Introduction to Machine Learning

Lecture 5
Linear Models II

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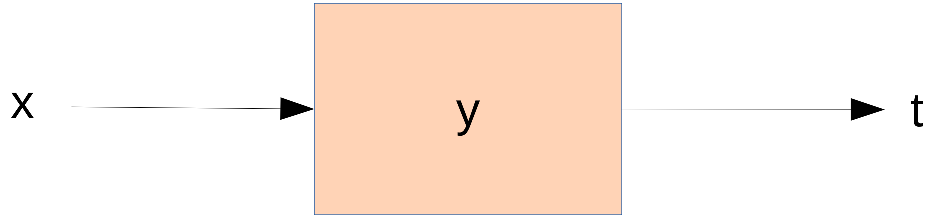
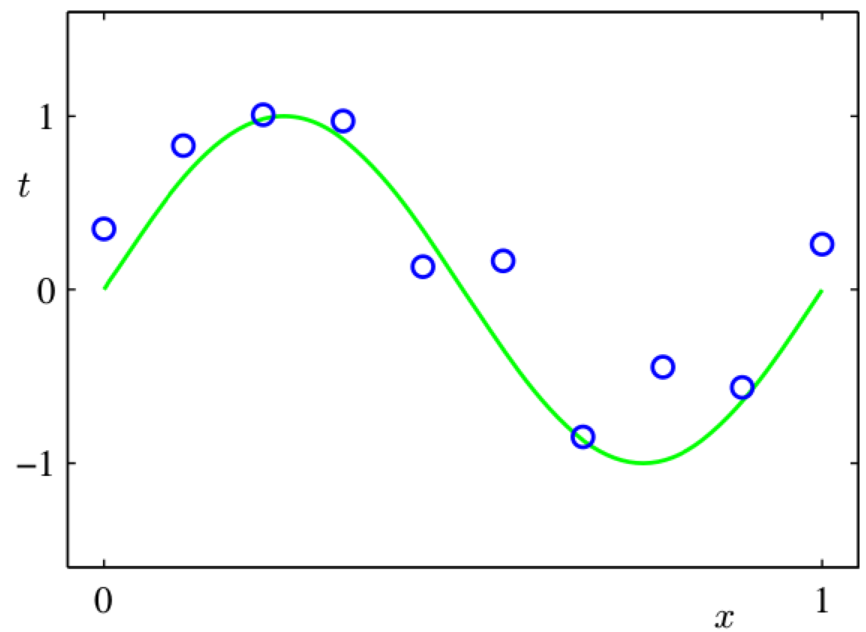
Polynomial curve fitting example



- Given N samples (training set) of {x, t}, learn function y
  - So we can predict t for a new x

Plot of a training data set of $N = 10$ points, shown as blue circles, each comprising an observation of the input variable x along with the corresponding target variable t. The green curve shows the function $\sin(2\pi x)$ used to generate the data. Our goal is to predict the value of t for some new value of x, without knowledge of the green curve.



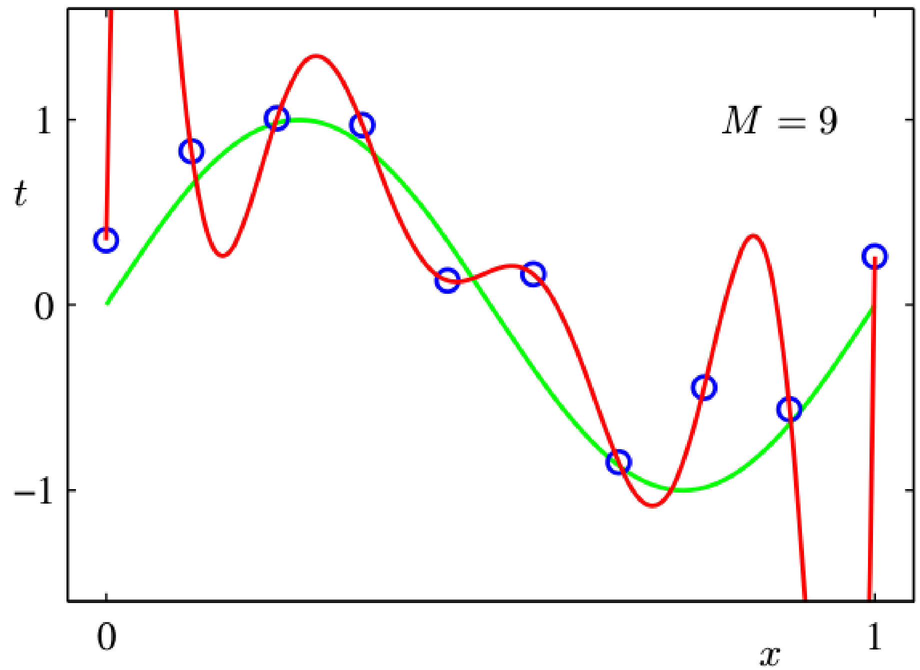


Table of the coefficients $\mathbf{w}^\star$ for polynomials of various order. Observe how the typical magnitude of the coefficients increases dramatically as the order of the polynomial increases.

	$M = 0$	$M = 1$	$M = 3$	$M = 9$
$w_0^\star$	0.19	0.82	0.31	0.35
$w_1^\star$		-1.27	7.99	232.37
$w_2^\star$			-25.43	-5321.83
$w_3^\star$			17.37	48568.31
$w_4^\star$				-231639.30
$w_5^\star$				640042.26
$w_6^\star$				-1061800.52
$w_7^\star$				1042400.18
$w_8^\star$				-557682.99
$w_9^\star$				125201.43

Regularization motivation

- As the coefficients get larger, the model becomes
  - More complex
  - Non-smooth
- Risk of overfitting

- Can we encourage coefficients to be smaller?
  - Give them a maximum size/magnitude.

$$\min_\beta \; (y - X\beta)^T(y - X\beta)$$

$$\text{s.t.} \quad \sum_{d=1}^{D} \beta_d^2 < C$$

$$(\text{or} \quad ||\beta||_2^2 < C)$$

[See ESL pg 63-64]

Brief aside on norms

- Norm: a function that assigns a strictly positive length or size to each vector

- *p*-norm (p>=1)

$$||x||_p = \left(\sum_i |x_i| \right)^{1/p}$$

- p=2 (l_2 norm), Euclidean norm

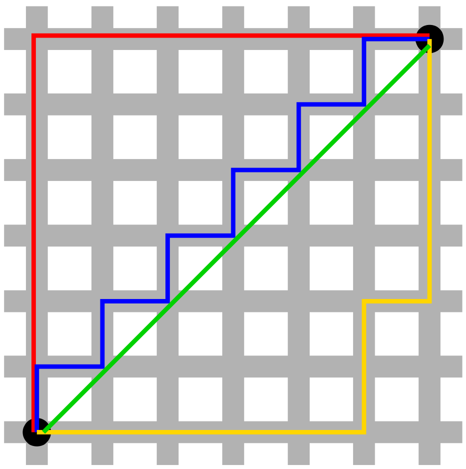
$$||x||_2 = \sqrt{\sum_i |x_i|^2}$$

- p=1 (l_1 norm), Taxicab (Manhattan) norm

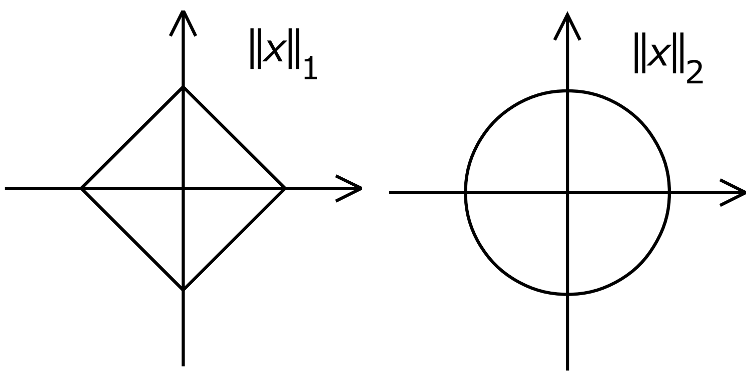
$$||x||_1 = \sum_i |x_i|$$

Brief aside on norms contd.

- Taxicab (Manhattan) norm



- Unit balls (circles) in L1 and L2



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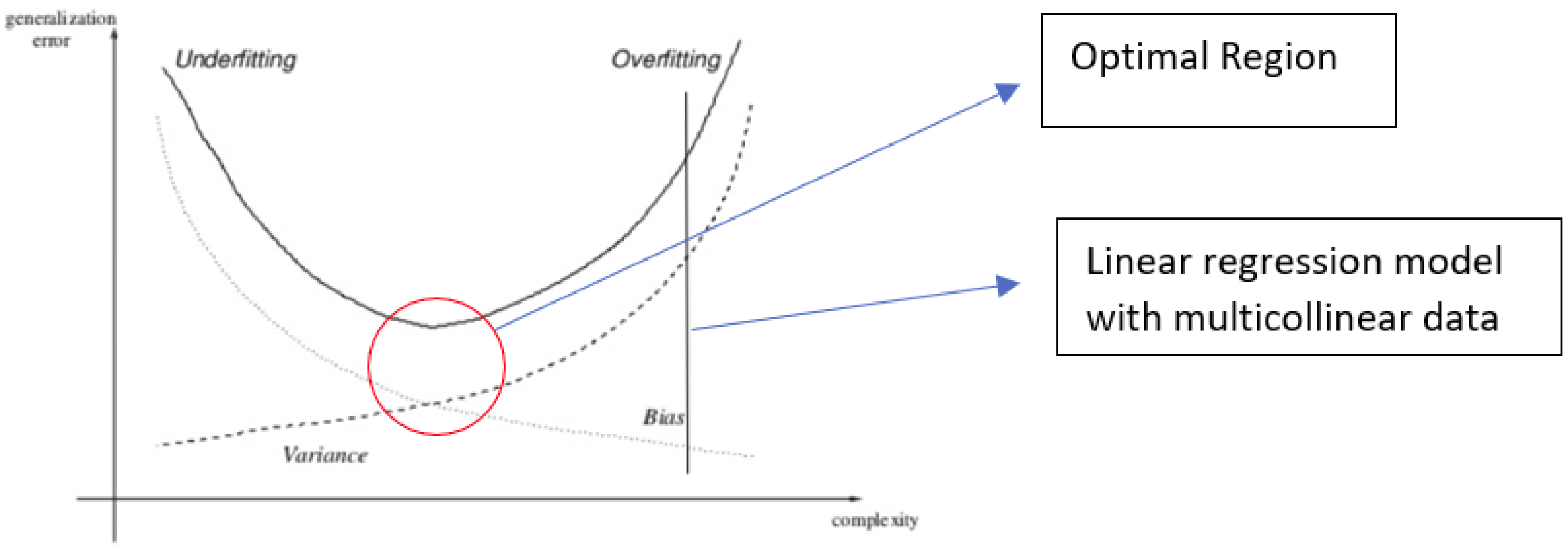
Regularization

- Introducing additional information/assumptions to
  - Solve an ill-posed problem
  - Prevent overfitting

- Reduces the variance substantially (with a slight increase in bias)



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l_2 regularization

- Known as Ridge regression, weight decay, Tikhonov regularization
- Solve

$$\mathrm{RSS} = \sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2.$$

$$\text{s.t.} \quad \sum_{p=1}\beta_p^2 < C$$

- Equivalently (add constraint as a penalty)

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}\beta_j^2$$

l_2 regularization

- Minimize wrt to β

$$\mathrm{RSS}(\lambda) = (\mathbf{y} - \mathbf{X}\beta)^T(\mathbf{y} - \mathbf{X}\beta) + \lambda\beta^T\beta,$$

- There is a closed form solution

$$\hat{\beta}^{\mathrm{ridge}} = (\mathbf{X}^T\mathbf{X} + \lambda\mathbf{I})^{-1}\mathbf{X}^T\mathbf{y},$$

- Adding the identity matrix makes the system non-singular

- Compare with least-squares estimate

$$\hat{\beta} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}.$$

What does l_2 regularization do?

- Pushes β towards zero
- λ controls how much we shrink them
  - Pick according to test performance (e.g., cross-validation)

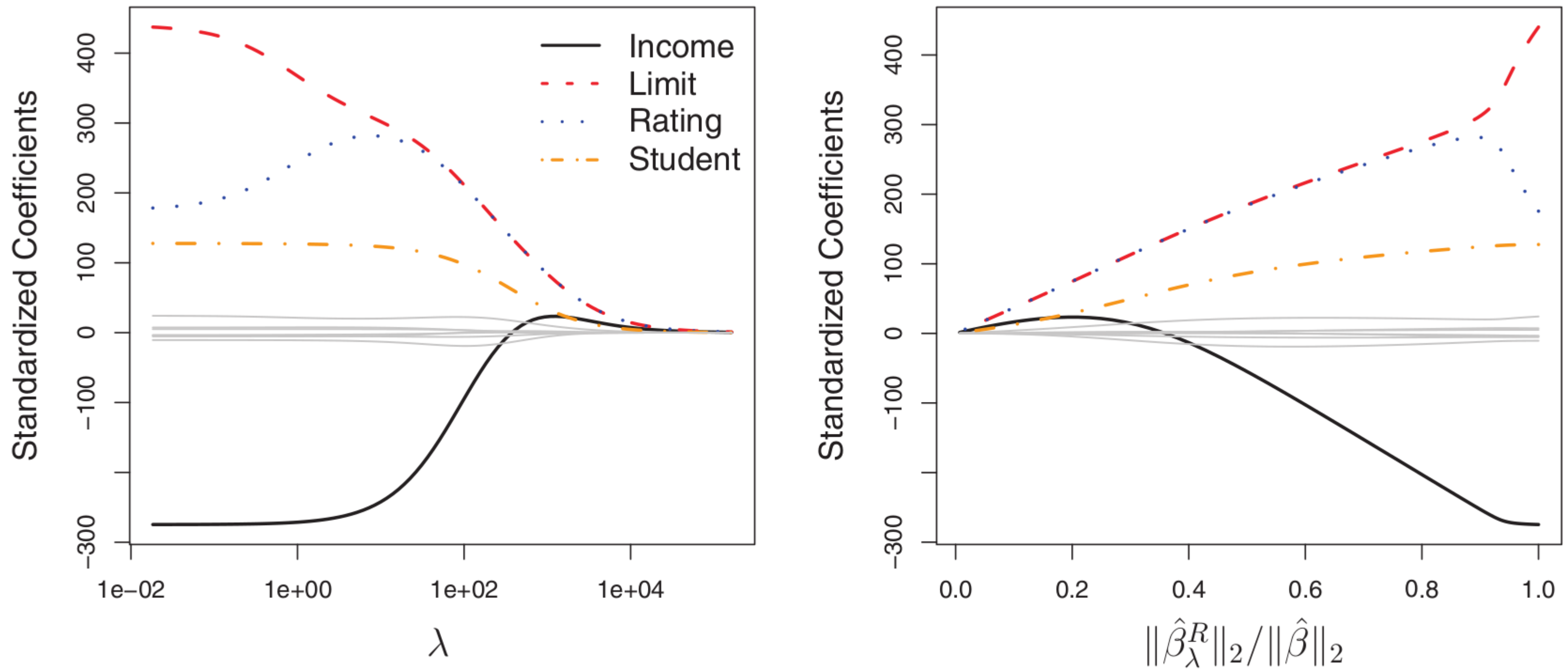


FIGURE 6.4. *The standardized ridge regression coefficients are displayed for the* Credit *data set, as a function of λ and $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$.*

Why does it help?

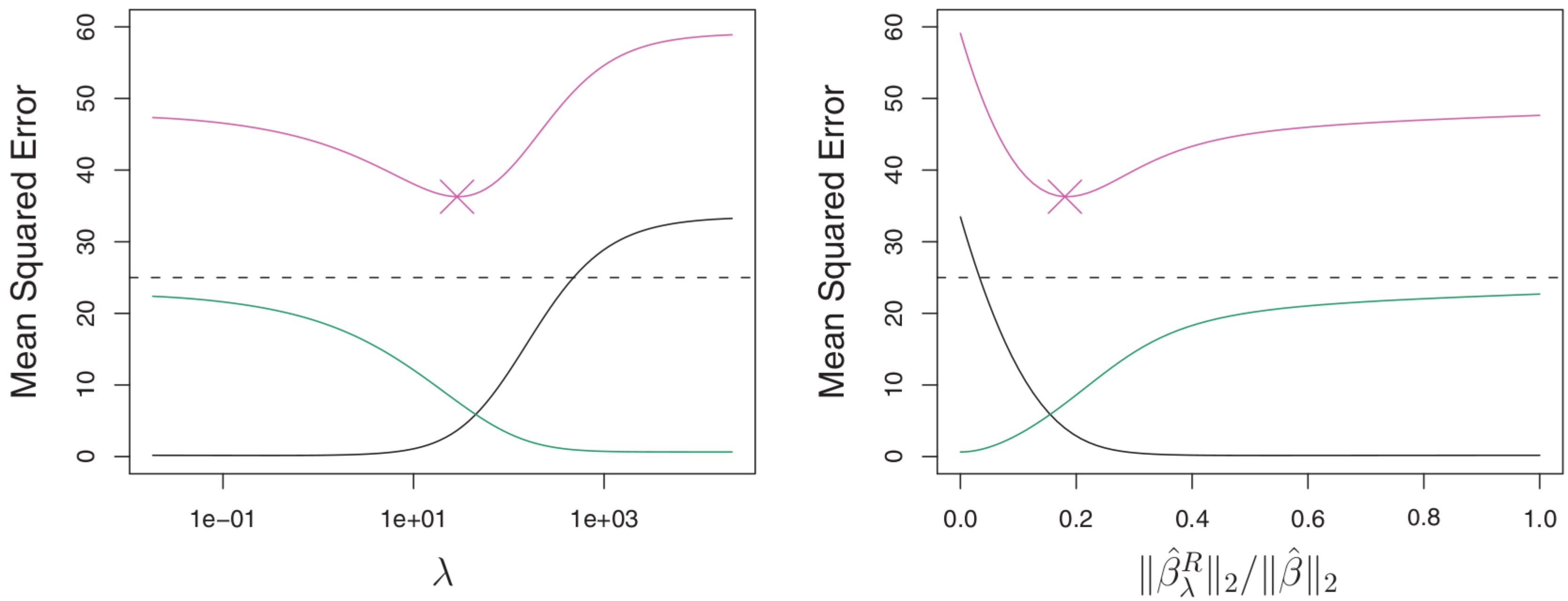


FIGURE 6.5. *Squared bias (black), variance (green), and test mean squared error (purple) for the ridge regression predictions on a simulated data set, as a function of* λ *and* $\|\hat{\beta}_\lambda^R\|_2/\|\hat{\beta}\|_2$. *The horizontal dashed lines indicate the minimum possible MSE. The purple crosses indicate the ridge regression models for which the MSE is smallest.*

Brief aside on normalization

- Ridge regression is not *scale invariant*
  - Multiply every feature by k, the solution is not simply multiplied by 1/k
  - Least-squares **is** *scale invariant*

- Normalization: Shifting, scaling data before feeding into the model
- Specifically, standardization
  - Make each feature zero mean, unit variance by
    - subtracting the mean
    - dividing by standard deviation

$$x \leftarrow \frac{x - \bar{x}}{\mathrm{sd}(x)}$$

- NOTE never peak at the test data
  - Calculate mean and sd on the training data, NOT the full dataset

l_1 regularization

- Known as Lasso, Basis Pursuit
- Use l_1 instead of l_2
- Solve

$$\sum_{i=1}^{n}\left(y_i - \beta_0 - \sum_{j=1}^{p}\beta_j x_{ij}\right)^2 + \lambda\sum_{j=1}^{p}|\beta_j|$$

- No more closed form solution
- But efficient algorithms available
  - Convex optimization problem

What does l_1 regularization do?

- Pushes β towards zero
- Sets some to exactly zero
  - Results in sparse solution
  - Automatic variable (feature) selection

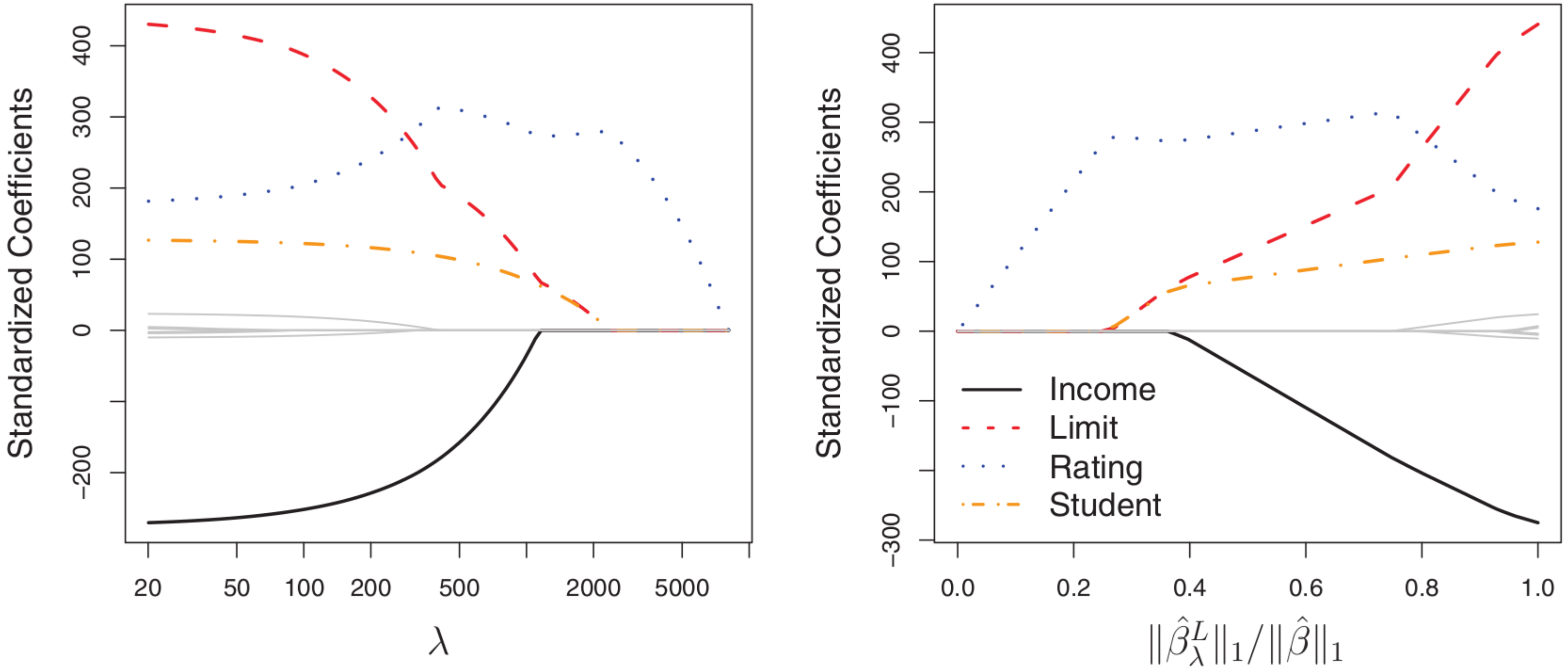


FIGURE 6.6. *The standardized lasso coefficients on the* `Credit` *data set are shown as a function of* λ *and* $\|\hat{\beta}^L_\lambda\|_1/\|\hat{\beta}\|_1$.

Why does l_1 lead to sparse solutions?

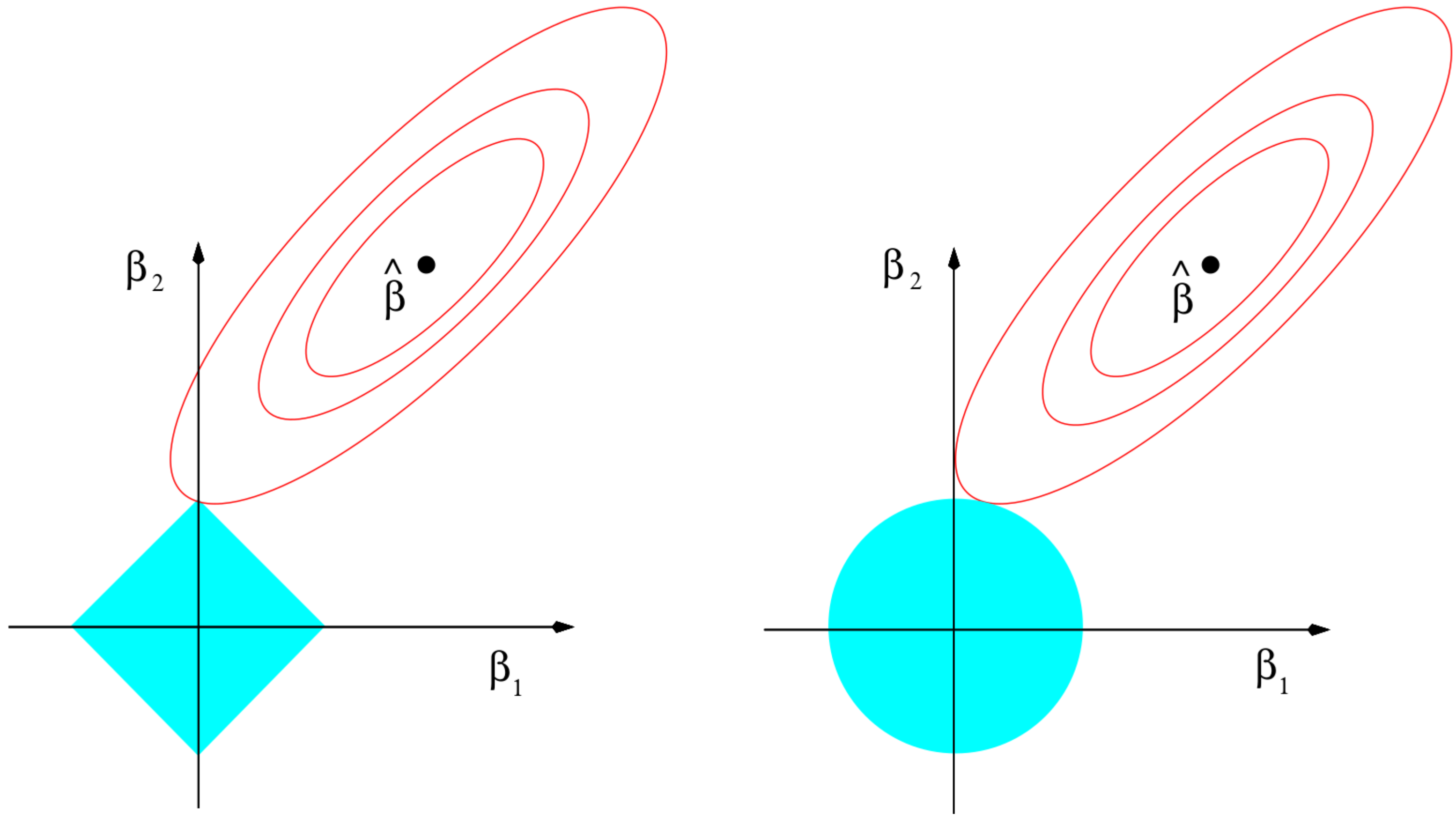


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \le t$ *and* $\beta_1^2 + \beta_2^2 \le t^2$, *respectively, while the red ellipses are the contours of the least squares error function.*

Ridge (l_2) vs. Lasso (l_1)

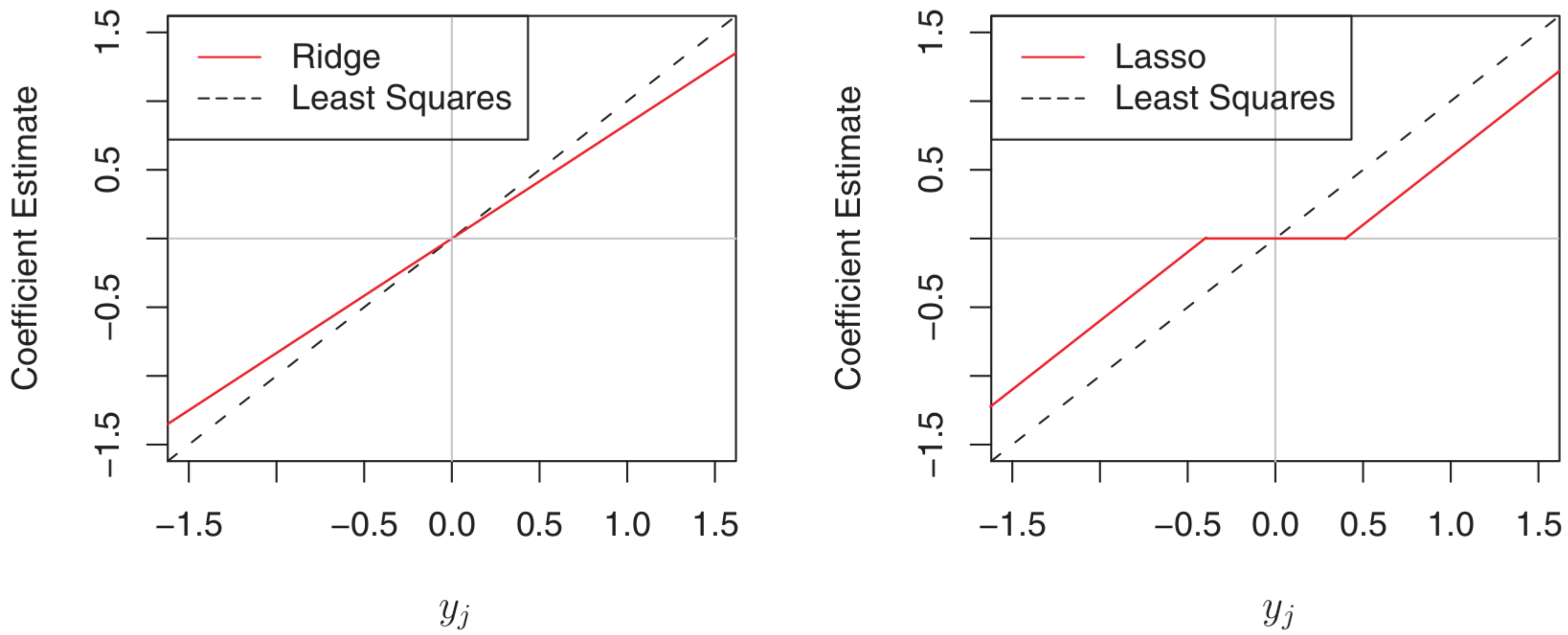
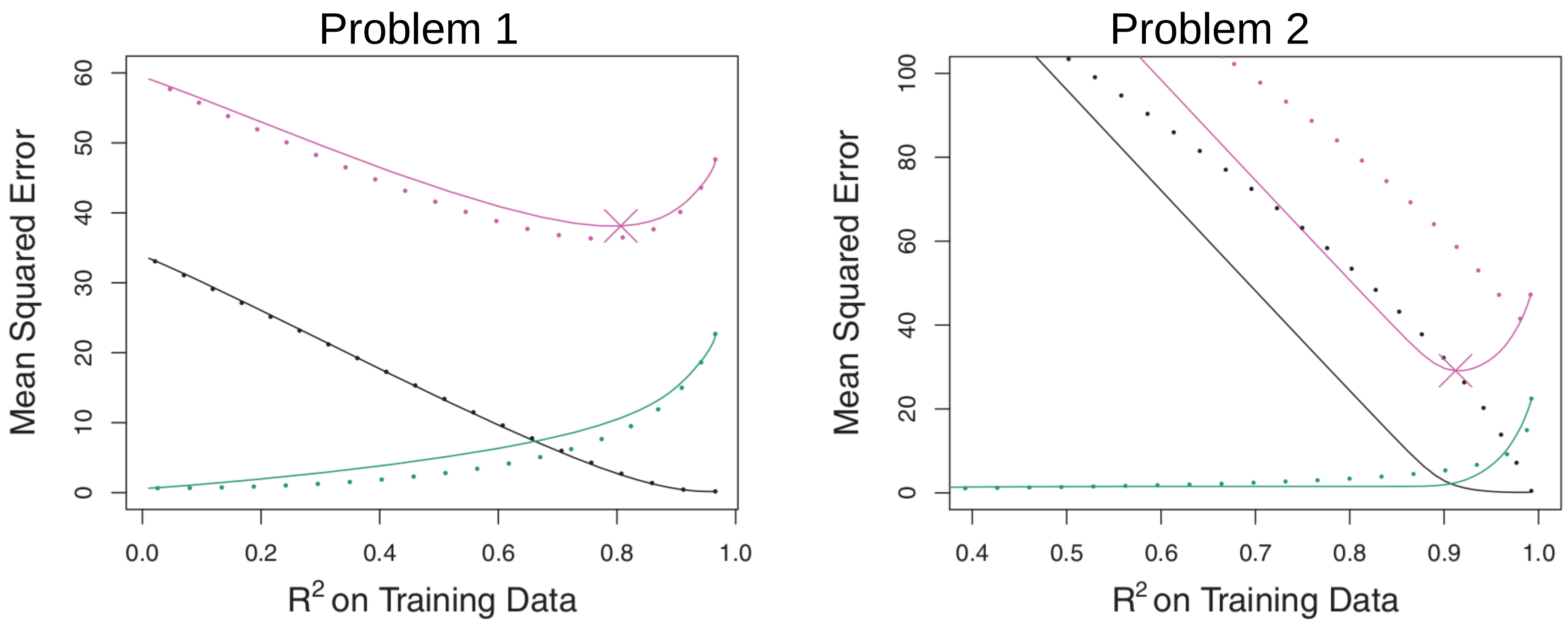


FIGURE 6.10. *The ridge regression and lasso coefficient estimates for a simple setting with $n = p$ and $\mathbf{X}$ a diagonal matrix with 1's on the diagonal.* Left: *The ridge regression coefficient estimates are shrunken proportionally towards zero, relative to the least squares estimates.* Right: *The lasso coefficient estimates are soft-thresholded towards zero.*

Ridge (l_2) vs. Lasso (l_1)

- Which one is better? Depends on the problem.
  - If some variables are not related to output at all, lasso might be better

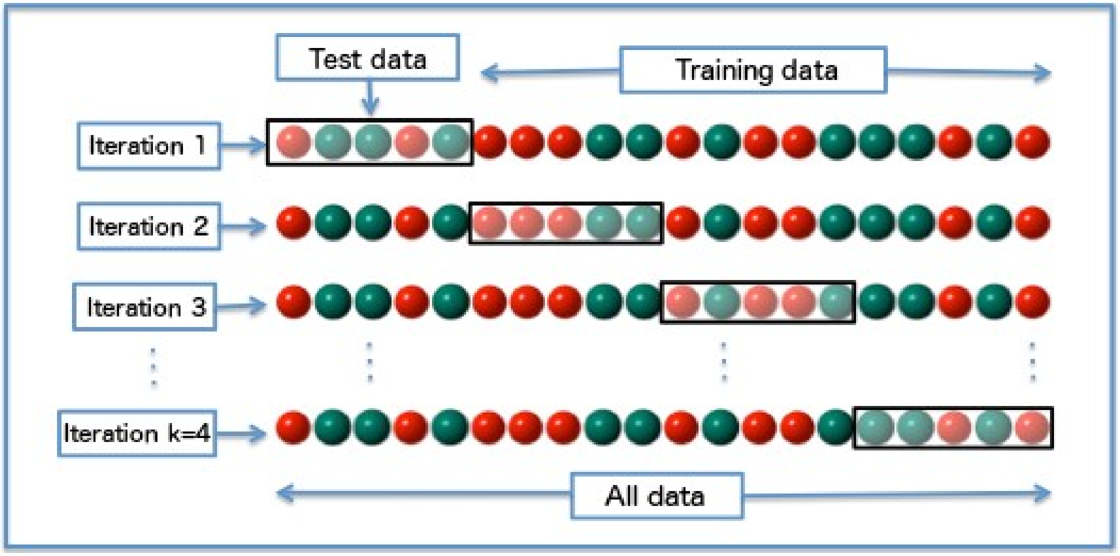


Legend:
Bias (black), variance (green), test error (purple)
Lasso (solid), Ridge (dotted)

Cross-validation

- Estimating the test-performance for a model
  - Pick hyper-parameters (e.g., λ)
- We talked about simple validation (holdout method)
  - Split into train/test, evaluate on test
    - Gives you a point estimate

- Various cross-validation techniques
- K-fold cross-validation



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Summary

- Regularization
- l_2 regularization
  - Non-sparse solutions
- l_1 regularization
  - Sparse solutions
- Picking λ
  - Cross-validation

- Exercises
  - Derive ridge regression solution
  - Do the lab in Section 6.6 of ISLR

References

[1] James, Witten, Hastie, and Tibshirani. An Introduction to Statistical Learning with Applications in R. Chapter 6.

[2] Hastie, Tibshirani, and Friedman. The Elements of Statistical Learning. Chapter 3.

[3] https://www.datasciencecentral.com/profiles/blogs/intuition-behind-bias-variance-trade-off-lasso-and-ridge

[4] https://en.wikipedia.org/wiki/Cross-validation_(statistics)

[5] https://en.wikipedia.org/wiki/Taxicab_geometry

[6] https://en.wikipedia.org/wiki/Norm_(mathematics)#Properties