Regularización

Machine Learning

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Agenda

1. Recap: Predicción y Overfit

2. Regularización
   - Recap: OLS Mechanics
   - Ridge
   - Lasso
   - $k > n$
   - Ridge and Lasso: Pros and Cons
   - Familia de regresiones penalizadas
   - Elastic Net

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Overfit y Predicción fuera de Muestra

- ML nos interesa la predicción fuera de muestra
- Overfit: modelos complejos predicen bien dentro de muestra, pero tienden a hacer un mal trabajo fuera de muestra
- Hay que elegir el modelo que "mejor" prediga fuera de muestra, i.e., que tenga un menor error fuera de muestra
- Como estimamos el error fuera de muestra?
  - Penalización ex-post: AIC, BIC, etc
  - Métodos de Remuestreo: Enfoque del conjunto de validación, LOOCV, Validación cruzada en K-partes.

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Regularización: Motivación

- Las técnicas econometricas estándar no están optimizadas para la predicción.
- OLS minimiza el error *"dentro de muestra"*, eligiendo βs de forma tal que

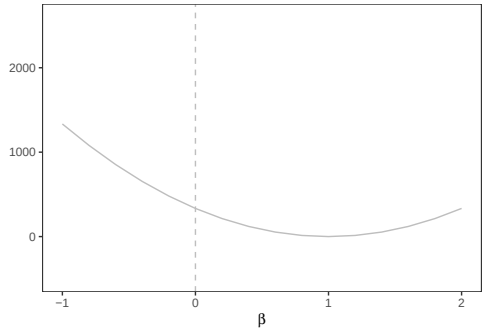
$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - \beta_0 - x_{i1}\beta_1 - \cdots - x_{ip}\beta_p)^2 \tag{1}$$

- o en forma matricial

$$min_{\beta} E(\beta) = (y - X\beta)'(y - X\beta) \tag{2}$$

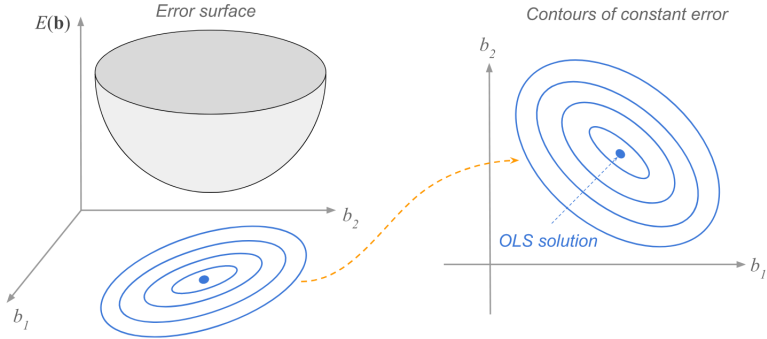
OLS 1 Dimension

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i \beta)^2 \tag{3}$$



Intuición en 2 Dimensiones (OLS)

$$min_\beta E(\beta) = \sum_{i=1}^{n} (y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2 \tag{4}$$



Fuente: https://allmodelsarewrong.github.io

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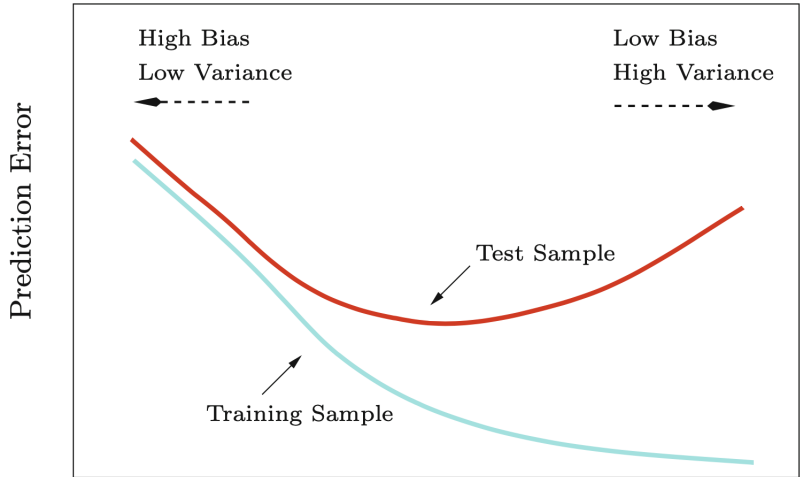
$$min_{\beta} E(\beta) = (y - X\beta)'(y - X\beta) \tag{2}$$

- Predicción queremos hacer un buen trabajo **fuera de muestra**

Regularización

- Asegurar cero sesgo dentro de muestra crea problemas fuera de muestra: trade-off Sesgo-Varianza



Regularización

- Las técnicas de machine learning fueron desarrolladas para hacer este trade-off de forma empírica.
- Vamos a proponer modelos del estilo

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - \beta_0 - x_{i1}\beta_1 - \cdots - x_{ip}\beta_p)^2 + \lambda \sum_{j=1}^{p} R(\beta_j) \tag{5}$$

- donde R es un regularizador que penaliza funciones que crean varianza

Ridge

- Para un $\lambda \geq 0$ dado, consideremos ahora el siguiente problema de optimización

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - \beta_0 - x_{i1}\beta_1 - \cdots - x_{ip}\beta_p)^2 + \lambda \sum_{j=1}^{p} (\beta_j)^2 \tag{6}$$

Ridge

- Para un $\lambda \geq 0$ dado, consideremos ahora el siguiente problema de optimización

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - \beta_0 - x_{i1}\beta_1 - \cdots - x_{ip}\beta_p)^2 + \lambda \sum_{j=1}^{p}(\beta_j)^2 \tag{6}$$

- o en forma matricial

$$min_\beta E(\beta) = (y - X\beta)'(y - X\beta) + \lambda\beta'\beta \tag{7}$$

Ridge: Intuición en 1 Dimension

- 1 predictor estandarizado
- El problema:

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda\beta^2 \tag{8}$$

- La solución?

Intuición en 2 Dimensiones (Ridge)

- En 2 dim

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2 + \lambda \left(\beta_1^2 + \beta_2^2\right) \tag{9}$$

- el dual es

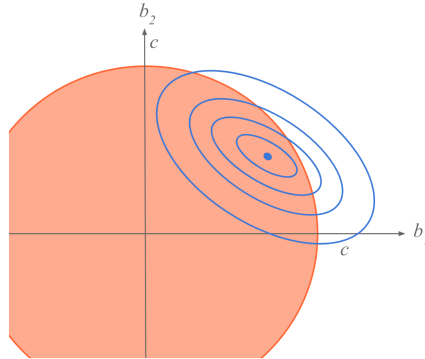
$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_{i1}\beta_1 - x_{i2}\beta_2)^2 \tag{10}$$

$$\text{sujeto a}$$

$$\left((\beta_1)^2 + (\beta_2)^2\right) \leq c$$

Intuición en 2 Dimensiones (Ridge)

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - x_{i1}\beta_1 - x_{i1}\beta_2)^2 \text{ s.a } \left((\beta_1)^2 + (\beta_2)^2\right) \leq c \tag{11}$$



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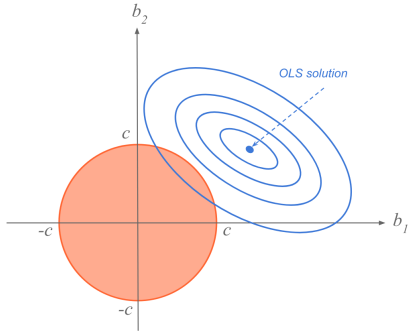
Intuición en 2 Dimensiones (Ridge)

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_{i1}\beta_1 - x_{i1}\beta_2)^2 \text{ s.a } \left((\beta_1)^2 + (\beta_2)^2\right) \leq c \tag{12}$$



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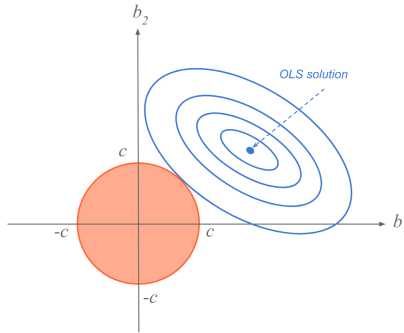

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Términos generales

- En regresión multiple (X es una matriz $n \times k$)
- Regresión: $y = X\beta + u$
- OLS

$$\hat{\beta}_{ols} = (X'X)^{-1}X'y$$

- Ridge

$$\hat{\beta}_{ridge} = (X'X + \lambda I)^{-1}X'y$$

Ridge vs OLS

- Ridge es sesgado $E(\hat{\beta}_{ridge}) \neq \beta$
- Pero la varianza es menor que la de OLS
- Para ciertos valores del parámetro $\lambda \Rightarrow MSE_{OLS} > MSE_{ridge}$

Example

photo from https://www.dailydot.com/parsec/batman-1966-labels-tumblr-twitter-vine/

Lasso

- Para un $\lambda \geq 0$ dado, consideremos el siguiente problema de optimización

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - \beta_0 - x_{i1}\beta_1 - \cdots - x_{ip}\beta_p)^2 + \lambda \sum_{j=1}^{p} |\beta_j| \tag{14}$$

- o en forma matricial

$$min_{\beta} E(\beta) = (y - X\beta)'(y - X\beta) + \lambda ||\beta||_1 \tag{15}$$

Lasso Intuición en 1 Dimension

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - x_i\beta)^2 + \lambda|\beta| \tag{16}$$

- Un solo predictor, un solo coeficiente
- Si $\lambda = 0$

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - x_i\beta)^2 \tag{17}$$

- y la solución es

$$\hat{\beta}_{OLS} \tag{18}$$

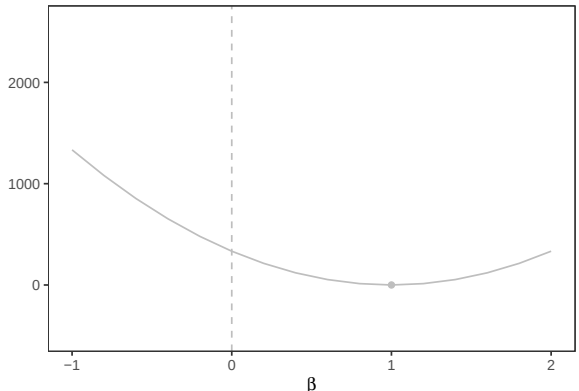
Intuición en 1 Dimension

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda|\beta| \tag{19}$$

Intuición en 1 Dimensión

$\hat{\beta} > 0$

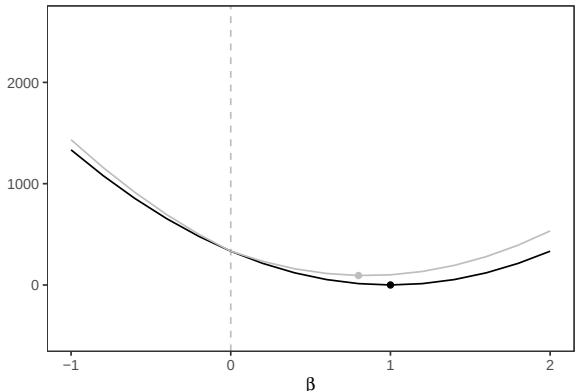
$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda\beta \tag{20}$$



Intuición en 1 Dimensión

$\hat{\beta} > 0$

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda\beta \tag{21}$$



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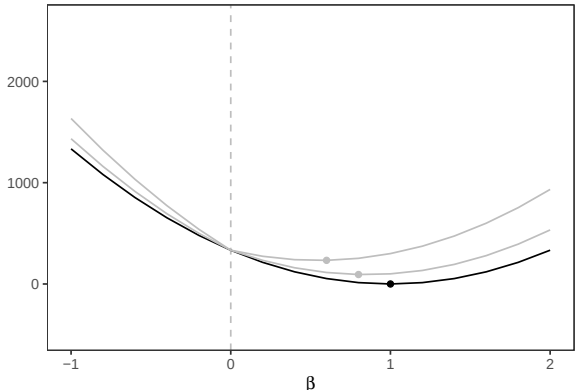

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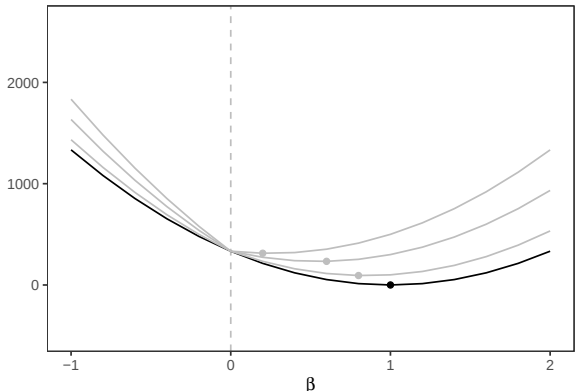
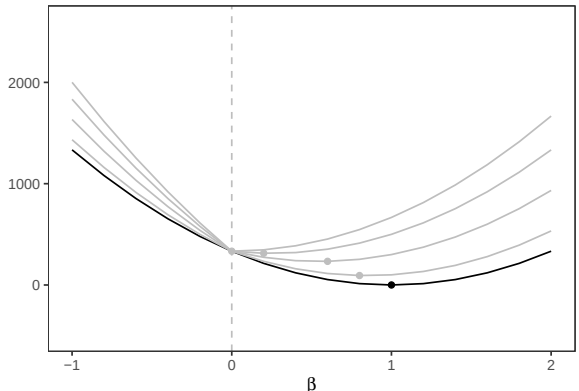


Intuición en 1 Dimensión

$\hat{\beta} > 0$

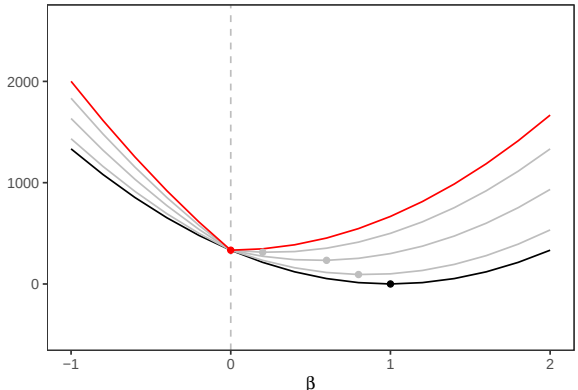
$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda\beta \tag{24}$$



Intuición en 1 Dimensión

$\hat{\beta} > 0$

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda\beta \tag{25}$$



Intuición en 1 Dimensión

$\hat{\beta} > 0$

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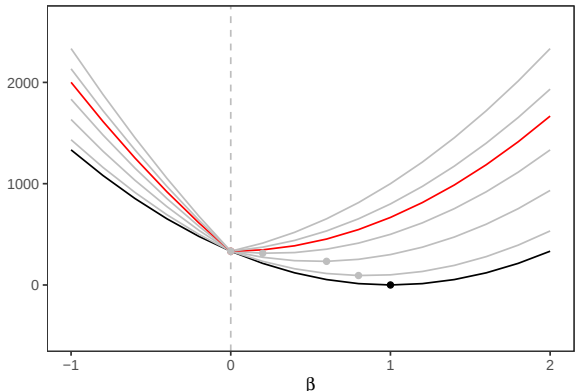


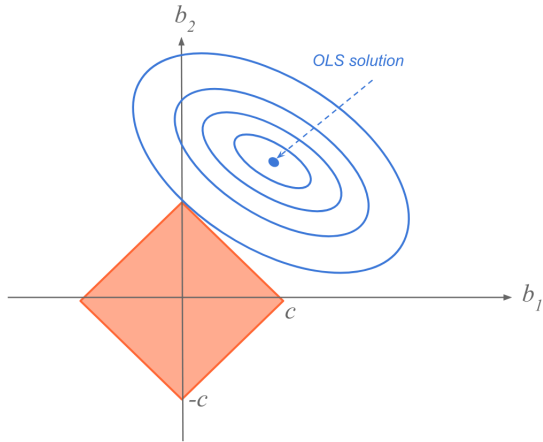
Intuición en 1 Dimension

Solución analitica

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_i\beta)^2 + \lambda|\beta| \tag{27}$$

Intuición en 2 Dimensiones (Lasso)

$$min_{\beta} E(\beta) = \sum_{i=1}^{n} (y_i - x_{i1}\beta_1 - x_{i1}\beta_2)^2 \text{ s.a } (|\beta_1| + |\beta_2|) \leq c \tag{28}$$



Example

photo from https://www.dailydot.com/parsec/batman-1966-labels-tumblr-twitter-vine/

More predictors than observations ($k > n$)

- What happens when we have more predictors than observations ($k > n$)?
  - OLS?
  - Ridge?
  - Lasso?

OLS when $k > n$

- Rank? Max number of rows or columns that are linearly independent
  - Implies $rank(X_{k\times n}) \leq min(k, n)$
- MCO we need $rank(X_{k\times n}) = k \implies k \leq n$
- If $rank(X_{k\times n}) = k$ then $rank(X'X) = k$
- If $k > n$, then $rank(X'X) \leq n < k$ then $(X'X)$ cannot be inverted
- Ridge and Lasso work when $k \geq n$

Ridge when $k > n$

$$min_\beta E(\beta) = \sum_{i=1}^{n}(y_i - x_{i1}\beta_1 - \cdots - x_{ik}\beta_k)^2 + \lambda \sum_{j=1}^{k}(\beta_j)^2 \tag{29}$$

- Solution $\rightarrow$ data augmentation
- Intuition: Ridge "adds" k additional points.
- Allows us to "deal" with $k \geq n$

Ridge when $k > n$

Adding k additional points

Lasso when $k > n$

- In the $k > n$ case, the lasso selects at most n variables before it saturates,
- This is because because of the nature of the convex optimization problem.

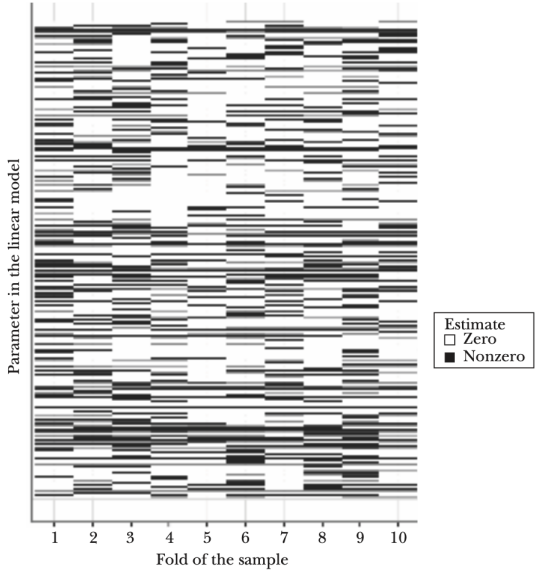
Ridge and Lasso: The good and the bad

- Objective 1: Accuracy
  - Minimize prediction error (in one step) $\rightarrow$ Ridge, Lasso
- Objective 2: Dimensionality
  - Reduce the predictor space $\rightarrow$ Lasso's free lunch
- More predictors than observations ($k > n$)
  - OLS fails
  - Ridge augments data
  - Lasso chooses at most n variables

Ridge and Lasso: The good and the bad

- When we have a group of highly correlated variables,
  - Lasso chooses only one.

Ridge and Lasso: The good and the bad



Ridge and Lasso: The good and the bad

- When we have a group of highly correlated variables,
  - Lasso chooses only one. Makes it unstable for prediction.
  - Ridge shrinks the coefficients of correlated variables toward each other.
  - For usual $n > k$ situations, if there are high correlations between predictors, it has been empirically observed that the prediction performance of the lasso is dominated by ridge regression (Tibshirani, 1996).

Family of penalized regressions

$$min_{\beta} R(\beta) = \sum_{i=1}^{n} (y_i - x_i'\beta)^2 + \lambda \sum_{s=2}^{p} |\beta_s|^q \tag{30}$$

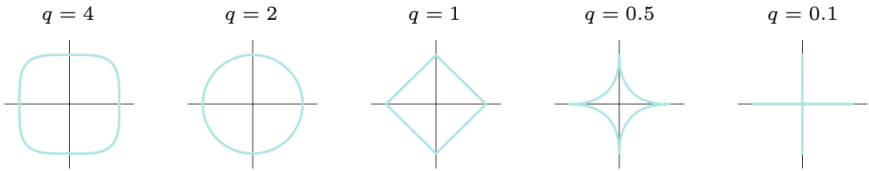


FIGURE 3.12. *Contours of constant value of* $\sum_j |\beta_j|^q$ *for given values of* q.

Elastic Net

- Elastic net: happy medium.
  - Good job at prediction and selecting variables

$$min_{\beta} EN(\beta) = \sum_{i=1}^{n}(y_i - \beta_0 - \sum_{j=1}^{p} x_{ij}\beta_j)^2 + \lambda \left(\alpha \sum_{j=1}^{p} |\beta_j| + \frac{(1-\alpha)}{2} \sum_{j=1}^{p} (\beta_j)^2 \right) \tag{31}$$

- Mixes Ridge and Lasso
- Lasso selects predictors
- Strict convexity part of the penalty (ridge) solves the grouping instability problem
- How to choose (λ, α)? $\rightarrow$ Bidimensional Crossvalidation
- Recomended lecture: Zou, H. & Hastie, T. (2005)

Example

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