Computational Data Analysis

Machine Learning

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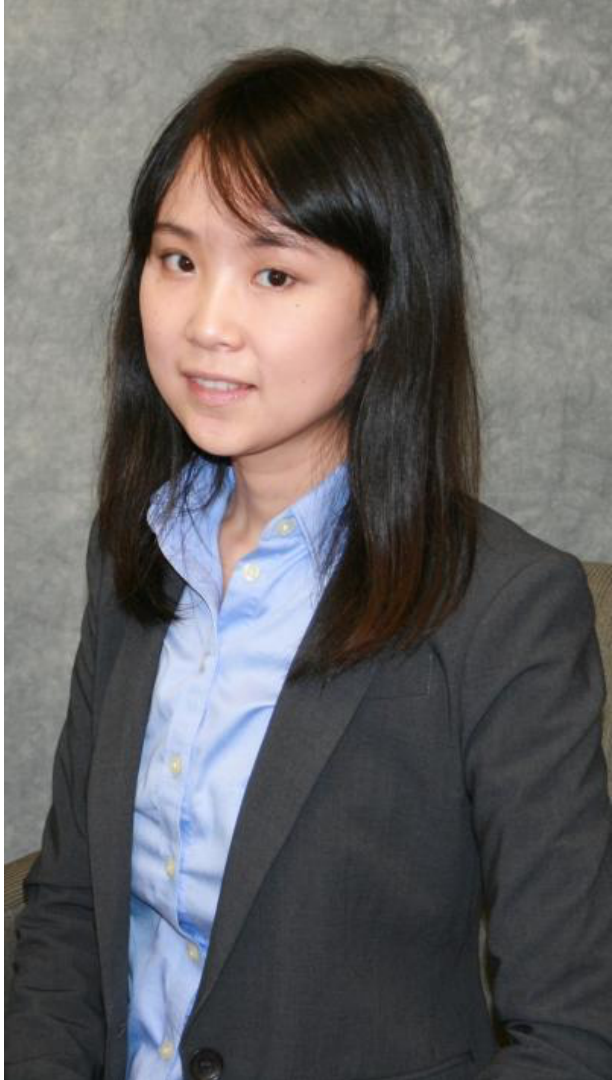
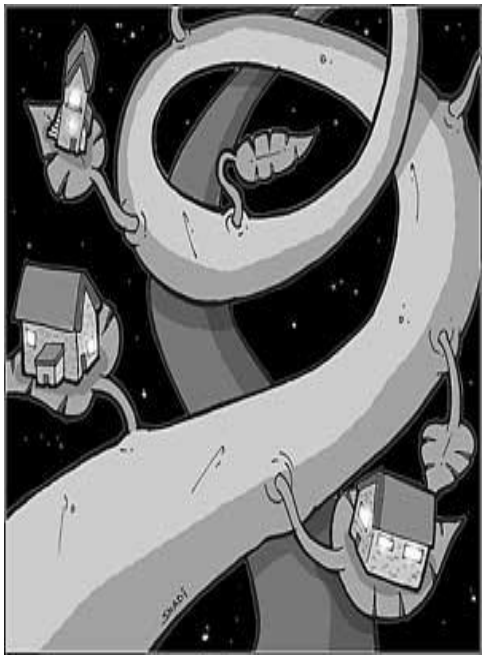


Regression and Random Forest

Machine learning for apartment hunting

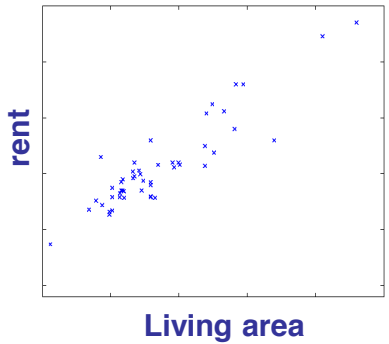


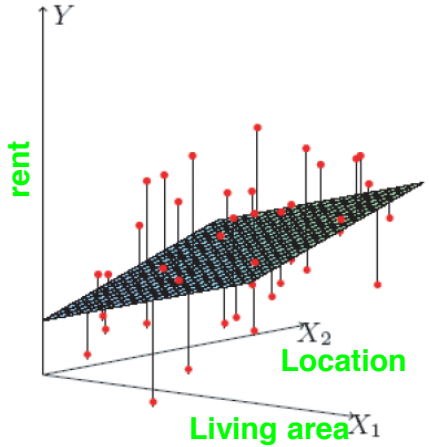
- Suppose you are to move to Atlanta
- And you want to find the **most reasonably priced** apartment satisfying your **needs:**

  square-ft., # of bedroom, distance to campus …

Living area (ft^2)	# bedroom	Rent ($)
230	1	600
506	2	1000
433	2	1100
109	1	500
…		
150	1	?
270	1.5	?

The learning problem





- Features:
  - Living area, distance to campus, # bedroom …
  - Denote as $x = (x_1, x_2, \dots, x_n)^\top$
- Target:
  - Rent
  - Denoted as y
- Training set:
  - $X = (x^1, x^2, \dots x^m)$
  - $y = (y^1, y^2, \dots, y^m)^\top$

Linear Regression Model

- Assume y is a linear function of x (features) plus noise ϵ

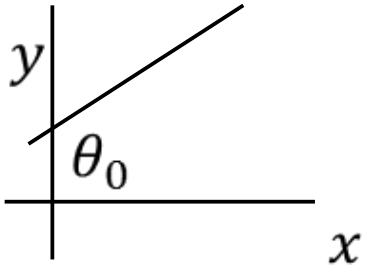
$$y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n + \epsilon$$

- where ϵ is an error term of unmodeled effects or random noise

- Let $\theta = (\theta_0, \theta_1, \ldots, \theta_n)^\top$, and augment data by one dimension

$$x \leftarrow (1, x)^\top$$

- Then $y = \theta^\top x + \epsilon$



Least mean square method

- Given m data points, find θ that minimizes the mean square error

$$\hat{\theta} = argmin_{\theta}\, L(\theta) = \frac{1}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)^2$$

- Our usual trick: set gradient to 0 and find parameter

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)x^i = 0$$

$$\Leftrightarrow -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i x^{i\top}\theta = 0$$

Matrix version of the gradient

- $\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m} y^i x^i + \frac{2}{m}\sum_{i=1}^{m} x^i x^{i\top}\theta = 0$

- Equivalent to

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}(x^1 \dots, x^m)(y^1 \dots, y^m)^\top + \frac{2}{m}(x^1, \dots x^m)(x^1, \dots x^m)^\top\theta = 0$$

- Define $X = (x^1, x^2, \dots x^m), y = (y^1, y^2, \dots, y^m)^\top$, gradient becomes

$$\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m} Xy + \frac{2}{m} XX^\top\theta = 0$$

$$\Rightarrow \hat{\theta} = (XX^\top)^{-1}Xy$$

Alternative way of obtaining θ

- The matrix inversion in $\hat{\theta} = (XX^\top)^{-1}Xy$ can be very expensive to compute

- $\frac{\partial L(\theta)}{\partial \theta} = -\frac{2}{m}\sum_{i=1}^{m}\left(y^i - \theta^\top x^i\right)x^i$

- Gradient descent

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^t + \frac{\alpha}{m}\sum_{i=1}^{m}\left(y^i - \hat{\theta}^{t\top} x^i\right)x^i$$

- Stochastic gradient descent (use one data point at a time)

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^t + \beta_t\left(y^i - \hat{\theta}^{t\top} x^i\right)x^i$$

A recap:

- Stochastic gradient update rule

$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \beta \left(y^{i} - \hat{\theta}^{t^{\top}} x^{i} \right) x^{i}$$

  - Pros: on-line, low per-step cost
  - Cons: coordinate, maybe slow-converging
- Gradient descent

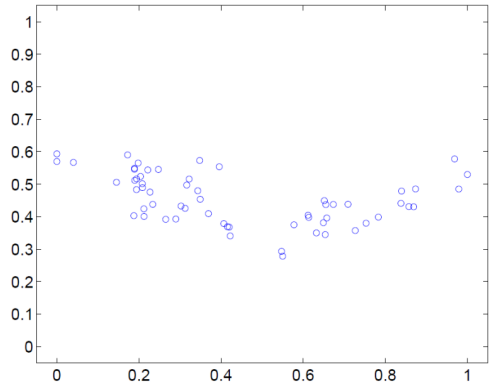
$$\hat{\theta}^{t+1} \leftarrow \hat{\theta}^{t} + \frac{\alpha}{m} \sum_{i=1}^{m} \left(y^{i} - \hat{\theta}^{t^{\top}} x^{i} \right) x^{i}$$

  - Pros: fast-converging, easy to implement
  - Cons: need to read all data
- Solve normal equations

$$(XX^{\top})\hat{\theta} = Xy$$

  - Pros: a single-shot algorithm! Easiest to implement.
  - Cons: need to compute inverse $(X^{T}X)^{-1}$, expensive, numerical issues (e.g., matrix is singular ..)

Nonlinear regression



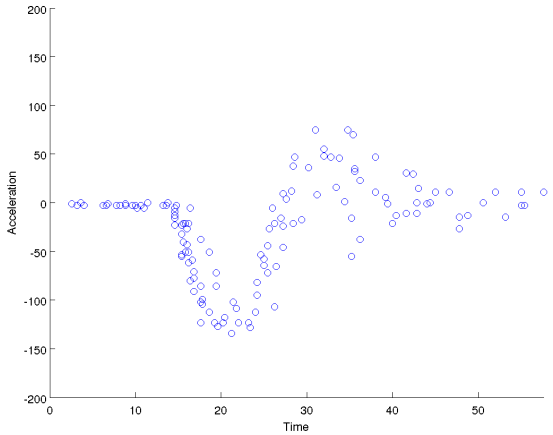
- Want to fit a polynomial regression model

$$y = \theta_0 + \theta_1 x + \theta_2 x^2 + \cdots + \theta_n x^n + \epsilon$$

- Let $\tilde{x} = (1, x, x^2, \ldots, x^n)^\top$ and $\theta = (\theta_0, \theta_1, \theta_2, \ldots, \theta_n)^\top$

$$\mathrm{y} = \theta^\top \tilde{x}$$

Example: head acceleration in accident

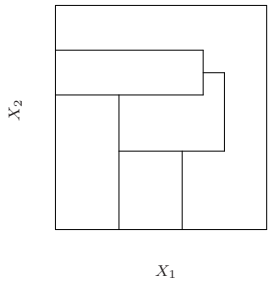


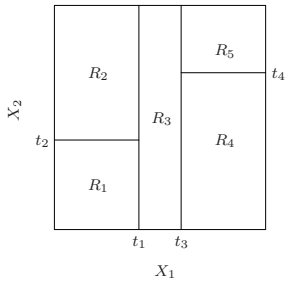
http://www.jari.jp/Portals/0/resource/pdf/AAI%20Summit/H25/4.%20MIROS.pdf

Regression tree

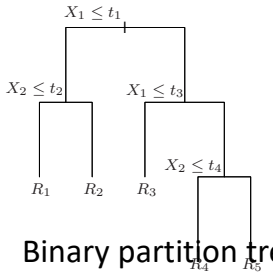
- Regression tree partition the feature space into a set of rectangles
- Fit a simple model (like a constant) in each one
- Popular method: CART

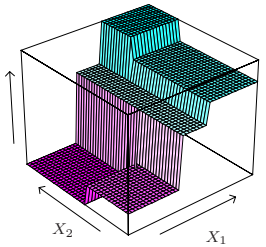
$$\hat{f}(X) = \sum_{m=1}^{5} c_m I\{(X_1, X_2) \in R_m\}.$$





$$\hat{c}_m = \text{ave}(y_i | x_i \in R_m)$$





Binary partition tree

Greedy procedure

- Greedy approach
- Start with all of the data
- Consider a splitting variable j and split point s, and define half-spaces

$$R_1(j,s) = \{X | X_j \leq s\} \text{ and } R_2(j,s) = \{X | X_j > s\}$$

- Solve the problem

$$\min_{j,\ s}\left[\min_{c_1}\sum_{x_i \in R_1(j,s)}(y_i - c_1)^2 + \min_{c_2}\sum_{x_i \in R_2(j,s)}(y_i - c_2)^2\right]$$

$$\hat{c}_1 = \text{ave}(y_i | x_i \in R_1(j,s))$$

$$\hat{c}_2 = \text{ave}(y_i | x_i \in R_2(j,s)).$$

Greedy procedure

- How large should the tree be
- Very large tree may over-fit the data; very small tree does not capture the important structure
- Determine the tree depth by controlling the fitting error-complexity tradeoff
- Grow a large tree, stop when a minimum node size has reached, then performing pruning by minimizing the cost function

error

$$C_\alpha(T) = \sum_{m=1}^{|T|} N_m Q_m(T) + \alpha|T|.$$

complexity

$$N_m = \#\{x_i \in R_m\},$$

$$\hat{c}_m = \frac{1}{N_m} \sum_{x_i \in R_m} y_i,$$

$$Q_m(T) = \frac{1}{N_m} \sum_{x_i \in R_m} (y_i - \hat{c}_m)^2,$$

Classification tree

- The classification outcome taking value 1,2,…, K
- The only change needed in the tree algorithm is to change the criteria for splitting nodes and pruning the tree

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k),$$

$$k(m) = \arg\max_k \hat{p}_{mk},$$

- Different measures of "error" $Q_m(T)$

Misclassification error: $\frac{1}{N_m} \sum_{i \in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}.$

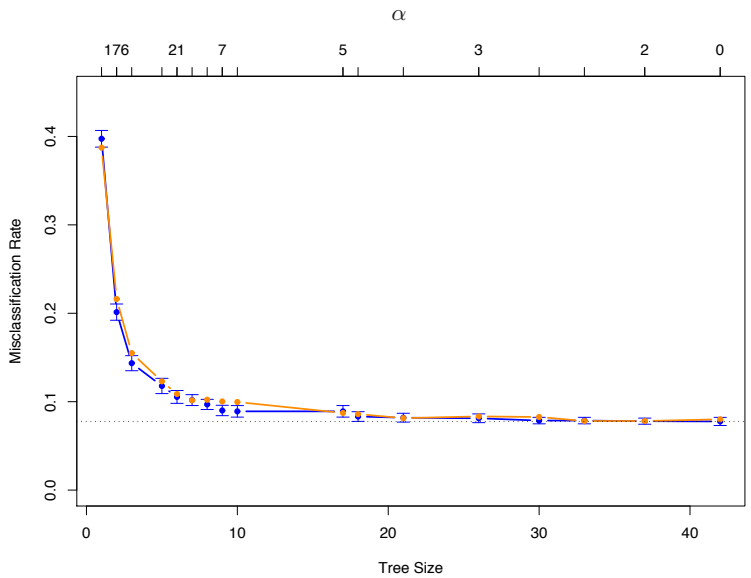
Gini index: $\sum_{k \neq k'} \hat{p}_{mk} \hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1 - \hat{p}_{mk}).$

Cross-entropy or deviance: $-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$

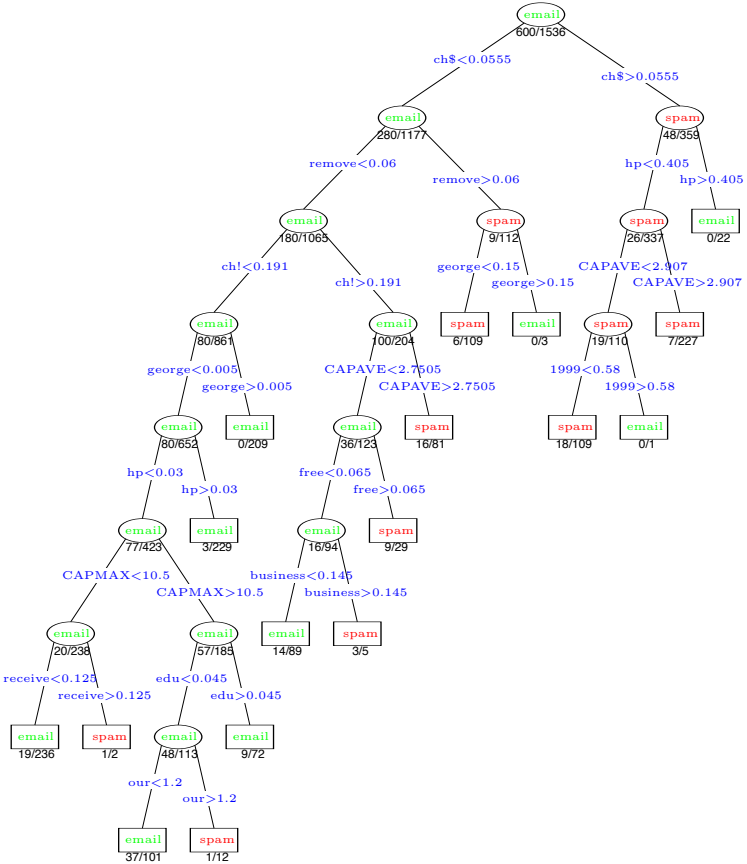
Example: Email spam

TABLE 9.3. *Spam data: confusion rates for the* 17*-node tree (chosen by cross–validation) on the test data. Overall error rate is* 9.3%.

	Predicted	
True	email	spam
email	57.3%	4.0%
spam	5.3%	33.4%

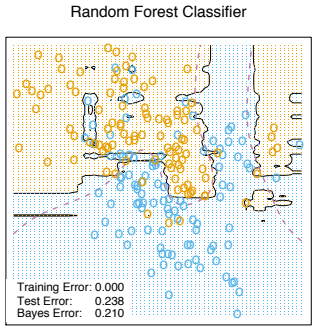


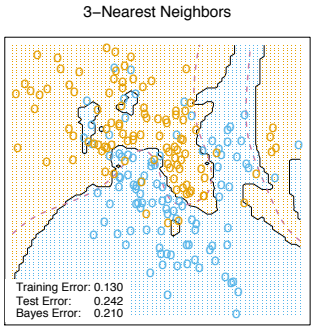
Example: Email spam

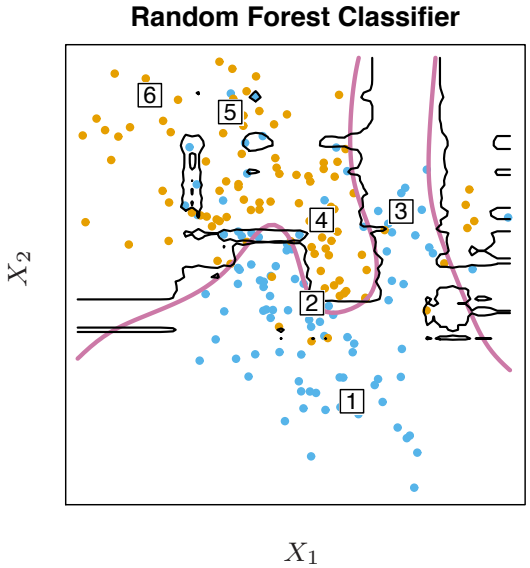


Random forest

- A main issue of the tree-based method is large variance
- Trees (if grown deep enough) have low bias: can capture complicated structure
- Trees are known to be very noisy
- They benefit greatly from averaging

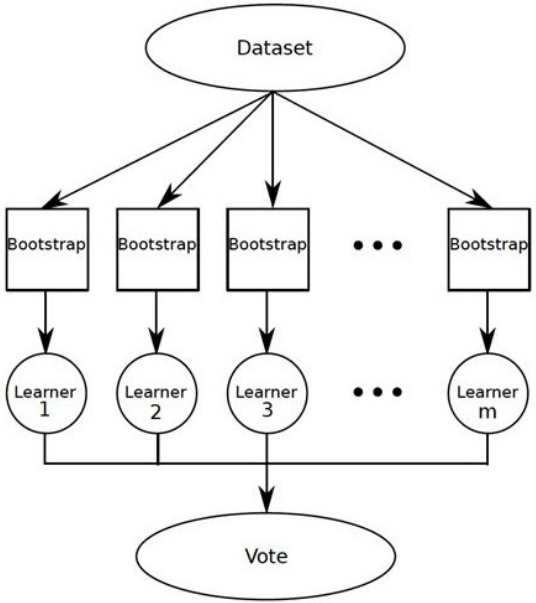






Overview

- Bagging or bootstrap aggregation is an approach to reduce variance of the prediction
- Random forest is a type of bagging algorithm that builds a large collection of de-correlated trees, and then average them.
- For many problems, performance of random forest is very similar to boosting, and they are simpler to train and tune.



California housing price

- Data set (Pace and Barry, 1997) is available from CMU StatLib
- Aggregated data from each of 20,460 neighborhood (1990 census data) in California
- 8 predictors
  - Median income
  - House density
  - Average occupancy
  - Location
  - Average number of rooms
  - Average number of bedrooms

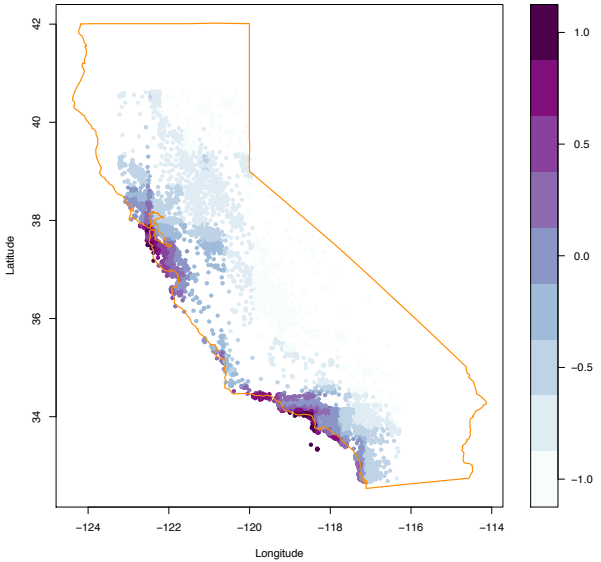
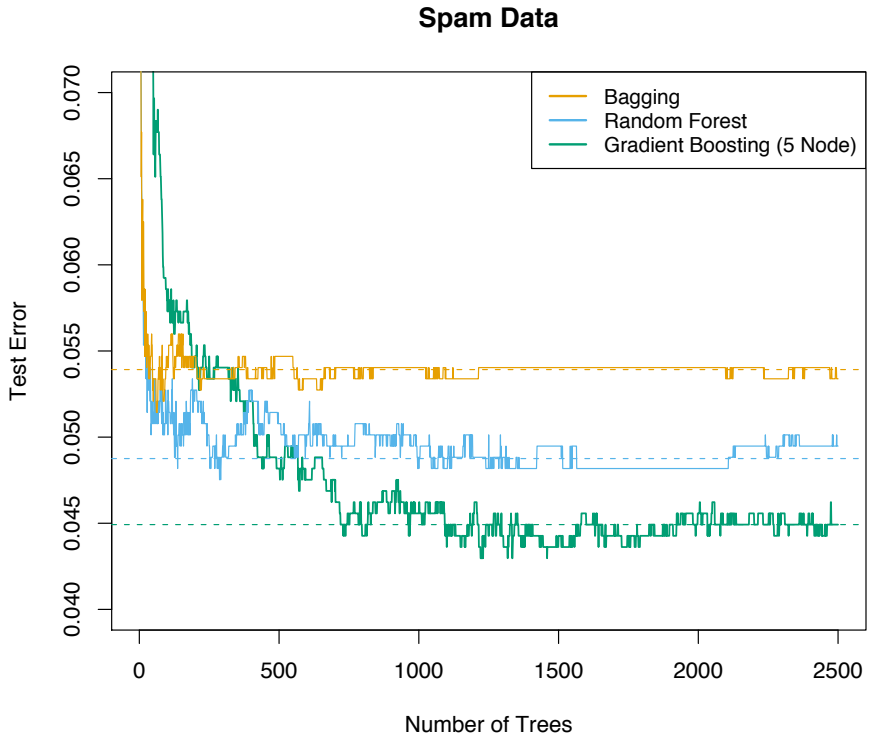


FIGURE 10.17. *Partial dependence of median house value on location in California. One unit is* $100,000, *at* 1990 *prices, and the values plotted are relative to the overall median of* $180,000.

California housing price




SUMMARY