L4 – Large-Scale Least-Squares

Large-Scale Data Analysis

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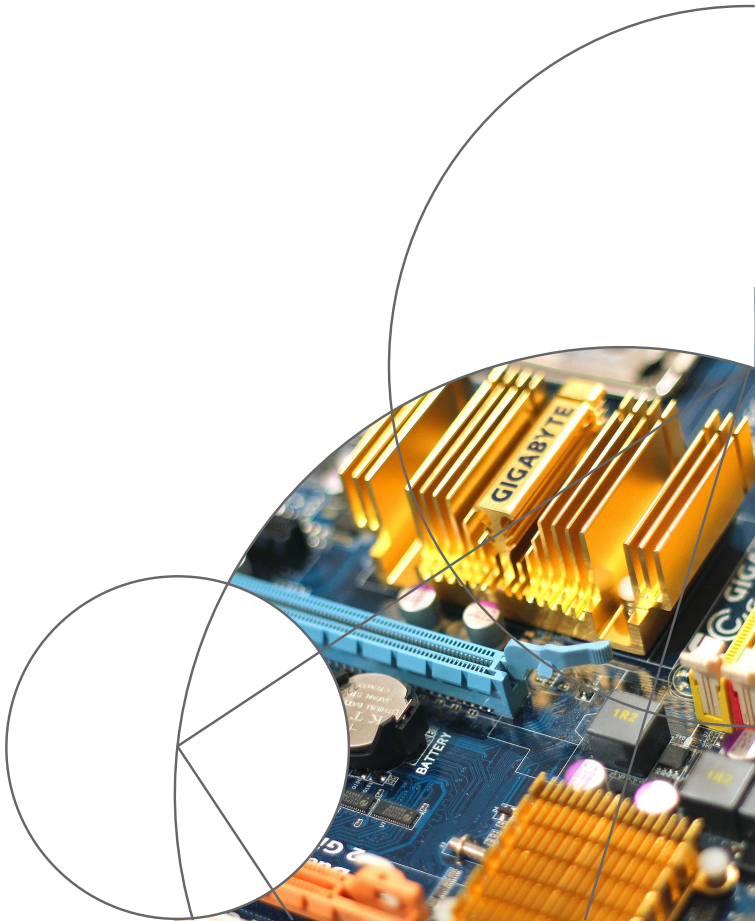
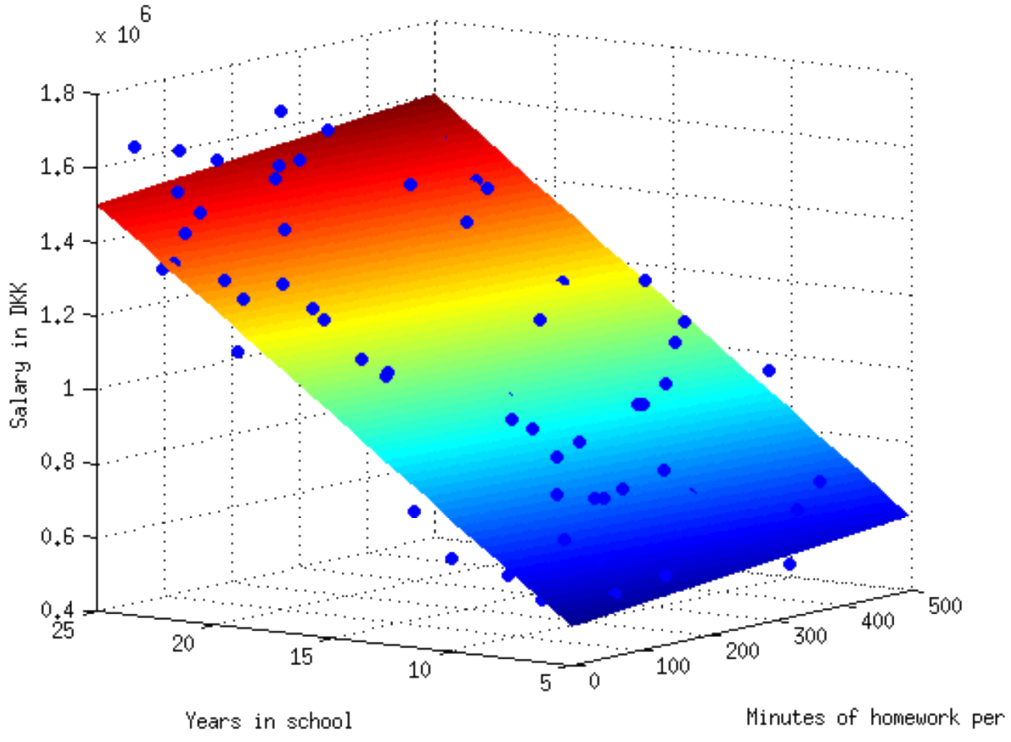


2 May 2019

Outline

Outline

Recap: Multivariate Linear Regression



General Form

- Given: Training set $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$.
- Goal: Linear model $f(\mathbf{z}; \mathbf{w}) = w_0 + w_1 z_1 + w_2 z_2 + \ldots + w_d z_d$ that is a good "fit".

Recap: Multivariate Linear Regression

- Given: Training set of the form $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$.
- Let's "augment" all patterns $\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n$. This yields an augmented data matrix $\mathbf{X} \in \mathbb{R}^{n \times (d+1)}$ and an associated target vector $\mathbf{y} \in \mathbb{R}^n$:

$$\mathbf{X} = \begin{bmatrix} 1 & x_{1,1} & x_{1,2} & \ldots & x_{1,d} \\ 1 & x_{2,1} & x_{2,2} & \ldots & x_{2,d} \\ \vdots & & & & \\ 1 & x_{n,1} & x_{n,2} & \ldots & x_{n,d} \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$

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- Linear regression aims at minimizing the following loss:

Squared Loss

$$\mathcal{L}(\mathbf{w}) = \frac{1}{n} \sum_{i=1}^{n} (f(\mathbf{x}_i; \mathbf{w}) - y_i)^2 = \frac{1}{n} (\mathbf{X}\mathbf{w} - \mathbf{y})^T (\mathbf{X}\mathbf{w} - \mathbf{y})$$

Simplifying the Objective

$$\mathcal{L}(\mathbf{w}) = \frac{1}{n}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$$

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\end{aligned}$$

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&= \frac{1}{n}(\mathbf{X}\mathbf{w})^T\mathbf{X}\mathbf{w} - \frac{1}{n}\mathbf{y}^T\mathbf{X}\mathbf{w} - \frac{1}{n}(\mathbf{X}\mathbf{w})^T\mathbf{y} + \frac{1}{n}\mathbf{y}^T\mathbf{y}
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\end{aligned}$$

with $\mathbf{y}^T\mathbf{X}\mathbf{w} = ((\mathbf{X}\mathbf{w})^T\mathbf{y})^T \in \mathbb{R}$

Gradient & Stationary Point

$$\mathcal{L}(\mathbf{w}) = \frac{1}{n}\mathbf{w}^T\mathbf{X}^T\mathbf{X}\mathbf{w} - \frac{2}{n}\mathbf{w}^T\mathbf{X}^T\mathbf{y} + \frac{1}{n}\mathbf{y}^T\mathbf{y}$$

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Toolbox (Table 1.4 in Rogers & Girolami)

1. $f(\mathbf{w}) = \mathbf{w}^T\mathbf{x} \Rightarrow \nabla f(\mathbf{w}) = \mathbf{x}$
2. $f(\mathbf{w}) = \mathbf{x}^T\mathbf{w} \Rightarrow \nabla f(\mathbf{w}) = \mathbf{x}$
3. $f(\mathbf{w}) = \mathbf{w}^T\mathbf{w} \Rightarrow \nabla f(\mathbf{w}) = 2\mathbf{w}$
4. $f(\mathbf{w}) = \mathbf{w}^T\mathbf{C}\mathbf{w} \Rightarrow \nabla f(\mathbf{w}) = 2\mathbf{C}\mathbf{w}$

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We have $\nabla\mathcal{L}(\mathbf{w}) = \frac{2}{n}\mathbf{X}^T\mathbf{X}\mathbf{w} - \frac{2}{n}\mathbf{X}^T\mathbf{y}$ and therefore:

$$\nabla\mathcal{L}(\mathbf{w}) = \mathbf{0}$$

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Recap: Multivariate Linear Regression

- Given: Training set of the form $\{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$.
- Goal: Find $(d+1)$-dimensional weight vector $\hat{\mathbf{w}} = [\hat{w}_0, \hat{w}_1, \ldots, \hat{w}_d]^T$ that minimizes $\mathcal{L}(\mathbf{w}) = \frac{1}{n}(\mathbf{X}\mathbf{w} - \mathbf{y})^T(\mathbf{X}\mathbf{w} - \mathbf{y})$, i.e., which is a solution for

$$\begin{aligned} & \nabla \mathcal{L}(\mathbf{w}) && = \mathbf{0} \\ \Leftrightarrow \quad & \mathbf{X}^T\mathbf{X}\mathbf{w} && = \mathbf{X}^T\mathbf{y} \end{aligned} \tag{1}$$

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Computation

1. Definition of data matrix $\mathbf{X} \in \mathbb{R}^{n \times (d+1)}$
2. There are different ways to compute an optimal weight vector $\hat{\mathbf{w}}$:
   1. Compute $\hat{\mathbf{w}} = (\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{y}$ (e.g., via `numpy.linalg.inv`)
   2. Directly solve system of equations (1) (e.g., via `numpy.linalg.solve`)
   3. ...
3. For new point $\mathbf{x}_{new} \in \mathbb{R}^d$: Compute $y_{new} = [1, \mathbf{x}_{new}^T]\hat{\mathbf{w}}$

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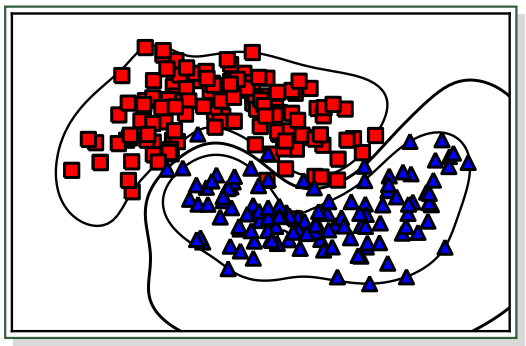
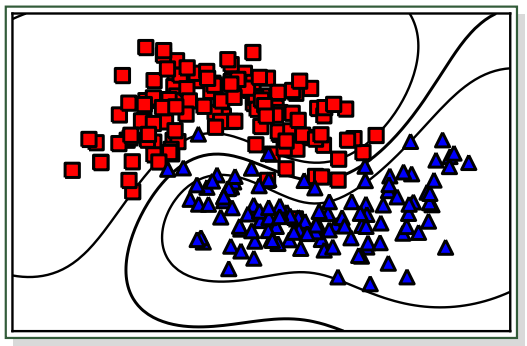
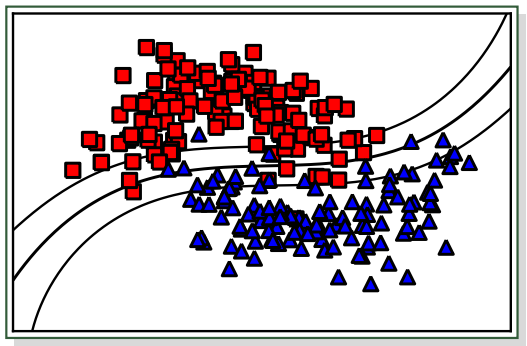
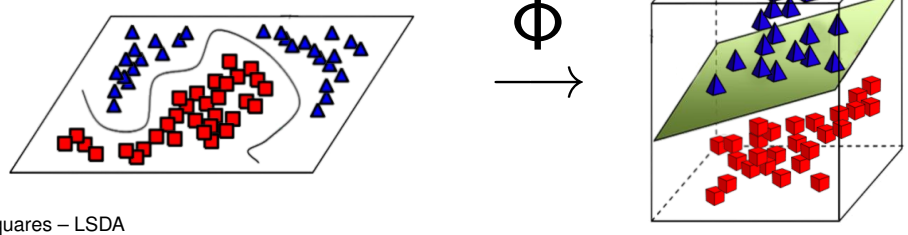
Question: What is the asymptotic runtime for approach (1)?

Outline

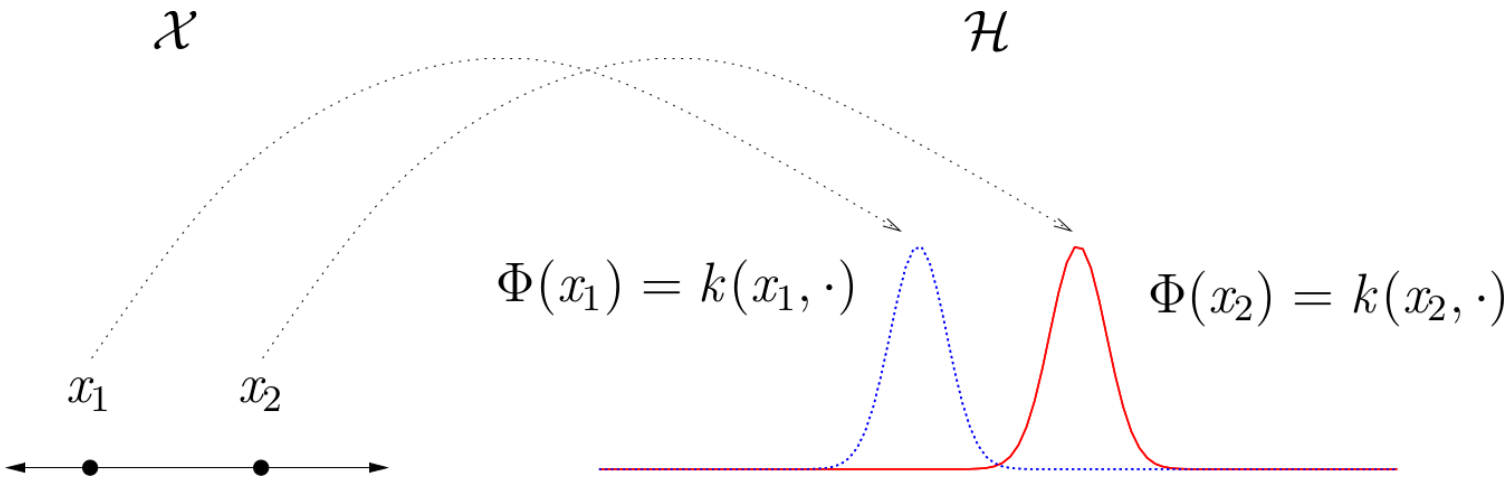
Recap: Kernel Methods

- Make use of kernel functions $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$. Examples:
  - Linear kernel $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle$.
  - Polynomial kernel $k(\mathbf{x}_i, \mathbf{x}_j) = \langle \mathbf{x}_i, \mathbf{x}_j \rangle^p$ for $p \in \mathbb{N}$.
  - RBF kernel $k(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\gamma \|\mathbf{x}_i - \mathbf{x}_j\|^2)$ with $\gamma > 0$.
- The kernel k is called positive semidefinite in case the associated kernel matrix $\mathbf{K}$ is positive semidefinite. In this case, the kernel gives rise to a feature map $\Phi : \mathcal{X} \to \mathcal{H}$ into a Hilbert Space $\mathcal{H}$.

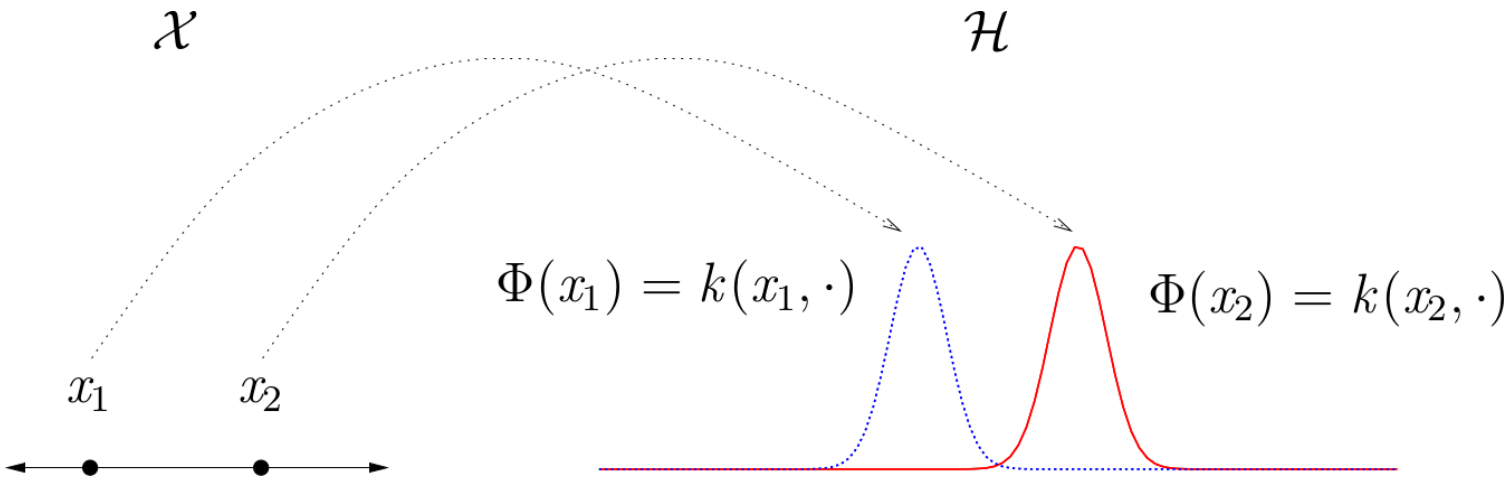


Recap: Kernel to Feature Map



1. Feature map: $\Phi : \mathcal{X} \to \mathbb{R}^{\mathcal{X}} := \{f : \mathcal{X} \to \mathbb{R}\}$ with $\Phi(\mathbf{x})(\cdot) = k(\cdot, \mathbf{x})$

Recap: Kernel to Feature Map

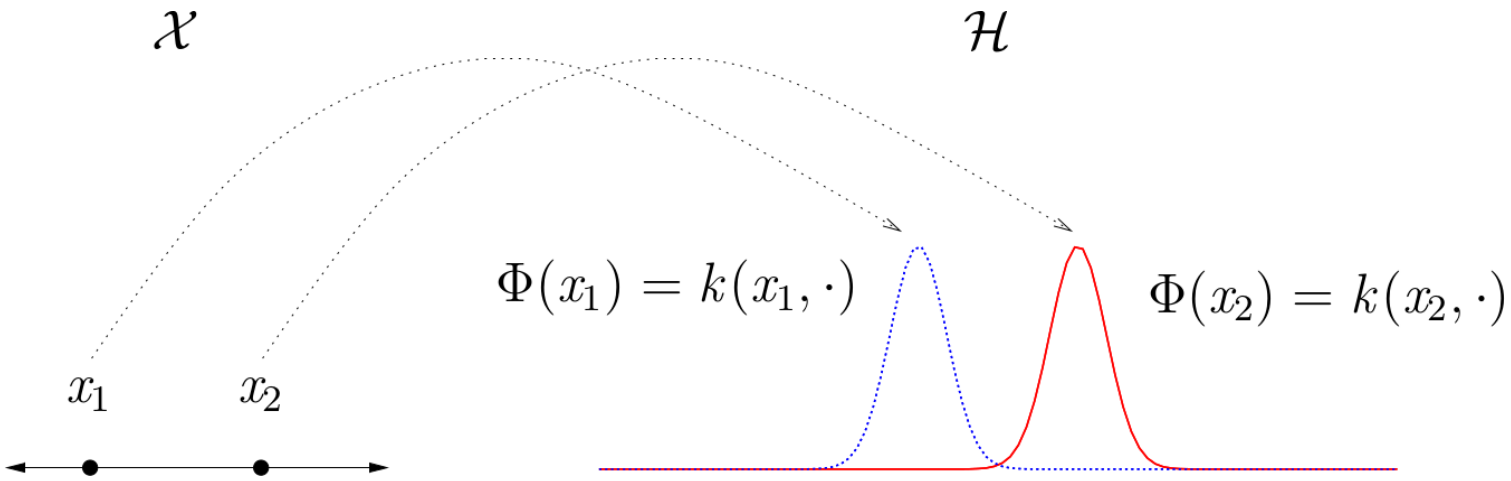


1. Feature map: $\Phi : \mathcal{X} \to \mathbb{R}^{\mathcal{X}} := \{f : \mathcal{X} \to \mathbb{R}\}$ with $\Phi(\mathbf{x})(\cdot) = k(\cdot, \mathbf{x})$
2. Vector space: $\text{span}\{k(\cdot, \mathbf{x}) \mid \mathbf{x} \in \mathcal{X}\}$ consisting of all functions of the form

$$f(\cdot) = \sum_{i=1}^{m} \alpha_i k(\cdot, \mathbf{x}_i)$$

for any $m \in \mathbb{N}$, $\mathbf{x}_1, \ldots, \mathbf{x}_m \in \mathcal{X}$, and $\alpha_1, \ldots, \alpha_m \in \mathbb{R}$.

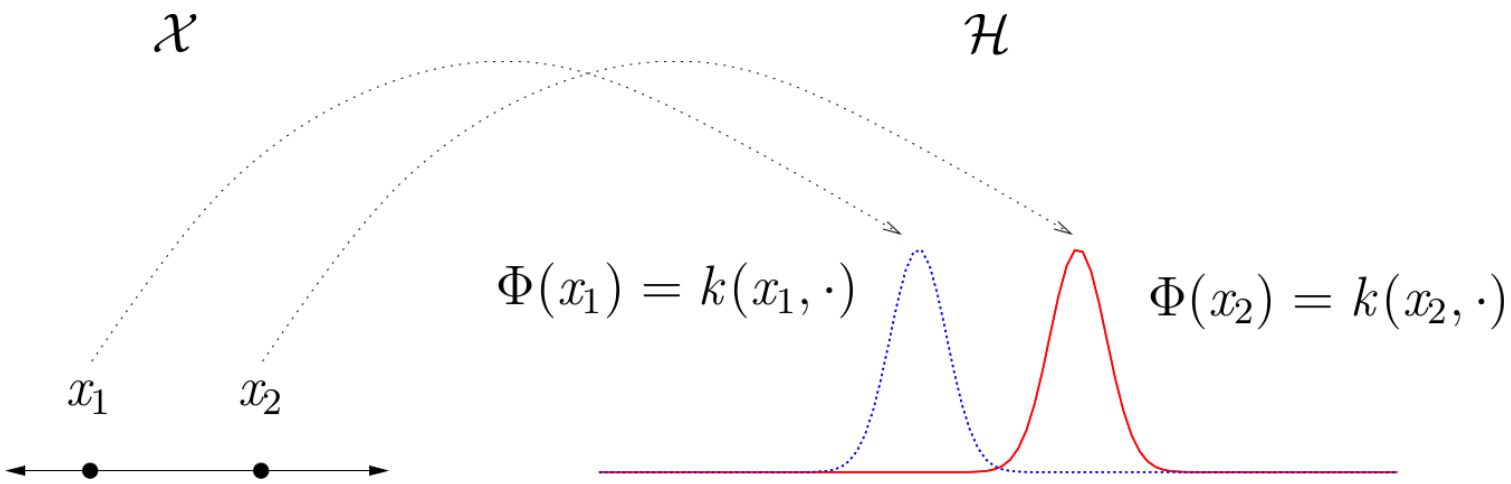
Recap: Kernel to Feature Map



3 Dot product: For $f(\cdot) = \sum_{i=1}^{m} \alpha_i k(\cdot, \mathbf{x}_i)$ and $g(\cdot) = \sum_{j=1}^{m'} \beta_j k(\cdot, \mathbf{x}'_j)$, let us define the following dot product:

$$\langle f, g \rangle := \sum_{i=1}^{m} \sum_{j=1}^{m'} \alpha_i \beta_j k(\mathbf{x}_i, \mathbf{x}'_j)$$

Recap: Kernel to Feature Map



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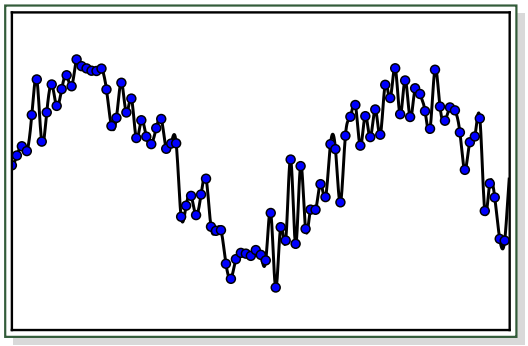
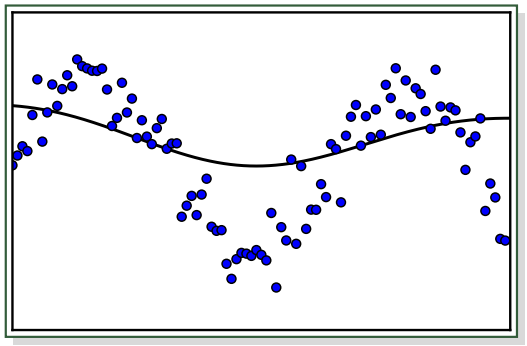
4 Reproducing kernel property: We have

$$\left\langle \Phi(\mathbf{x}), \Phi(\mathbf{x}') \right\rangle = \left\langle k(\cdot, \mathbf{x}), k(\cdot, \mathbf{x}') \right\rangle = k(\mathbf{x}, \mathbf{x}')$$

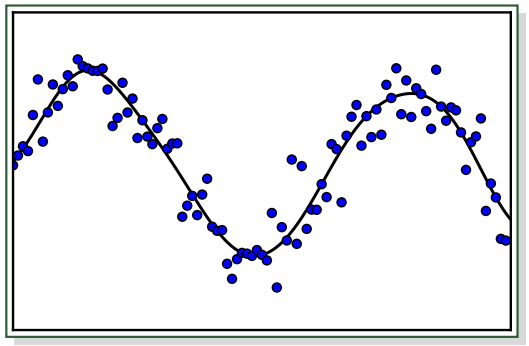
Recap: Regularization Networks



$\lambda = \text{small}$



$\lambda = \text{large}$



$\lambda = \text{middle}$

Regularized Least-Squares

Let $\mathcal{X} = \mathbb{R}^d$, $T = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$, and $\lambda > 0$. Goal: Find a model $f \in \mathcal{H}$ in the hypothesis space $\mathcal{H}$ that minimizes

$$\underset{f \in \mathcal{H}}{\text{minimize}} \underbrace{\frac{1}{n} \sum_{i=1}^{n} (f(\mathbf{x}_i) - y_i)^2}_{\text{Small Loss}} + \underbrace{\lambda \|f\|^2}_{\text{Small Complexity}} \tag{2}$$

Here: Models of the form $f(\cdot) = \sum_{j=1}^{m} \alpha_j k(\cdot, \mathbf{z}_j)$ with arbitrary m, arbitrary $\alpha \in \mathbb{R}^m$, and arbitrary $\mathbf{z}_1, \ldots, \mathbf{z}_m \in \mathcal{X}$. The norm $\|f\|^2$ measures the complexity of a model.

Optimal Solution

Regularized Least-Squares

Let $\mathcal{X} = \mathbb{R}^d$, $T = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$, and $\lambda > 0$. Goal: Find a model $f \in \mathcal{H}$ in the hypothesis space $\mathcal{H}$ that minimizes

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The representer theorem guarantees that the solution for this problem can be written as

$$f(\cdot) = \sum_{i=1}^{n} c_i k(\cdot, \mathbf{x}_i)$$

for some $\mathbf{c} \in \mathbb{R}^n$. Thus: We only need the training patterns $\mathbf{x}_1, \ldots, \mathbf{x}_n$ to represent an optimal solution!

Schölkopf, Herbrich, and Smola.
A Generalized Representer Theorem. COLT, 2001.

Optimal Solution

The complexity term $\|f\|^2$ can be rewritten in the following way:

$$\begin{aligned}
\|f\|^2 &= \langle f, f \rangle \\
&= \left\langle \sum_{i=1}^{n} c_i k(\cdot, x_i), \sum_{i=1}^{n} c_i k(\cdot, x_i) \right\rangle \\
&= \sum_{i=1}^{n} \sum_{j=1}^{n} c_i c_j k(x_i, x_j) \\
&= \mathbf{c}^T \mathbf{K} \mathbf{c}
\end{aligned}$$

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- We can therefore rewrite (2) in the following way:

$$\underset{\mathbf{c}\in\mathbb{R}^n}{\text{minimize}} \quad \frac{1}{n}(\mathbf{y}-\mathbf{K}\mathbf{c})^T(\mathbf{y}-\mathbf{K}\mathbf{c})+\lambda\mathbf{c}^t\mathbf{K}\mathbf{c}$$

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- $\nabla^2 F(\mathbf{c})$ is positive semidefinite. Why?

Optimal Solution

- Thus, F is convex in $\mathbf{c}$. We can find a global minimum by setting the gradient to $\mathbf{0}$:

$$\begin{aligned} & \nabla F(\mathbf{c}) && = \mathbf{0} \\ \Leftrightarrow \quad & -\tfrac{2}{n}\mathbf{K}^T(\mathbf{y}-\mathbf{K}\mathbf{c}) + 2\lambda\mathbf{K}\mathbf{c} && = \mathbf{0} \\ \Leftrightarrow \quad & (\mathbf{K}^T\mathbf{K} + n\lambda\mathbf{K})\mathbf{c} && = \mathbf{K}^T\mathbf{y} \\ \Leftrightarrow \quad & (\mathbf{K} + n\lambda\mathbf{I})\mathbf{c} && = \mathbf{y} \end{aligned}$$

For the last step, we assumed that $\mathbf{K}$ is invertible. If $\mathbf{K}$ is not invertible, then the following solution still depicts one of the optimal solutions.

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- Thus, an optimal solution can be found by computing

$$\mathbf{c}^* = (\mathbf{K}+n\lambda\mathbf{I})^{-1}\mathbf{y}$$

Runtime and Space Analysis

Regularized Least-Squares

Let $\mathcal{X} = \mathbb{R}^d$, $T = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \subset \mathbb{R}^d \times \mathbb{R}$, and $\lambda > 0$. Goal: Find a model $f \in \mathcal{H}$ in the hypothesis space $\mathcal{H}$ that minimizes

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- What is the runtime and space complexity for this approach?
  - Space: $O(n^2)$ space for $\mathbf{K} + n\lambda \mathbf{I}$
  - Runtime: $O(n^3)$ for computing the inverse of this matrix (plus runtime needed for the computation of the kernel matrix).
    Note that solving such a system of linear equations generally takes $O(n^3)$ time.

Trick I: Linear Kernel

- For a linear kernel, we $\mathbf{K} = \mathbf{X}\mathbf{X}^T$ with $\mathbf{X} \in \mathbb{R}^{n \times d}$ containing the patterns as rows. We can therefore rewrite the task:

$$\begin{aligned}
&\underset{\mathbf{c} \in \mathbb{R}^n}{\text{minimize}} && \frac{1}{n}(\mathbf{y} - \mathbf{K}\mathbf{c})^T(\mathbf{y} - \mathbf{K}\mathbf{c}) + \lambda \mathbf{c}^t \mathbf{K}\mathbf{c} \\
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Note: No $n \times n$ kernel matrix is computed! An offset parameter can be added by prepending a column of ones to $\mathbf{X}$, see before!

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- Hence: Instead of spending $\mathcal{O}(n^3)$ for each λ, we only need to spend $\mathcal{O}(n^3)$ once and can then test each λ in only $\mathcal{O}(n^2)$ time!

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- Let $R = \{i_1, \ldots, i_r\} \subseteq \{1, \ldots, n\}$ a subset of indices. Then, search for models of the form

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WARNING: In practice, do not invert the matrices (numerical issues!). Instead, directly solve the linear system of equations (e.g., via `numpy.linalg.solve`).

Nyström Approximation

- The matrix

$$\widetilde{\mathbf{K}} = (\mathbf{K}_R)^T (\mathbf{K}_{R,R})^{-1} \mathbf{K}_R \in \mathbb{R}^{n \times n} \tag{3}$$

  is called the Nyström approximation of the kernel matrix $\mathbf{K}$.

Nyström Approximation

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$$\widetilde{\mathbf{K}} = (\mathbf{K}_R)^T (\mathbf{K}_{R,R})^{-1} \mathbf{K}_R \in \mathbb{R}^{n \times n} \tag{3}$$
is called the Nyström approximation of the kernel matrix $\mathbf{K}$.
- A good assignment for r depends on the dataset! The larger, the better.

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Question: Difference of this approach compared to using only a subset of r training instances?

Demo Time!

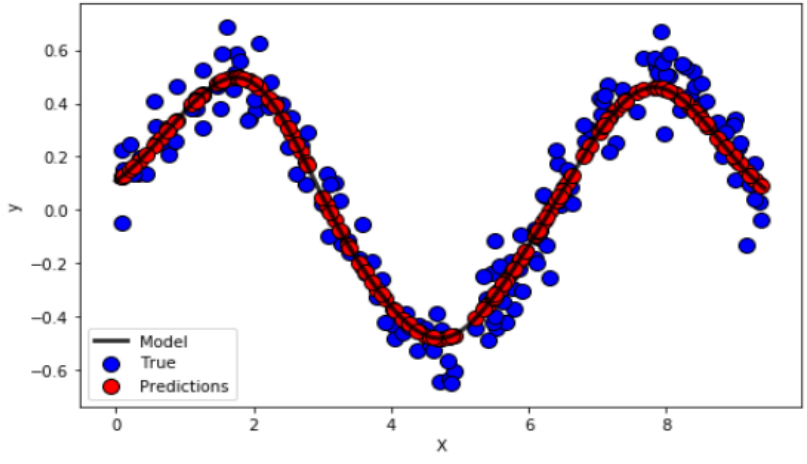
jupyter Least_Squares (autosaved)

Logout

File Edit View Insert Cell Kernel Widgets Help Trusted Python 3

Run Code

```
from sklearn.model_selection import train_test_split

X, y = get_dataset(n=500)
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.33, random_state=1)

plt.figure(figsize=(8,5))

model = LeastSquaresRegression(kernel="fast_rbf", lam=0.01, gamma=1, r=None)
model.fit(X_train, y_train)
preds = model.predict(X_test)

# plot test points and predictions
plt.scatter(X_test, y_test, s=100, c="b", edgecolor="k", linewidths=1, label="True")
plt.scatter(X_test, preds, s=100, c="r", edgecolor="k", linewidths=1, label="Predictions")

# plot model
x = numpy.linspace(X.min(), X.max(), 500)
plt.plot(x, model.predict(x), "-k", alpha=0.8, linewidth=3.0, label="Model")

plt.xlabel("X")
plt.ylabel("y")
plt.legend(loc=0)

plt.show()
```



Outline

Do we Need Hundreds of Classifiers to Solve Real World Classification Problems?

Manuel Fernández-Delgado MANUEL.FERNANDEZ.DELGADO@USC.ES
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Editor: Russ Greiner

Abstract

We evaluate **179 classifiers** arising from **17 families** (discriminant analysis, Bayesian, neural networks, support vector machines, decision trees, rule-based classifiers, boosting, bagging, stacking, random forests and other ensembles, generalized linear models, nearest-neighbors, partial least squares and principal component regression, logistic and multinomial regression, multiple adaptive regression splines and other methods), implemented in Weka, R (with and without the caret package), C and Matlab, including all the relevant classifiers available today. We use **121 data sets**, which represent **the whole UCI** data base (excluding the large-scale problems) and other own real problems, in order to achieve significant conclusions about the classifier behavior, not dependent on the data set collection. **The classifiers most likely to be the bests are the random forest** (RF) versions, the best of which (implemented in R and accessed via caret) achieves 94.1% of the maximum accuracy overcoming 90% in the 84.3% of the data sets. However, the difference is not statistically significant with the second best, the SVM with Gaussian kernel

Now!

http://jmlr.csail.mit.edu/papers/volume15/delgado14a/delgado14a.pdf

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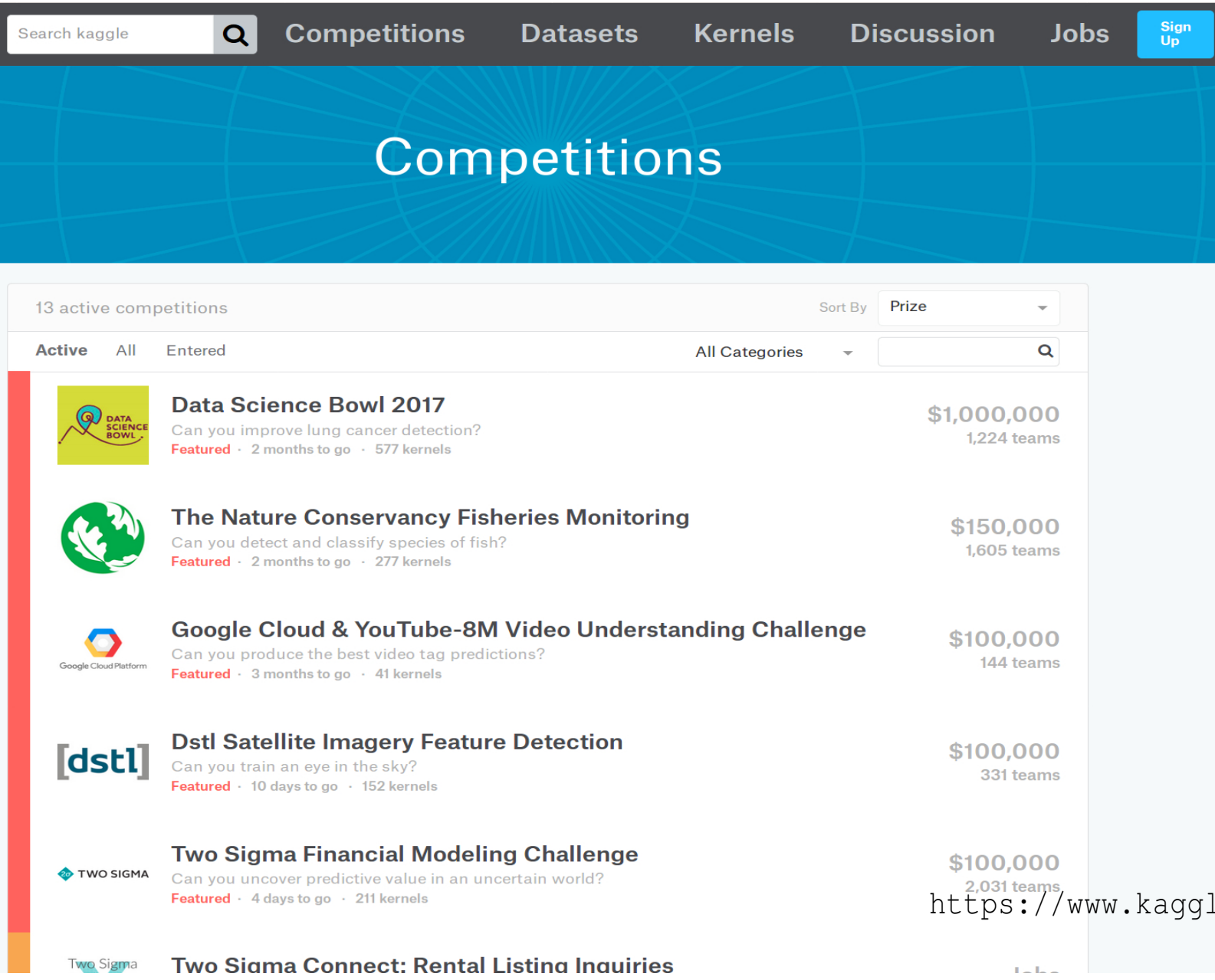
Data Analysis: Real-World Competitions



https://www.kaggle.com

Now!

https://dnc1994.com/2016/05/rank-10-percent-in-first-kaggle-competition-en/

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How to Rank 10% in Your First Kaggle Competition

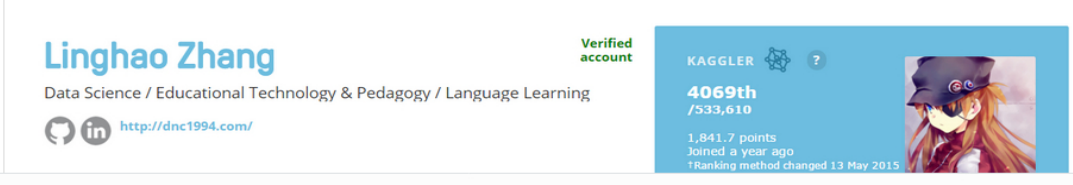
Posted on 2016-05-10 | In Data Science | 22 Comments

Introduction

Kaggle is the best place to learn from other data scientists. Many companies provide data and prize money to set up data science competitions on Kaggle. Recently I had my first shot on Kaggle and **ranked 98th (~ 5%) among 2125 teams**. Being my Kaggle debut, I feel quite satisfied with the result. Since many Kaggle beginners set 10% as their first goal, I want to share my two cents on how to achieve that.

This post is also available in Chinese.

Updated on Oct 28th, 2016: I made many wording changes and added several updates to this post. Note that Kaggle has went through some major changes since I published this post, especially with its ranking system. Therefore some descriptions here might not apply anymore.



Now!

https://dnc1994.com/2016/05/rank-10-percent-in-first-kaggle-competition-en/

Model Selection

When the features are set, we can start training models. Kaggle competitions usually favor **tree-based models**:

- **Gradient Boosted Trees**
- Random Forest
- Extra Randomized Trees

The following models are slightly worse in terms of general performance, but are suitable as base models in ensemble learning (will be discussed later):

- SVM
- Linear Regression
- Logistic Regression
- Neural Networks

Note that this does not apply to computer vision competitions which are pretty much dominated by neural network models.

All these models are implemented in **Sklearn**.

Here I want to emphasize the greatness of **Xgboost**. The outstanding performance of gradient boosted trees and Xgboost's efficient implementation makes it very popular in Kaggle competitions. Nowadays almost every winner uses Xgboost in one way or another.

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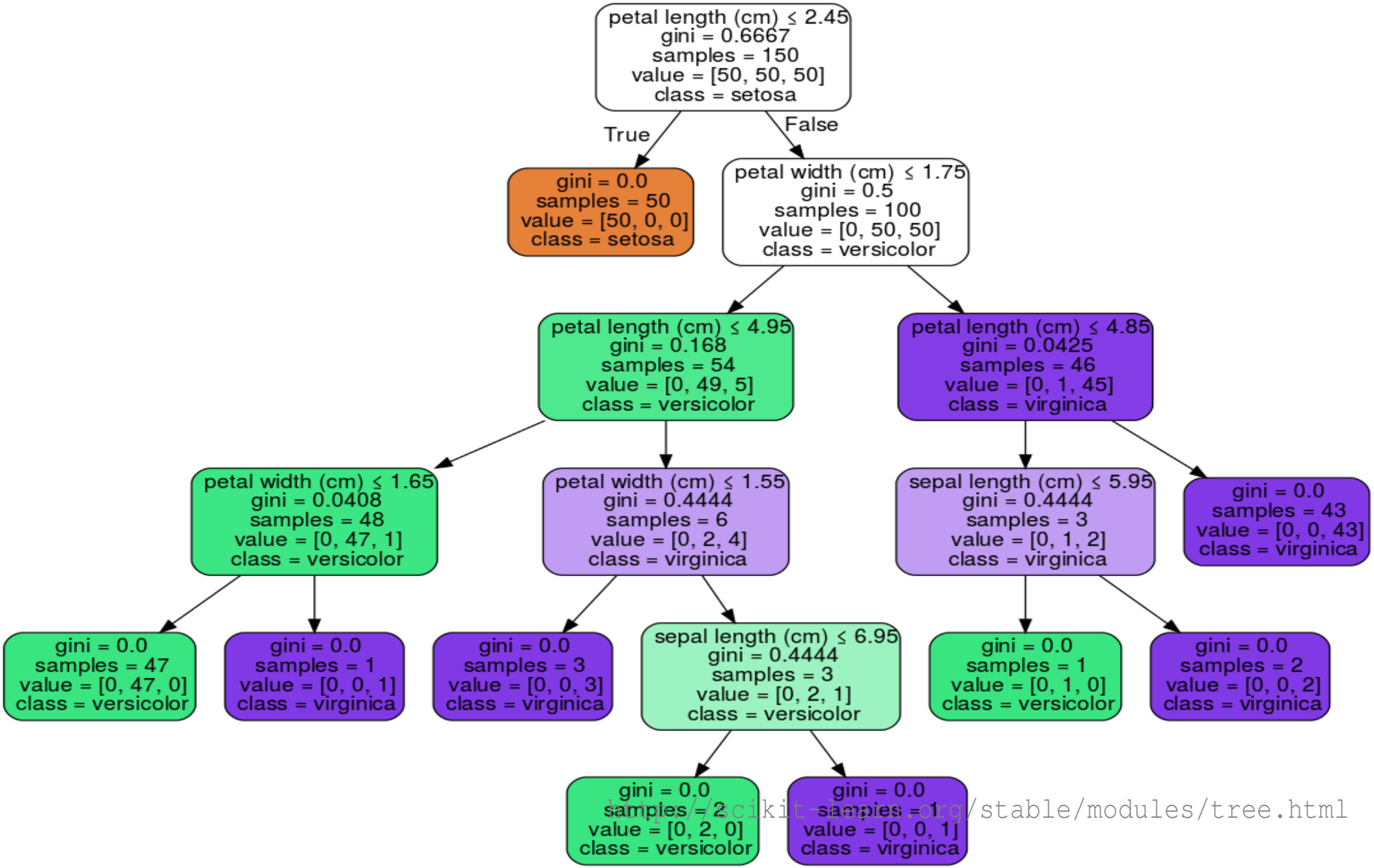
Example: Iris Flower Classification Tree

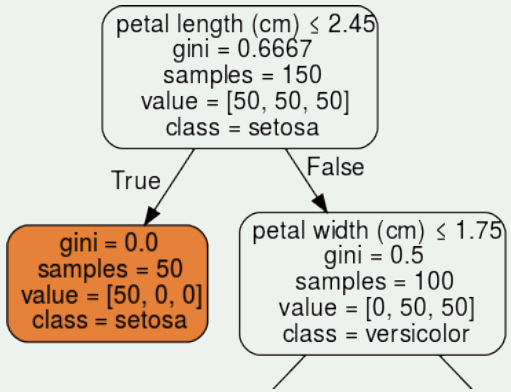


http://scikit-learn.org/stable/modules/tree.html

Classification and Regression Trees (CARTs)

Structure & Training

- Every internal node is associated with one coordinate $i \in \{1, \ldots, d\}$ and a threshold θ.
- At each inner node, the training data $S = \{(\mathbf{x}_1, y_1), \ldots\}$ at that node are split into



$$L_{i,\theta} = \{(\mathbf{x}, y) \in S \,|\, x_i \leq \theta\} \text{ and } R_{i,\theta} = \{(\mathbf{x}, y) \in S \,|\, x_i > \theta\},$$

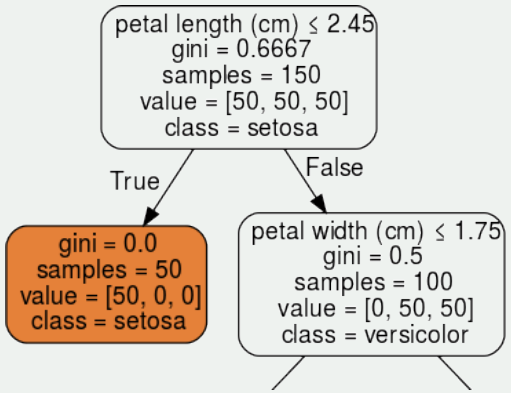
which are passed to the left/right child for further processing.

- Construction: The optimal tree cannot be found efficiently. Therefore, trees are built using a heuristic.
- The leaf nodes, indexed by $\tau = 1, \ldots, M$, define regions $\mathcal{R}_\tau \subseteq \mathbb{R}^d$.

Building CARTs

Basic Idea

- Every inner node is associated with one coordinate $i \in \{1, \ldots, d\}$ and a threshold θ.
- At each inner node, the associated data $S = \{(\mathbf{x}_1, y_1), \ldots\}$ are split into $L_{i,\theta}$ and $R_{i,\theta}$ such that the information gain



$$G_{i,\theta}(S) = Q(S) - \frac{|L_{i,\theta}|}{|S|} Q(L_{i,\theta}) - \frac{|R_{i,\theta}|}{|S|} Q(R_{i,\theta})$$

  is maximized, where Q is some impurity measure.
- If the number $|S|$ of points at a node is smaller than a user-defined value or if S is pure (i.e., all point have the same label), the node becomes a leaf (further stopping rules exist!).

Simplified Objective

Note that

$$\underset{i,\theta}{\text{maximize}}\ G_{i,\theta}(S) = Q(S) - \frac{|L_{i,\theta}|}{|S|}Q(L_{i,\theta}) - \frac{|R_{i,\theta}|}{|S|}Q(R_{i,\theta})$$

is equivalent to

$$\underset{i,\theta}{\text{minimize}}\ |L_{i,\theta}|Q(L_{i,\theta}) + |R_{i,\theta}|Q(R_{i,\theta})$$

Let's build a tree!

Recursive Tree Construction

Procedure: BUILDTREE(S,m)

Require: $S = \{(\mathbf{x}_1, y_1), \ldots\}$ and number m.

Ensure: Tree $\mathcal{T}$ built for the input patterns in S.

1: **if** $|S| \leq m$ **then**
2: **return** leaf node storing the labels $\{y_1, \ldots, y_{|S|}\}$
3: **end if**
4: **if** $y_i = y_j$ for all $(\mathbf{x}_i, y_i), (\mathbf{x}_j, y_j) \in S$ **then**
5: **return** leaf node storing the labels $\{y_1, \ldots, y_{|S|}\}$
6: **end if**
7: Find $(i^*, \theta^*) = \text{argmax}_{i,\theta}\, G_{i,\theta}(S)$
8: $\mathcal{T}_l$ = BUILDTREE($L_{i,\theta}$, m)
9: $\mathcal{T}_r$ = BUILDTREE($R_{i,\theta}$, m)
10: Generate node that stores the splitting information (i^*, θ^*) and pointers to its subtrees $\mathcal{T}_l$ and $\mathcal{T}_r$. Let $\mathcal{T}$ denote the resulting tree.
11: **return** $\mathcal{T}$

Regression Trees

Construction: What are "optimal" splits?

- Impurity measure: For regression problems, a common choice is

$$Q(S) = \sum_{(\mathbf{x},y)\in S} (y - \hat{y})^2,$$

  where $\bar{y} = \frac{1}{|S|} \sum_{(\mathbf{x},y)\in S} y$

- Find optimal splitting dimension i^* and threshold θ^* w.r.t.

$$\underset{i,\theta}{\text{minimize}} \; |L_{i,\theta}| Q(L_{i,\theta}) + |R_{i,\theta}| Q(R_{i,\theta})$$

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How to compute the optimal dimension and threshold?

1. Naive approach, $\mathcal{O}(d \cdot |S|^2)$ time: For each i, do:
   - Consider all possible thresholds (e.g., $\{\mathbf{x}_i | \mathbf{x} \in S\}$).
   - For each threshold θ: Compute $|L_{i,\theta}| Q(L_{i,\theta})$ and $|R_{i,\theta}| Q(R_{i,\theta})$.

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   - For each threshold θ: Compute $|L_{i,\theta}| Q(L_{i,\theta})$ and $|R_{i,\theta}| Q(R_{i,\theta})$.
2. Better approach, $\mathcal{O}(d \cdot |S| \log |S|)$ time: For each i, do:
   - Sort all instances $(\mathbf{x}, y)$ in S according to the patterns i-th dimension.
   - Scan this sorted list and update these values incrementally!

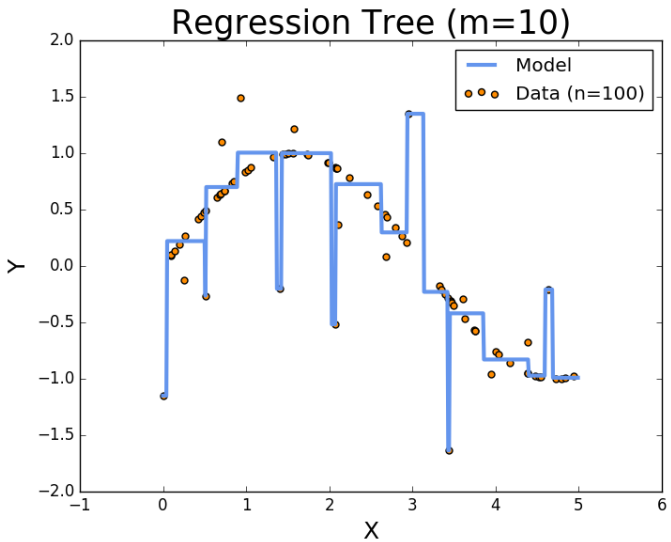
Regression Trees

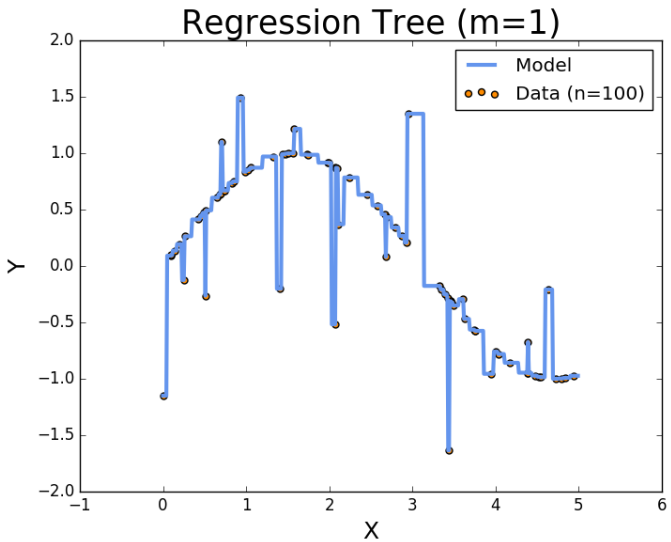
Prediction

- Training data $S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_n, y_n)\} \in \mathbb{R}^d \times \mathbb{R}$
- Each leaf node $\tau = 1, \ldots, M$ of the tree $\mathcal{T}$ corresponds to a region $R_\tau \subseteq \mathbb{R}^d$
- The output $\hat{y} = \mathcal{T}(\mathbf{x})$ given a new input instance $\mathbf{x}$ is

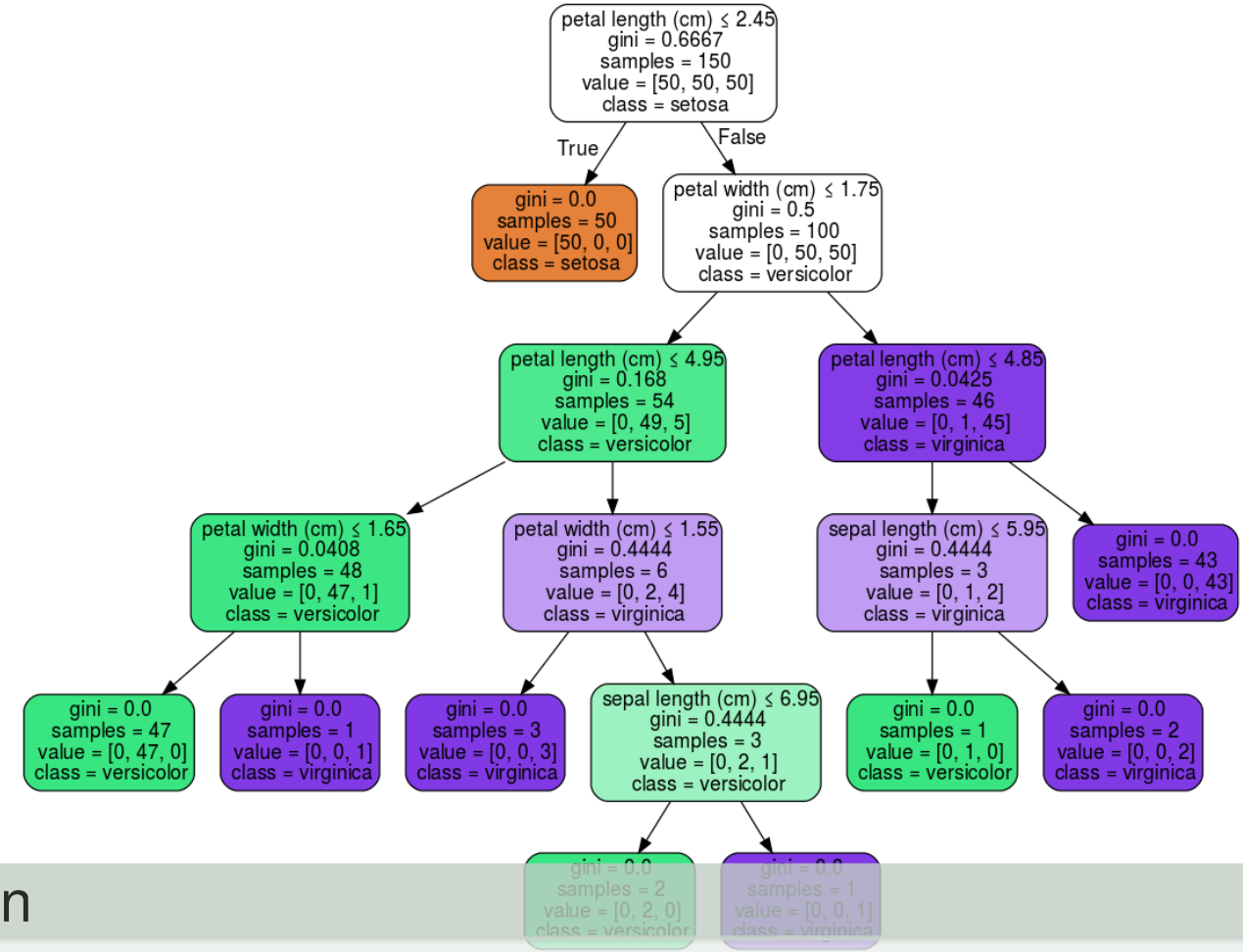
$$\mathcal{T}(\mathbf{x}) = \sum_{\tau=1}^{M} c_\tau \mathbb{I}\{\mathbf{x} \in \mathcal{R}_\tau\} \ ,$$

where $c_\tau = \frac{1}{|R_\tau \cap S|} \sum_{\mathbf{x}_j \in \mathcal{R}_\tau \cap S} y_j$ (thus: mean of all labels stored in leaf).





Classification Trees



Prediction

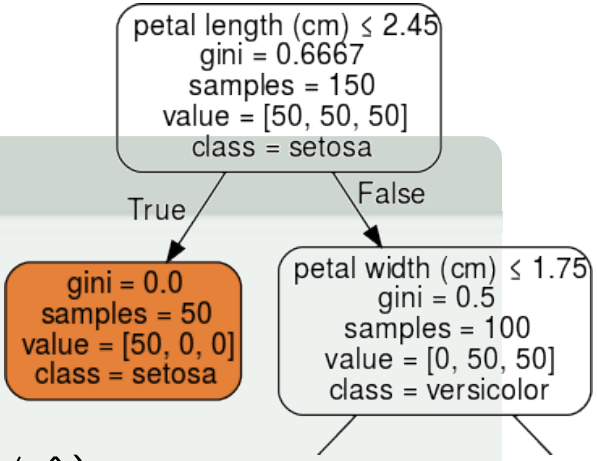
1. Traverse the tree $\mathcal{T}$ to find the leaf that contains the query $\mathbf{x}$.
2. Each leaf node $\tau = 1, \ldots, M$ of the tree $\mathcal{T}$ corresponds to a region $R_\tau \subset \mathbb{R}^d$
3. Use majority class in leaf as prediction $\mathcal{T}(\mathbf{x})$.

Classification Trees

Construction

As before: We need to define an impurity measure $Q(S)$.
Let p_{Sk} be the fraction of points belonging to class k in S.

1. Misclassification error: Let $\hat{y} = \text{argmax}_k\, p_{Sk}$ be the dominant class in S. Then $Q(S) = \frac{1}{|S|} \sum_{(\mathbf{x}_j, y_j) \in S} \mathbb{I}(y_j \neq \hat{y})$
2. Gini index: $Q(S) = \sum_{k=1}^{K} p_{Sk}(1 - p_{Sk})$
3. ...



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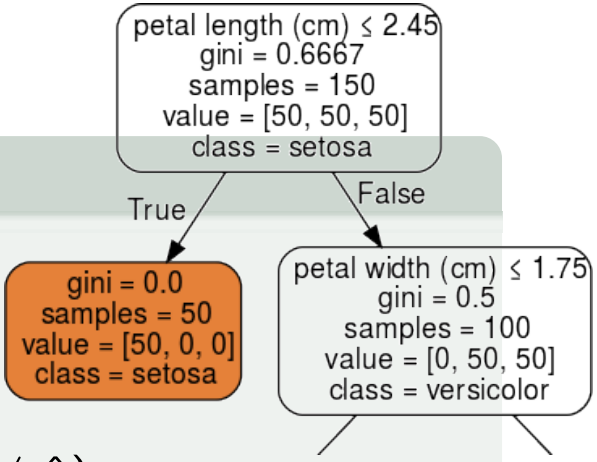

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3. ...

At home: Check Gini indices for all three nodes.

Outline

Summary & Outlook

Today

1. Large-Scale Least-Squares

Outlook

- Today (Practical Sessions): VirtualBox, Google Colab, HW1/HW2
- Tuesday (Lecture): Large-Scale Random Forests & Boosted Trees I (FG)
- Thursday (Lecture): Neural Networks (CI)

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