Supervised Learning with Tabular Data

Gov 2018

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Generalized Additive Models (GAM)

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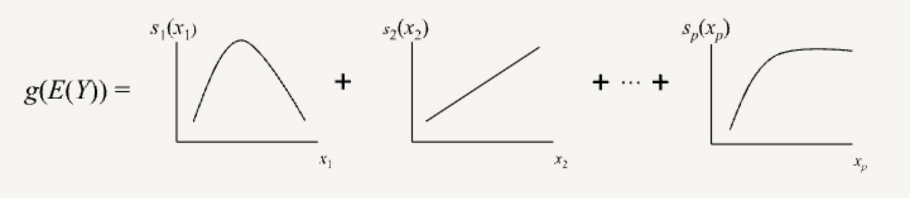
- Relationships between IV and DV follow some smooth patterns (linear or non-linear).
- We can estimate these smooth relationships simultaneously and then predict $E(Y|X)$ by simply adding them up.

Example

$$E(Y|X) = a + b \cdot x^2 + c \cdot x + \cdots + \exp(x) + \epsilon$$



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- Can use a combination of linear and flexible terms (e.g. to estimate constant treatment effect while controlling flexibly for other variables)
- Also works for generalized linear models: $E[Y_i] = g^{-1}\left(\beta_0 + 27(X_{i1}) + \cdots + f_K(X_{iK})\right)$, where $g(\cdot)$ is an exponential link function

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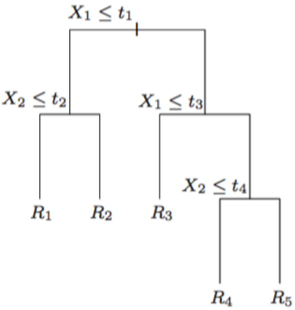
Tree-Based Methods

Classification and Regression Trees (CART) recursively partition the input space



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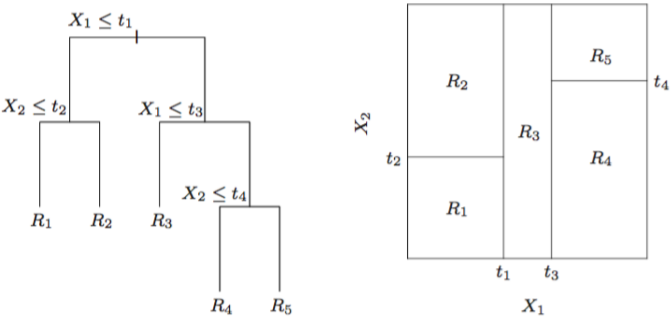

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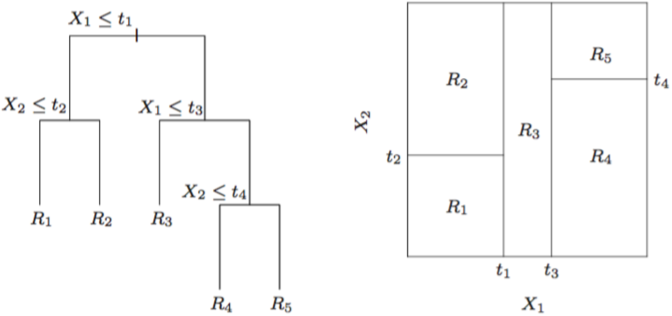

$$f(x) = \mathbb{E}[\mathbf{y}|X] = \sum_{m=1}^{M} \bar{y}_m \mathbb{1}\{x \in R_m\}$$

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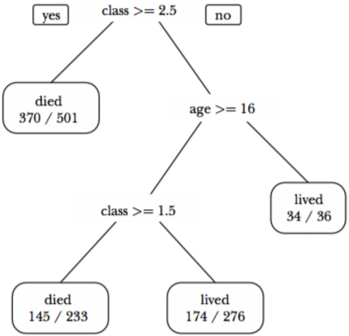
  - Titanic example from Varian (2014, JEP): rich children survived



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- Finding the optimal partitioning is NP-complete (i.e., computation time grows too quickly as the size of the problem grows)
- Greedy algorithm (not thinking ahead, missing high-level interaction): locally optimal choice at each stage (not necessarily leads to a global optimum)

CART Algorithm

- At each stage, axis parallel splits is done by:

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

where $R_1(j,s)=\{X|X_j\le s\}$ and $R_2(j,s)=\{X|X_j\ge s\}$, and c_m is the mean of $y_i|i\in R_m(j,s)$.

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- CART is very popular and easy to implement (`rpart` package in R)
- However, the greedy algorithm often leads to poor prediction. It also has a problem of over-fitting (pruning is needed), and thus highly variable.

Model Selection

- What variables should we include in a given model?
- Ridge and Lasso regressions: the knowledge of λ value.
- GAM depends on the selection of smoothing function.
- CART requires pruning to achieve optimal performance.
- $\cdots$

1. Regression with Continuous Outcome
    - Generalized Additive Models (GAM)
    - CART
    - Motivation of Model Selection

2. Model Selection and Combination
    - Model Selection
    - Benign Overfitting
    - Model Aggregation
    - Evaluation Metrics, Cross-Validation

Goals

- Model assessment: Estimate generalization error
  - How good will this model be when I use it out-of-sample?
  - Is it better/worse than random choice?
  - Is it better/worse than human coders? (inter-coder reliability)
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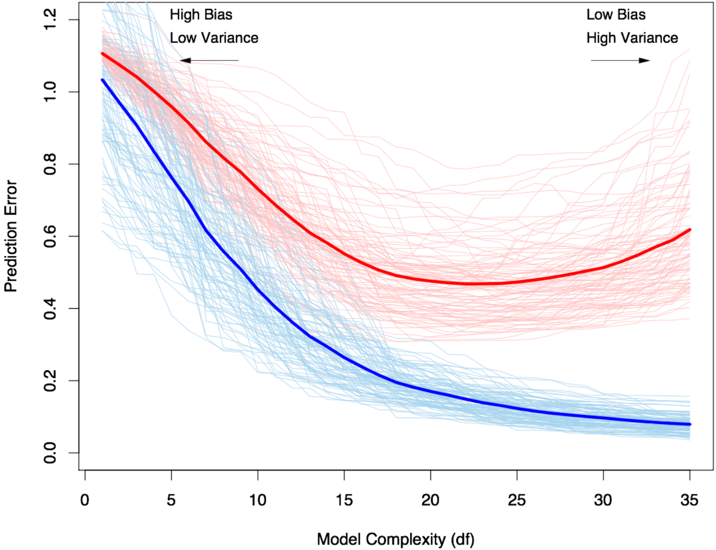
- Model aggregation: Combining candidate models into something better

Training Error vs. Test Error



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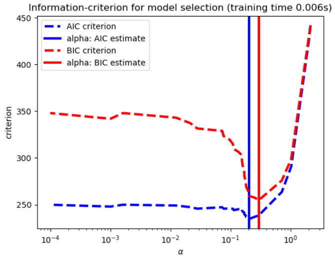

Training Error vs. Test Error

- We don't have a luxury of having a large data as a test set
- Estimating error variance $\hat{\sigma}$ to calculate loglik is problematic with high-dimensional setting ($n < p$)
- Cross-validation: Holding out a subset of the training observations from the training process

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- When is this positive? All possible distributions $g(x) \neq f(x)$.

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- In inequality:

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- Proof:

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-KL(f||g) &= -\int_{-\infty}^{\infty} f(x) \log\left(\frac{f(x)}{g(x)}\right) \\
&= \int_{-\infty}^{\infty} f(x) \log\left(\frac{g(x)}{f(x)}\right) \\
&\leq \int_{-\infty}^{\infty} f(x) \left(\frac{g(x)}{f(x)} - 1\right) \\
&= \int_{-\infty}^{\infty} (g(x) - f(x)) \\
&= 1 - 1 \\
&= 0
\end{aligned}$$

KL divergence is not a proper distance measure

- Kullback-Leibler divergence is not a distance metric!
- Distances must be nonnegative, symmetric, and satisfy triangle inequality: distance from A to C must be less than (A to B) + (B to C)

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- Or documents, if they are represented as distributions of word coordinates in a continuous embedding space

  "The limited but real influence of elite rhetoric in the 2009–2010 health care debate" , Hopkins, 2018, Political behavior

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- The problem: we don't know the true population distribution

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- Interpretation: KL divergence is directly related to the expected log likelihood (under the candidate model) of a randomly drawn observation from the true DGP

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- We have many random draws from true DGP: validation set!
- As sample size goes to infinity, size of validation set generally also goes to infinity (not true for leave-one-out CV)

Benign Overfitting

- A new statistical phenomenon: good prediction with zero training error (such as a deep learning method) .
- When a perfect fit to training data in linear regression is compatible with accurate prediction.
- Over-parameterization is essential for benign overfitting in some setting: more features than sample size.
- "Benign overfitting in linear regression", Bartlett et al, PNAS, 2020.
- Most of situations we don't have benign overfitting - unless you can justify the choice.
- AI models such as Chat GPT relies on massive over-fitting that are benign.

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  - Use some aggregation rule (e.g. mean, majority vote) to combine

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- Assumed DGP: first randomly choose a model, then generate all data points from that model

$$Z \sim \text{Cat}(\pi)$$
$$Y_i \sim f_Z(y|X_i = x_i)$$

taking $\mathbf{X}$ as given

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  - Take weighted average of predictions

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- Easy to implement (`randomForest` package in R) and often very good off-the-shelf performance

Bootstrapping: More Perspectives

Each bootstrap draw is a sample split

- Observation i is in validation set with probability $(1 - 1/N)^N \approx 1 - 1/e \approx 0.632$
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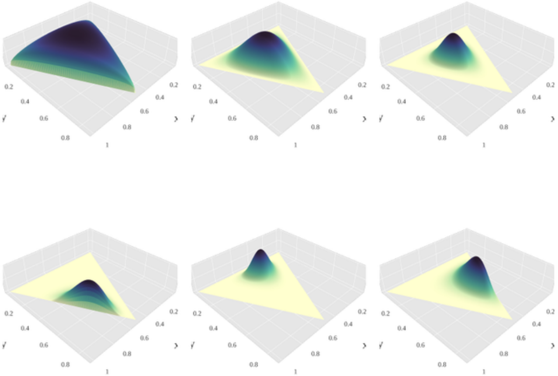
Each bootstrap draw is a reweighting of the original data

- For each draw, $w_i \in \{0, 1/N, \cdots, 1\})$
- Weights must sum to 1
- In other words, weights are a distribution over the $N - 1$ simplex

Bootstrapping: More Perspectives



Bayesian bootstrap:

- The Dirichlet distribution is also a distribution over the $N-1$ simplex
- $\mathbf{w} = [w_1, \cdots, w_N]$
- $\mathbf{w} \sim \text{Dirichlet}([1, \ldots, 1]^\top)$
- $E[\mathbf{w}] = [1/N, \ldots, 1/N]^\top$
- Procedure: Sample $\mathbf{w}$, then do the original analysis. Repeat.

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- These bases can be combined to form an even better approximation to the true conditional expectation function

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- Why? What happens if the true model is among the candidates?
- Asymptotically at least as accurate as the best possible input

Boosting

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    - For out-of-sample data, generate final predictions as $\hat{\mathbf{Y}} = \sum_m \alpha_m \hat{\mathbf{Y}}^m$

Boosting

- Again, the sequential models $m = 1, \dots, M$ create basis functions
- We greedily approximate the true conditional expectation with these bases
- Make the best approximation possible using $m = 1$
- Then fine-tune it with $m = 2, \dots$
- Models evolve in an adaptive way to remove bias
- Later models focus on examples that were misclassified in earlier rounds (hard to classify, e.g. near best decision boundary)

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6. Presumably you have a good proxy for generalization performance from "in-sample" (all labeled data) data to "out-of-sample" (test data, new observations to predict, or true DGP)

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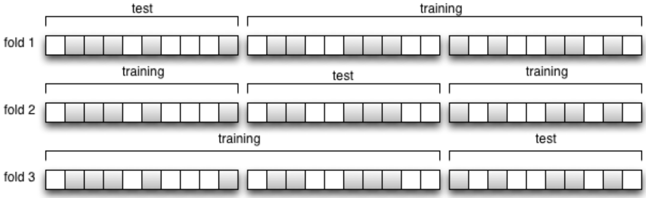

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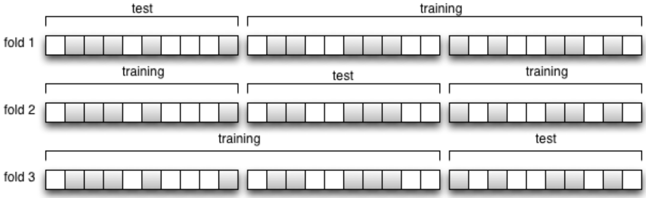

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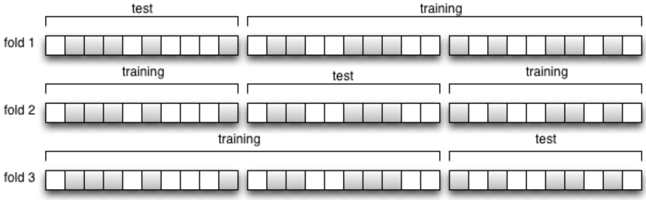

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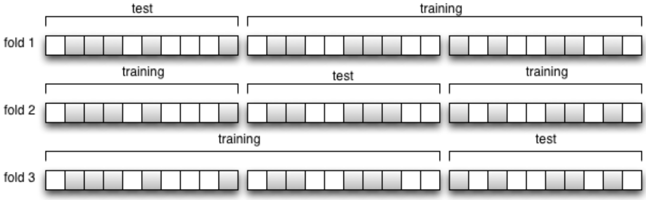

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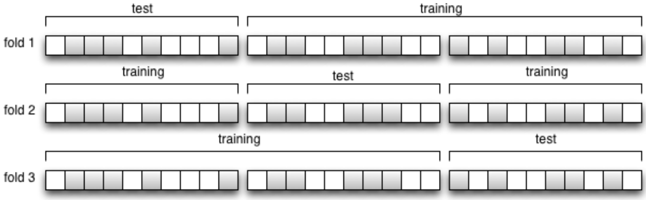

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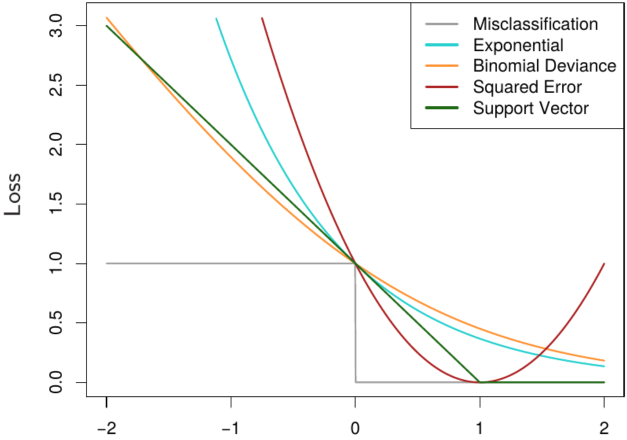

- Loss for observation with $y_i = +1$ (vs -1). x-axis is $y \cdot f(x)$. This is also related to Hinge Loss.

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- Precision: Among observations that are predicted to be positive, proportion that are actually positive: $D/(C + D)$
- Accuracy: $(A + D)/(A + B + C + D)$

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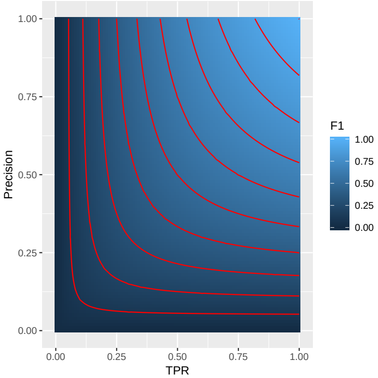

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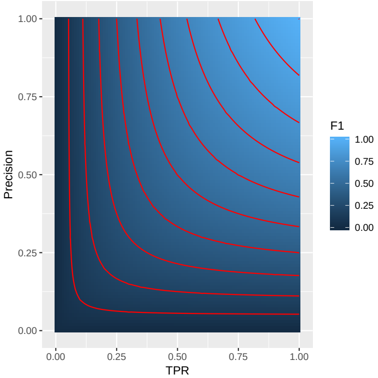

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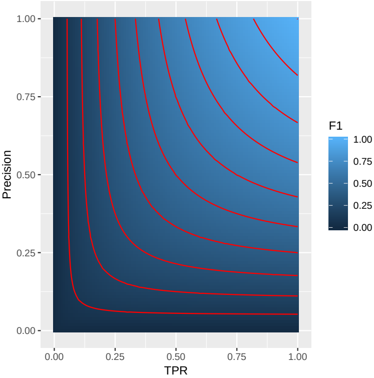

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- Greatest gain can be made by improving whichever performance measure is currently worst

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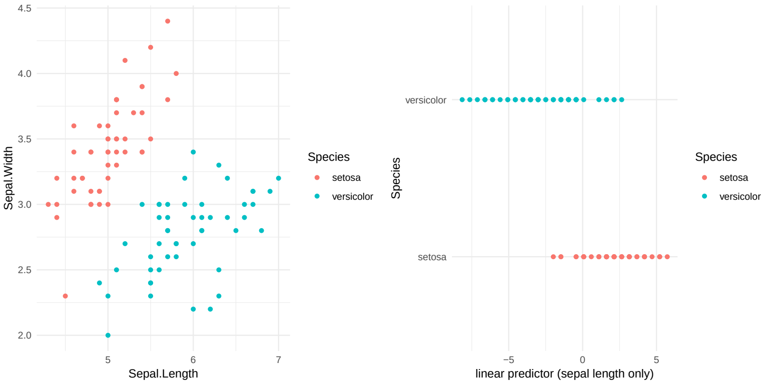

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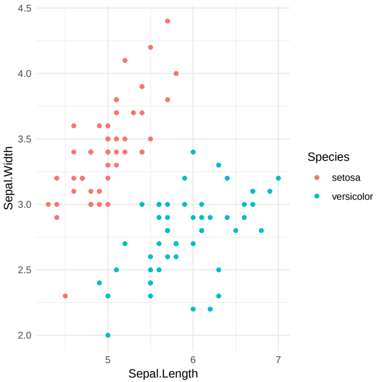

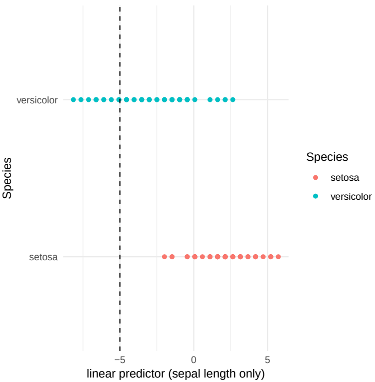

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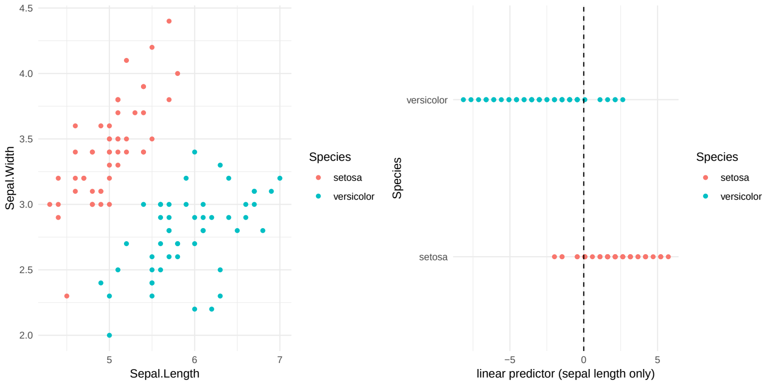

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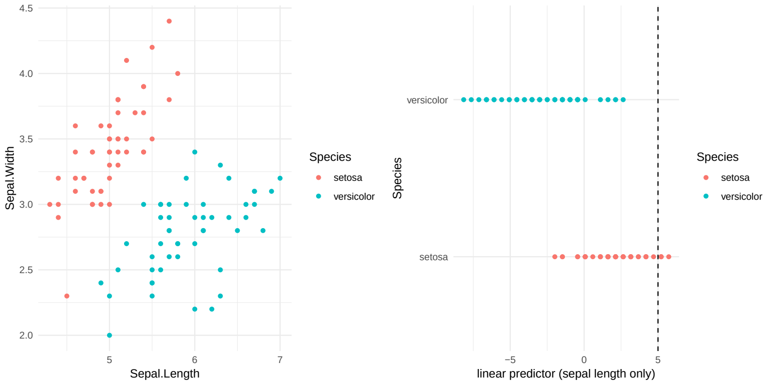

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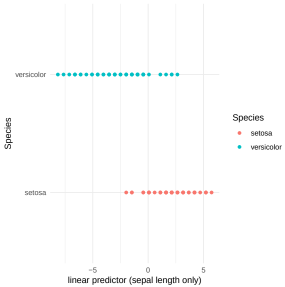

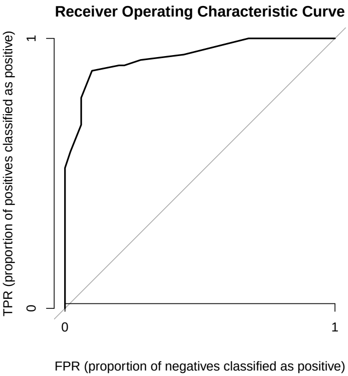

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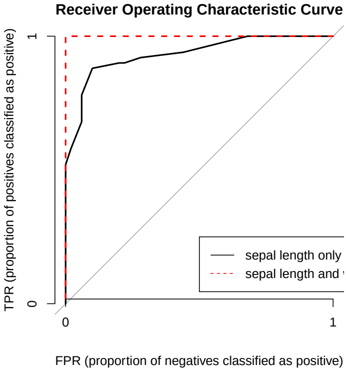

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- ROC will be better if we use more variables.

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$$\begin{aligned} AUC &= \int_{-\infty}^{\infty} P(\hat{Y}_i > \theta|Y_i = +1) \cdot (-f(\theta|Y_i = -1))d\theta \\ &= \int_{\infty}^{-\infty} P(\hat{Y}_i > \theta|Y_i = +1) \cdot f(\theta|Y_i = -1)d\theta \\ &= E[Z > Z'] \end{aligned}$$

Where Z (Z') is randomly drawn predictions from positive (negative) class and reversing sign is because increasing θ decreases FPR

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  - For more, see Nadeau, Claude and Yoshua Bengio. 2003. "Inference for the Generalization Error." *Machine Learning*, 53(3).