Multiclass Classification, Structured Prediction, & Decision Trees

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Margin for Multiclass

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

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

• Want margin to be large and positive $(w^T x^{(n)})$ 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 $y \neq y^{(n)}$.

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Multiclass SVM: separable case

Binary

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

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

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

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

$$\min_{w} \quad \frac{1}{2} \|w\|^2 \tag{6}$$

s.t.
$$m_{n,y}(w) \geqslant 1 \quad \forall (x^{(n)}, y^{(n)}) \in \mathcal{D}, y \neq y^{(n)}$$
 (7)

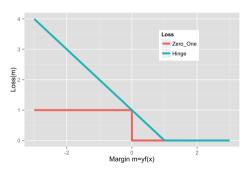
Exercise: write the objective for the non-separable case

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Recap: hingle loss for binary classification

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

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



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Generalized hinge loss

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

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

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

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

$$\implies \langle w, \Psi(x, y) \rangle \leqslant \langle w, \Psi(x, \hat{y}) \rangle \tag{11}$$

$$\Rightarrow \Delta(y,\hat{y}) \leq \Delta(y,\hat{y}) - \langle w, (\Psi(x,y) - \Psi(x,\hat{y})) \rangle$$
 When are they equal? (12)

• Generalized hinge loss:

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

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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:

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

- $\Delta(y, y')$ 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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- Problem: Multiclass classification $\mathcal{Y} = \{1, ..., k\}$
- Solution 1: One-vs-All
 - Train k models: $h_1(x), \ldots, h_k(x) : \mathcal{X} \to \mathbb{R}$.
 - 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: $h(x,y): \mathfrak{X} \times \mathcal{Y} \to \mathsf{R}$.
 - 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

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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.

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Introduction to Structured Prediction

Example: Part-of-speech (POS) Tagging

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

X	[START]	He	eats	apples
	× ₀	× ₁	<i>x</i> ₂	<i>x</i> ₃
У	[START]	Pronoun	Verb	Noun
	<i>y</i> ₀	<i>y</i> ₁	<i>y</i> ₂	<i>y</i> ₃

- $\mathcal{V} = \{\text{all English words}\} \cup \{[\text{START}], "."\}$
- $X = V^n$, n = 1, 2, 3, ... [Word sequences of any length]
- $\mathcal{P} = \{START, Pronoun, Verb, Noun, Adjective\}$
- $y = \mathcal{P}^n$, n = 1, 2, 3, ...[Part of speech sequence of any length]

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Multiclass Hypothesis Space

- Discrete output space: 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

$$\mathcal{F} = \left\{ x \mapsto \argmax_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$

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

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Structured Prediction

Part-of-speech tagging

• Multiclass hypothesis space:

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

$$\mathcal{F} = \left\{ x \mapsto \arg\max_{y \in \mathcal{Y}} h(x, y) \mid h \in \mathcal{H} \right\}$$
 (15)

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

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Unary features

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

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

- 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:

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

where we define the sequence feature vector by

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

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```
Given a dataset \mathcal{D} = \{(x, v)\}:
Initialize w \leftarrow 0:
for iter = 1, 2, ..., T do
      for (x, y) \in \mathcal{D} do
            \hat{y} = \operatorname{arg\,max}_{\mathbf{v}' \in \mathbf{y}(\mathbf{x})} \mathbf{w}^T \psi(\mathbf{x}, \mathbf{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 y(x).

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Structured hinge loss

Recall the generalized hinge loss

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

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

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

where L is the sequence length.

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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.

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

Solution Dynamic programming (similar to the Viterbi algorithm)

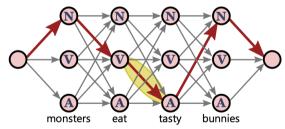
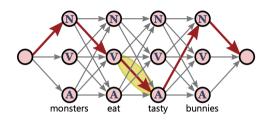


Figure by Daumé III. A course in machine learning. Figure 17.1.

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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?

The argmax problem in general

Efficient problem-specific algorithms:

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

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

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

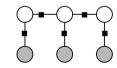
$$p(y|x) = \frac{1}{Z(x)} \exp(w^{\top} \psi(x, y)).$$

- 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: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



Logistic Regression





Linear-chain CRFs

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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:

$$I(w) = -\frac{1}{N} \sum_{i=1}^{N} \log p(y^{(i)}|x^{(i)}) + \frac{1}{2}\lambda ||w||^{2}$$

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

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Loss function:

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

• Gradient:

$$\frac{\partial I(w)}{\partial w_k} = -\frac{1}{N} \sum_{i} \sum_{t} \sum_{k} \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N} \sum_{i} \frac{\partial}{\partial w_k} \log \sum_{y' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y_t', y_{t-1}')) + \sum_{k} \lambda w_k \qquad (20)$$

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

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

$$\frac{1}{N} \sum_{i} \frac{\partial}{\partial w_{k}} \log \sum_{v' \in Y} \exp(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1}))$$
(21)

$$= \frac{1}{N} \sum_{i} \left[\sum_{y' \in Y} \exp\left(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y'_{t}, y'_{t-1})\right) \right]^{-1}$$
 (22)

$$\left[\sum_{y'\in Y} \exp\left(\sum_{t} \sum_{k'} w_{k'} \psi_{k'}(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)})\right) \sum_{t} \psi_{k}(x^{(i)}, y_t', y_{t-1}')\right]$$
(23)

$$= \frac{1}{N} \sum_{i} \sum_{t} \sum_{y' \in X} \rho(y'_t, y'_{t-1} | x) \psi_k(x^{(i)}, y'_t, y'_{t-1})$$
(24)

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• It is the expectation of $\psi_k(x^{(i)}, y'_t, y'_{t-1})$ under the model distribution $p(y'_t, y'_{t-1}|x)$.

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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).

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Examples

- 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.

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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.

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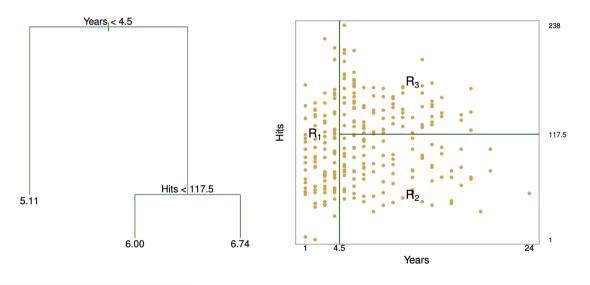
Decision Trees

Overview: Decision Trees

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

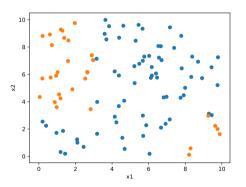
Decision Trees

Regression trees: Predicting basketball players' salaries



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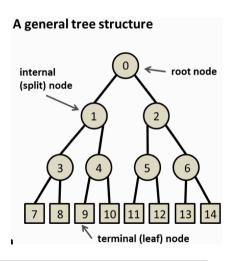
Classification trees



- 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 $x_i \leqslant t$
- 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.

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Constructing the tree

Goal Find boxes $R_1, ..., R_J$ 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

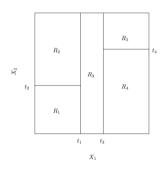
• We only split regions defined by previous non-terminal nodes

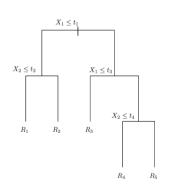
Prediction Our prediction is the mean value of a terminal node: $\hat{y}_{R_m} = \text{mean}(y_i \mid x_i \in R_m)$

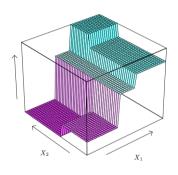
- A greedy algorithm is the one that make the best **local** decisions, without lookahead to evaluate their downstream consequences
- This procedure is not very likely to result in the globally optimal tree

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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:

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

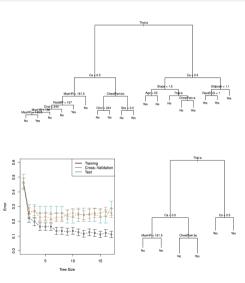
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Decision Trees and Overfitting

- 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):
 - **1** 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.

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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
$$R_1:8+/2 R_2:2+/8-$$

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

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

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

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

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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

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

• Entropy / Information gain

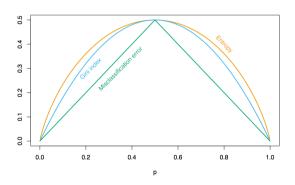
$$-\sum_{k=1}^K \hat{p}_{mk} \log \hat{p}_{mk}.$$

• 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)



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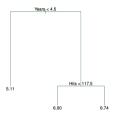
Quantifying the Impurity of a Split

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

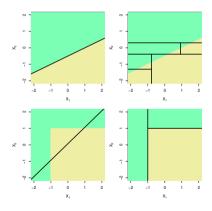


- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable large trees, maybe not so much

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Discussion: Trees vs. Linear Models

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



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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)

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