_1 + w_2 = 2\sqrt{2} + 3.5$ corresponds to the empirical risk minimizers.
- Empirical risk increase as we move away from these parameter settings
- Intersection of $w_1 + w_2 = 2\sqrt{2}$ and the norm ball $\|w\|_2 \leqslant 2$ is ridge solution.
- Note that $w_1 = w_2$ at the solution

Equal Features, ℓ_1 Constraint



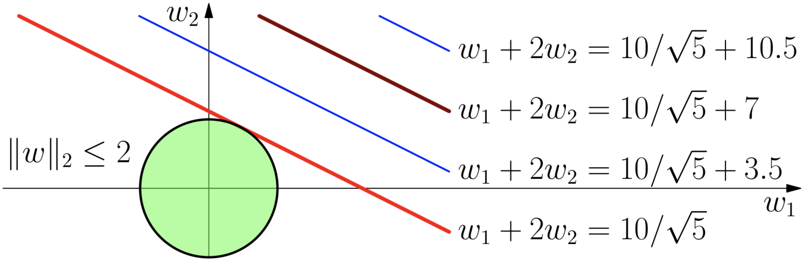
- Suppose the line $w_1 + w_2 = 5.5$ corresponds to the empirical risk minimizers.
- Intersection of $w_1 + w_2 = 2$ and the norm ball $\|w\|_1 \leqslant 2$ is lasso solution.
- Note that the solution set is $\{(w_1, w_2) : w_1 + w_2 = 2, w_1, w_2 \geqslant 0\}$.

Linearly Dependent Features

Linearly Related Features

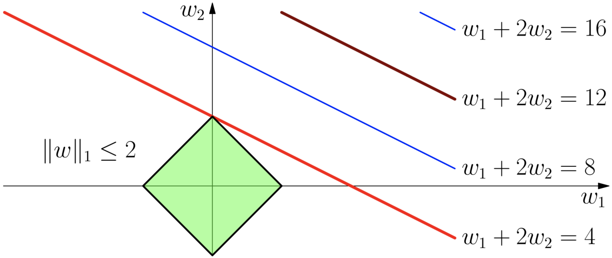
- Linear prediction functions: $f(x) = w_1 x_2 + w_2 x_2$
- Same setup, now suppose $x_2 = 2x_1$.
- Then all functions with $w_1 + 2w_2 = k$ are the same.
  - give same predictions and have same empirical risk
- What function will we select if we do ERM with ℓ_1 or ℓ_2 constraint?
- Compare a solution that just uses w_1 to a solution that just uses w_2...

Linearly Related Features, ℓ_2 Constraint



- $w_1 + 2w_2 = 10/\sqrt{5} + 7$ corresponds to the empirical risk minimizers.
- Intersection of $w_1 + 2w_2 = 10\sqrt{5}$ and the norm ball $\|w\|_2 \leqslant 2$ is ridge solution.
- At solution, $w_2 = 2w_1$.

Linearly Related Features, ℓ_1 Constraint



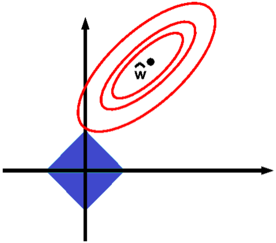
- Intersection of $w_1 + 2w_2 = 4$ and the norm ball $\|w\|_1 \leqslant 2$ is lasso solution.
- Solution is now a corner of the ℓ_1 ball, corresonding to a sparse solution.

Linearly Dependent Features: Take Away

- For identical features
  - ℓ_1 regularization spreads weight arbitrarily (all weights same sign)
  - ℓ_2 regularization spreads weight evenly
- Linearly related features
  - ℓ_1 regularization chooses variable with larger scale, 0 weight to others
  - ℓ_2 prefers variables with larger scale – spreads weight proportional to scale

Empirical Risk for Square Loss and Linear Predictors

- Recall our discussion of linear predictors $f(x) = w^T x$ and square loss.
- Sets of w giving same empirical risk (i.e. level sets) formed ellipsoids around the ERM.



- With x_1 and x_2 linearly related, $X^T X$ has a 0 eigenvalue.
- So the level set $\left\{ w \mid (w - \hat{w})^T X^T X (w - \hat{w}) = nc \right\}$ is no longer an ellipsoid.
- It's a degenerate ellipsoid – that's why level sets were pairs of lines in this case

KPM Fig. 13.3

Correlated Features

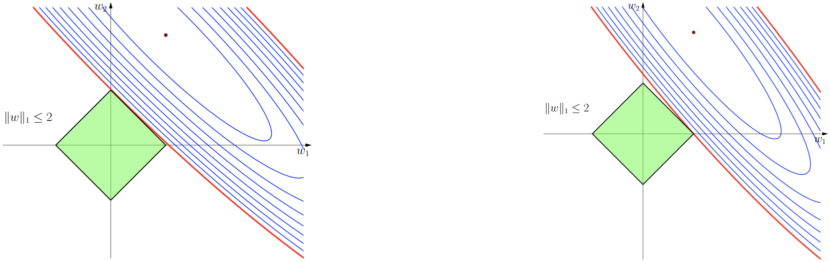
Correlated Features – Same Scale

- Suppose x_1 and x_2 are highly correlated and the same scale.
- This is quite typical in real data, after normalizing data.

- Nothing degenerate here, so level sets are ellipsoids.

- But, the higher the correlation, the closer to degenerate we get.
- That is, ellipsoids keep stretching out, getting closer to two parallel lines.

Correlated Features, ℓ_1 Regularization



- Intersection could be anywhere on the top right edge.
- Minor perturbations (in data) can drastically change intersection point – very unstable solution.
- Makes division of weight among highly correlated features (of same scale) seem arbitrary.
  - If $x_1 \approx 2x_2$, ellipse changes orientation and we hit a corner. (Which one?)

The Case Against Sparsity

A Case Against Sparsity

- Suppose there's some unknown value $\theta \in \mathbf{R}$.
- We get 3 noisy observations of θ:

$$x_1, x_2, x_3 \sim \mathcal{N}(\theta, 1) \ \text{(i.i.d)}$$

- What's a good estimator $\hat{\theta}$ for θ?
- Would you prefer $\hat{\theta} = x_1$ or $\hat{\theta} = \frac{1}{3}(x_1 + x_2 + x_3)$?

Estimator Performance Analysis

- $\mathbb{E}[x_1] = \theta$ and $\mathbb{E}\left[\frac{1}{3}(x_1 + x_2 + x_3)\right] = \theta$. So both unbiased.
- $\text{Var}[x_1] = 1$.
- $\text{Var}\left[\frac{1}{3}(x_1 + x_2 + x_3)\right] = \frac{1}{9}(1 + 1 + 1) = \frac{1}{3}$.
- Average has a smaller variance — the independent errors cancel each other out.
- Similar thing happens in regression with correlated features:
  - e.g. If 3 features are correlated, we could keep just one of them.
  - But we can potentially do better by using all 3.

Example with highly correlated features

- Model in words:
  - y is some unknown linear combination of z_1 and z_2.
  - But we don't observe z_1 and z_2 directly.
  - We get 3 noisy observations of z_1, call them x_1, x_2, x_3.
  - We get 3 noisy observations of z_2, call them x_4, x_5, x_6.
- We want to predict y from our noisy observations.
- That is, we want an estimator $\hat{y} = f(x_1, x_2, x_3, x_4, x_5, x_6)$ for estimating y.

Example from Section 4.2 in Hastie et al's *Statistical Learning with Sparsity*.

Example with highly correlated features

- Suppose (x, y) generated as follows:

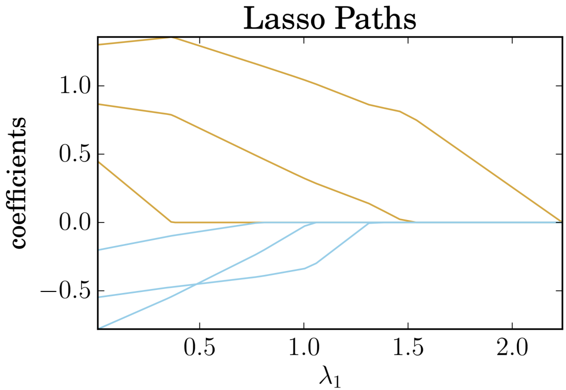
$$\begin{aligned} z_1, z_2 &\sim \mathcal{N}(0,1) \text{ (independent)} \\ \varepsilon_0, \varepsilon_1, \ldots, \varepsilon_6 &\sim \mathcal{N}(0,1) \text{ (independent)} \\ y &= 3z_1 - 1.5z_2 + 2\varepsilon_0 \\ x_j &= \begin{cases} z_1 + \varepsilon_j/5 & \text{for } j = 1,2,3 \\ z_2 + \varepsilon_j/5 & \text{for } j = 4,5,6 \end{cases} \end{aligned}$$

- Generated a sample of $((x_1, \ldots, x_6), y)$ pairs of size $n = 100$.
- That is, we want an estimator $\hat{y} = f(x_1, x_2, x_3, x_4, x_5, x_6)$ that is good for estimating y.
- **High feature correlation**: Correlations within the groups of x's is around 0.97.

Example from Section 4.2 in Hastie et al's *Statistical Learning with Sparsity*.

Example with highly correlated features

- Lasso regularization paths:



- Lines with the same color correspond to features with essentially the same information
- Distribution of weight among them seems almost arbitrary

Hedge Bets When Variables Highly Correlated

- When variables are highly correlated (and same scale – assume we've standardized features),
  - we want to give them roughly the same weight.
- Why?
  - Let their errors cancel out
- How can we get the weight spread more evenly?

Elastic Net

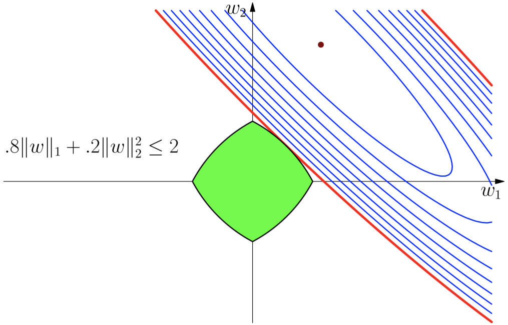
Elastic Net

- The **elastic net** combines lasso and ridge penalties:

$$\hat{w} = \underset{w \in \mathbf{R}^d}{\arg\min} \frac{1}{n} \sum_{i=1}^{n} \left\{ w^T x_i - y_i \right\}^2 + \lambda_1 \|w\|_1 + \lambda_2 \|w\|_2^2$$

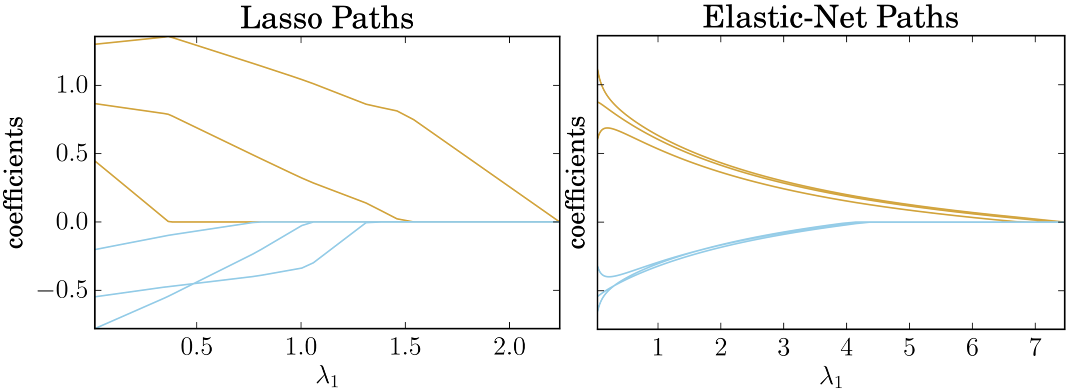
- We expect correlated random variables to have similar coefficients.

Highly Correlated Features, Elastic Net Constraint



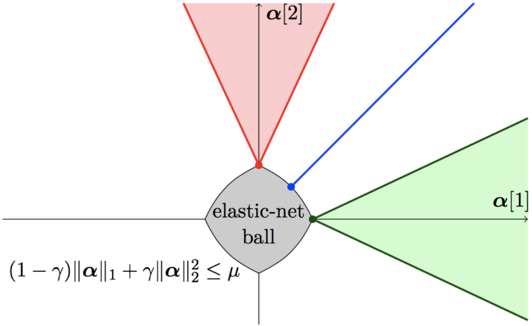
- Elastic net solution is closer to $w_2 = w_1$ line, despite high correlation.

Elastic Net Results on Model



- Lasso on left; Elastic net on right.
- Ratio of ℓ_2 to ℓ_1 regularization roughly $2:1$.

Elastic Net - "Sparse Regions"



- Suppose design matrix X is orthogonal, so $X^T X = I$, and contours are circles (and features uncorrelated)
- Then OLS solution in green or red regions implies elastic-net constrained solution will be at corner

Fig from Mairal et al.'s Sparse Modeling for Image and Vision Processing Fig 1.9

Elastic Net – A Theorem for Correlated Variables

Theorem

Let $\rho_{ij} = \widehat{corr}(x_i, x_j)$. Suppose features $x_1, \ldots, x_d$ are standardized and $\hat{w}_i$ and $\hat{w}_j$ are selected by elastic net, with $\hat{w}_i \hat{w}_j > 0$. Then

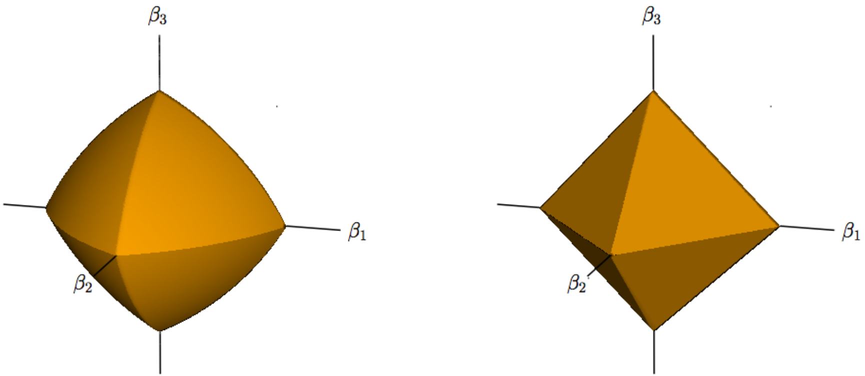
$$|\hat{w}_i - \hat{w}_j| \leqslant \frac{\|y\|_2 \sqrt{2}}{\sqrt{n}\lambda_2} \sqrt{1 - \rho_{ij}}.$$

Proof.

See Theorem 1 in Zou and Hastie's 2005 paper "Regularization and variable selection via the elastic net." Or see these notes that adapt their proof to our notation. □

Extra Pictures

Elastic Net vs Lasso Norm Ball



From Figure 4.2 of Hastie et al's *Statistical Learning with Sparsity*.

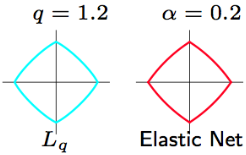


FIGURE 3.13. *Contours of constant value of $\sum_j |\beta_j|^q$ for $q = 1.2$ (left plot), and the elastic-net penalty $\sum_j (\alpha\beta_j^2 + (1-\alpha)|\beta_j|)$ for $\alpha = 0.2$ (right plot). Although visually very similar, the elastic-net has sharp (non-differentiable) corners, while the $q = 1.2$ penalty does not.*

From Hastie et al's *Elements of Statistical Learning*.