Model Inference and Averaging

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Consider two random variables, X and Y, representing the value of two assets. How should a person invest in these two assets to minimize the amount of potential risk?

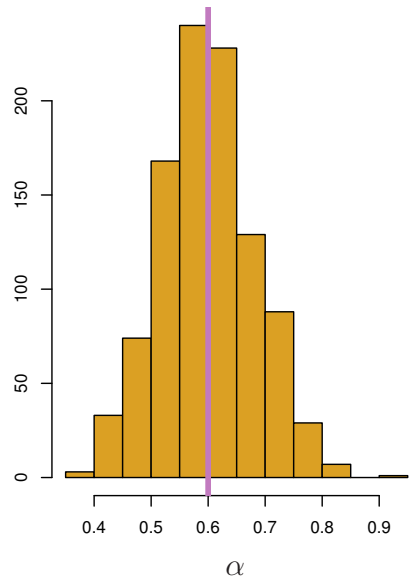
Given only one month of prices of these assets, how would you set up your portfolio?

$$\hat{\alpha} = \frac{\hat{\sigma}_Y^2 - \hat{\sigma}_{XY}}{\hat{\sigma}_X^2 + \hat{\sigma}_Y^2 - 2\hat{\sigma}_{XY}}$$

$$\bar{\alpha} = \frac{1}{B}\sum_{s=1}^{B} \hat{\alpha}^{*s}$$

$$SE_B(\hat{\alpha}) = \sqrt{\frac{1}{B-1}\sum_{r=1}^{B}\left(\hat{\alpha}^{*r} - \frac{1}{B}\sum_{s=1}^{B}\hat{\alpha}^{*s}\right)^2}$$

[1]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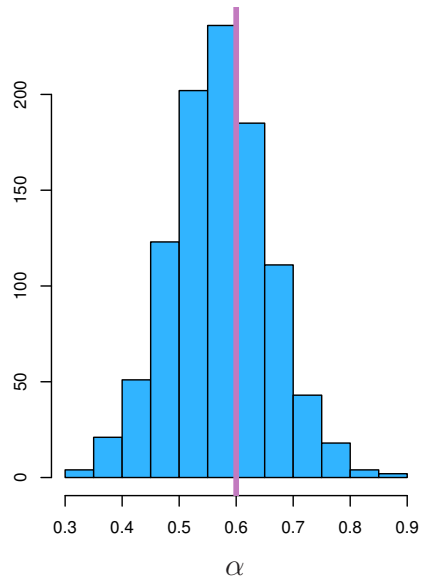
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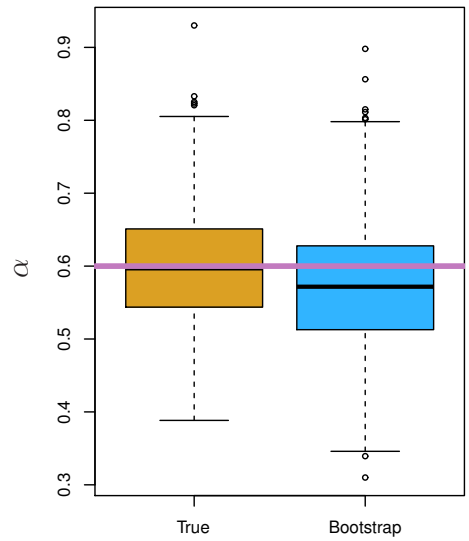
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Bootstrap

Denote training data $\mathbf{Z} = \{z_1, z_2, \ldots, z_N\}$, with $z_i = (x_i, y_i), i = 1, 2, \ldots, N$.

Lets fit a cubic spline with three knots placed at the quartiles. This will result in a seven-dimensional linear space

$$\mu(x) = \sum_{j=1}^{7} \beta_j h_j(x)$$

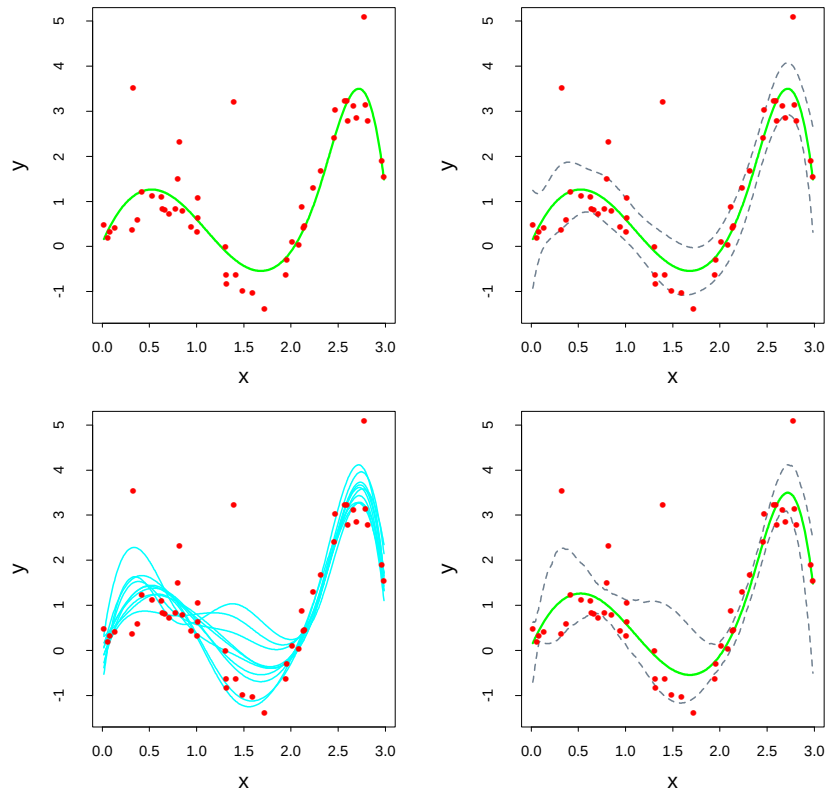


FIGURE 8.2. *(Top left:) B-spline smooth of data. (Top right:) B-spline smooth plus and minus* $1.96\times$ *standard error bands. (Bottom left:) Ten bootstrap replicates of the B-spline smooth. (Bottom right:) B-spline smooth with* 95% *standard error bands computed from the bootstrap distribution.*

Let **H** be the $N \times 7$ matrix with ij^{th} element $h_j(x_i)$. The estimate of β using squared error is given by:

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

This is then used to determine:

$$\hat{\mu}(x) = \sum_{j=1}^{7} \hat{\beta}_j h_j(x)$$

with estimated covariance matrix:

$$\hat{\mathbb{V}}(\hat{\beta}) = (\mathbf{H}^T\mathbf{H})^{-1}\hat{\sigma}^2$$

We are using here an estimate for the noise variance given by:

$$\hat{\sigma}^2 = \sum_{i=1}^{N} (y_i - \hat{\mu}(x_i))^2 / N$$

which is then used to determine the standard error of a prediction $\hat{\mu}(x) = h(x)^T \hat{\beta}$ as:

$$\hat{se}(\hat{\mu}(x)) = (h(x)^T (\mathbf{H}^T \mathbf{H})^{-1} h(x))^{\frac{1}{2}} \hat{\sigma}$$

To bootstrap, draw B datasets each of size N with replacement from the training data.

To each bootstrapped data set $\mathbf{Z}^*$, fit a cubic spline $\hat{\mu}^*(x)$.
Using $B = 200$, we can determine a 95% confidence interval.
This is an example of a **non-parametric bootstrap.**

Parametric Bootstrap

Lets assume that the model errors are Gaussian, this leads us to:

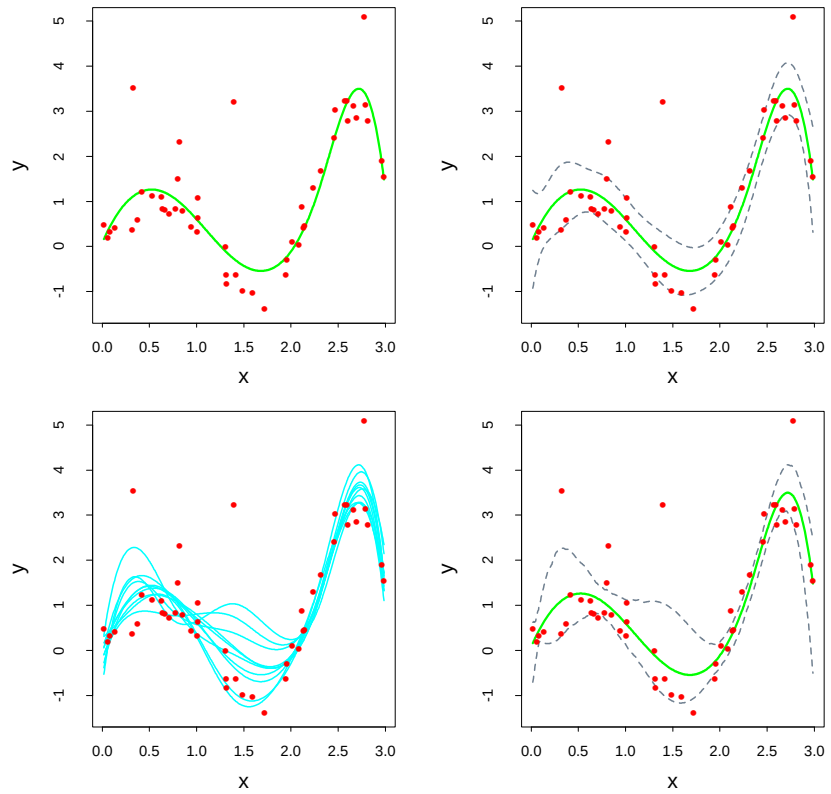
$$Y = \mu(X) + \varepsilon; \varepsilon \sim N(0, \sigma^2),$$

$$\mu(x) = \sum_{j=1}^{7} \beta_j h_j(x)$$

We simulate new responses by adding Gaussian noise to the predicted values,

$$y_i^* = \hat{\mu}^*(x_i) + \varepsilon_i^*; \varepsilon_i^* \sim N(*0, \hat{\sigma}^2); i = 1, \ldots, N$$

The process is repeated B times and the the resulting bootstrap datasets, $(x_1, y_1^*), \ldots, (x_N, y_N^*)$ have the smoothing spline fit on each.



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Simple Example

Assume we have a mixture of two normal random variables, X_1 and X_2.

Looking at their histogram, we can see that a single normal would be a very bad fit.

We attempt to model this using a mixture of two normal distributions given by:

$$Y = (1 - \Delta) Y_1 + \Delta Y_2$$

where $\Delta \in \{0, 1\}$, with $\mathbb{P}(\Delta = 1) = \pi$.

If we let $\phi_\theta(x)$ be the normal density with parameters θ, then the density of Y is:

$$g_Y(y) = (1 - \pi)\phi_{\theta_1}(y) + \pi\phi_{\theta_2}(y)$$

If we want to fit this using MLE, we need to estimate the parameters:

$$\theta = (\pi, \theta_1, \theta_2) = (\pi, \mu_1, \sigma_1^2, \mu_2, \sigma_2^2)$$

The log-likelihood based on the N cases is:

$$\ell(\theta; \mathbf{Z}) = \sum_{i=1}^{N} \log[(1-\pi)\phi_{\theta_1}(y_i) + \pi\phi_{\theta_2}(y_i)]$$

which is difficult to maximize

We can simplify it by introducing a new variable Δ_i (an unobserved latent variable) that takes values either 1 or 0.

$$\ell_0(\theta; \mathbf{Z}, \Delta) = \sum_{i=1}^{N} [(1 - \Delta_i) \log \phi_{\theta_1}(y_i) + \Delta_i \log \phi_{\theta_2}(y_i)]$$
$$+ \sum_{i=1}^{N} [(1 - \Delta_i) \log(1 - \pi) + \Delta_i \log \pi]$$

Since the values of the Δ_i's are unknown, we substitute for each Δ_i its expected value:

$$\gamma_i(\theta) = \mathbb{E}[\Delta_i|\theta, \mathbf{Z}] = \mathbb{P}(\Delta_i = 1|\theta, \mathbf{Z})$$

Algorithm 8.1: EM Algorithm for Two-component Gaussian Mixture

1. Take initial guesses for the parameters $\hat{\mu}_1$, $\hat{\sigma}_1^2$, $\hat{\mu}_2$, $\hat{\sigma}_2^2$, $\hat{\pi}$
2. *Expectation Step:* compute the responsibilites

$$\hat{\gamma}_i = \frac{\hat{\pi}\phi_{\hat{\theta}_2}(y_i)}{(1-\hat{\pi})\phi_{\hat{\theta}_1}(y_i) + \hat{\pi}\phi_{\hat{\theta}_2}(y_i)}, i = 1, \ldots, N$$

3. *Maximization Step:* compute the weighted means and variances.

$$\hat{\mu}_1 = \frac{\sum_{i=1}^N (1-\hat{\gamma}_i) y_i}{\sum_{i=1}^N (1-\hat{\gamma}_i)}, \qquad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^N (1-\hat{\gamma}_i)(y_i - \hat{\mu}_1)^2}{\sum_{i=1}^N (1-\hat{\gamma}_i)}$$

$$\hat{\mu}_2 = \frac{\sum_{i=1}^N \hat{\gamma}_i y_i}{\sum_{i=1}^N \hat{\gamma}_i}, \qquad \hat{\sigma}_1^2 = \frac{\sum_{i=1}^N \hat{\gamma}_i (y_i - \hat{\mu}_2)^2}{\sum_{i=1}^N \hat{\gamma}_i}$$

   and the mixing probability $\hat{\pi} = \sum_{i=1}^N \hat{\gamma}_i / N$
4. Iterate steps 2 and 3 until convergence.[2]

Mixture of M Normals

We introduce new unknown random variables ($\mathbf{Y}$) and use them to create a simpler expression of the likelihood.

$$p(\mathbf{X}, \mathbf{Y}|\Theta) = p(\mathbf{Y}|\mathbf{X}, \Theta)\frac{p(\mathbf{X}, \mathbf{Y}|\Theta)}{p(\mathbf{Y}|\mathbf{X}, \Theta)} \tag{1}$$

- E-Step: $P^{(t)}(y) = P(y|x, \Theta^{(t)})$
- M-Step: $\Theta^{(t+1)} = \underset{\Theta}{\operatorname{argmax}} \left(\mathbb{E}_{P^{(t)}}[\ln P(y, x|\Theta)]\right)$

For a mixture of normals we have the lower bound:

$$\lambda(X, \Theta) \geq \sum_{i=1}^{N} \sum_{j=1}^{M} p^{(t)}(j|x_i, \Theta^{(t)}) \ln \frac{p_j g(x_i; \mu_j, \sigma_j^2)}{p^{(t)}(j|x_i, \Theta^{(t)})} = b_t$$

where $g\left(x_i; \mu_j^{(t)}, \sigma_j^{2(t)}\right)$ denotes the Gaussian pdf.

Our Expectation Step is expressed as:

$$p^{(t)}(j|x_i, \Theta^{(t)}) = \frac{p_j^{(t)} g(x_i; \mu_j^{(t)}, \sigma_j^{2(t)})}{\sum_{j=1}^{M} p_j^{(t)} g(x_i; \mu_j^{(t)}, \sigma_j^{2(t)})}$$

Since b_t is a lower bound for the log-likelihood, if we maximize b_t we will improve the log-likelihood as well. Looking at b_t we can see:

$$b_t = \sum_{i=1}^{N}\sum_{j=1}^{M} p^{(t)}(j|x_i, \Theta^{(t)}) \ln p_j g(x_i; \mu_j, \sigma_j^2) - \sum_{i=1}^{N}\sum_{j=1}^{M} p^{(t)}(j|x_i, \Theta^{(t)}) \ln p^{(t)}(j|x_i, \Theta^{(t)})$$

$$\hat{\Theta} = \Theta^{(t+1)} = \underset{\Theta}{\operatorname{argmax}} \sum_{i=1}^{N}\sum_{j=1}^{M} p^{(t)}(j|x_i, \Theta^{(t)}) \ln p_j g(x_i; \mu_j, \sigma_j^2) \quad (2)$$

To ease writing out formulas we will define the function

$$q(j,i) = p_j g(x_i; \mu_j, \sigma_j^2)$$

This function has the following partial derivatives with respect to the parameters,

$$\frac{\partial q}{\partial \mu_j} = q(j,i)\left(\frac{x_i - \mu_j}{\sigma_j^2}\right)$$

$$\frac{\partial q}{\partial \sigma_j} = q(j,i)\left(\frac{(x_i - \mu_j)^2 - \sigma_j^2}{\sigma_j^3}\right)$$

$$\frac{\partial q}{\partial p_j} = g(x_i; \mu_j, \sigma_j^2)$$

As the term will appear often, we will substitute $p^{(t)}(j|x_i, \Theta^{(t)})$ with the simpler but less descriptive expression $p(j|i)$

$$\frac{\partial b_t}{\partial \mu_j} = \sum_{i=1}^{N} p(j|i) \frac{1}{q(j,i)} q(j,i) \left(\frac{x_i - \mu_j}{\sigma_j^2} \right)$$

$$0 = \sum_{i=1}^{N} p(j|i) \left(\frac{x_i - \mu_j}{\sigma_j^2} \right)$$

$$\mu_j^{(t+1)} = \frac{\sum_{i=1}^{N} p(j|i) x_i}{\sum_{i=1}^{N} p(j|i)}$$

Using this estimate for the value of μ_j for the next iteration we have:

$$\frac{\partial b_t}{\partial \sigma_j} = \sum_{i=1}^{N} p(j|i) \frac{1}{q(j,i)} q(j,i) \left(\frac{(x_i - \mu_j)^2 - \sigma_j^2}{\sigma_j^3} \right)$$

$$0 = \sum_{i=1}^{N} p(j|i) \left(\frac{(x_i - \mu_j)^2 - \sigma_j^2}{\sigma_j^3} \right)$$

$$\sigma_j^{(t+1)} = \sqrt{\frac{\sum_{i=1}^{N} p(j|i)(x_i - \mu_j^{(t+1)})^2}{\sum_{i=1}^{N} p(j|i)}}$$

The final step is to look at the partials with respect to the mixing probabilities:

$$\frac{\partial b_t}{\partial p_j} = \sum_{i=1}^{N} p(j|i) \frac{1}{q(j,i)} g(x_i; \mu_j, \sigma_j^2)$$

$$0 = \sum_{i=1}^{N} \frac{p(j|i)}{p_j}$$

This is a very problematic condition, as the only way this is equal to 0, is if each of the observed conditional probabilities are all equal to 0.

The reason for this difficulty lies in the fact that we have not enforced the constraint $\sum_{j=1}^{M} p_j = 1$. To this end we can express the probabilities through another set of variables $(\gamma_1, \ldots, \gamma_M)$ using a softmax function to ensure these conditions are met.

$$p_k = \frac{e^{\gamma_k}}{\sum_{j=1}^{M} e^{\gamma_j}} \tag{3}$$

We can now take the partial derivatives of our lower bound function with respect to these variables using

$$\frac{\partial p_j}{\partial \gamma_k} = \begin{cases} p_k - p_k^2 : k = j \\ -p_k p_j : k \neq j \end{cases}$$

Now, the partial derivatives with respect to γ_k are:

$$\frac{\partial b_t}{\partial \gamma_k} = \sum_{i=1}^{N} \sum_{\substack{j=1 \\ j \neq k}}^{M} p(j|i) \frac{1}{q(j,i)} g(x_i; \mu_j, \sigma_j^2)(-p_k p_j) + \sum_{i=1}^{N} p(k|i) \frac{1}{q(k,i)} g(x_i; \mu_k, \sigma_k^2)(p_k - p_k^2)$$

$$0 = \sum_{i=1}^{N} p(k|i) \frac{1}{q(k,i)} g(x_i; \mu_k, \sigma_k^2)(p_k) - \sum_{i=1}^{N} \sum_{j=1}^{M} p(j|i) \frac{1}{q(j,i)} g(x_i; \mu_j, \sigma_j^2)(p_k p_j)$$

$$0 = \sum_{i=1}^{N} p(k|i) - N p_k$$

$$p_k^{(t+1)} = \frac{\sum_{i=1}^{N} p(k|i)}{N}$$

for $k \in \{1, \ldots, M\}$.

1. Determine initial estimates for the parameters $\Theta^{(0)}$.
2. E-Step: Calculate the membership probabilities based on current parameter estimates

$$p^{(t)}(j|x_i, \Theta^{(t)}) = \frac{p_j^{(t)} g(x_i; \mu_j^{(t)}, \sigma_j^{2(t)})}{\sum_{j=1}^{M} p_j^{(t)} g(x_i; \mu_j^{(t)}, \sigma_j^{2(t)})} = p(j|i) \tag{4}$$

3. M-Step: Calculate improved estimates for the parameters based on these membership probabilities

$$\mu_j^{(t+1)} = \frac{\sum_{i=1}^{N} p(j|i) x_i}{\sum_{i=1}^{N} p(j|i)} \tag{5}$$

$$\sigma_j^{(t+1)} = \sqrt{\frac{\sum_{i=1}^{N} p(j|i)(x_i - \mu_j^{(t+1)})^2}{\sum_{i=1}^{N} p(j|i)}} \tag{6}$$

$$p_j^{(t+1)} = \frac{\sum_{i=1}^{N} p(j|i)}{N} \tag{7}$$

4. Check if condition for stopping is satisfied. We use for our condition $(\hat{\Theta}^{(t+1)} - \hat{\Theta}^{(t)})^2 < \varepsilon$
5. If the condition is not met, repeat steps 2 and 3 with $\hat{\Theta}^{(t+1)} \rightarrow \hat{\Theta}^{(t)}$

Algorithm 8.2: The EM Algorithm

1. Start with initial guesses for the parameters $\hat{\theta}^{(0)}$.
2. *Expectation Step:* at the j^{th} step, compute

$$Q(\theta', \hat{\theta}^{(j)}) = \mathbb{E}[\ell_0(\theta'; \mathbf{T})|\mathbf{Z}, \hat{\theta}^{(j)}]$$

   as a function of the dummy argument θ'
3. *Maximization Step:* determine the new estimate $\hat{\theta}^{(j+1)}$ as the maximizer of $Q(\theta', \hat{\theta}^{(j)})$ over θ'
4. Iterate steps 2 and 3 until convergence.

[2]

Bagging

Bagging or bootstrap aggregation averages the prediction over a collection of bootstrap samples.

For each bootstrap sample $\mathbf{Z}^{*b}, b = 1, 2, \ldots, B$, we fit our model giving prediction $\hat{f}^{*b}(x)$. The bagging estimate is defined by

$$\hat{f}_{\text{bag}}(x) = \frac{1}{B} \sum_{b=1}^{B} \hat{f}^{*b}(x)$$

Bumping

Similar to bagging, but instead of averaging the predictions, we choose the best one.

$$\hat{b} = \arg\min_{b} \sum_{i=1}^{N} [y_i - \hat{f}^{*b}(x_i)]^2$$

and then:

$$\hat{f}_{bump}(x) = \hat{f}^{*\hat{b}}(x)$$

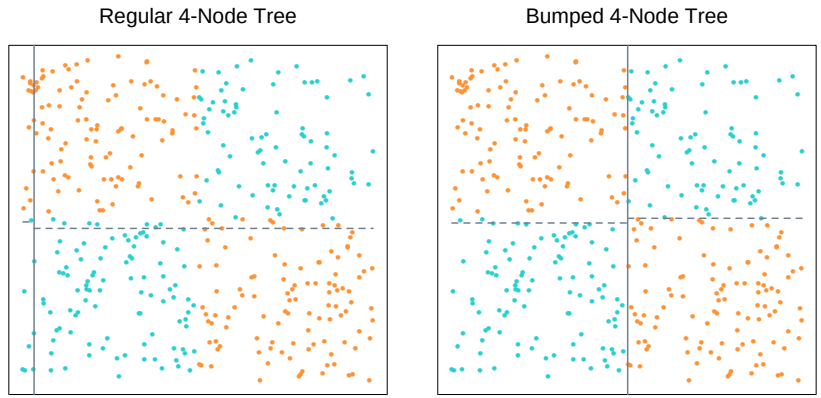

FIGURE 8.13. *Data with two features and two classes (blue and orange), displaying a pure interaction. The left panel shows the partition found by three splits of a standard, greedy, tree-growing algorithm. The vertical grey line near the left edge is the first split, and the broken lines are the two subsequent splits. The algorithm has no idea where to make a good initial split, and makes a poor choice. The right panel shows the near-optimal splits found by bumping the tree-growing algorithm* 20 *times.*

[1] Trevor Hastie Gareth James, Daniela Witten and Robert Tibshirani. *An Introduction to Statistical Learning with Applications in R*. Number v. 6. Springer, 2013.

[2] Robert Tibshirani Trevor Hastie and Jerome Friedman. *The Elements of Stastical Learning: Data Mining, Inference, and Prediction*. Number v.2 in Springer Series in Statistics. Springer, 2009.