Introduction to Machine Learning

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Outline

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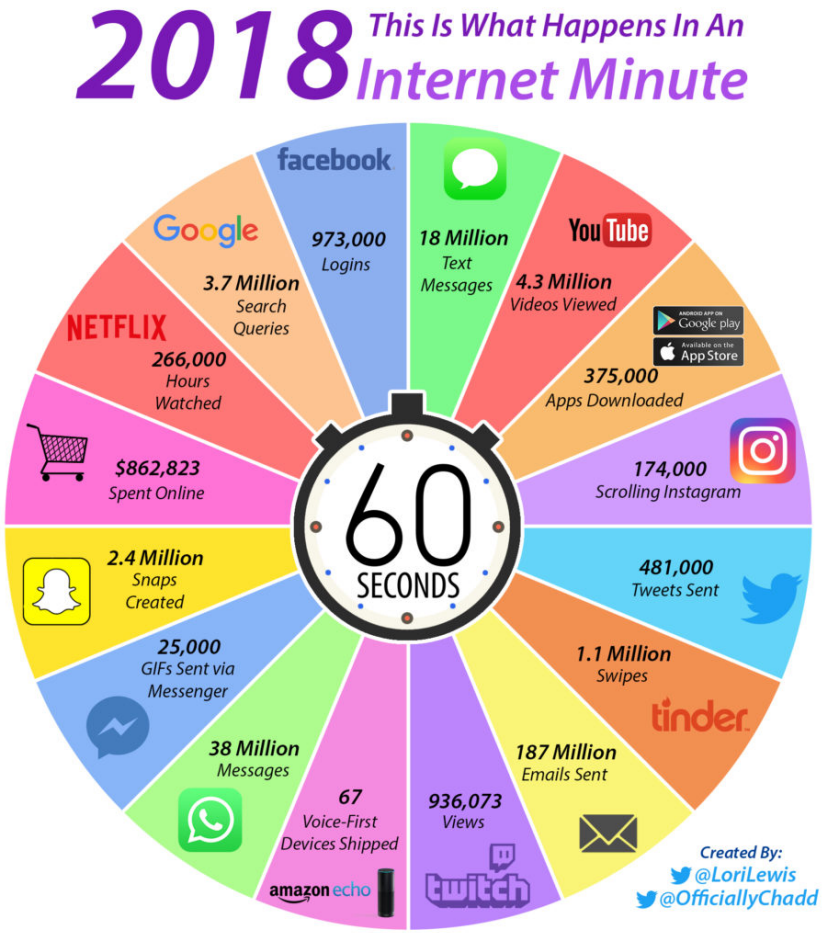
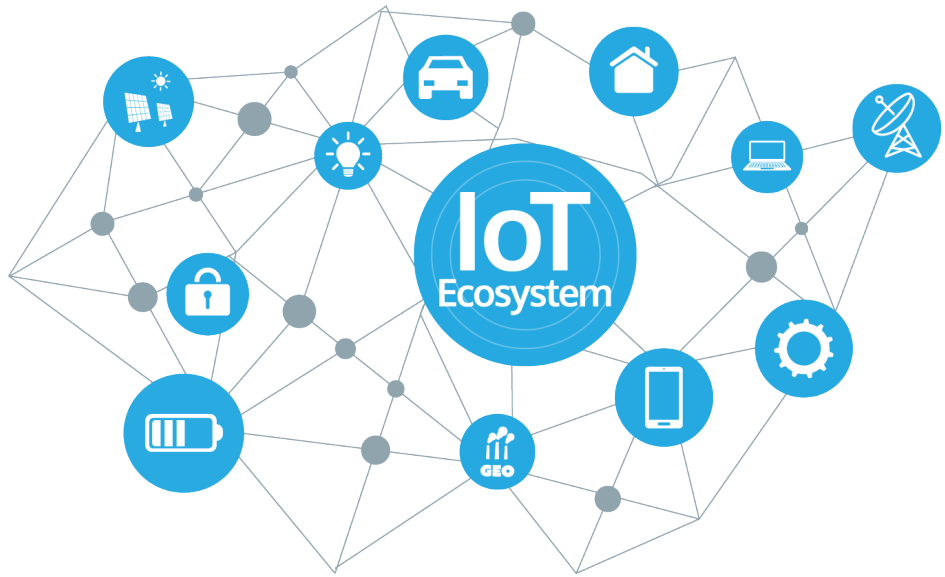
Our Reality: We Are Drowning In Data

- Every click, every network packet and every online interaction is recorded and will outlive us.





Data Science

- The umbrella field of data science aims to harness this massive amount of data to glean insights, drive industry and improve the human experience.

Societal Ramifications and Applications

- Health care (drug re-purposing, RNA sequencing)
- Automated knowledge discovery (scientific literature mining)
- Ease of mass surveillance (social credit systems, geographic tracking)
- Targeted advertising (political elections, big nudging)

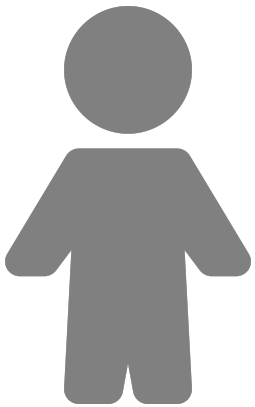
Pattern Recognition and Machine Learning

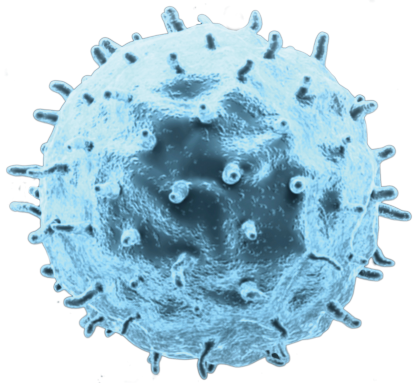
- This talk focuses on gaining insight into the underlying algorithms and structures that produce models capable of tackling such problems.
- We will explore in-depth a heuristical algorithm - the supervised Decision Tree.

Outline

Entities

- The world around us can be succinctly described as comprised of entities.





Entities

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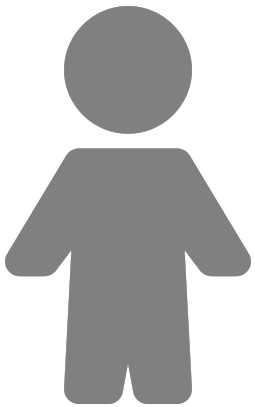
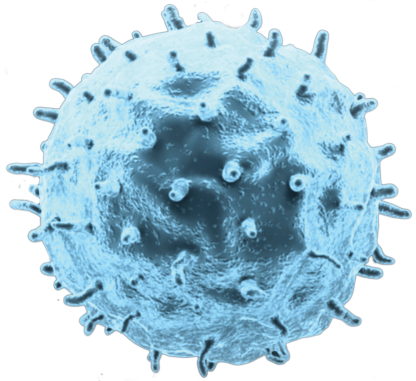
- Entities interact (relate) with other entities and in the process possibly form new entities.





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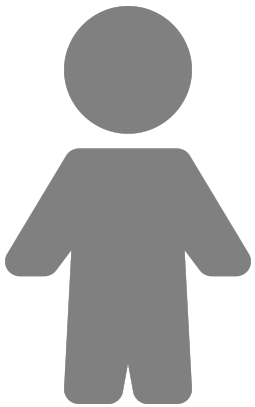
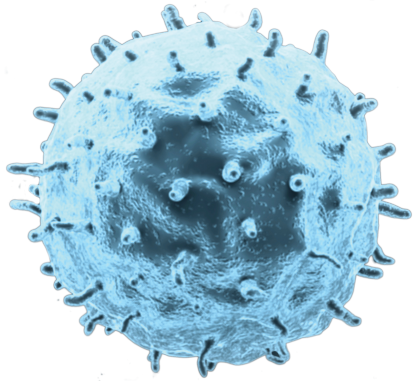
- Entities are composed of attributes.





Entities

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- Entities interact (relate) with other entities and in the process possibly form new entities.
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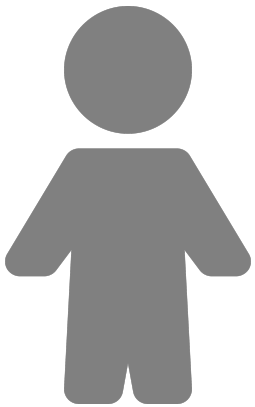
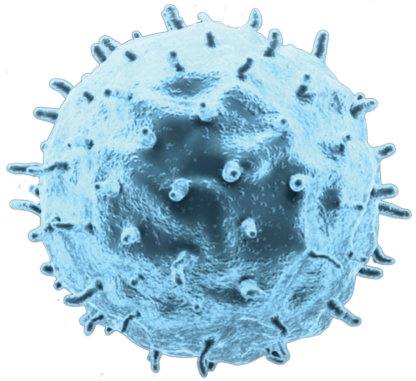
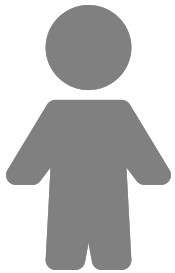
- An instance of an entity is a particular manifestation of the attributes that comprise the entity.





Instances of Entities

- A collection of instances $x_i \in \mathbb{D}$ from an entity domain $\mathbb{D}$ forms a sample from the domain.



	account_balance	income	age	has_defaulted	credit_worthy
x_1	57103	50000	25	0	?
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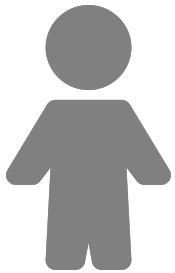

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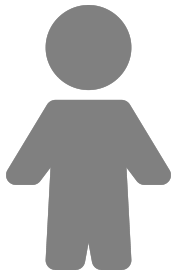
- The dimension d of $\mathbb{D}$ is the number of attributes describing its entity.
- We assume attributes (observations, features) of a given instance $x_{i,\,j}$ $(0 \leq j < d)$ are real numbers.



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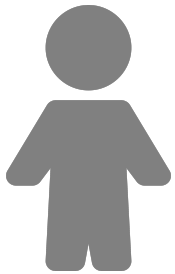

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Supervised Learning

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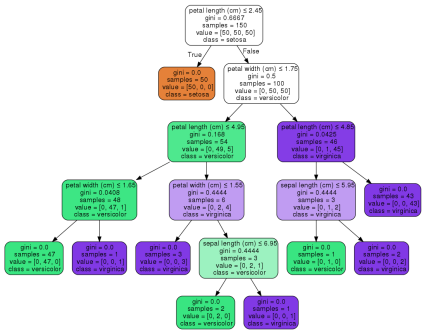

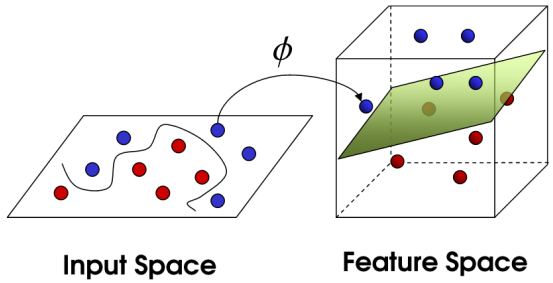

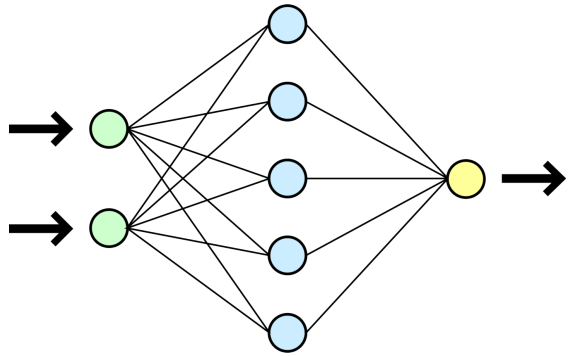

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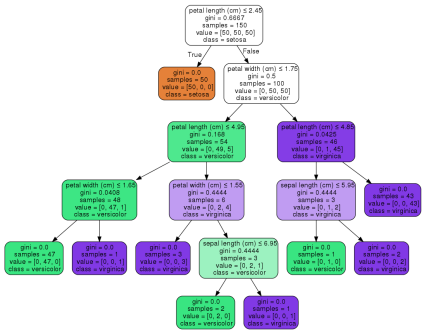
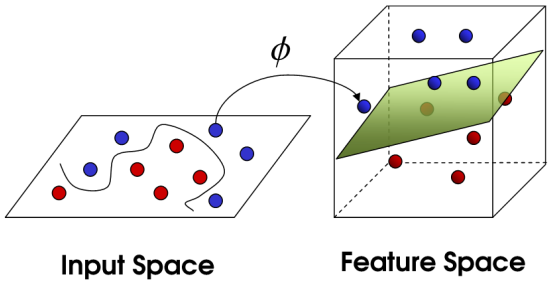
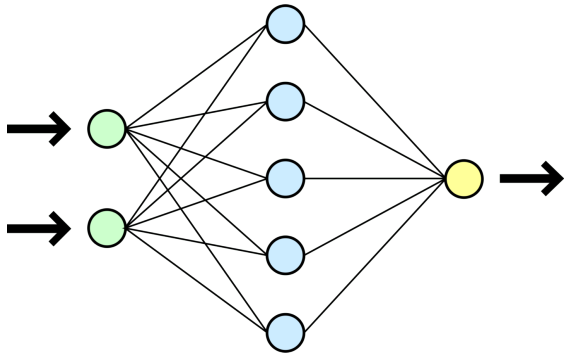
- In the supervised setting, a machine learning algorithm finds (learns) a mapping from observations X to outputs y.







Supervised Learning

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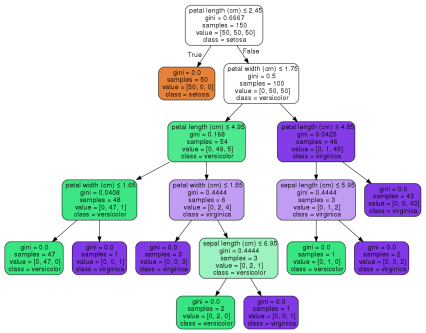
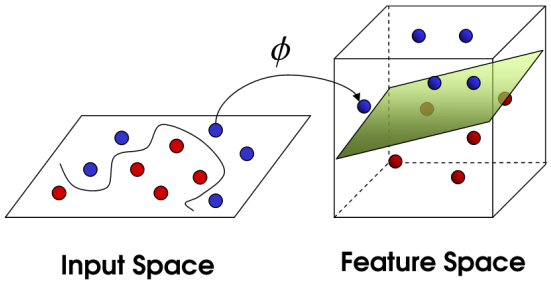
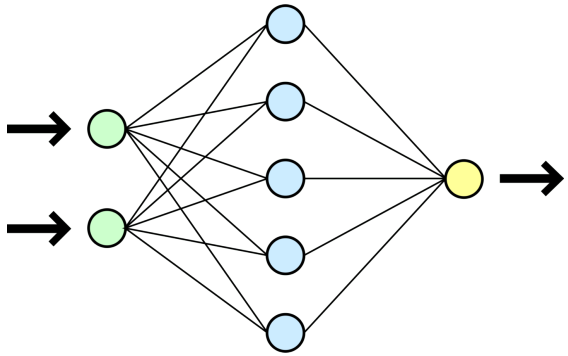
- The rest of this talk explores how such a mapping (classifier, model) can be learned.

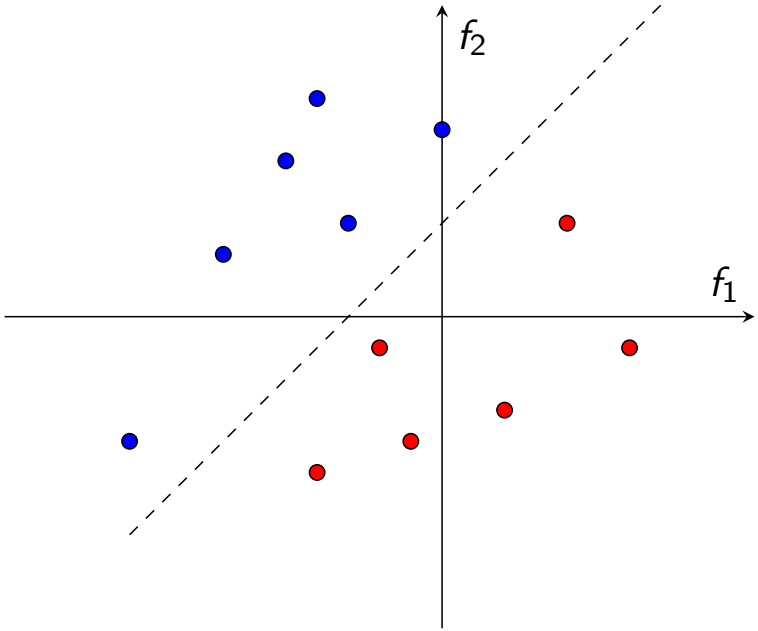




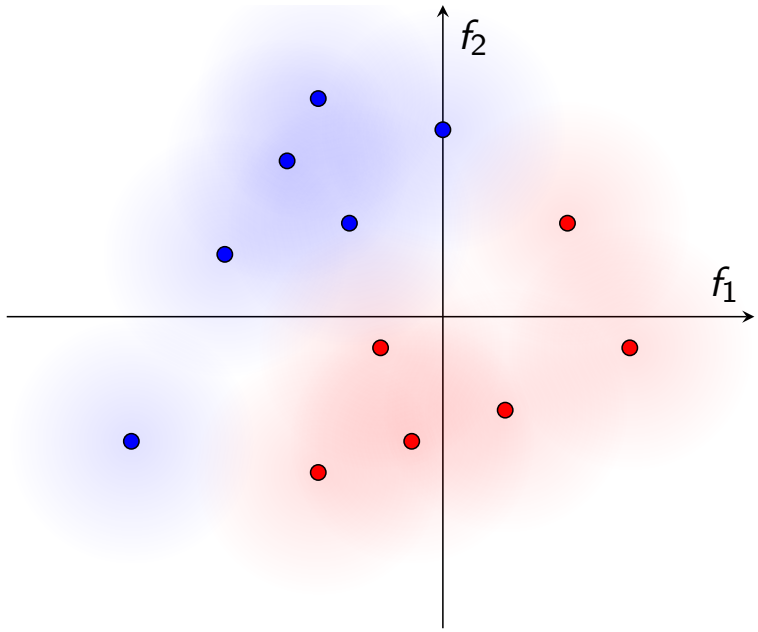


Learning a Supervised Model

- Supervised Learning algorithms differ by the space of hypothesis $\mathbb{H}$ they search when selecting an $h \in \mathbb{H}$ with optimal predictive ability.



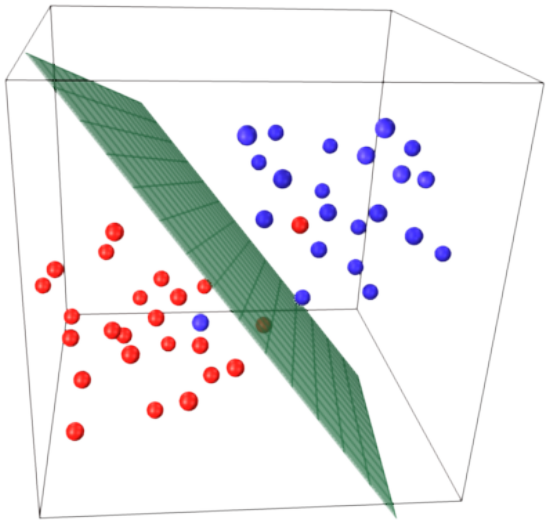
(a) Discriminative Classifier



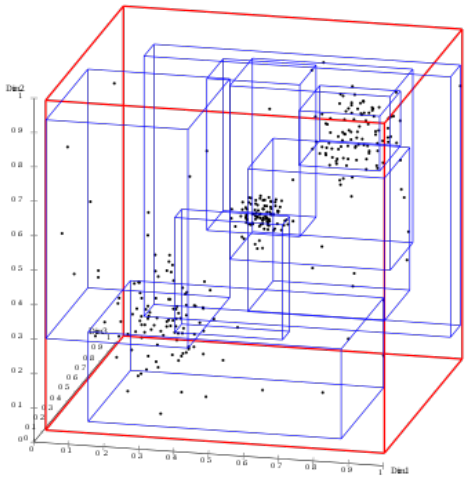
(b) Generative (probabilistic) Classifier

Discriminative Models

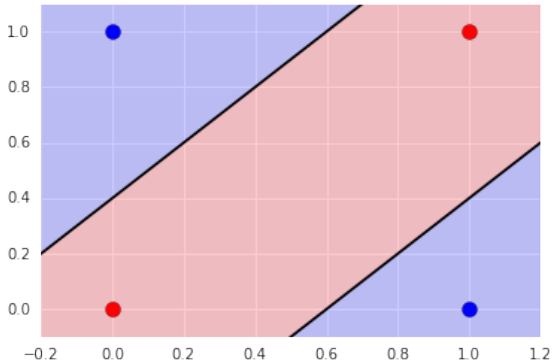
- Discriminative algorithms search the hypothesis space of geometric decision boundaries separating classes.



(a) Hyperplanes



(b) Hyper-rectangles



(c) Nested-Hyperplanes

Outline

Generalization Ability

- Recall that a hypothesis function (model) h is the output of our learning algorithm applied to our training sample X.

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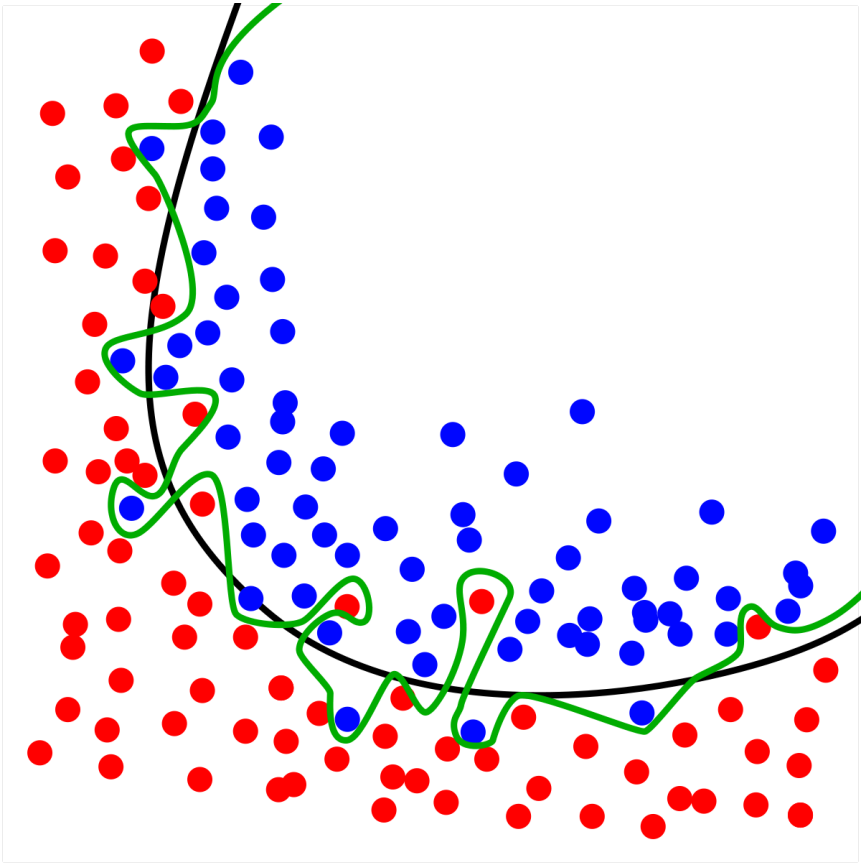
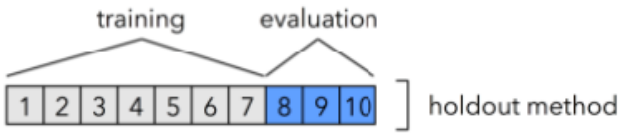
- How can we ensure that our selected h is consistent with $\mathbb{D}$ (i.e. generalizes)?



Generalization Ability

- Recall our training set:

$$\begin{bmatrix} x_{11} & x_{12} & x_{13} & \cdots & x_{1d} \\ x_{21} & x_{22} & x_{23} & \cdots & x_{2d} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ x_{n1} & x_{d2} & x_{d3} & \cdots & x_{nd} \end{bmatrix} \rightarrow \begin{bmatrix} y_1 \\ y_2 \\ \vdots \\ y_n \end{bmatrix}$$



(a) Hold-out Subset

(b) Cross Validation (partitioning)

Hold Out Validation

Back to our loan example: a supervised algorithm trained on a training partition $T \subset X$ and evaluated on a test partition $X \setminus T$ building a model h:

$$h(T)$$
$$\begin{bmatrix} \text{give} \\ \text{deny} \\ \text{deny} \\ \text{give} \\ \text{give} \\ \text{deny} \end{bmatrix}$$

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\begin{array}{cc}
h(T) & \\
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\end{array}
\quad
\begin{array}{cc}
h(X \setminus T) & \\
\left[\begin{array}{c} \text{give} \\ \\ \\ \\ \\ \end{array}\right] & \text{True Positive (TP)}
\end{array}
$$

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h(X \setminus T) & \\
\left[\begin{array}{c} \text{give} \\ \text{give} \\ \\ \\ \\ \end{array}\right] & \begin{array}{l} \text{True Positive (TP)} \\ \text{False Positive (FP)} \end{array}
\end{array}
$$

Hold Out Validation

Back to our loan example: a supervised algorithm trained on a training partition $T \subset X$ and evaluated on a test partition $X \setminus T$ building a model h:

$$\begin{matrix} h(T) \\ \begin{bmatrix} \text{give} \\ \text{deny} \\ \text{deny} \\ \text{give} \\ \text{give} \\ \text{deny} \end{bmatrix} \end{matrix} \rightarrow \begin{matrix} h(X \setminus T) \\ \begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \\ \\ \\ \end{bmatrix} \end{matrix} \begin{matrix} \\ \text{True Positive (TP)} \\ \text{False Positive (FP)} \\ \\ \\ \\ \\ \end{matrix}$$

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$$
\begin{array}{c}
h(T) \\
\begin{bmatrix} \text{give} \\ \text{deny} \\ \text{deny} \\ \text{give} \\ \text{give} \\ \text{deny} \end{bmatrix}
\end{array}
\quad \rightarrow \quad
\begin{array}{c}
h(X \setminus T) \\
\begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \\ \\ \\ \end{bmatrix}
\end{array}
\begin{array}{l}
\\
\text{True Positive (TP)} \\
\text{False Positive (FP)} \\
\text{True Negative (TN)} \\
\\
\\
\\
\end{array}
$$

Hold Out Validation

Back to our loan example: a supervised algorithm trained on a training partition $T \subset X$ and evaluated on a test partition $X \setminus T$ building a model h:

$$
\begin{array}{ccc}
h(T) & & h(X \setminus T) \\
\begin{bmatrix} \text{give} \\ \text{deny} \\ \text{deny} \\ \text{give} \\ \text{give} \\ \text{deny} \end{bmatrix} & \rightarrow & \begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \text{give} \\ \\ \end{bmatrix}
\begin{array}{l} \text{True Positive (TP)} \\ \text{False Positive (FP)} \\ \text{True Negative (TN)} \end{array}
\end{array}
$$

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\end{array}
\quad \rightarrow \quad
\begin{array}{c}
h(X \setminus T) \\
\begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \text{give} \\ \\ \\ \end{bmatrix}
\end{array}
\quad
\begin{array}{l}
\\
\text{True Positive (TP)} \\
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\text{True Positive (TP)} \\
\\
\\
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$$

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\end{array}
\rightarrow
\begin{array}{c}
h(X \setminus T) \\
\begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \text{give} \\ \text{deny} \\ \\ \end{bmatrix}
\end{array}
\begin{array}{l}
\\
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\\
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$$

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$$
\begin{array}{c}
h(T) \\
\begin{bmatrix} \text{give} \\ \text{deny} \\ \text{deny} \\ \text{give} \\ \text{give} \\ \text{deny} \end{bmatrix}
\end{array}
\quad \rightarrow \quad
\begin{array}{cc}
h(X \setminus T) & \\
\begin{bmatrix} \text{give} \\ \text{give} \\ \text{deny} \\ \text{give} \\ \text{deny} \\ \\ \end{bmatrix} &
\begin{array}{l} \text{True Positive (TP)} \\ \text{False Positive (FP)} \\ \text{True Negative (TN)} \\ \text{True Positive (TP)} \\ \text{False Negative (FN)} \end{array}
\end{array}
$$

Hold Out Validation

Back to our loan example: a supervised algorithm trained on a training partition $T \subset X$ and evaluated on a test partition $X \setminus T$ building a model h:

$h(T)$		$h(X \setminus T)$	
give		give	True Positive (TP)
deny		give	False Positive (FP)
deny	$\rightarrow$	deny	True Negative (TN)
give		give	True Positive (TP)
give		deny	False Negative (FN)
deny		give	

Hold Out Validation

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	PP	PN
P	2	1
N	2	1

Hold Out Validation

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$h(T)$		$h(X \setminus T)$	
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give		give	True Positive (TP)
give		deny	False Negative (FN)
deny		give	False Positive (FP)

	PP	PN
P	2	1
N	2	1

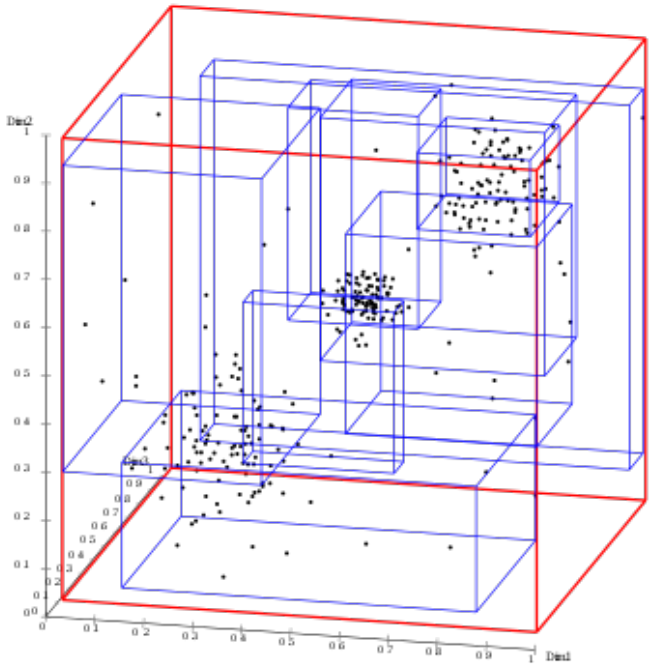
$$\text{Accuracy} = \frac{TP + TN}{N} = \frac{3}{6}$$

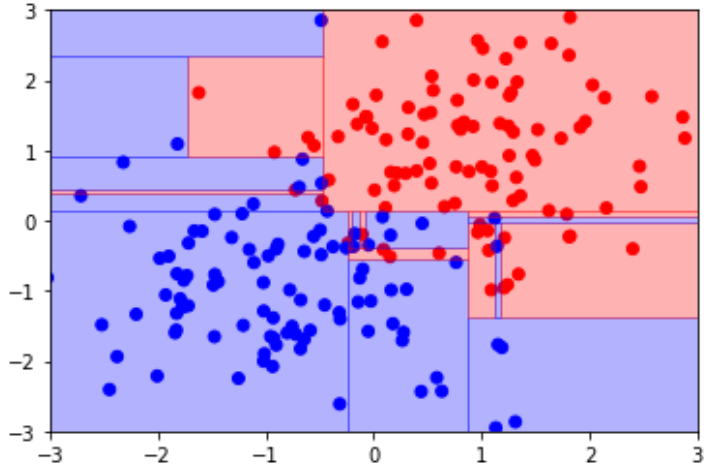
$$\text{Recall} = \frac{TP}{TP + FN} = \frac{2}{3}$$

Outline

The Supervised Decision Tree

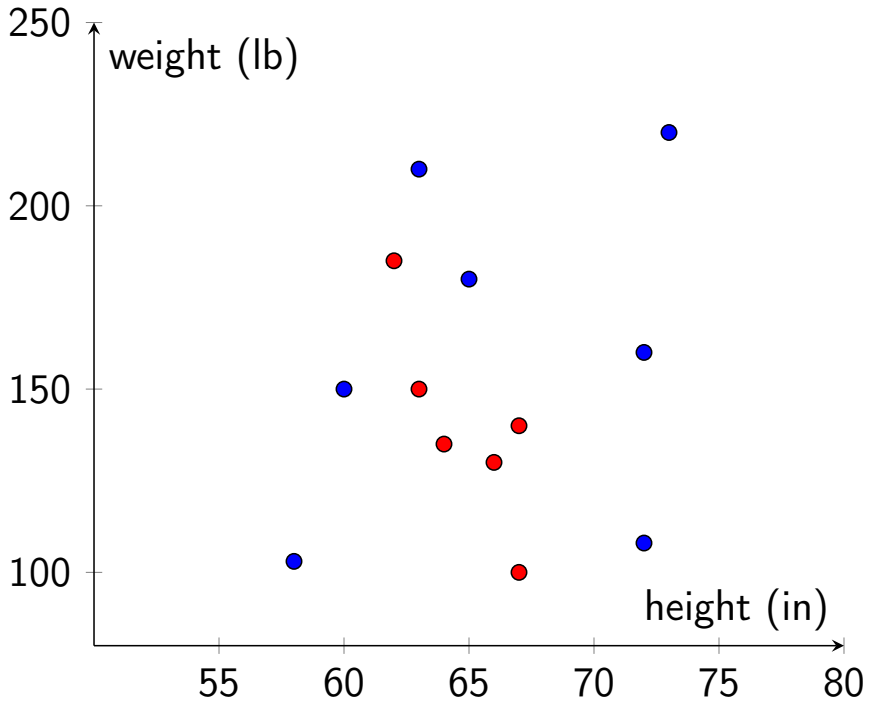
- Decision Trees are a class of discriminative learning algorithm searching the hypothesis space of hyper-rectangles.
- Given a labeled training sample X, a Decision Tree produces a model h mapping partitioned hyper-rectangles in $\mathbb{R}^d$ to target classes.





Decision Tree Induction

- Decision Trees build a model by recursively applying a simple heuristic: select a cut-point on the attribute that maximizes the class purity in the regions resulting from the cut-points partitioning.



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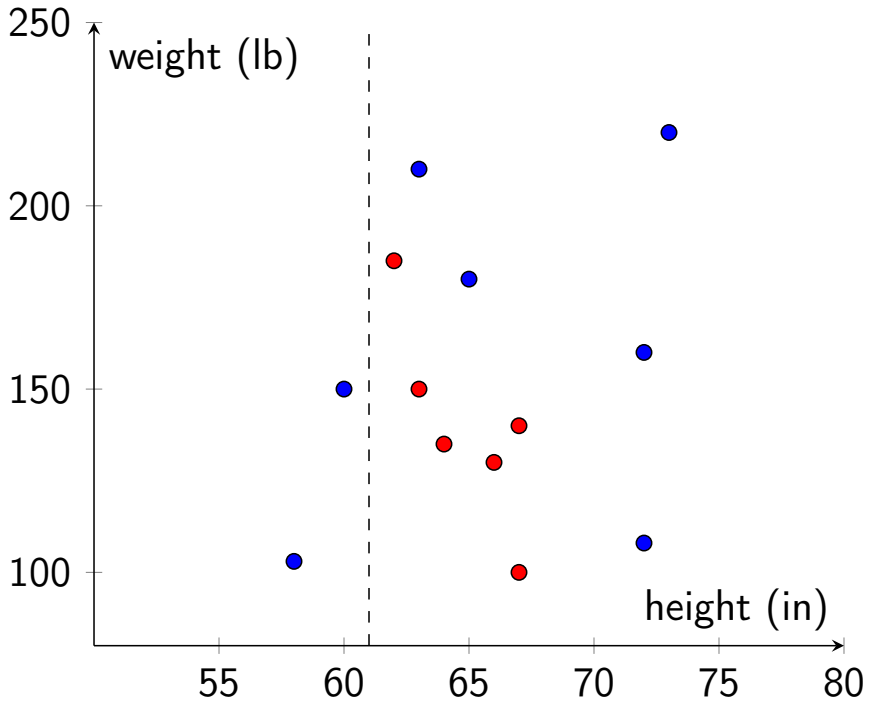

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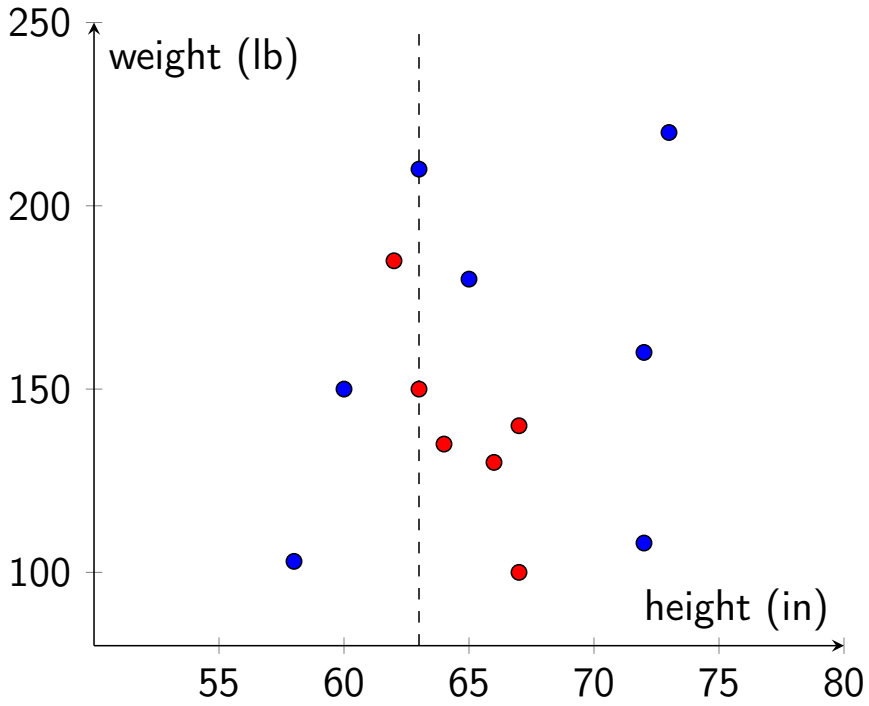

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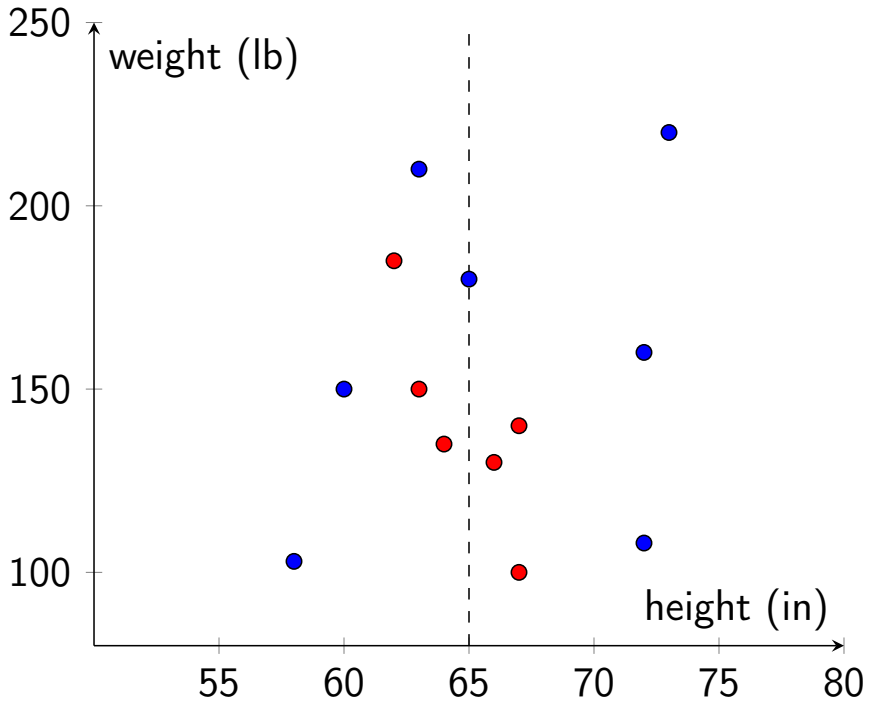

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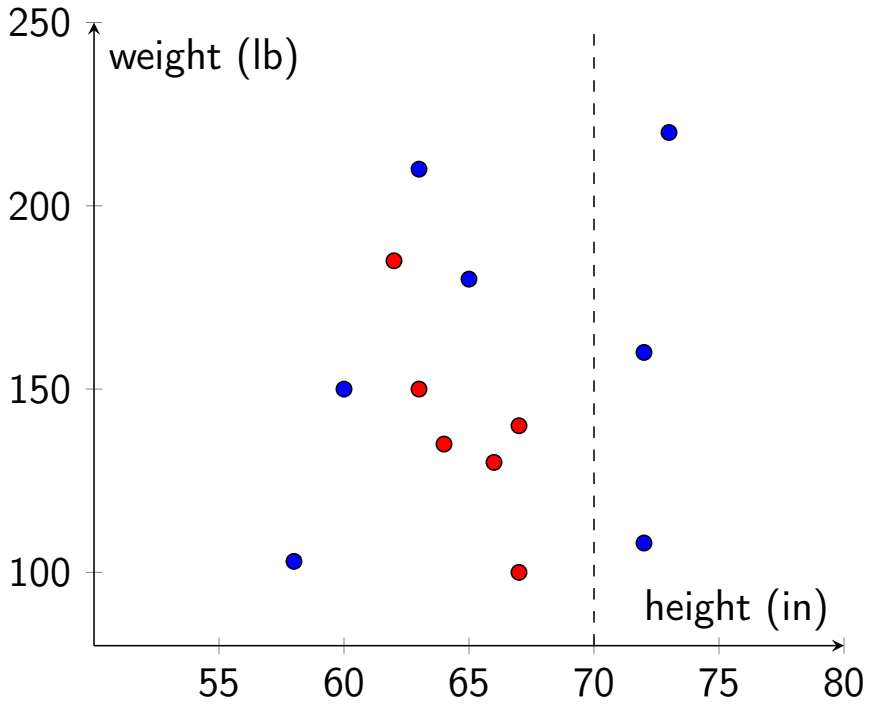

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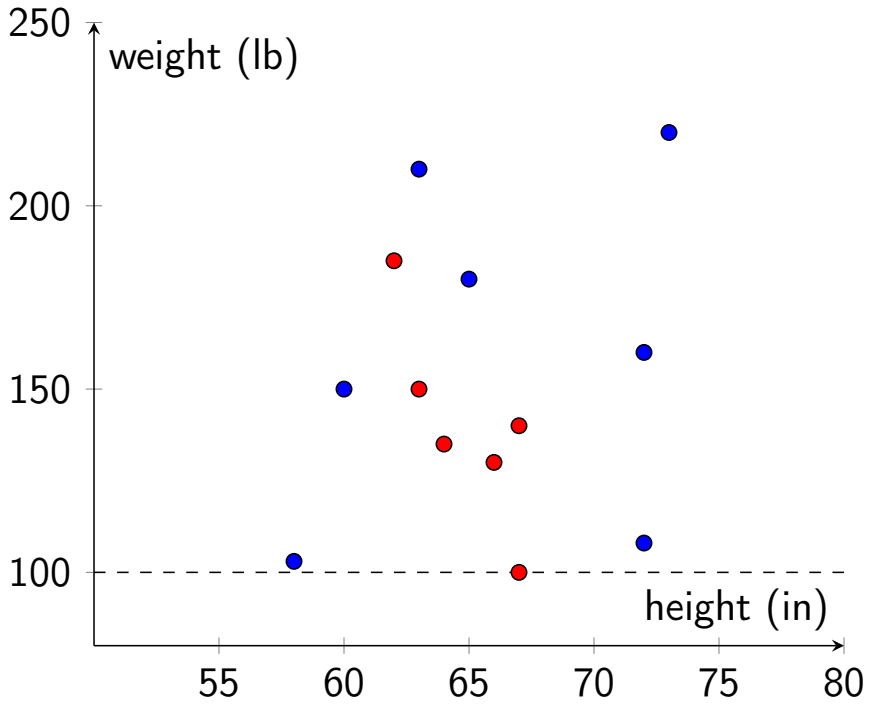

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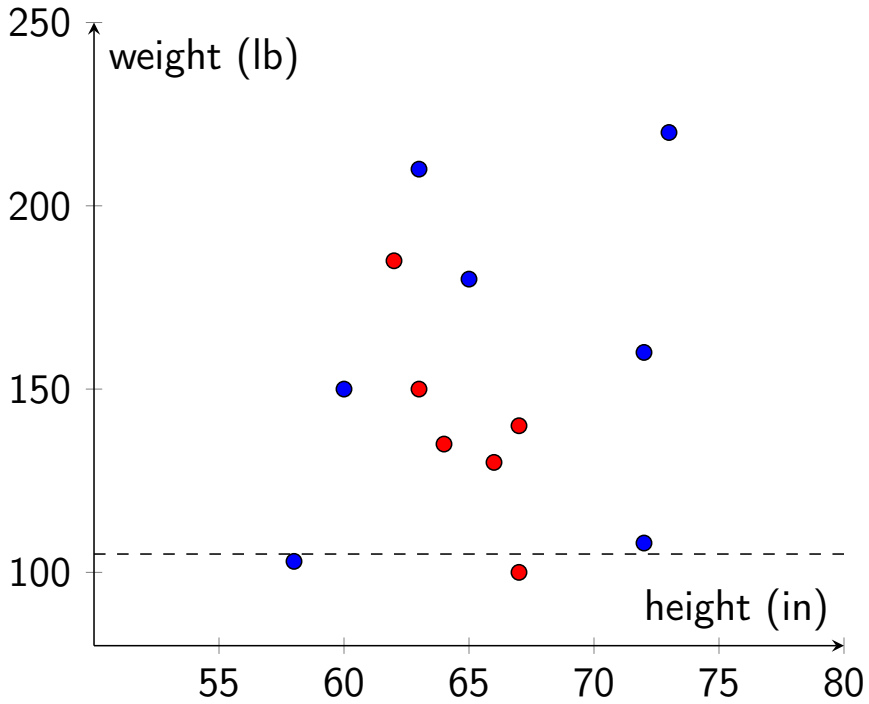

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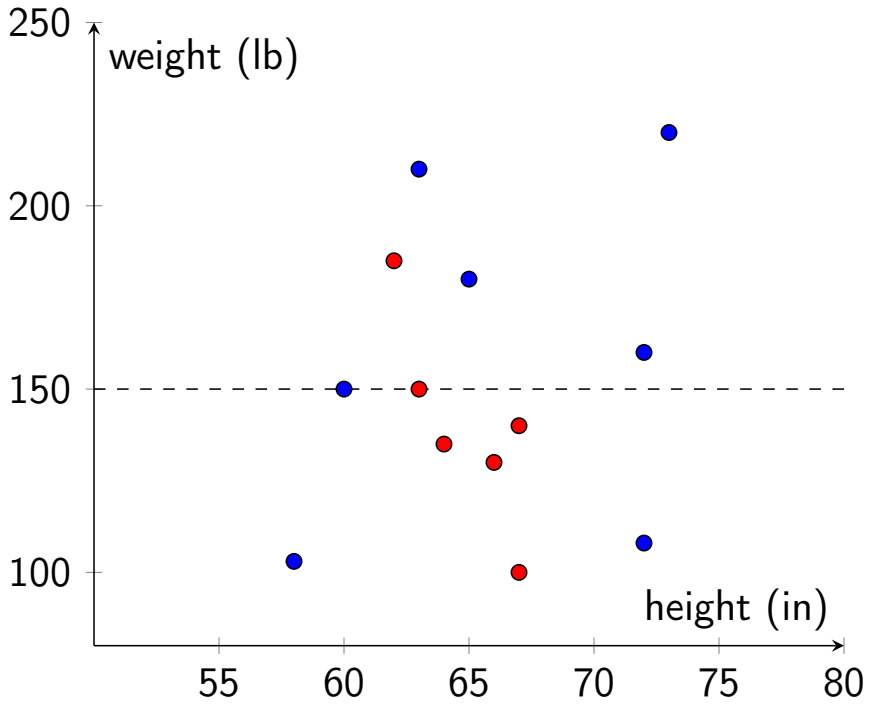

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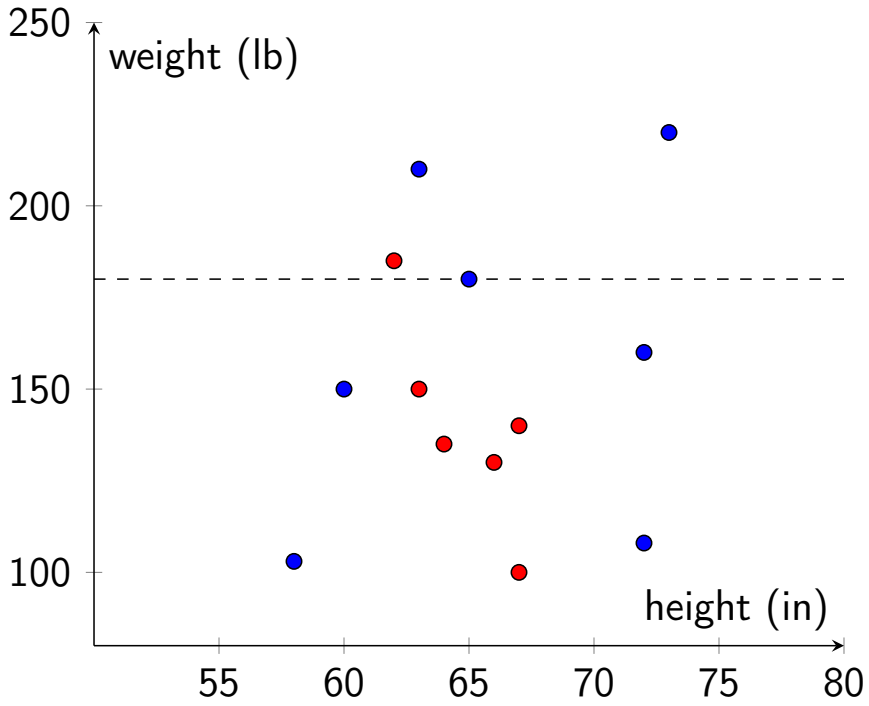

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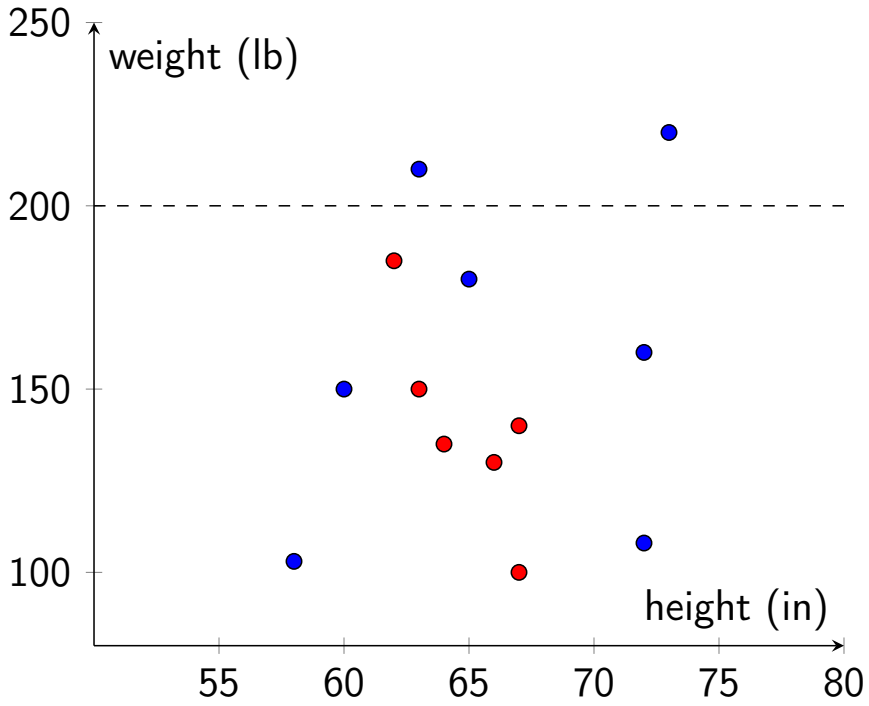

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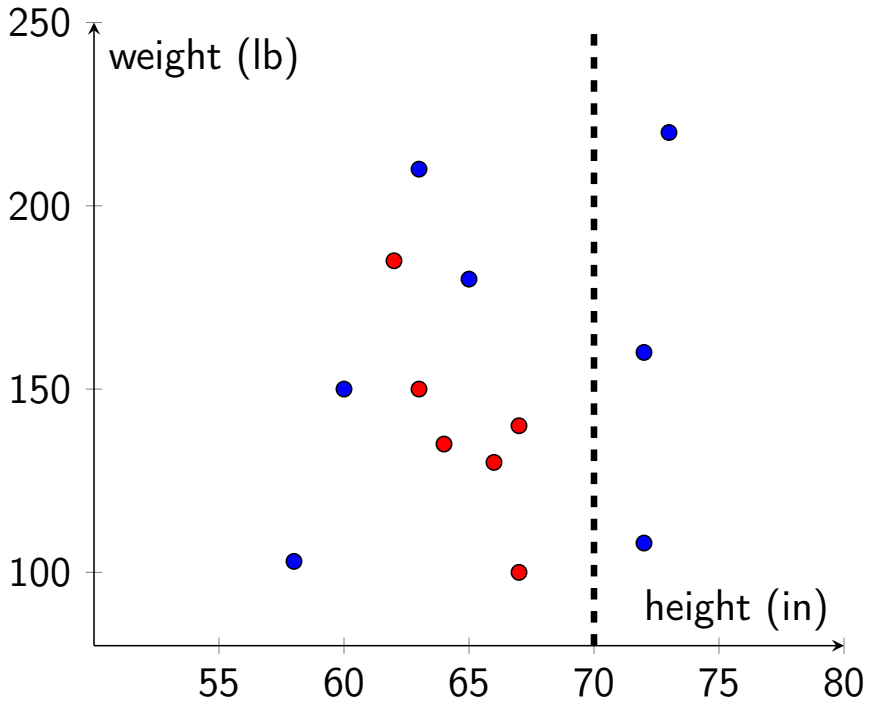

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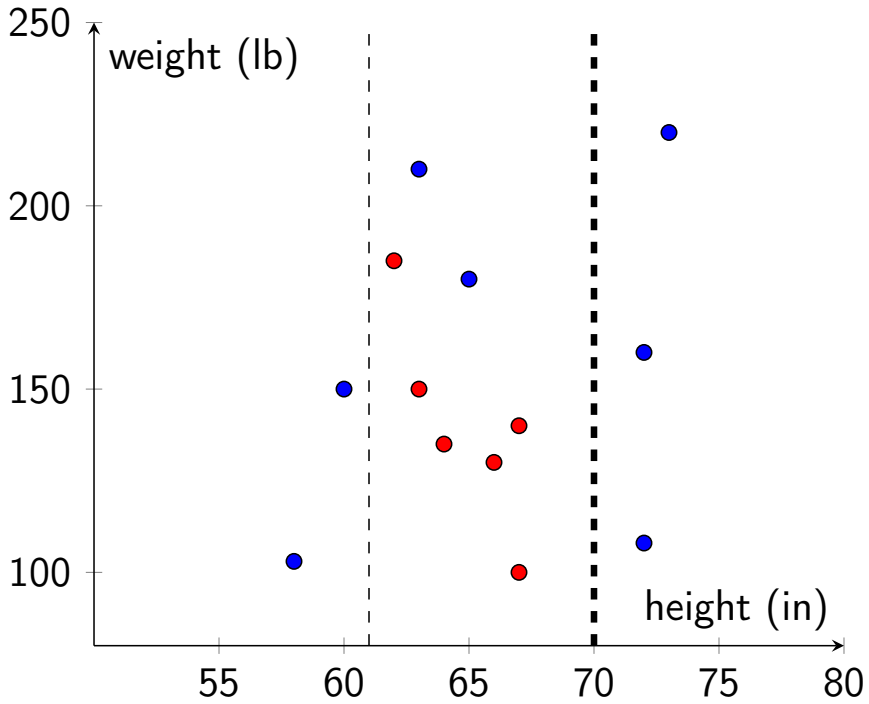

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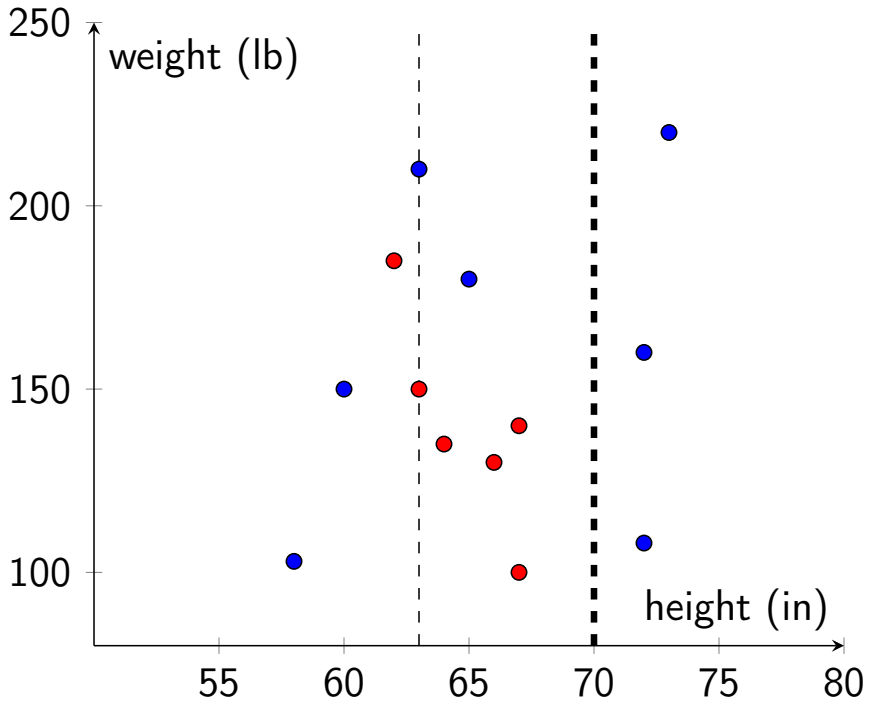

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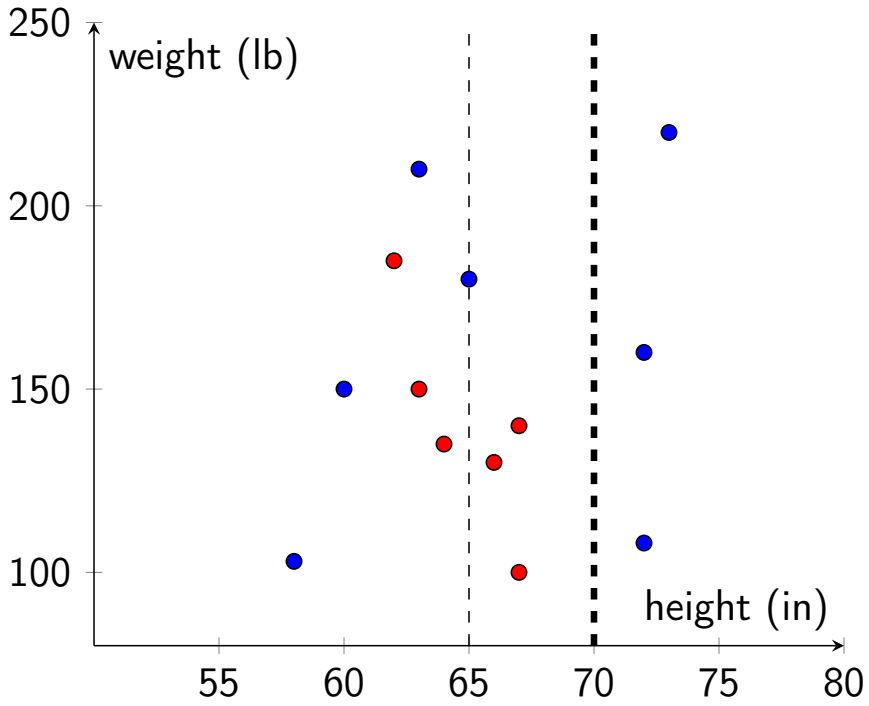

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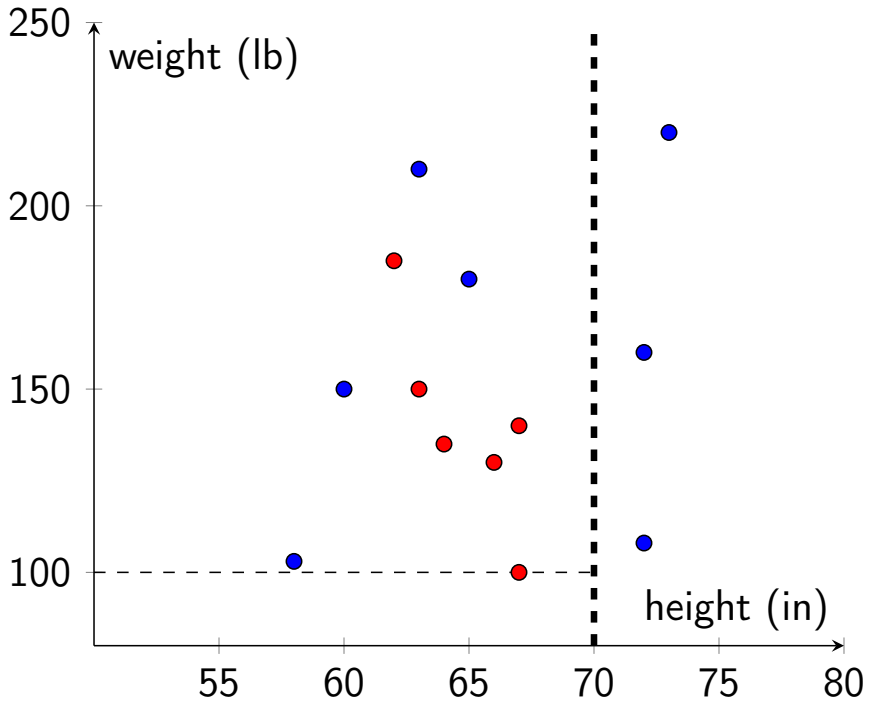

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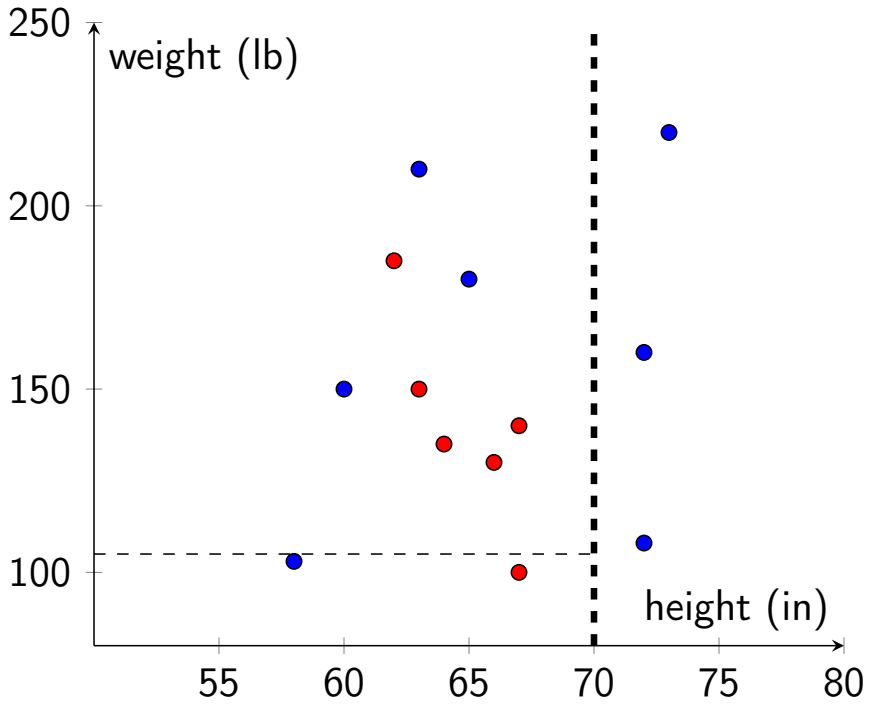

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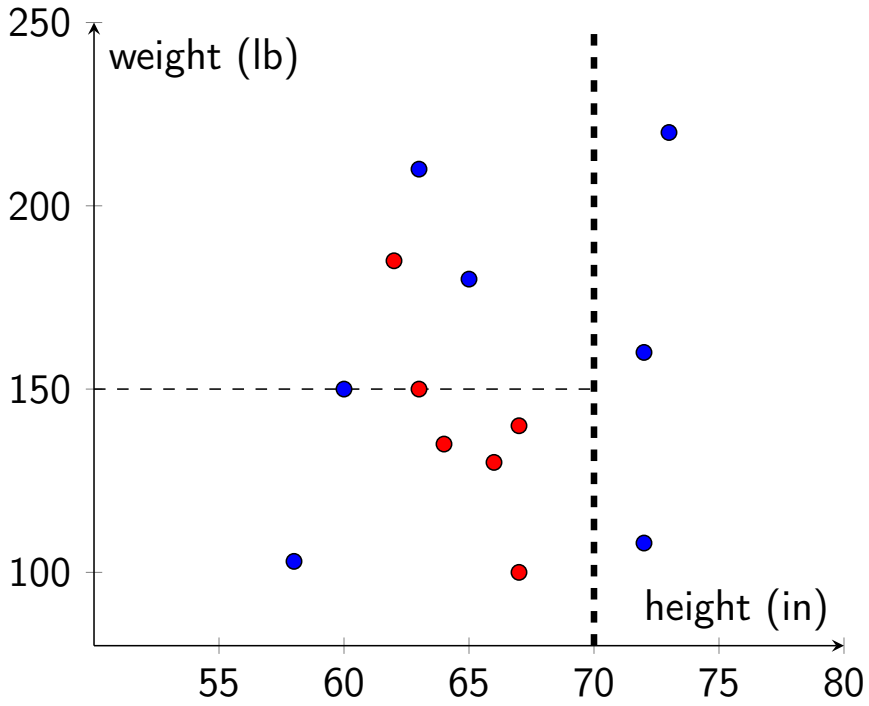

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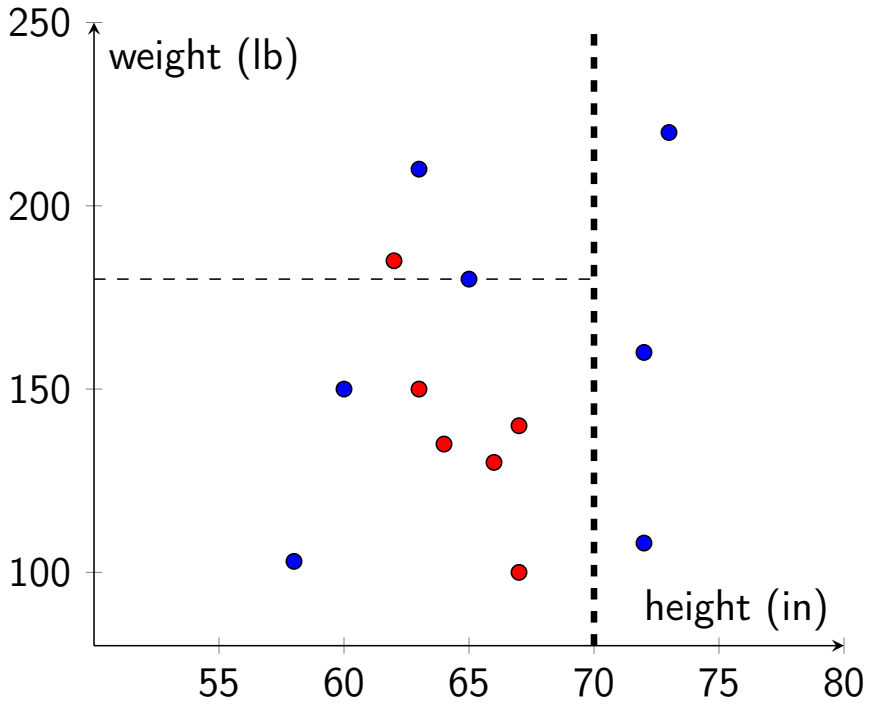

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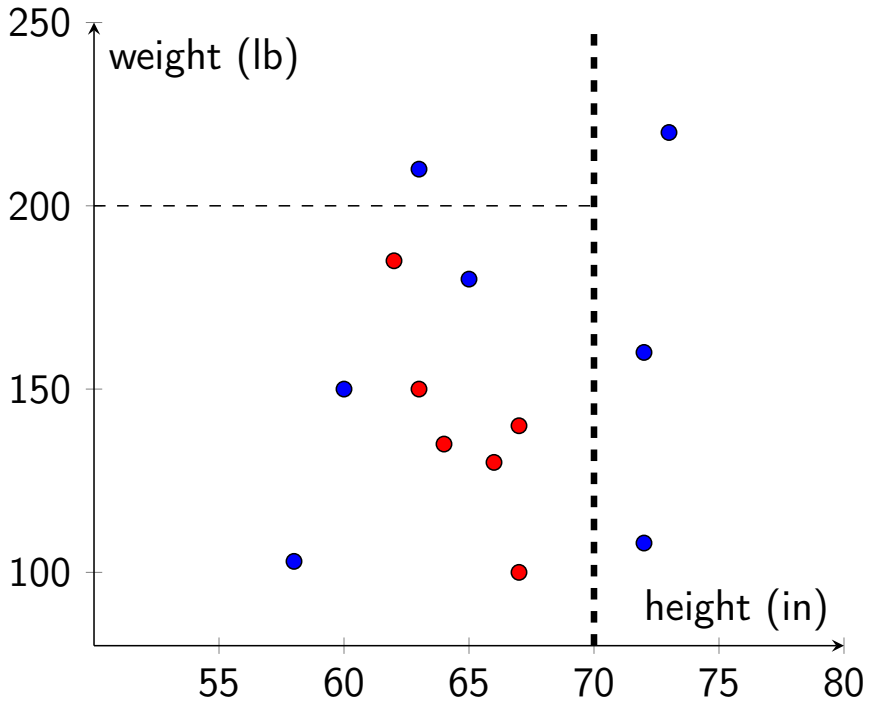

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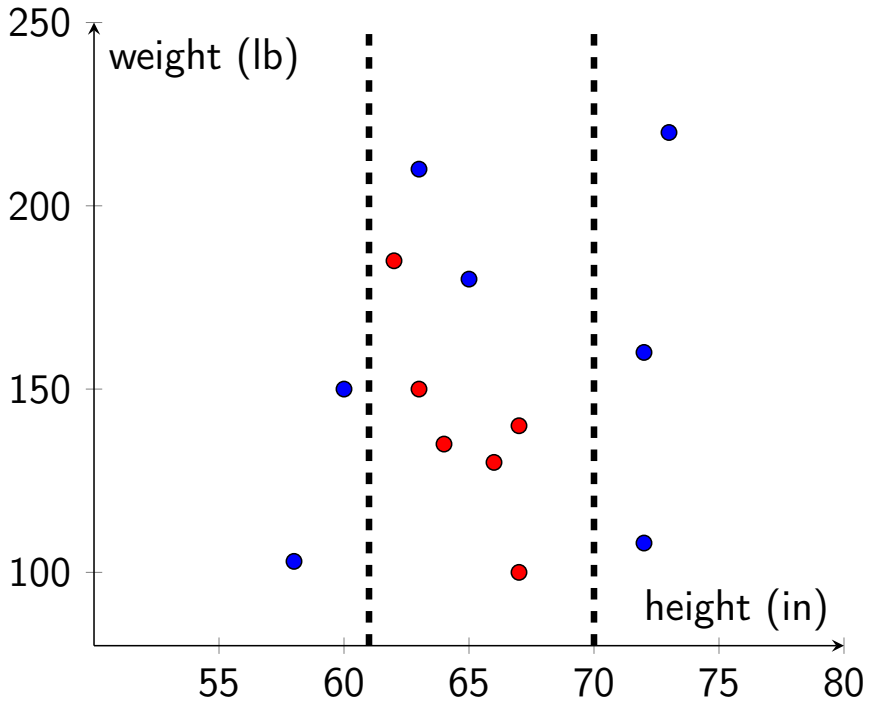

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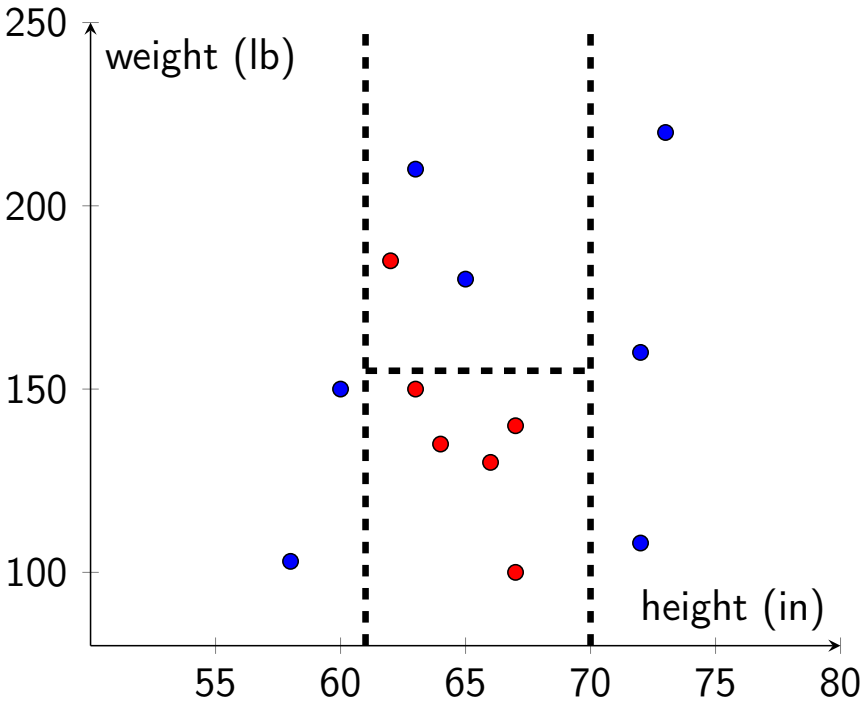
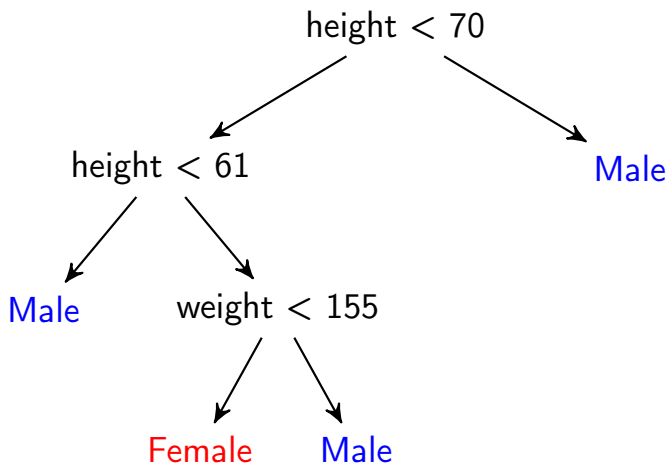
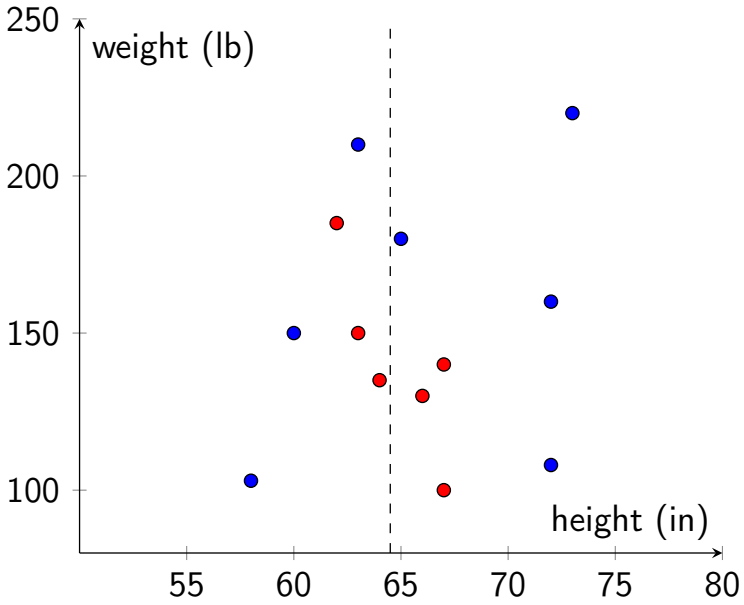




The Impurity Criterion: A Heuristic

- A potential split (partition) induces two class distributions derived from the class distribution of the parent partition.



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$$P_{\text{L,male}} = \frac{3}{6} \qquad P_{\text{R,male}} = \frac{4}{7}$$

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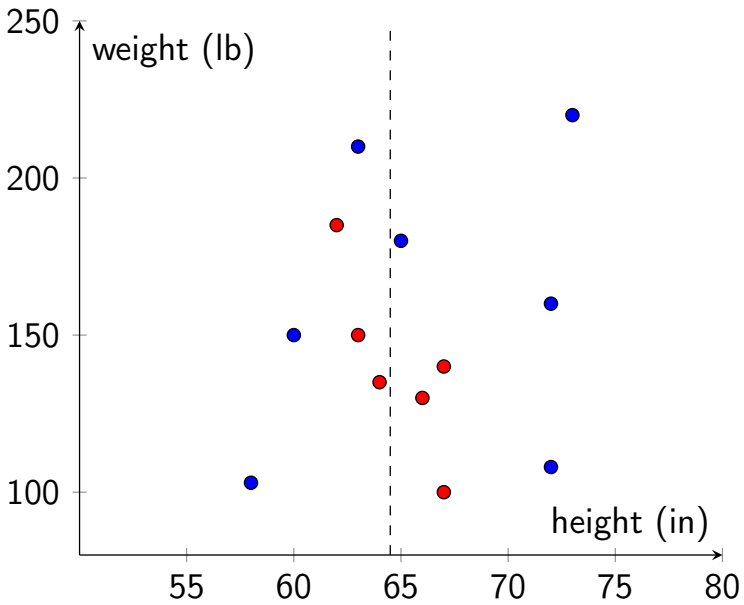

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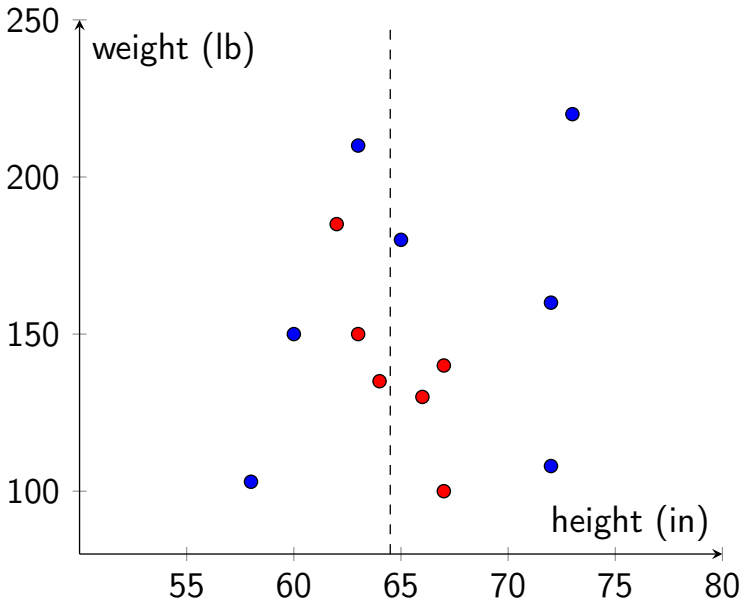

$$\text{Gini}_R = 1 - \sum_{p_c \in P_R} p_c^2$$

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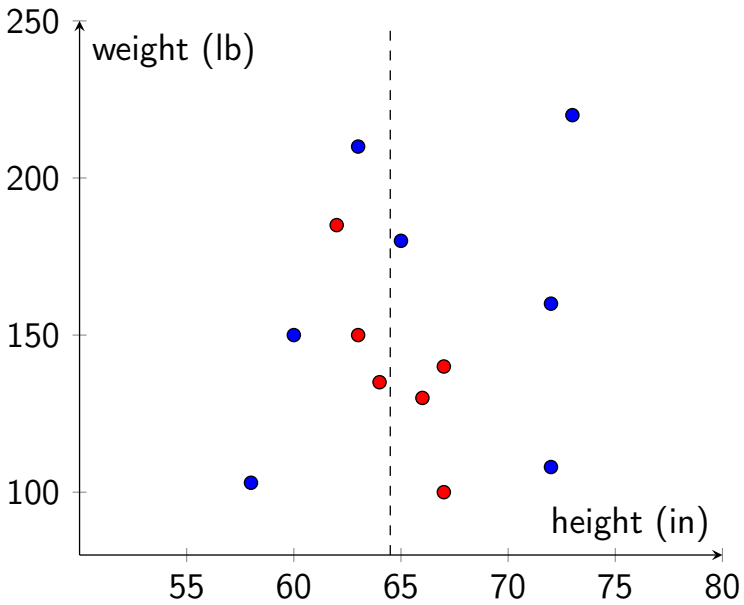

$$\text{Gini}_R = 1 - \sum_{p_c \in P_R} p_c^2$$

$$\text{Gini}_R = 1 - P_R(\text{Male})^2 - P_R(\text{Female})^2$$

Conclusion

Thank you for your attention!
Questions?

https://bit.ly/2tPVPfv

aymulyar@vcu.edu
www.andriymulyar.com