Multiclass Classification, Structured Prediction, & Decision Trees

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Margin for Multiclass

Binary

- Margin for $(x^{(n)}, y^{(n)})$:

$$y^{(n)} w^T x^{(n)} \tag{1}$$

- Want margin to be large and positive ($w^T x^{(n)}$ has same sign as $y^{(n)}$)

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Multiclass

- Class-specific margin for $(x^{(n)}, y^{(n)})$:

$$h(x^{(n)}, y^{(n)}) - h(x^{(n)}, y). \tag{2}$$

- Difference between scores of the correct class and each other class
- Want margin to be large and positive for all $y \neq y^{(n)}$.

Multiclass SVM: separable case

Binary

$$\min_{w} \quad \frac{1}{2}\|w\|^2 \tag{3}$$

$$\text{s.t.} \quad \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}} \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D} \tag{4}$$

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Multiclass As in the binary case, take 1 as our target margin.

$$m_{n,y}(w) \stackrel{\text{def}}{=} \underbrace{\left\langle w, \Psi(x^{(n)}, y^{(n)}) \right\rangle}_{\text{score of correct class}} - \underbrace{\left\langle w, \Psi(x^{(n)}, y) \right\rangle}_{\text{score of other class}} \tag{5}$$

$$\begin{aligned} \min_w \quad & \frac{1}{2}\|w\|^2 && (6) \\ \text{s.t.} \quad & m_{n,y}(w) \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D}, y \neq y^{(n)} && (7) \end{aligned}$$

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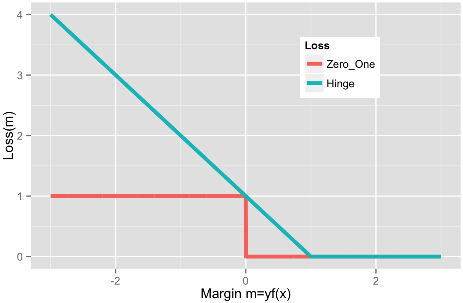
Exercise: write the objective for the non-separable case

Recap: hingle loss for binary classification

- Hinge loss: a convex upperbound on the 0-1 loss

$$\ell_{\text{hinge}}(y,\hat{y}) = \max(0, 1 - yh(x)) \tag{8}$$



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- Upper bound on $\Delta(y, y')$.

$$\hat{y} \overset{\text{def}}{=} \underset{y' \in \mathcal{Y}}{\arg\max} \left\langle w, \Psi(x, y') \right\rangle \tag{10}$$

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$$\Longrightarrow \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, (\Psi(x, y) - \Psi(x, \hat{y})) \rangle \qquad \text{When are they equal?} \tag{12}$$

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- Generalized hinge loss:

$$\ell_{\text{hinge}}(y,x,w) \overset{\text{def}}{=} \max_{y' \in \mathcal{Y}} \left(\Delta(y,y') - \left\langle w, \left(\Psi(x,y) - \Psi(x,y')\right)\right\rangle\right) \tag{13}$$

Multiclass SVM with Hinge Loss

- Recall the hinge loss formulation for binary SVM (without the bias term):

$$\min_{w \in \mathrm{R}^d} \frac{1}{2}||w||^2 + C \sum_{n=1}^{N} \max\left(0, 1 - \underbrace{y^{(n)} w^T x^{(n)}}_{\text{margin}}\right).$$

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- The multiclass objective:

$$\min_{w\in\mathbb{R}^d} \frac{1}{2}||w||^2 + C\sum_{n=1}^{N} \max_{y'\in\mathcal{Y}}\left(\Delta(y, y') - \underbrace{\left\langle w, \left(\Psi(x, y) - \Psi(x, y')\right)\right\rangle}_{\text{margin}}\right)$$

  - $\Delta(y, y')$ as target margin for each class.
  - If margin $m_{n,y'}(w)$ meets or exceeds its target $\Delta(y^{(n)}, y')$ $\forall y \in \mathcal{Y}$, then no loss on example n.

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  - Predict with $\arg\max_{y \in \mathcal{Y}} h_y(x)$.
  - Gave simple example where this fails for linear classifiers
- Solution 2: Multiclass loss
  - Train one model: $h(x, y) : \mathcal{X} \times \mathcal{Y} \to \mathrm{R}$.
  - Prediction involves solving $\arg\max_{y \in \mathcal{Y}} h(x, y)$.

Does it work better in practice?

- Paper by Rifkin & Klautau: "In Defense of One-Vs-All Classification" (2004)
  - Extensive experiments, carefully done
    - albeit on relatively small UCI datasets
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    - (or at least, the advantages claimed by earlier papers for multiclass methods were not compelling)
- Compared
  - many multiclass frameworks (including the one we discuss)
  - one-vs-all for SVMs with RBF kernel
  - one-vs-all for square loss with RBF kernel (for classification!)
- All performed roughly the same

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- The framework we have developed for multiclass
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- Generalizes to situations where k is very large and one-vs-all is intractable.
- Key idea is that we can generalize across outputs y by using features of y.

Introduction to Structured Prediction

Example: Part-of-speech (POS) Tagging

- Given a sentence, give a part of speech tag for each word:

x	$\underbrace{\text{[START]}}_{x_0}$	$\underbrace{\text{He}}_{x_1}$	$\underbrace{\text{eats}}_{x_2}$	$\underbrace{\text{apples}}_{x_3}$
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- $\mathcal{P} = \{\text{START}, \text{Pronoun}, \text{Verb}, \text{Noun}, \text{Adjective}\}$
- $\mathcal{Y} = \mathcal{P}^n, \ n = 1, 2, 3, \ldots$[Part of speech sequence of any length]

Multiclass Hypothesis Space

- Discrete output space: $\mathcal{Y}(x)$
  - Very large but has structure, e.g., linear chain (sequence labeling), tree (parsing)
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- Multiclass hypothesis space

$$\mathcal{F} = \left\{ x \mapsto \operatorname*{arg\,max}_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$

- Final prediction function is an $f \in \mathcal{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.

Structured Prediction

- Part-of-speech tagging

$x:$	he	eats	apples
$y:$	pronoun	verb	noun

- Multiclass hypothesis space:

$$h(x,y) = w^T \Psi(x,y) \tag{14}$$

$$\mathcal{F} = \left\{ x \mapsto \operatorname*{arg\,max}_{y \in \mathcal{Y}} h(x,y) \mid h \in \mathcal{H} \right\} \tag{15}$$

- A special case of multiclass classification
- How to design the feature map Ψ? What are the considerations?

Unary features

- A **unary feature** only depends on
  - the label at a single position, y_i, and x
- Example:

$$\begin{aligned}
\phi_1(x, y_i) &= \mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Verb}] \\
\phi_2(x, y_i) &= \mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Noun}] \\
\phi_3(x, y_i) &= \mathbb{1}[x_{i-1} = \text{He}]\mathbb{1}[x_i = \text{runs}]\mathbb{1}[y_i = \text{Verb}]
\end{aligned}$$

Markov features

- A **markov feature** only depends on
  - two adjacent labels, y_{i-1} and y_i, and x
- Example:

$$\begin{aligned} \theta_1(x, y_{i-1}, y_i) &= \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Verb}] \\ \theta_2(x, y_{i-1}, y_i) &= \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Noun}] \end{aligned}$$

- Reminiscent of Markov models in the output space
- Possible to have higher-order features

Local Feature Vector and Compatibility Score

- At each position i in sequence, define the **local feature vector** (unary and markov):

$$\begin{aligned}\Psi_i(x, y_{i-1}, y_i) \quad = \quad & (\phi_1(x, y_i), \phi_2(x, y_i), \ldots, \\ & \theta_1(x, y_{i-1}, y_i), \theta_2(x, y_{i-1}, y_i), \ldots)\end{aligned}$$

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- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.

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- And **local compatibility score** at position i: $\langle w, \Psi_i(x, y_{i-1}, y_i)\rangle$.

- The compatibility score for (x, y) is the sum of local compatibility scores:

$$\sum_i \langle w, \Psi_i(x, y_{i-1}, y_i)\rangle = \left\langle w, \sum_i \Psi_i(x, y_{i-1}, y_i)\right\rangle = \langle w, \Psi(x, y)\rangle, \tag{16}$$

where we define the **sequence feature vector** by

$$\Psi(x, y) = \sum_i \Psi_i(x, y_{i-1}, y_i). \qquad \text{decomposable}$$

Structured perceptron

```
Given a dataset $\mathcal{D} = \{(x, y)\}$;
Initialize $w \leftarrow 0$;
for $iter = 1, 2, \ldots, T$ do
    for $(x, y) \in \mathcal{D}$ do
        $\hat{y} = \arg\max_{y' \in \mathcal{Y}(x)} w^T \psi(x, y')$;
        if $\hat{y} \neq y$ then // We've made a mistake
            $w \leftarrow w + \Psi(x, y)$ ; // Move the scorer towards $\psi(x, y)$
            $w \leftarrow w - \Psi(x, \hat{y})$ ; // Move the scorer away from $\psi(x, \hat{y})$
        end
    end
end
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```

Identical to the multiclass perceptron algorithm except the $\arg\max$ is now over the structured output space $\mathcal{Y}(x)$.

Structured hinge loss

- Recall the generalized hinge loss

$$\ell_{\text{hinge}}(y,\hat{y}) \overset{\text{def}}{=} \max_{y' \in \mathcal{Y}(x)} \left(\Delta(y,y') + \left\langle w, \left(\Psi(x,y') - \Psi(x,y)\right)\right\rangle\right) \tag{17}$$

- What is $\Delta(y,y')$ for two sequences?

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- What is $\Delta(y, y')$ for two sequences?
- **Hamming loss** is common:

$$\Delta(y, y') = \frac{1}{L} \sum_{i=1}^{L} \mathbb{1}[y_i \neq y_i']$$

where L is the sequence length.

Structured SVM

Exercise:

- Write down the objective of structured SVM using the structured hinge loss.
- Stochastic sub-gradient descent for structured SVM
- Compare with the structured perceptron algorithm

The argmax problem for sequences

Problem To compute predictions, we need to find $\arg\max_{y \in \mathcal{Y}(x)} \langle w, \Psi(x, y) \rangle$, and $|\mathcal{Y}(x)|$ is exponentially large.

Figure by Daumé III. A course in machine learning. Figure 17.1.

The argmax problem for sequences

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Observation $\Psi(x, y)$ decomposes to $\sum_i \Psi_i(x, y)$.

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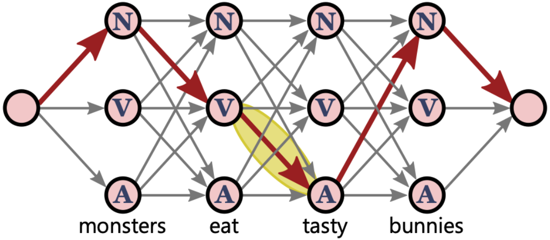
Solution Dynamic programming (similar to the Viterbi algorithm)



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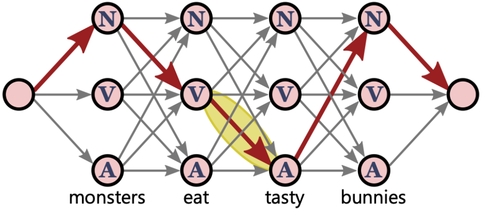
Structured SVM inference (linear chain)



- Initiate $\alpha_j(1) = w^\top \psi(y_1 = j, x_1)$

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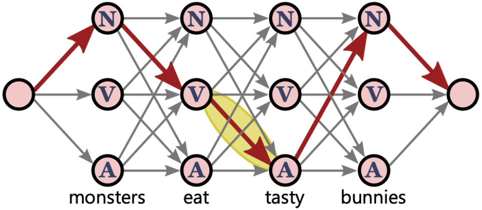

- Initiate $\alpha_j(1) = w^\top \psi(y_1 = j, x_1)$
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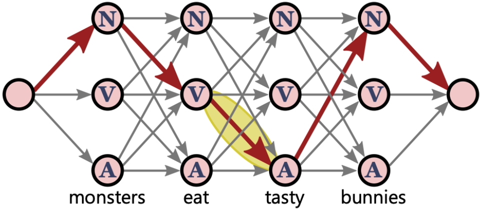

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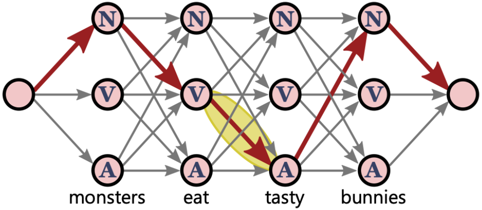

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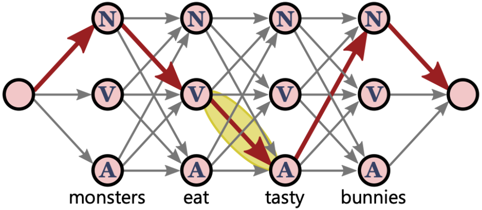

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What's the running time?

The argmax problem in general

Efficient problem-specific algorithms:

problem	structure	algorithm
constituent parsing	binary trees with context-free features	CYK
dependency parsing	spanning trees with edge features	Chu-Liu-Edmonds
image segmentation	2d with adjacent-pixel features	graph cuts

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General algorithm:

- Integer linear programming (ILP)

$$\max_z a^T z \quad \text{s.t. linear constraints on } z \tag{18}$$

- z: indicator of substructures, e.g., $\mathbb{I}\{y_i = \text{article and } y_{i+1} = \text{noun}\}$
- constraints: z must correspond to a valid structure

Conditional random field (CRF)

- Recall that we can write logistic regression in a general form:

$$p(y|x) = \frac{1}{Z(x)} \exp(w^\top \psi(x,y)).$$

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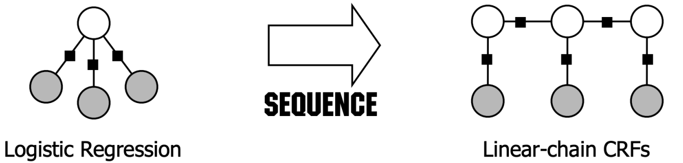
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



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- Compared to Structured SVM, CRF has a probabilistic interpretation.
- We can draw samples in the output space.
- How do we learn w? Maximum log likelihood, and regularization term: $\lambda\|w\|^2$.
- $p(y|x) = \frac{1}{Z(x)}\exp(w^\top \psi(x,y))$.
- Loss function:

$$\begin{aligned} l(w) &= -\frac{1}{N}\sum_{i=1}^{N}\log p(y^{(i)}|x^{(i)}) + \frac{1}{2}\lambda\|w\|^2 \\ &= -\frac{1}{N}\sum_i\sum_t\sum_k w_k\psi_k(y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_i \log Z(x^{(i)}) + \frac{1}{2}\sum_k \lambda w_k^2 \end{aligned}$$

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- Gradient:

$$\frac{\partial l(w)}{\partial w_k} = -\frac{1}{N}\sum_i \sum_t \sum_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) \tag{19}$$

$$+\frac{1}{N}\sum_i \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_t \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_t, y'_{t-1})) + \sum_k \lambda w_k \tag{20}$$

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- To compute the gradient, we need to infer expectation under the model distribution $p(y|x)$.
- Compare the learning algorithms: in structured SVM we need to compute the argmax, whereas in CRF we need to compute the model expectation.
- Both problems are NP-hard for general graphs.

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- In general graphs, we rely on approximate inference (e.g. loopy belief propagation).

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- Semantic segmentation
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- Multi-label learning
  An image may contain multiple class labels, e.g. a bus is likely to co-occur with a car.

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- Structured prediction: Structured SVM, CRF. Data containing structure. Extremely large output space. Text and image applications. More in-depth content in a probabilistic graphical model (PGM) course.

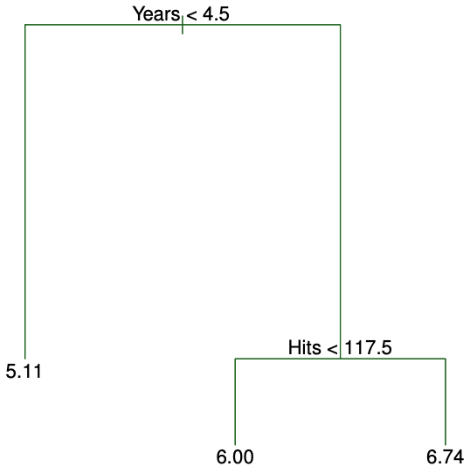
Decision Trees

Overview: Decision Trees

- Our first inherently non-linear classifier: decision trees.
- Ensemble methods: bagging and boosting.

Decision Trees

Regression trees: Predicting basketball players' salaries



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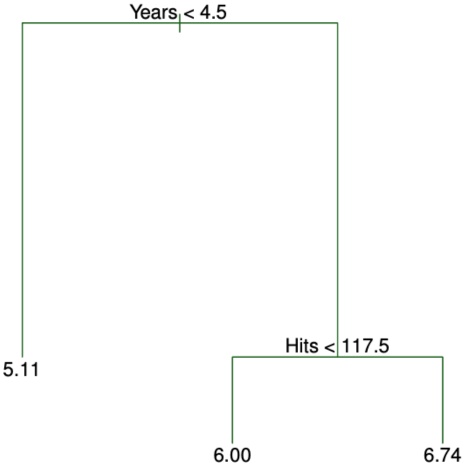
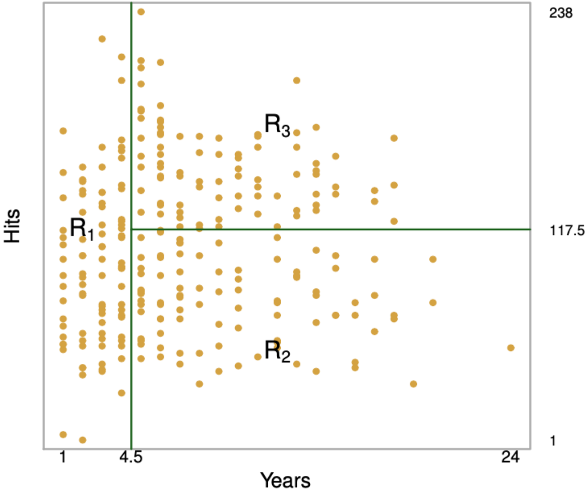
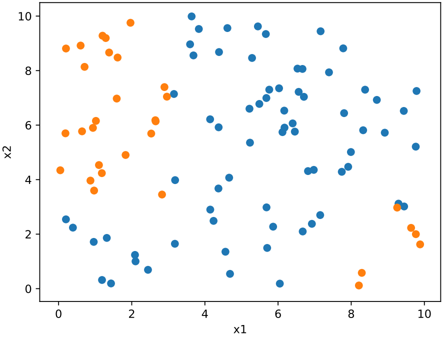




Classification trees



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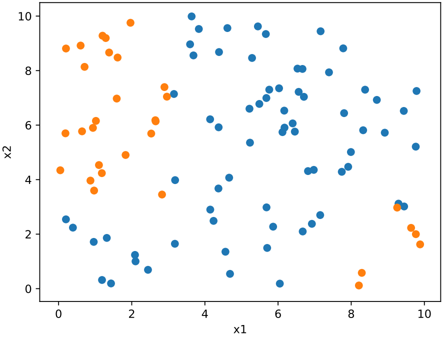
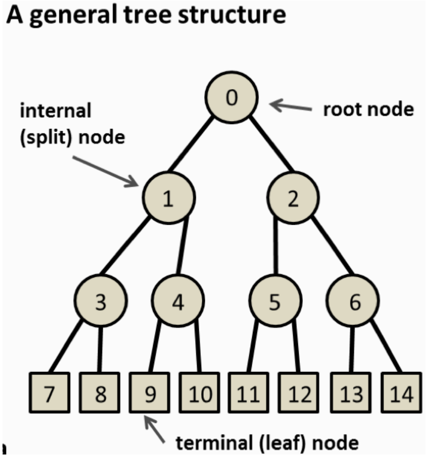


- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



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From Criminisi et al. MSR-TR-2011-114, 28 October 2011.

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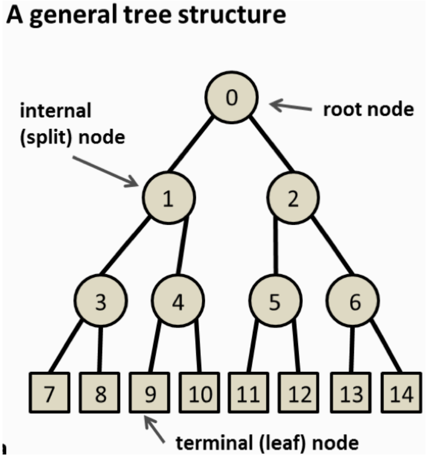

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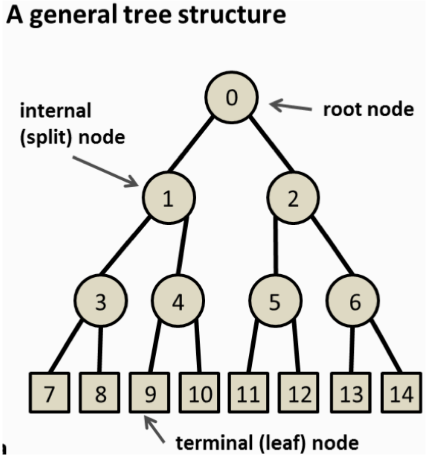

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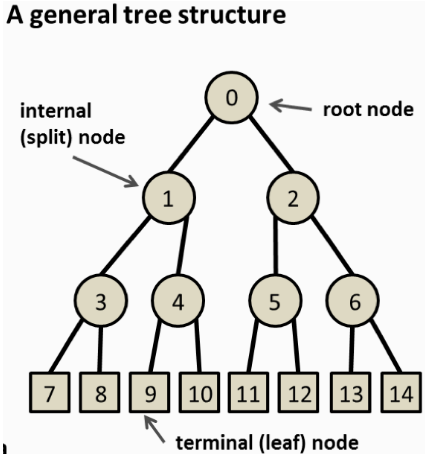

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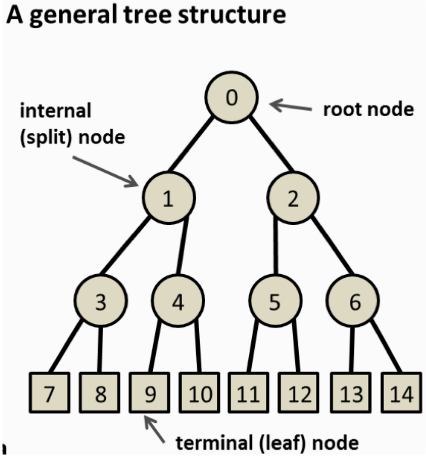

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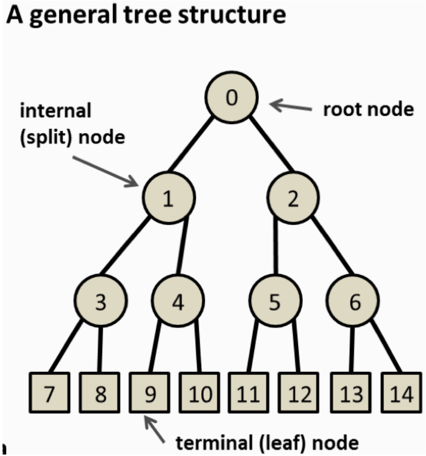

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- Predictions are made in terminal nodes

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Constructing the tree

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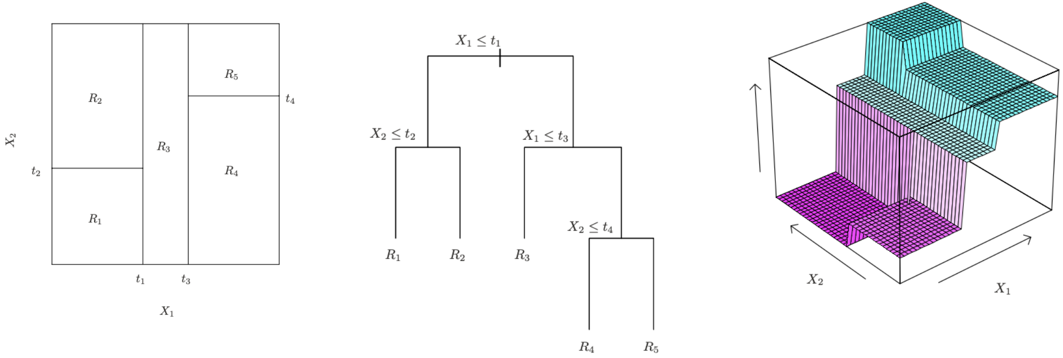
Prediction in a Regression Tree



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- It is common to split half way between two adjacent values:

$$s_j \in \left\{ \frac{1}{2}\left(x_{j(r)} + x_{j(r+1)}\right) \mid r = 1, \ldots, n-1 \right\}. \qquad n-1 \text{ splits} \qquad (25)$$

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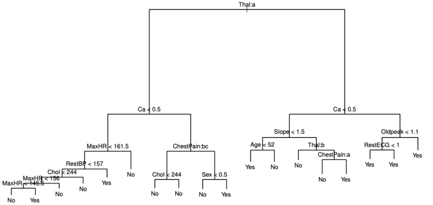
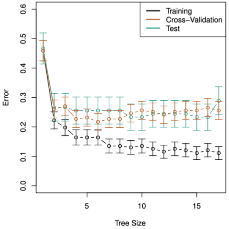
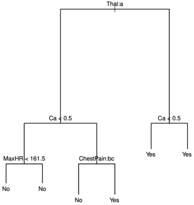
    2. *Prune* the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

Pruning: Example







What Makes a Good Split for Classification?

Our plan is to predict the **majority label** in each region.

Which of the following splits is better?

Split 1	$R_1 : 8+/2-$	$R_2 : 2+/8-$
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Intuition: we want to produce *pure* nodes, i.e. nodes where most instances have the same class.

Misclassification error in a node

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- We predict the majority class in node m:

$$k(m) = \arg\max_k \hat{p}_{mk}$$

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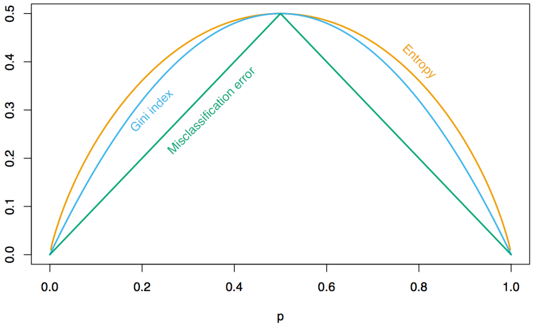
  - Entropy / Information gain
    $$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$$
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

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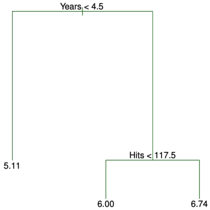
- Let $Q(R_L)$ and $Q(R_R)$ be the node impurity measures for each node.
- We aim to find a split that minimizes the *weighted average of node impurities*:

$$\frac{N_L Q(R_L) + N_R Q(R_R)}{N_L + N_R}$$

Discussion: Interpretability of Decision Trees



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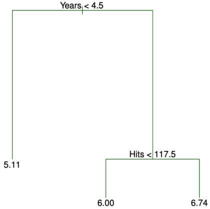
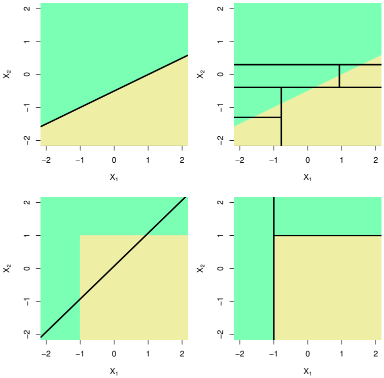


- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

Discussion: Trees vs. Linear Models

Trees may have to work hard to capture linear decision boundaries, but can easily capture certain nonlinear ones:



Discussion: Review

Decision trees are:

- Non-linear: the decision boundary that results from splitting may end up being quite complicated

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Additional pros:

- Interpretable and simple to understand

Cons:

- Struggle to capture linear decision boundaries
- They have high variance and tend to overfit: they are sensitive to small changes in the training data (The ensemble techniques we discuss next can mitigate these issues)