Machine Learning

An overview of supervised methods

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Outline

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Statistics vs. Machine Learning

Statistics

- Interpretable models
- Precision and Uncertainty
- Exposure vs. adjustments
- Distributions

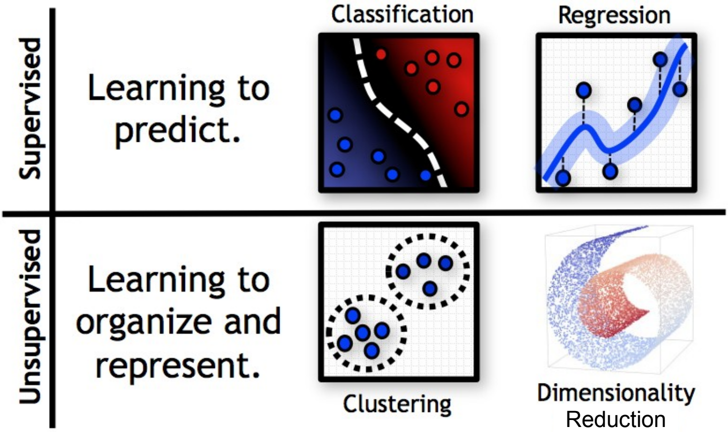
Machine Learning

- Larger, often black-box models
- Prediction
- Features
- Optimization, Algorithms

Fields converge, especially as datasets grow

Machine Learning

Tasks



Supervised Learning

- Training data: $\mathcal{T} = \{(\mathbf{x_i}, y_i), i = 1 \ \ldots \ N\}$ with d attributes $\mathbf{x}$
- Classification: $y \in \mathcal{Y} = \{1 \ \ldots \ K\}$
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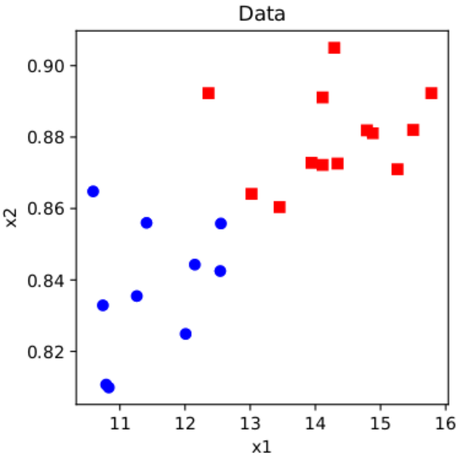
Support Vector Machines

- A binary support vector machine is a linear classifier that takes labels in the set {-1,1}.
- decision function:

$$f_{SVM}(\mathbf{x}) = \text{sign}(\mathbf{w}^T\mathbf{x} + b)$$

Support Vector Machines



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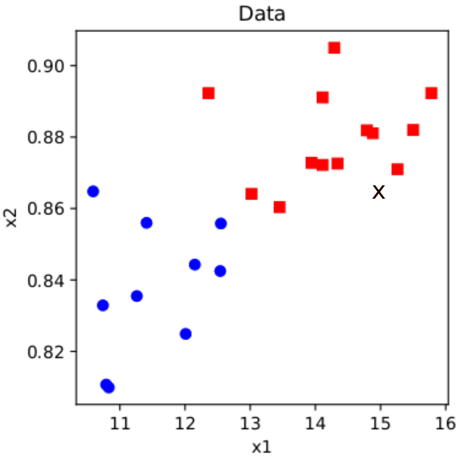

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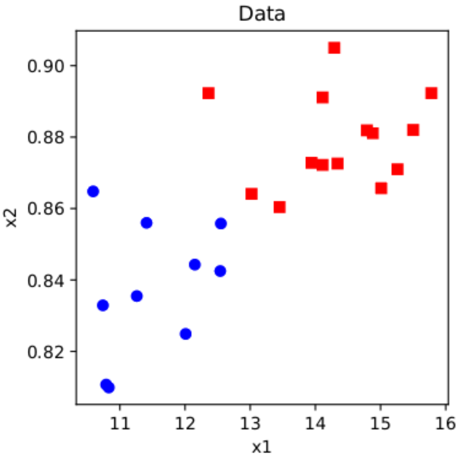

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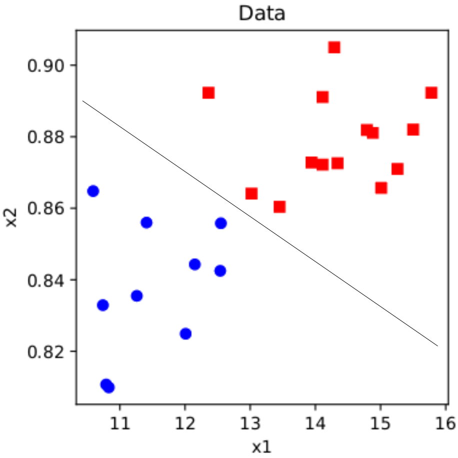

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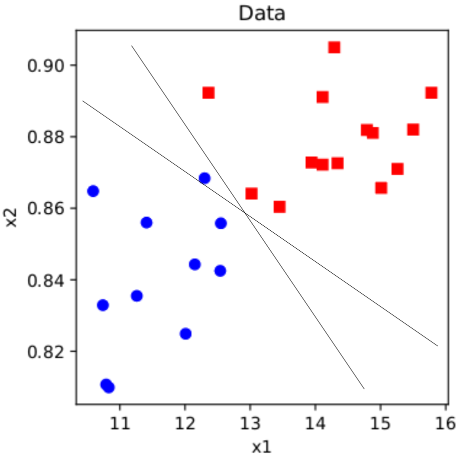
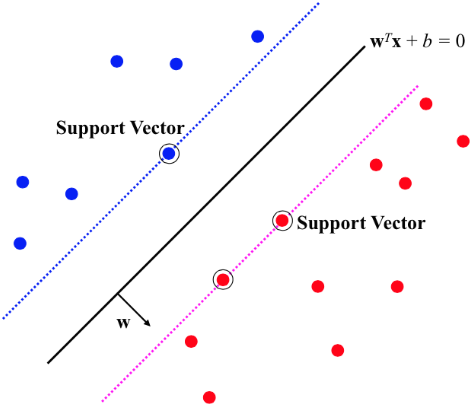


Support Vector Machines

SVMs choose parameters that give the "maximum margin" property.



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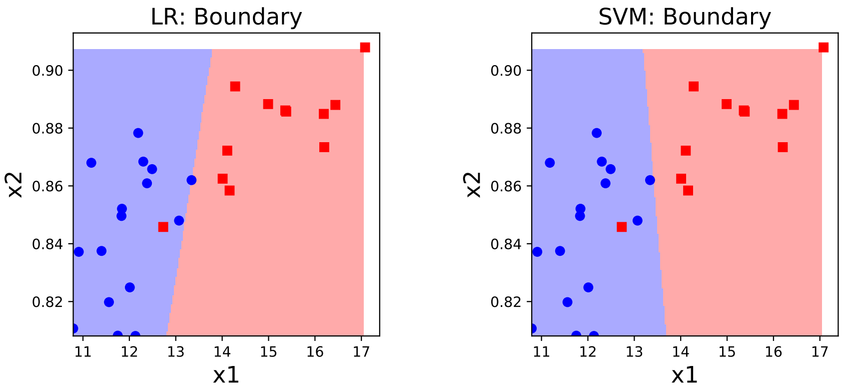
- the decision boundary for logistic regression can be written the same way

Support Vector Machines

and Logistic Regression



Support Vector Machines

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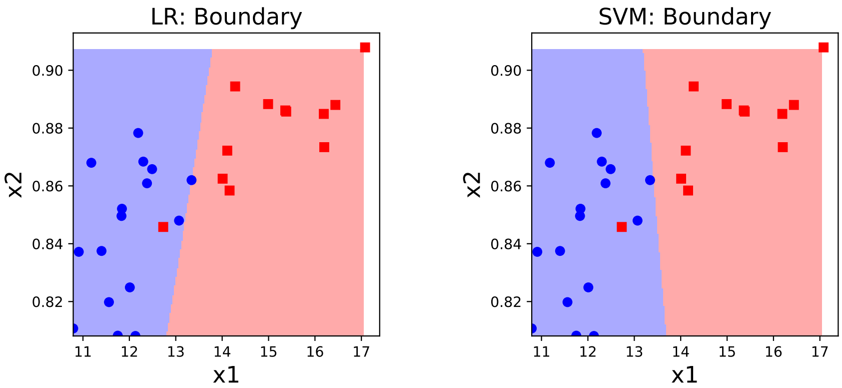
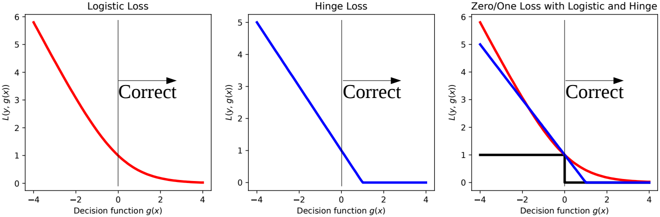


So how do SVM and LR differ?

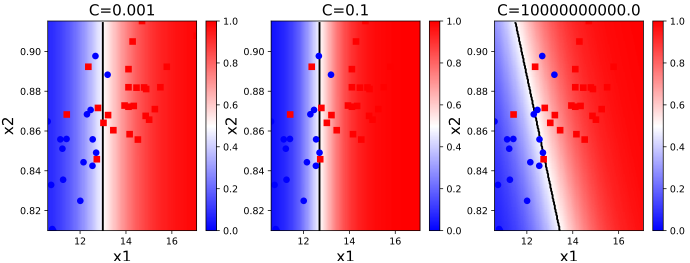
Support Vector Machines

They optimize different loss functions.



Support Vector Machines

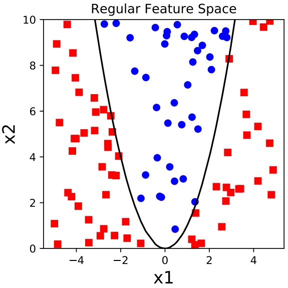
C: relaxation parameter allows some points to fall in the margin.

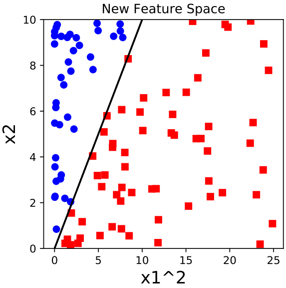


C	0.001	0.1	1e10
Train Accuracy	0.595	0.929	0.888
Test Accuracy	0.459	**0.905**	0.867

Support Vector Machines

- What if the decision boundary isn't linear?
- We can non-linear transform **x**, then train in the (hopefully linear) transformed space
- SVMs use Kernels to do this.





Support Vector Machines

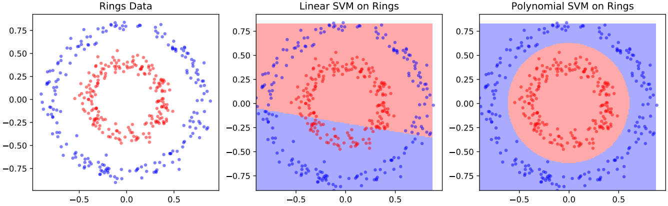
The SVM function can be written as an inner product:

$$\mathbf{w}^T\mathbf{x}_i + b = \sum_j^N \alpha_j \mathbf{x}_j^T \mathbf{x}_i + b$$

$$K(\mathbf{x}, \mathbf{x}') = \mathbf{x}^T\mathbf{x}'$$

- B-order Polynomial Kernel: $K_p(\mathbf{x}, \mathbf{x}') = (\mathbf{x}^T\mathbf{x}' + 1)^B$
- Gaussian/RBF Kernel: $K_G(\mathbf{x}, \mathbf{x}') = exp(-\gamma||\mathbf{x} - \mathbf{x}'||_2^2)$
- "Kernel trick" makes this quick

Support Vector Machines



Support Vector Machines

Conclusions

- SVMs use of the hinge loss function can make them generalize better than Logistic Regression.
- SVMs use Kernel functions to make non-linear boundaries.
- The C parameter must be tuned to generate reliable predictions.

Decision Trees

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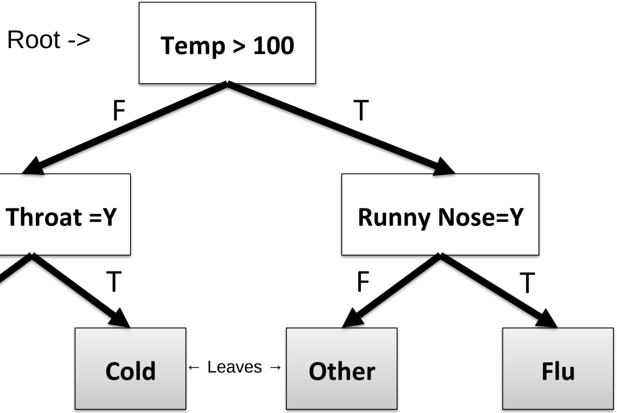
- leaf nodes label examples with a class or average value.

Decision Trees

Example



Decision Trees

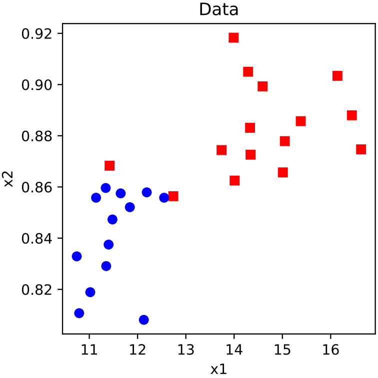
Learning

- Recursively finds a variable that best divides data into two outcomes
- "best variable" is determined heuristically
  - Gini impurity (CART)
  - Information Gain (ID3, C4.5)
- Heuristics: produce splits as homogenous as possible in terms of labels
- stop criterion: max depth, purity of labels in each leaf

Decision Trees

Boundary

What does a decision tree boundary look like?



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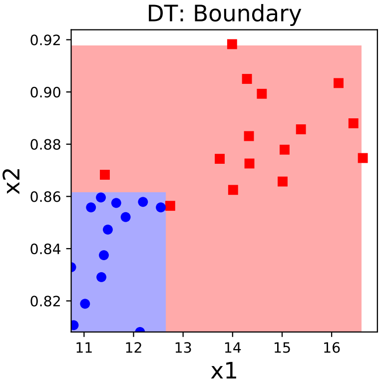

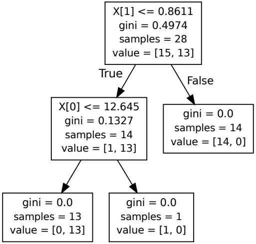

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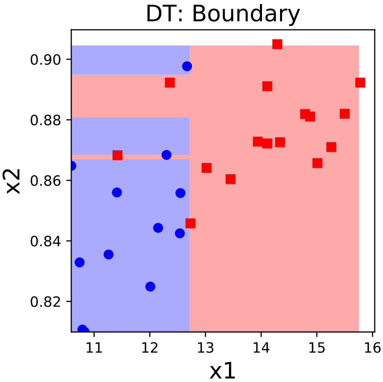

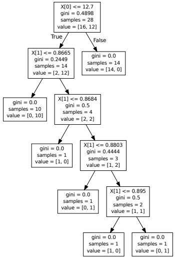

Decision Trees

Other Properties

- Splitting on singe variables can require very large trees to accurately model decision boundaries
- Greedy (optimal trees are hard to find)
- Given sufficient depth, a decision tree can approximate any classification function to arbitrary accuracy

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- Many versions of same model, different types of models
- Final output: weighted average or vote

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- A simple majority vote can improve classification performance by *decreasing variance* in this setting.
- How do we train such an ensemble?

Bagging

- Bootstrap aggregation
- Attempts to train independent classifiers by sampling the training set.
- Sample $\mathcal{T}$ k times with replacement
- Train k classifiers $f_1(\mathbf{x})$ ... $f_k(\mathbf{x})$ on subsets
- Useful for high-variance, high-capacity models (i.e. decision trees)
- Internal error estimate: use the portion of data that wasnt built to create model as a test set (out of bag data)

Random Forests

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- Extension: only consider random sub-set of features when deciding which variables to split on
- When given new data, pass it to all trees in forest, and estimate class based on most popular outcome

Random Forests

- Good predictive performance and avoids overfitting

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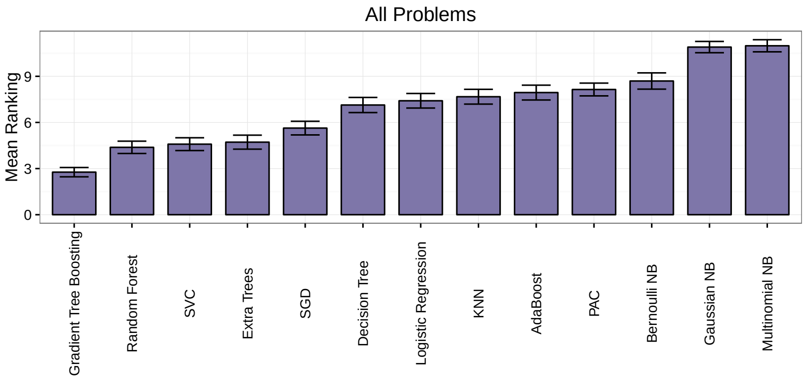
- Good predictive performance and avoids overfitting
- Importance: estimate of single variable contribution to classification

Ensemble Examples

Analysis of 14 methods on 165 open-source classification datasets (PSB 2018)



Conclusions

- We covered SVM, Decision Trees, Random Forests
- Other supervised learning algorithms
  - K-Nearest Neighbors
  - Neural Networks / Deep Learning
  - Naïve Bayes
- Thursday: Unsupervised Learning
  - K-Means
  - Heirarchical Clustering
  - PCA