Regression

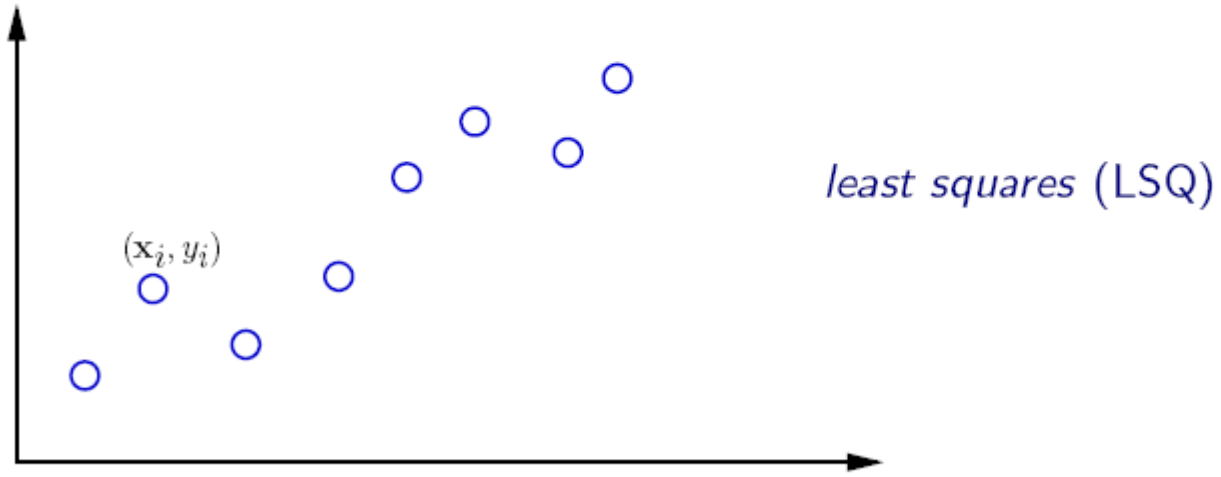
Linear Regression
Regression Trees

Characteristics of classification models

model	linear	parametric	global	stable
decision tree	no	no	no	no
logistic regression	yes	yes	yes	yes
discriminant analysis	yes/no	yes	yes	yes
k-nearest neighbor	no	no	no	no
naïve Bayes	no	yes/no	yes	yes

Linear fitting to data

- We want to fit a linear function to an observed set of points $X = [\mathbf{x}_1, \ldots, \mathbf{x}_N]$ with associated labels $Y = [y_1, \ldots, y_N]$.
  - Once we fit the function, we can use it to *predict* the y for new $\mathbf{x}$.
- Find the function that minimizes sum (or average) of square distances between actual ys in the training set and predicted ones.



slide thanks to Greg Shakhnarovich (CS195-5, Brown Univ., 2006)

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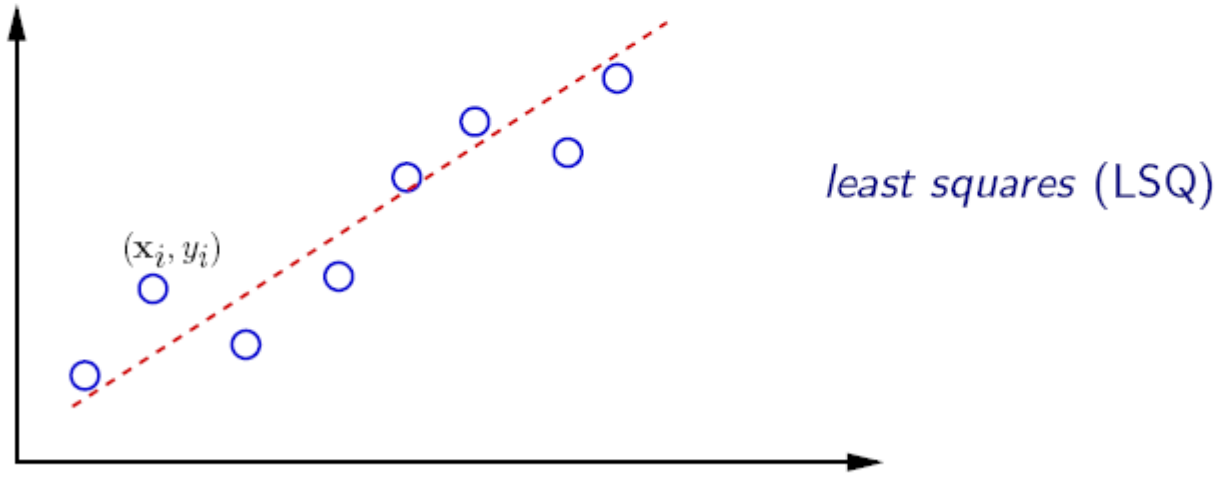

least squares (LSQ)

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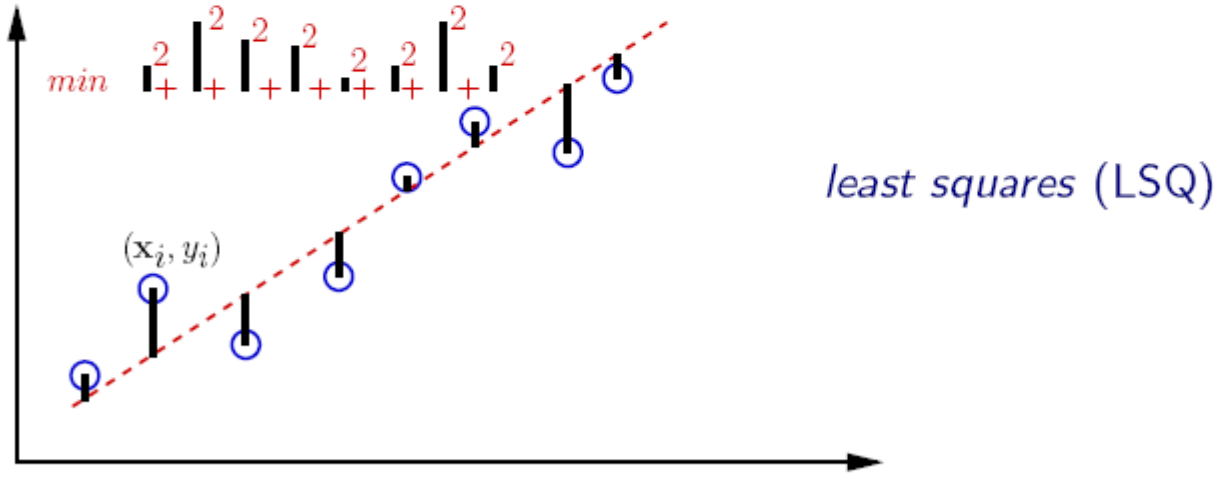

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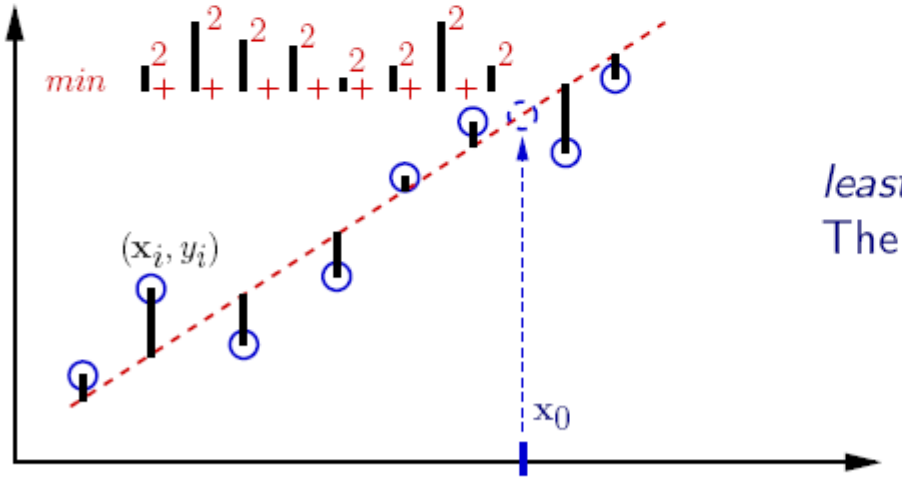
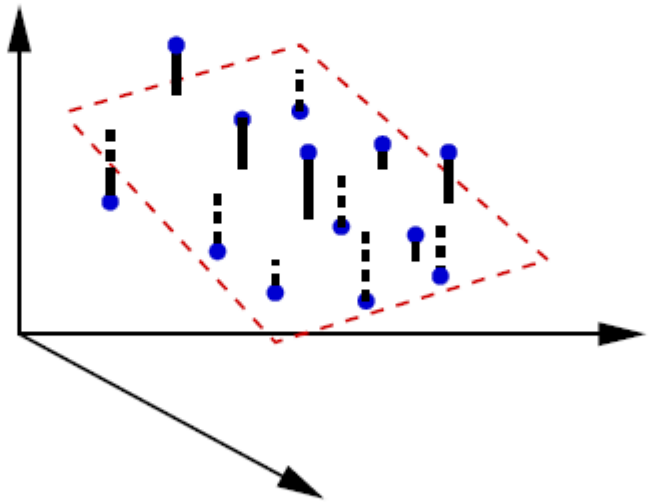


least squares (LSQ)
The fitted line is used as a predictor

slide thanks to Greg Shakhnarovich (CS195-5, Brown Univ., 2006)

Linear functions

- General form: $f(\mathbf{x}; \mathbf{w}) = w_0 + w_1 x_1 + \ldots + w_d x_d$
- 1D case ($\mathcal{X} = \mathbb{R}$): a line
- $\mathcal{X} = \mathbb{R}^2$: a plane



- *Hyperplane* in general, d-D case.

slide thanks to Greg Shakhnarovich (CS195-5, Brown Univ., 2006)

Loss function

- Suppose target labels come from set Y
  - Binary classification: $Y = \{ 0, 1 \}$
  - Regression: $Y = \Re$ (real numbers)
- A loss function maps decisions to costs:
  - $L(y, \hat{y})$ defines the penalty for predicting $\hat{y}$ when the true value is y.
- Standard choice for classification:
  0/1 loss (same as misclassification error)

$$L_{0/1}(y, \hat{y}) = \begin{cases} 0 & \text{if } y = \hat{y} \\ 1 & \text{otherwise} \end{cases}$$

- Standard choice for regression:
  squared loss

$$L(y, \hat{y}) = (\hat{y} - y)^2$$

Least squares linear fit to data

- Most popular estimation method is least squares:
  - Determine linear coefficients **w** that minimize sum of squared loss (SSL).
  - Use standard (multivariate) differential calculus:
    - differentiate SSL with respect to **w**
    - find zeros of each partial differential equation
    - solve for each w_i
- In one dimension:

$$\text{SSL} = \sum_{j=1}^{N} (y_j - (w_0 + w_1 \cdot x_j))^2 \qquad N = \text{number of samples}$$

$$w_1 = \frac{\text{cov}[x, y]}{\text{var}[x]} \qquad w_0 = \bar{y} - w_1 \cdot \bar{x} \qquad \bar{x},\bar{y} = \text{means of training } x, y$$

$$\hat{y}_t = w_0 + w_1 \cdot x_t \qquad \text{for test sample } x_t$$

Least squares linear fit to data

- Multiple dimensions
  - To simplify notation and derivation, add a new feature $x_0 = 1$ to feature vector $\mathbf{x}$:

$$\hat{y} = w_0 \cdot 1 + \sum_{i=1}^{d} w_i \cdot x_i = \mathbf{w} \cdot \mathbf{x}$$

  - Calculate SSL and determine $\mathbf{w}$:

$$\text{SSL} = \sum_{j=1}^{N} (y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 = (\mathbf{y} - \mathbf{X}\mathbf{w})^{\mathsf{T}} \cdot (\mathbf{y} - \mathbf{X}\mathbf{w})$$

$\mathbf{y}$ = vector of all training responses y_j

$\mathbf{X}$ = matrix of all training samples $\mathbf{x}_j$

$$\mathbf{w} = (\mathbf{X}^{\mathsf{T}}\mathbf{X})^{-1}\mathbf{X}^{\mathsf{T}}\mathbf{y}$$

$$\hat{y}_t = \mathbf{w} \cdot \mathbf{x}_t \qquad \text{for test sample } \mathbf{x}_t$$

Least squares linear fit to data

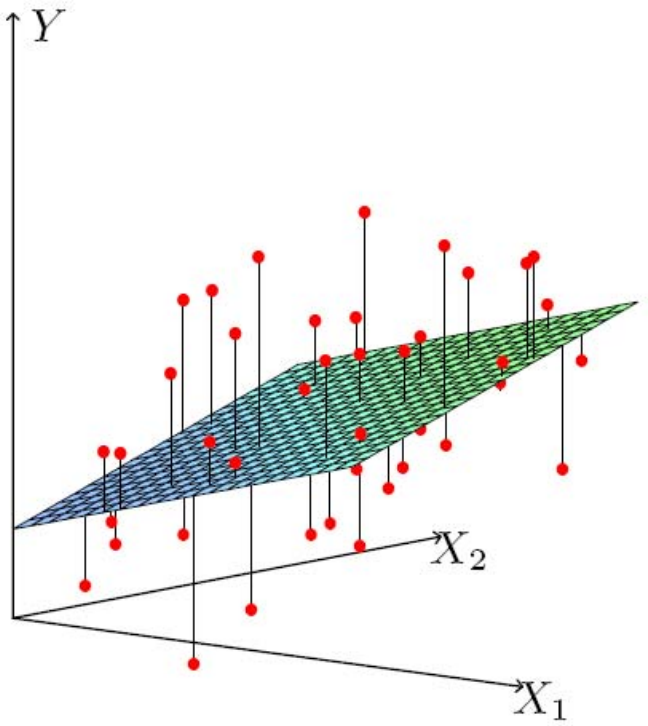


FIGURE 3.1. *Linear least squares fitting with* $X \in \mathbb{R}^2$. *We seek the linear function of* X *that minimizes the sum of squared residuals from* Y.

Least squares linear fit to data

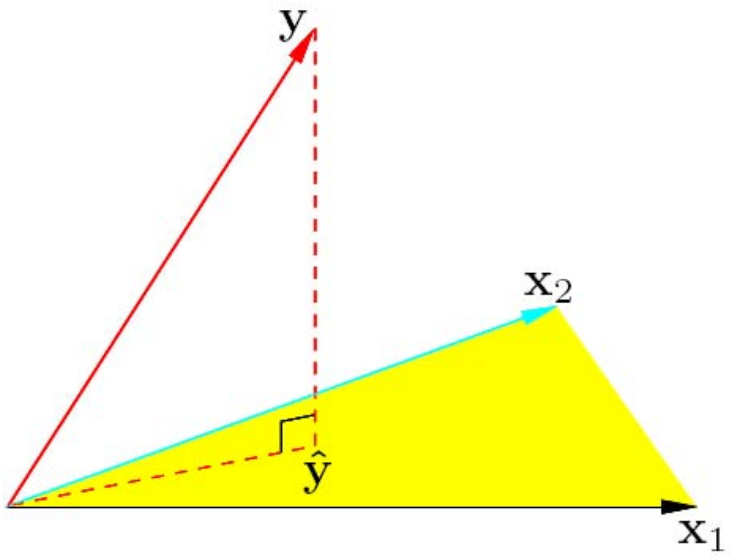
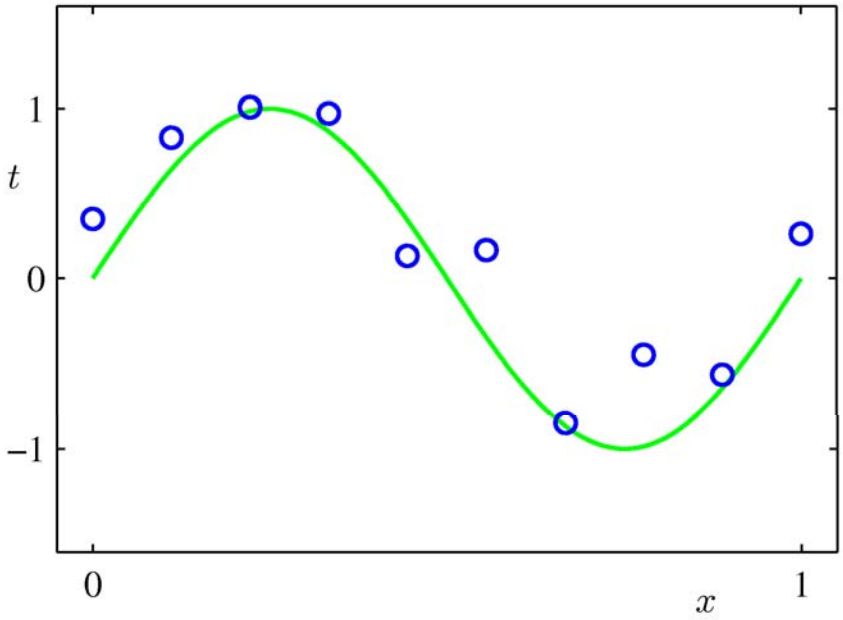


FIGURE 3.2. *The N-dimensional geometry of least squares regression with two predictors. The outcome vector* $\mathbf{y}$ *is orthogonally projected onto the hyperplane spanned by the input vectors* $\mathbf{x}_1$ *and* $\mathbf{x}_2$*. The projection* $\hat{\mathbf{y}}$ *represents the vector of the least squares predictions*

Extending application of linear regression

- The inputs **X** for linear regression can be:
  - Original quantitative inputs
  - Transformation of quantitative inputs, e.g. log, exp, square root, square, etc.
  - Polynomial transformation
    - example: $y = w_0 + w_1 \cdot x + w_2 \cdot x^2 + w_3 \cdot x^3$
  - Basis expansions
  - Dummy coding of categorical inputs
  - Interactions between variables
    - example: $x_3 = x_1 \cdot x_2$
- This allows use of linear regression techniques to fit much more complicated non-linear datasets.

Example of fitting polynomial curve with linear model



$$y(x, \mathbf{w}) = w_0 + w_1 x + w_2 x^2 + \ldots + w_M x^M = \sum_{j=0}^{M} w_j x^j$$

Prostate cancer dataset

- 97 samples, partitioned into:
  - 67 training samples
  - 30 test samples
- Eight predictors (features):
  - 6 continuous (4 log transforms)
  - 1 binary
  - 1 ordinal
- Continuous outcome variable:
  - `lpsa`: log(prostate specific antigen level)

Correlations of predictors in prostate cancer dataset

	lcavol	lweight	age	lbph	svi	lcp	gleason
lweight	0.300						
age	0.286	0.317					
lbph	0.063	0.437	0.287				
svi	0.593	0.181	0.129	−0.139			
lcp	0.692	0.157	0.173	−0.089	0.671		
gleason	0.426	0.024	0.366	0.033	0.307	0.476	
pgg45	0.483	0.074	0.276	−0.030	0.481	0.663	0.757

lcavol	log cancer volume
lweight	log prostate weight
age	age
lbph	log amount of benign prostatic hypertrophy
svi	seminal vesicle invasion
lcp	log capsular penetration
gleason	Gleason score
pgg45	percent of Gleason scores 4 or 5

Fit of linear model to prostate cancer dataset

TABLE 3.2. *Linear model fit to the prostate cancer data. The Z score is the coefficient divided by its standard error (3.12). Roughly a Z score larger than two in absolute value is significantly nonzero at the* $p = 0.05$ *level.*

Term	Coefficient	Std. Error	Z Score
`Intercept`	2.46	0.09	27.60
`lcavol`	0.68	0.13	5.37
`lweight`	0.26	0.10	2.75
`age`	−0.14	0.10	−1.40
`lbph`	0.21	0.10	2.06
`svi`	0.31	0.12	2.47
`lcp`	−0.29	0.15	−1.87
`gleason`	−0.02	0.15	−0.15
`pgg45`	0.27	0.15	1.74

Regularization

- Complex models (lots of parameters) often prone to overfitting.
- Overfitting can be reduced by imposing a constraint on the overall magnitude of the parameters.
- Two common types of regularization (shrinkage) in linear regression:
  - L_2 regularization (a.k.a. ridge regression). Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} w_i^2$$

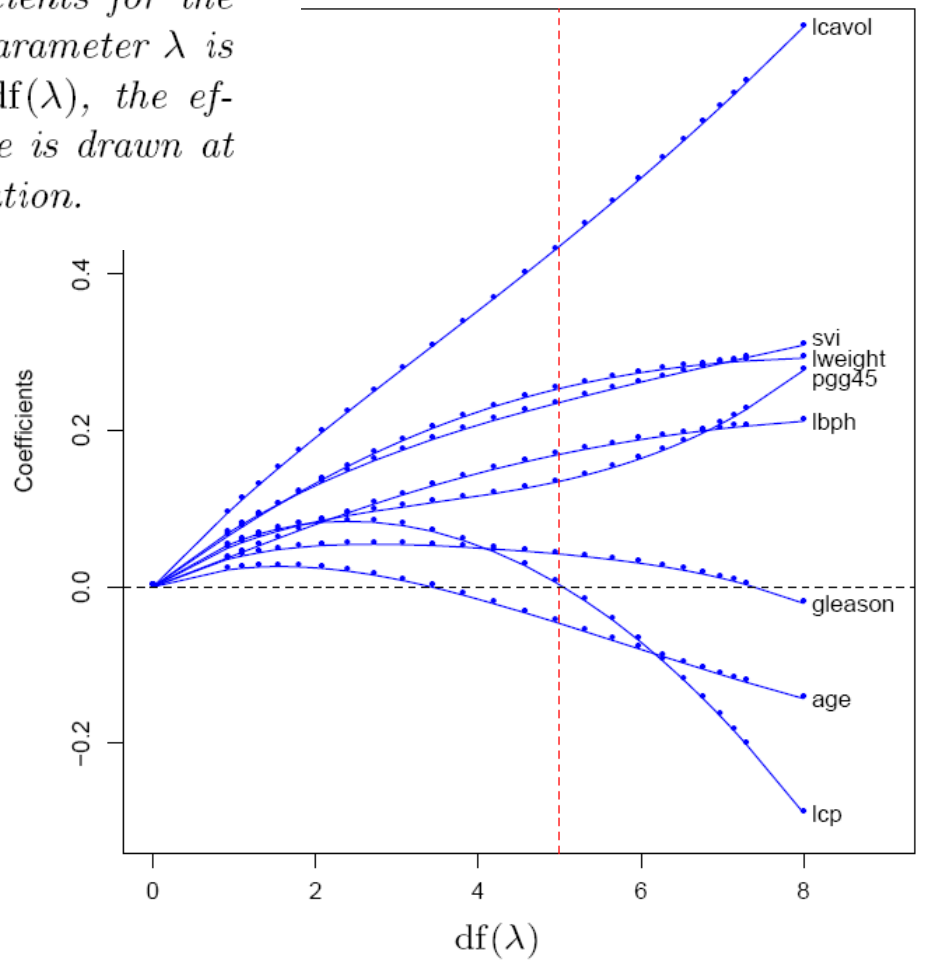
    - λ is the regularization parameter: bigger λ imposes more constraint

  - L_1 regularization (a.k.a. lasso). Find **w** which minimizes:

$$\sum_{j=1}^{N}(y_j - \sum_{i=0}^{d} w_i \cdot x_i)^2 + \lambda \sum_{i=1}^{d} |w_i|$$

Example of L_2 regularization

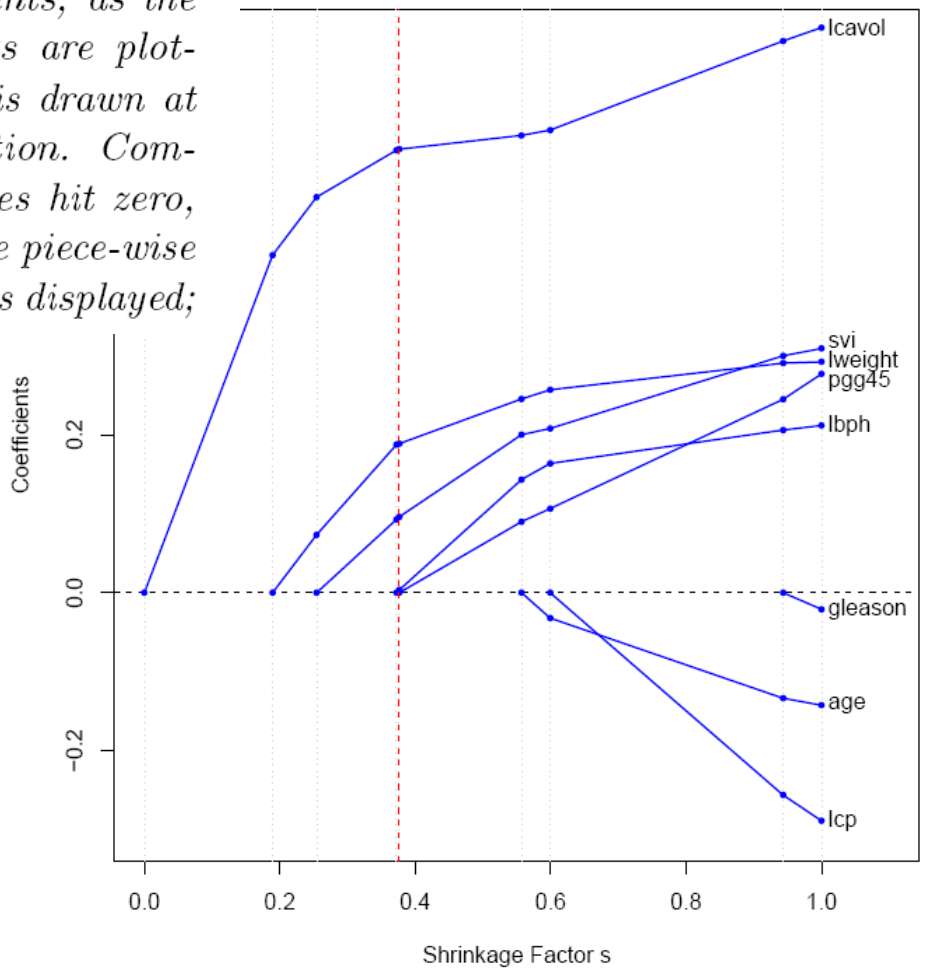
FIGURE 3.8. *Profiles of ridge coefficients for the prostate cancer example, as the tuning parameter λ is varied. Coefficients are plotted versus $\mathrm{df}(\lambda)$, the effective degrees of freedom. A vertical line is drawn at $\mathrm{df} = 5.0$, the value chosen by cross-validation.*



L2 regularization shrinks coefficients towards (but not to) zero, and towards each other.

Example of L_1 regularization

FIGURE 3.10. *Profiles of lasso coefficients, as the tuning parameter t is varied. Coefficients are plotted versus* $s = t/\sum_1^p |\hat{\beta}_j|$. *A vertical line is drawn at* $s = 0.36$, *the value chosen by cross-validation. Compare Figure 3.8 on page 9; the lasso profiles hit zero, while those for ridge do not. The profiles are piece-wise linear, and so are computed only at the points displayed;*



L1 regularization shrinks coefficients to zero at different rates; different values of λ give models with different subsets of features.

Example of subset selection

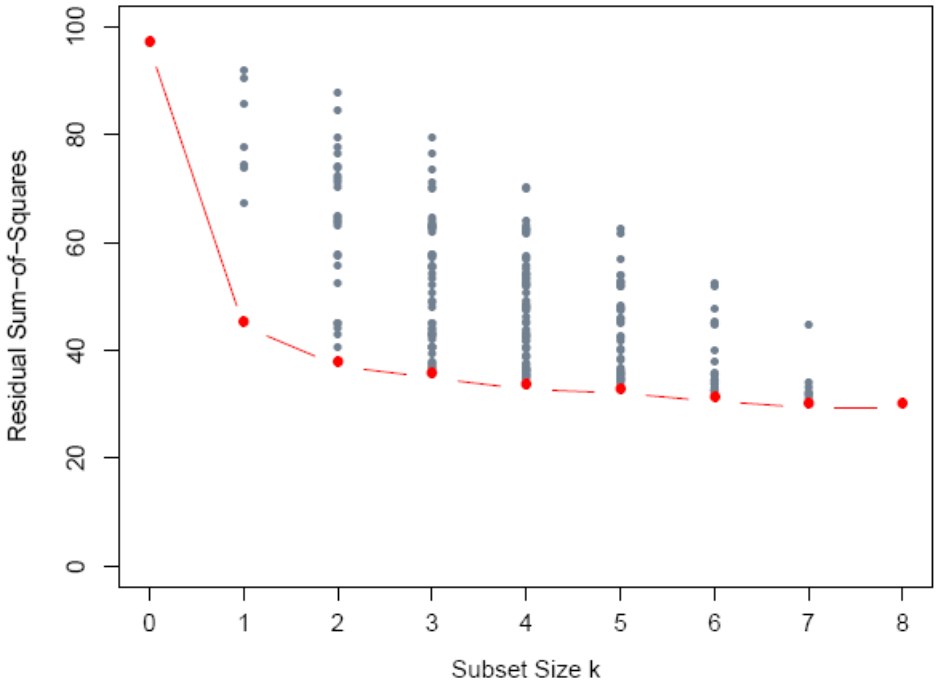


FIGURE 3.5. *All possible subset models for the prostate cancer example. At each subset size is shown the residual sum-of-squares for each model of that size.*

Comparison of various selection and shrinkage methods

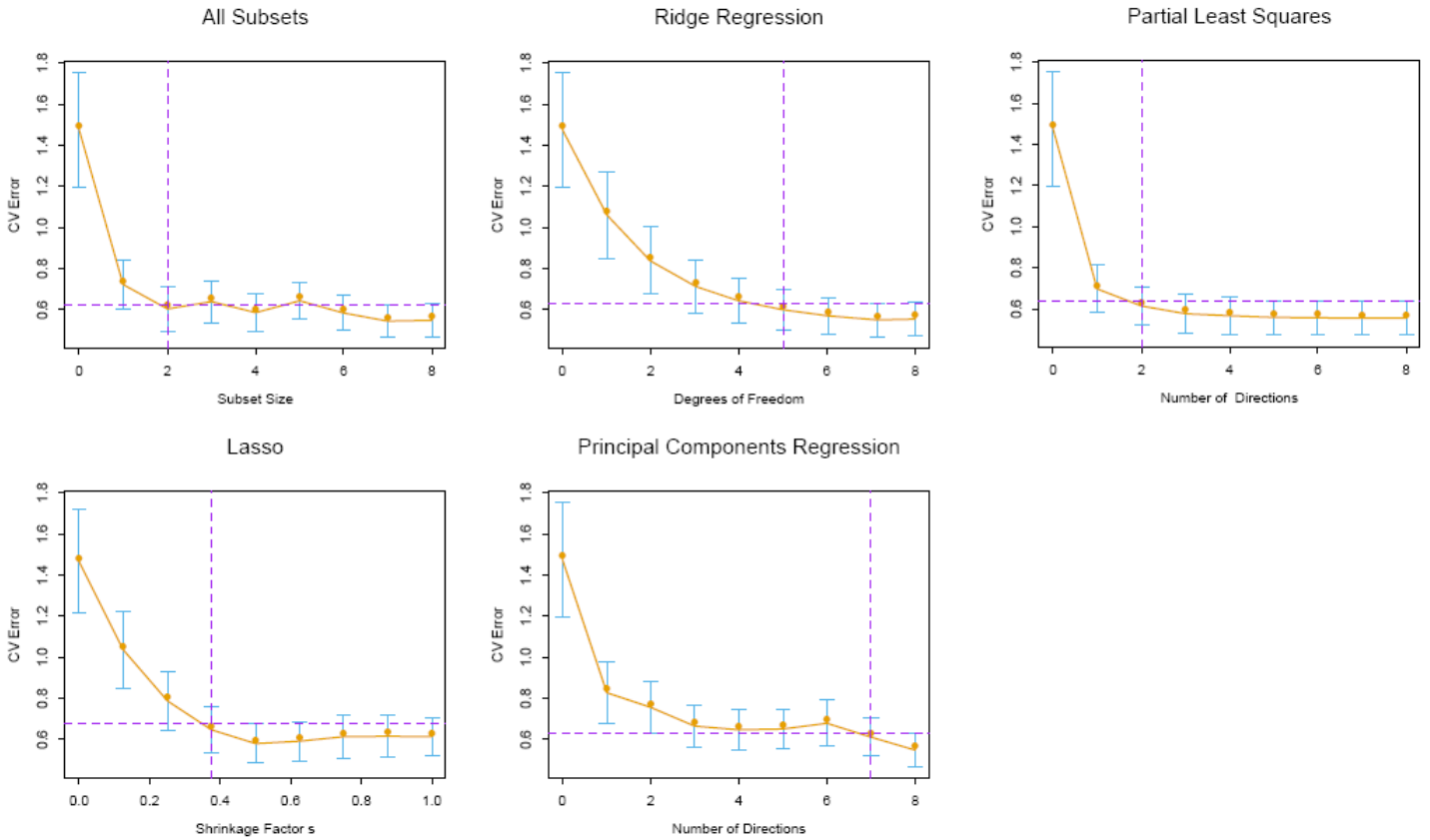


FIGURE 3.7. *Estimated prediction error curves and their standard errors for the various selection and shrinkage methods. Each curve is plotted as a func-*

L_1 regularization gives sparse models, L_2 does not

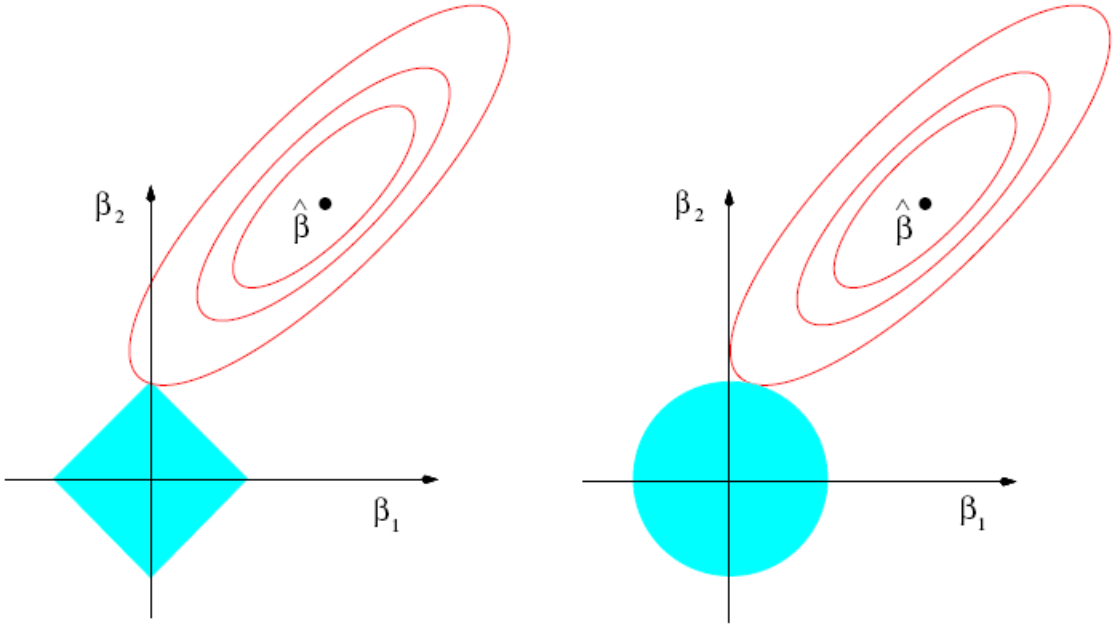


FIGURE 3.11. *Estimation picture for the lasso (left) and ridge regression (right). Shown are contours of the error and constraint functions. The solid blue areas are the constraint regions* $|\beta_1| + |\beta_2| \leq t$ *and* $\beta_1^2 + \beta_2^2 \leq t^2$, *respectively, while the red ellipses are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

Other types of regression

- In addition to linear regression, there are:
  - many types of non-linear regression
    - regression trees
    - nearest neighbor
    - neural networks
    - support vector machines
  - locally linear regression
  - etc.

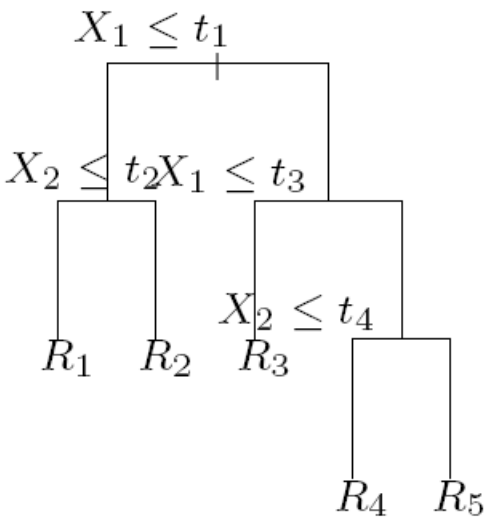
Regression trees

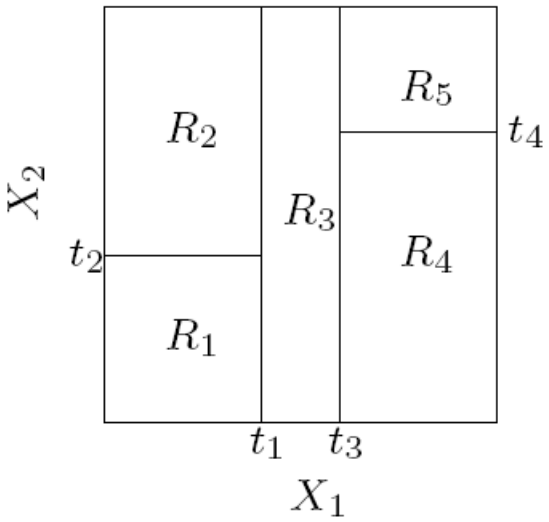
- Model very similar to classification trees
- Structure:

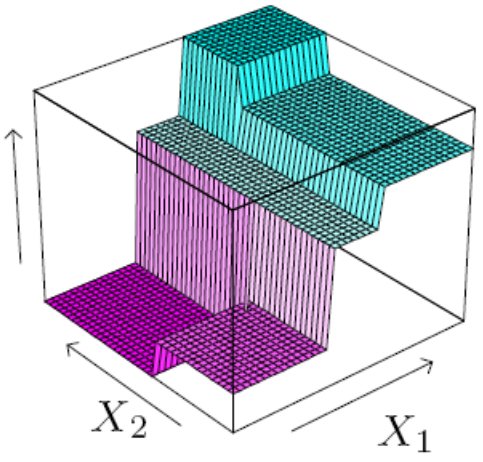
  binary splits on single attributes
- Prediction:

  mean value of training samples in leaf
- Induction:
  - greedy
  - loss function: sum of squared loss

Regression trees







$R_2 < R_1 < R_3 < R_4 < R_5$

Regression tree loss function

- Assume:
  - Attribute and split threshold for candidate split are selected
  - Candidate split partitions samples at parent node into child node sample sets C_1 and C_2
  - Loss for the candidate split is:

$$\sum_{x_i \in C_1} (y_i - \bar{y}_{C_1})^2 + \sum_{x_i \in C_2} (y_i - \bar{y}_{C_2})^2$$

$\bar{y}_{C_1}, \bar{y}_{C_2}$ are mean values of samples in child nodes C_1, C_2

Characteristics of regression models

model	linear	parametric	global	stable	continuous
linear regression	yes	yes	yes	yes	yes
regression tree	no	no	no	no	no

MATLAB interlude

matlab_demo_08.m