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^Tx⁽ⁿ⁾ has same sign as y⁽ⁿ⁾)
Multiclass
Class-specific margin for (x⁽ⁿ⁾, y⁽ⁿ⁾):

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

$$\min_{w} \quad \frac{1}{2} \|w\|^{2} \qquad (3)$$

s.t.
$$\underbrace{y^{(n)}w^{T}x^{(n)}}_{\cdot} \ge 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D} \qquad (4)$$

margin

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

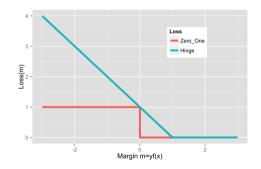
Exercise: write the objective for the non-separable case

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Recap: hingle loss for binary classification

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

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



(8)

Generalized hinge loss

• What's the zero-one loss for multiclass classification?

$$\Delta(\mathbf{y},\mathbf{y}') = \mathbb{I}\left\{\mathbf{y}\neq\mathbf{y}'\right\} \tag{9}$$

- In general, can also have different cost for each class.
- Upper bound on $\Delta(y, y')$.

$$\hat{y} \stackrel{\text{def}}{=} \arg\max_{y' \in \mathcal{Y}} \langle w, \Psi(x, y') \rangle \tag{10}$$
$$\longrightarrow \langle w, \Psi(x, y) \rangle \leq \langle w, \Psi(x, \hat{y}) \rangle \tag{11}$$

$$\implies \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, (\Psi(x, y) - \Psi(x, \hat{y})) \rangle \qquad \text{When are they equal?}$$
(11)
$$\implies \Delta(y, \hat{y}) \leqslant \Delta(y, \hat{y}) - \langle w, (\Psi(x, y) - \Psi(x, \hat{y})) \rangle \qquad \text{When are they equal?}$$
(12)

• Generalized hinge loss:

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

Multiclass SVM with Hinge Loss

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

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

• The multiclass objective:

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

- $\Delta(y, y')$ 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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Recap: What Have We Got?

- Problem: Multiclass classification $\mathcal{Y} = \{1, \dots, k\}$
- Solution 1: One-vs-All
 - Train k models: $h_1(x), \ldots, h_k(x) : \mathfrak{X} \to \mathsf{R}$.
 - 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: $h(x, y) : \mathfrak{X} \times \mathfrak{Y} \to \mathsf{R}$.
 - 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
 - Suggests one-vs-all works just as well in practice
 - (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

Why Are We Bothering with Multiclass?

- The framework we have developed for multiclass
 - compatibility features / scoring functions
 - multiclass margin
 - target margin / multiclass loss
- 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	[START]	$\underbrace{\operatorname{He}}_{x_1}$	eats _{x2}	$\underbrace{apples}_{x_3}$
у	[START]	$\underbrace{Pronoun}_{y_1}$	\underbrace{Verb}_{y_2}	Noun y ₃

- $\mathcal{V} = \{ all \ English \ words \} \cup \{ [START], "." \} \}$
- $\mathcal{X} = \mathcal{V}^n$, n = 1, 2, 3, ... [Word sequences of any length]
- $\mathcal{P} = \{ \mathsf{START}, \mathsf{Pronoun}, \mathsf{Verb}, \mathsf{Noun}, \mathsf{Adjective} \}$
- $\mathcal{Y} = \mathcal{P}^n$, $n = 1, 2, 3, \dots$ [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)
 - Size depends on input x
- Base Hypothesis Space: $\mathcal{H} = \{h : \mathcal{X} \times \mathcal{Y} \to \mathsf{R}\}$
 - h(x, y) gives compatibility score between input x and output y
- 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 $f \in \mathfrak{F}$.
- For each $f \in \mathcal{F}$ there is an underlying compatibility score function $h \in \mathcal{H}$.

Structured Prediction

• Part-of-speech tagging

<i>x</i> :	he	eats	apples
<i>y</i> :	pronoun	verb	noun

• Multiclass hypothesis space:

$$h(x, y) = w^{T} \Psi(x, y)$$
(14)
$$\mathcal{F} = \left\{ x \mapsto \operatorname*{arg\,max}_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$
(15)

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

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

$$\begin{aligned} \varphi_1(x, y_i) &= \mathbb{1}[x_i = \operatorname{runs}]\mathbb{1}[y_i = \operatorname{Verb}] \\ \varphi_2(x, y_i) &= \mathbb{1}[x_i = \operatorname{runs}]\mathbb{1}[y_i = \operatorname{Noun}] \\ \varphi_3(x, y_i) &= \mathbb{1}[x_{i-1} = \operatorname{He}]\mathbb{1}[x_i = \operatorname{runs}]\mathbb{1}[y_i = \operatorname{Verb}] \end{aligned}$$

Markov features

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

$$\theta_1(x, y_{i-1}, y_i) = \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Verb}]$$

$$\theta_2(x, y_{i-1}, y_i) = \mathbb{1}[y_{i-1} = \text{Pronoun}]\mathbb{1}[y_i = \text{Noun}]$$

- 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):

$$\Psi_{i}(x, y_{i-1}, y_{i}) = (\phi_{1}(x, y_{i}), \phi_{2}(x, y_{i}), \dots, \\ \theta_{1}(x, y_{i-1}, y_{i}), \theta_{2}(x, y_{i-1}, y_{i}), \dots)$$

- 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:

$$\sum_{i} \langle w, \Psi_{i}(x, y_{i-1}, y_{i}) \rangle = \left\langle w, \sum_{i} \Psi_{i}(x, y_{i-1}, y_{i}) \right\rangle = \langle w, \Psi(x, y) \rangle, \quad (16)$$

where we define the sequence feature vector by

1

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

Structured perceptron

```
Given a dataset \mathcal{D} = \{(x, y)\};
Initialize w \leftarrow 0:
for iter = 1, 2, ..., T do
     for (x, y) \in \mathcal{D} do
           \hat{y} = \arg \max_{y' \in \Psi(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

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

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

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

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

where L is the sequence length.

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.

Observation $\Psi(x, y)$ decomposes to $\sum_{i} \Psi_i(x, y)$.

Solution Dynamic programming (similar to the Viterbi algorithm)

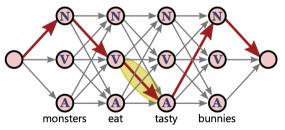
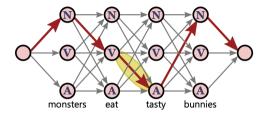


Figure by Daumé III. A course in machine learning. Figure 17.1.

Structured SVM inference (linear chain)



- Initiate $\alpha_j(1) = w^\top \psi(y_1 = j, x_1)$
- Recursion $\alpha_j(t) = \max_i \alpha_i(t-1) + w^\top \psi(y_t = j, y_{t-1} = i, x_t)$
- Pointer $\gamma(t,j) = \arg \max_i \alpha_i(t-1) + w^\top \psi(y_t = j, y_{t-1} = i, x_t)$
- Backtrack: $r(T) = \arg \max_i \alpha_i(T), r(t) = \gamma(t, r(t+1))$

What's the running time?

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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

General algorithm:

• Integer linear programming (ILP)

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

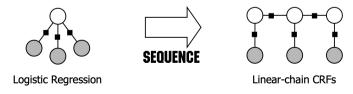
(18)

- 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

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

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

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



- 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:

$$I(w) = -\frac{1}{N} \sum_{i=1}^{N} \log p(y^{(i)}|x^{(i)}) + \frac{1}{2}\lambda ||w||^{2}$$
$$= -\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} w_{k} \psi_{k}(y_{t}^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N} \sum_{i} \log Z(x^{(i)}) + \frac{1}{2} \sum_{k} \lambda w_{k}^{2}$$

• Loss function:

$$I(w) = -\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} w_{k} \psi_{k}(x^{(i)}, y^{(i)}_{t}, y^{(i)}_{t-1}) + \frac{1}{N} \sum_{i} \log Z(x^{(i)}) + \frac{1}{2} \sum_{k} \lambda w_{k}^{2}$$

• Gradient:

$$\frac{\partial I(w)}{\partial w_{k}} = -\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} \psi_{k}(x^{(i)}, y^{(i)}_{t}, y^{(i)}_{t-1})$$

$$+ \frac{1}{N} \sum_{i} \frac{\partial}{\partial w_{k}} \log \sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1})) + \sum_{k} \lambda w_{k}$$
(19)
(19)

- What is $\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} \psi_{k}(x^{(i)}, y^{(i)}_{t}, y^{(i)}_{t-1})$?
- It is the expectation $\psi_k(x^{(i)}, y_t, y_{t-1})$ under the empirical distribution $\tilde{p}(x, y) = \frac{1}{N} \sum_i \mathbb{1}[x = x^{(i)}] \mathbb{1}[y = y^{(i)}].$

• What is
$$\frac{1}{N} \sum_{i} \frac{\partial}{\partial w_{k}} \log \sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1}))?$$

$$\frac{1}{N} \sum_{i} \frac{\partial}{\partial w_{k}} \log \sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1})))$$

$$= \frac{1}{N} \sum_{i} \left[\sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1})) \right]^{-1}$$

$$\left[\sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y^{(i)}_{t}, y^{(i)}_{t-1})) \sum_{t} \psi_{k}(x^{(i)}, y'_{t}, y'_{t-1}) \right]$$

$$= \frac{1}{N} \sum_{i} \sum_{t} \sum_{y' \in Y} p(y'_{t}, y'_{t-1} | x) \psi_{k}(x^{(i)}, y'_{t}, y'_{t-1})$$
(21)
$$(21)$$

• It is the expectation of $\psi_k(x^{(i)}, y'_t, y'_{t-1})$ under the model distribution $p(y'_t, y'_{t-1}|x)$. Mengye Ren (NYU) CSCI-GA 2565 Nov 7, 2023

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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.

CRF Inference

- In the linear chain structure, we can use the forward-backward algorithm for inference, similar to Viterbi.
- Initiate $\alpha_j(1) = \exp(w^\top \psi(y_1 = j, x_1))$
- Recursion: $\alpha_j(t) = \sum_i \alpha_i(t-1) \exp(w^\top \psi(y_t = j, y_{t-1} = i, x_t))$
- Result: $Z(x) = \sum_{j} \alpha_{j}(T)$
- Similar for the backward direction.
- Test time, again use Viterbi algorithm to infer argmax.
- The inference algorithm can be generalized to belief propagation (BP) in a tree structure (exact inference).
- In general graphs, we rely on approximate inference (e.g. loopy belief propagation).

- POS tag Relationship between constituents, e.g. NP is likely to be followed by a VP.
- Semantic segmentation Relationship between pixels, e.g. a grass pixel is likely to be next to another grass pixel, and a sky pixel is likely to be above a grass pixel.
- Multi-label learning

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

Conclusion

Multiclass algorithms

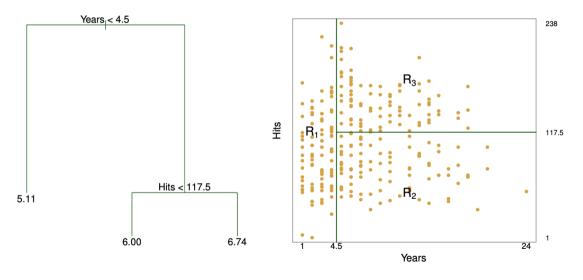
- Reduce to binary classification, e.g., OvA, AvA
 - Good enough for simple multiclass problems
 - They don't scale and have simplified assumptions
- Generalize binary classification algorithms using multiclass loss
 - Multi-class perceptron, multi-class logistics regression, multi-class SVM
- Structured 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

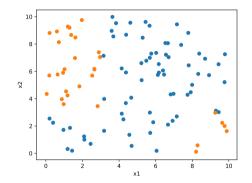
- Our first inherently non-linear classifier: decision trees.
- Ensemble methods: bagging and boosting.

Decision Trees

Regression trees: Predicting basketball players' salaries



Classification trees



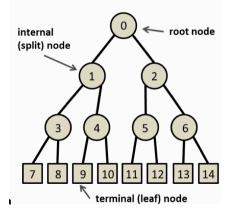
- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

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Decision trees setup





- We focus on *binary* trees (as opposed to multiway trees where nodes can have more than two children)
- Each node contains a subset of data points
- The data splits created by each node involve only a *single* feature
- For continuous variables, the splits are always of the form $x_i \leq t$
- For discrete variables, we partition values into two sets (not covered today)
- Predictions are made in terminal nodes

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

Constructing the tree

Goal Find boxes R_1, \ldots, R_J that minimize $\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \hat{y}_{R_j})^2$, subject to complexity constraints.

Problem Finding the optimal binary tree is computationally intractable.

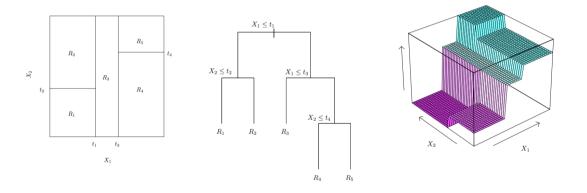
Solution Greedy algorithm: starting from the root, and repeating until a stopping criterion is reached (e.g., max depth), find the non-terminal node that results in the "best" split

• We only split regions defined by previous non-terminal nodes

Prediction Our prediction is the mean value of a terminal node: $\hat{y}_{R_m} = \text{mean}(y_i | x_i \in R_m)$

- A greedy algorithm is the one that make the best **local** decisions, without lookahead to evaluate their downstream consequences
- This procedure is not very likely to result in the globally optimal tree

Prediction in a Regression Tree



Finding the Best Split Point

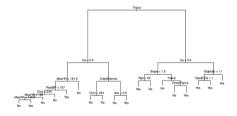
- We enumerate all features and all possible split points for each feature. There are infinitely many split points, but...
- Suppose we are now considering splitting on the *j*-th feature x_j , and let $x_{j(1)}, \ldots, x_{j(n)}$ be the sorted values of the *j*-th feature.
- We only need to consider split points between two adjacent values, and any split point in the interval $(x_{j(r)}, x_{(j(r+1)})$ will result in the same loss
- It is common to split half way between two adjacent values:

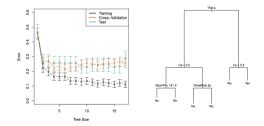
$$s_j \in \left\{ \frac{1}{2} \left(x_{j(r)} + x_{j(r+1)} \right) \mid r = 1, \dots, n-1 \right\}.$$
 $n-1$ splits (25)

Decision Trees and Overfitting

- What will happen if we keep splitting the data into more and more regions?
 - Every data point will be in its own region-overfitting.
- When should we stop splitting? (Controlling the complexity of the hypothesis space)
 - Limit total number of nodes.
 - Limit number of terminal nodes.
 - Limit tree depth.
 - Require minimum number of data points in a terminal node.
 - Backward pruning (the approach used in CART; Breiman et al 1984):
 - **(**) Build a really big tree (e.g. until all regions have ≤ 5 points).
 - Prune the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

Pruning: Example





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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 $R_1: 8 + /2 R_2: 2 + /8 -$ Split 2 $R_1: 6 + /4 R_2: 4 + /6 -$

How about here?

Split 1 $R_1: 8 + /2 - R_2: 2 + /8 -$ Split 2 $R_1: 6 + /4 - R_2: 0 + /10 -$

Intuition: we want to produce *pure* nodes, i.e. nodes where most instances have the same class.

Misclassification error in a node

- Let's consider the multiclass classification case: $\mathcal{Y} = \{1, 2, \dots, K\}$.
- Let node m represent region R_m , with N_m observations
- We denote the proportion of observations in R_m with class k by

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{\{i:x_i \in R_m\}} \mathbb{1}[y_i = k].$$

• We predict the majority class in node *m*:

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

Node Impurity Measures

- Three measures of node impurity for leaf node m:
 - Misclassification error

$$1 - \hat{p}_{mk(m)}$$

• The Gini index encourages \hat{p}_{mk} to be close to 0 or 1

$$\sum_{k=1}^{K} \hat{p}_{mk}(1-\hat{p}_{mk}).$$

• Entropy / Information gain

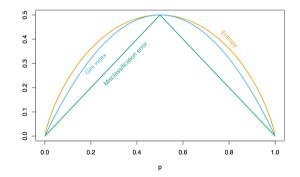
$$-\sum_{k=1}^{K}\hat{p}_{mk}\log\hat{p}_{mk}.$$

• The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

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Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

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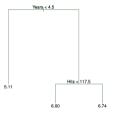
Quantifying the Impurity of a Split

Scoring a potential split that produces the nodes R_L and R_R :

- Suppose we have N_L points in R_L and N_R points in R_R .
- 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:

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

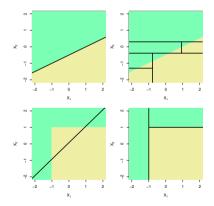
Discussion: Interpretability of Decision Trees



- 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
- Non-metric: they do not rely on the geometry of the space (inner products or distances)
- Non-parametric: they make no assumptions about the distribution of the data

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)