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.

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

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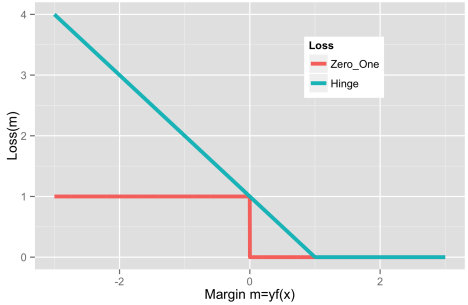
Exercise: write the objective for the non-separable case

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 $\Delta(y, y')$.

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- Generalized hinge loss:

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

Multiclass SVM with Hinge Loss

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

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

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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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- 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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  - $h(x, y)$ gives compatibility score between input x and output y
- Multiclass hypothesis space

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

- 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:

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

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

- 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):

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

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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
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  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

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

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

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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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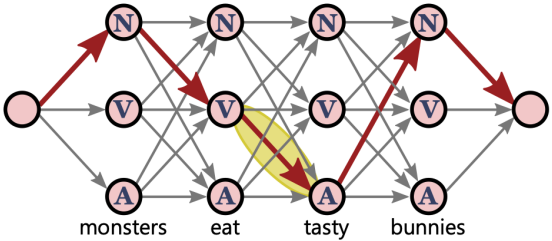
Solution Dynamic programming (similar to the Viterbi algorithm)



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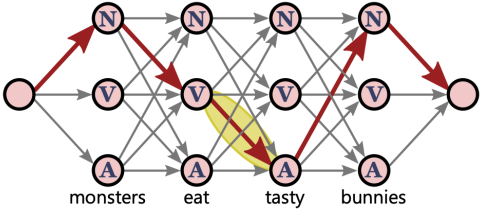
Structured SVM inference (linear chain)



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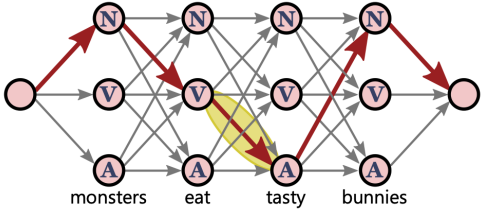

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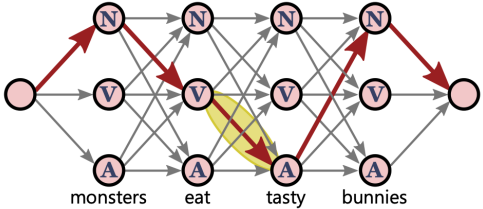

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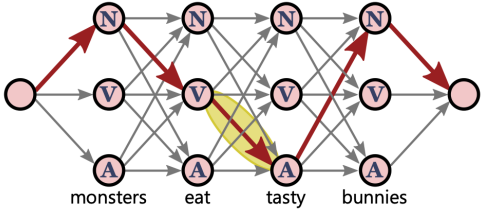

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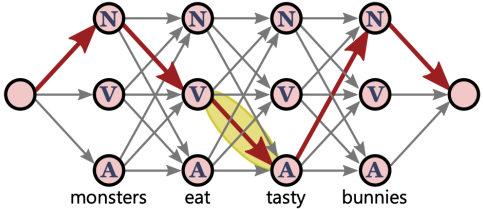

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What's the running time?

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

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)

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

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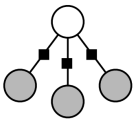
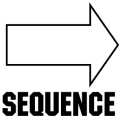
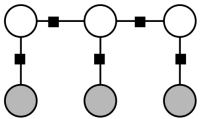
- Example: linear chain $\{y_t\}$
- We can incorporate unary and Markov features: $p(y|x) = \frac{1}{Z(x)} \exp(\sum_t w^\top \psi(x, y_t, y_{t-1}))$



Logistic Regression





Linear-chain CRFs

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- We can draw samples in the output space.

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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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- Loss function:

$$l(w) = -\frac{1}{N}\sum_i \sum_t \sum_k w_k \psi_k(x^{(i)}, y_t^{(i)}, y_{t-1}^{(i)}) + \frac{1}{N}\sum_i \log Z(x^{(i)}) + \frac{1}{2}\sum_k \lambda w_k^2$$

- Gradient:

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

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

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

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

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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.

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

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- 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

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- Generalize binary classification algorithms using multiclass loss
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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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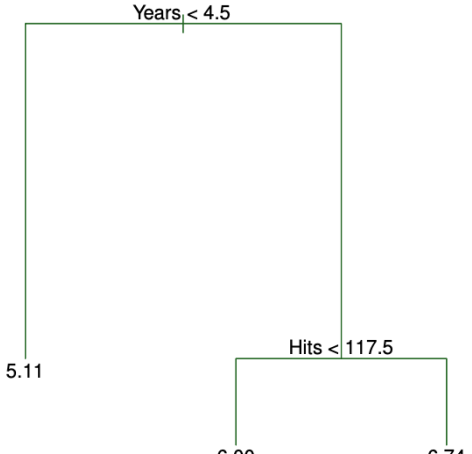
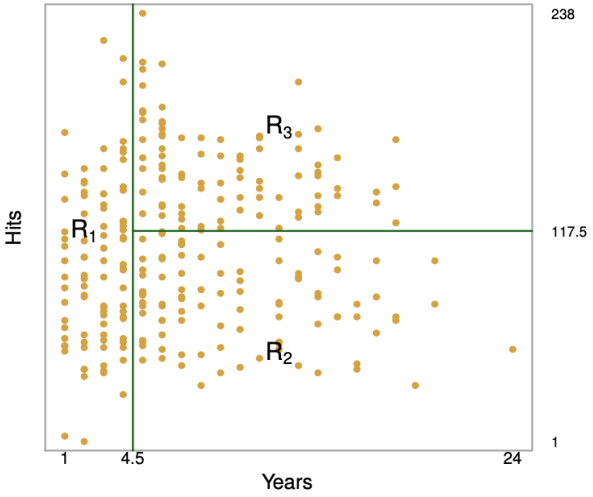
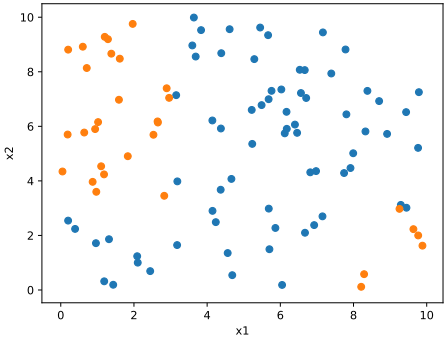




Classification trees



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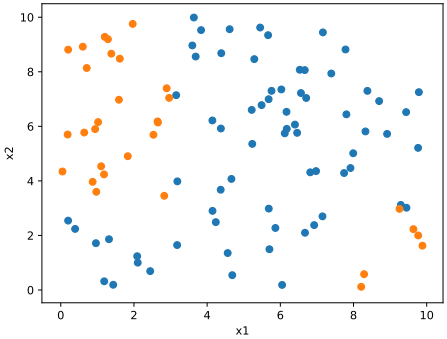
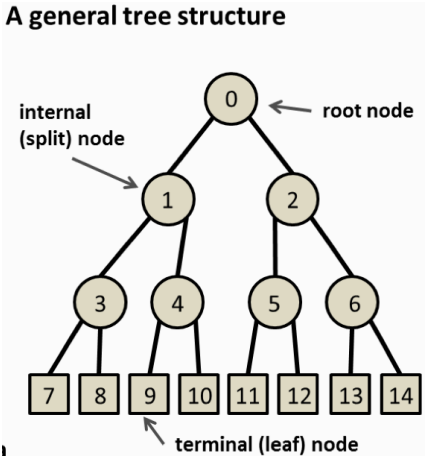


- Can we classify these points using a linear classifier?
- Partition the data into axis-aligned regions recursively (on the board)

Decision trees setup



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

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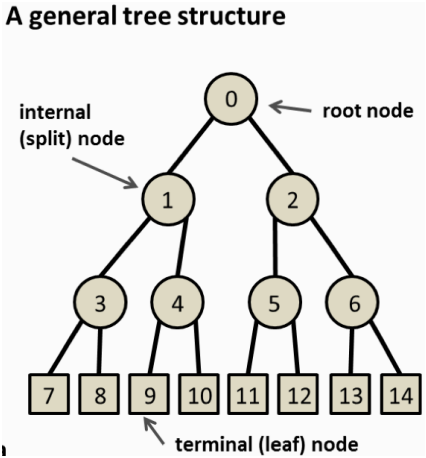

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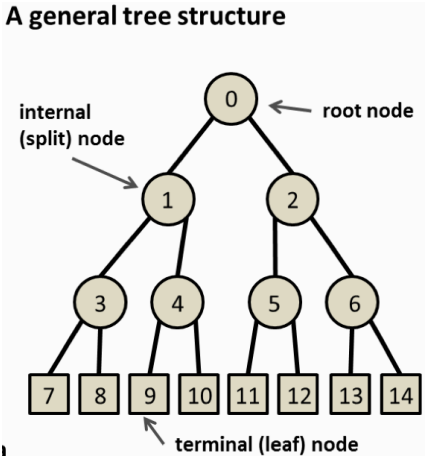

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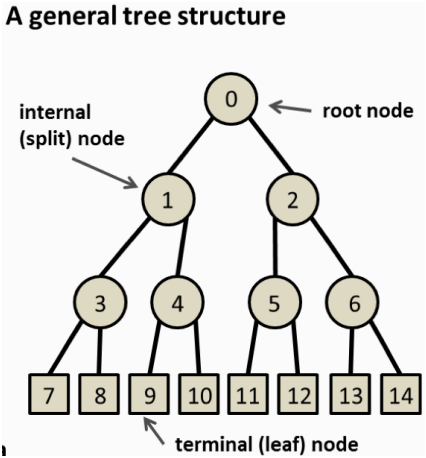

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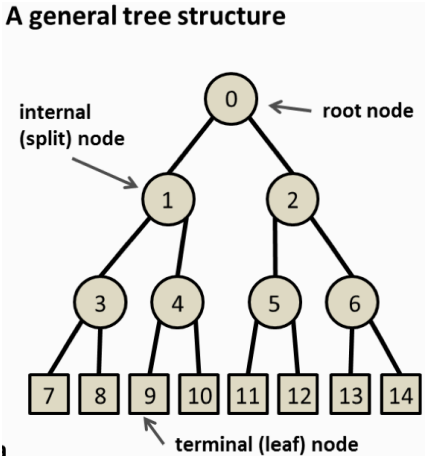

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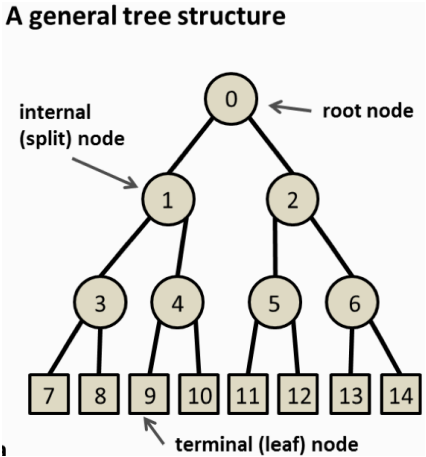

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- Predictions are made in terminal nodes

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.

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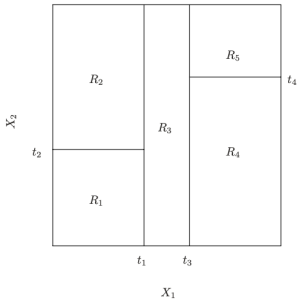
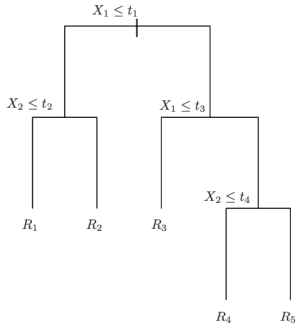
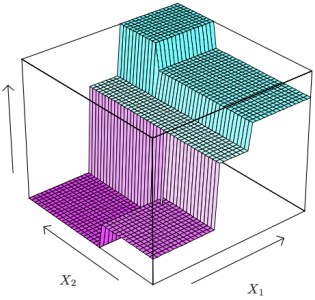
Prediction in a Regression Tree







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

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

Decision Trees and Overfitting

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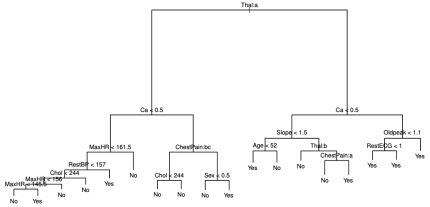
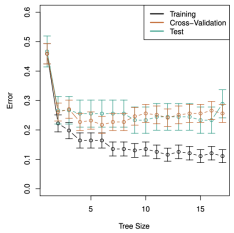
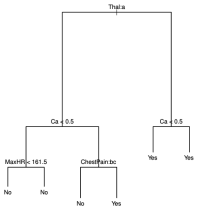
    2. *Prune* the tree back greedily, potentially all the way to the root, until validation performance starts decreasing.

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

- Let's consider the multiclass classification case: $\mathcal{Y} = \{1, 2, \ldots, K\}$.
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- We predict the majority class in node m:

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

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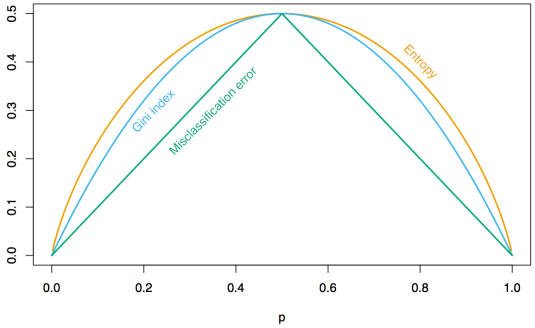
- The Gini index and entropy are numerically similar to each other, and both work better in practice than the misclassification error.

Impurity Measures for Binary Classification

(p is the relative frequency of class 1)



HTF Figure 9.3

Quantifying the Impurity of a Split

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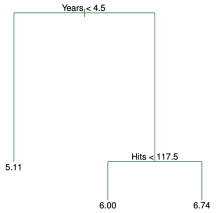
- Let $Q(R_L)$ and $Q(R_R)$ be the node impurity measures for each node.
- We aim to find a split that minimizes the *weighted average of node impurities*:

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

Discussion: Interpretability of Decision Trees



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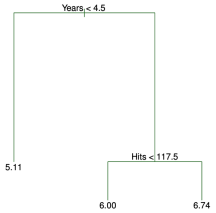
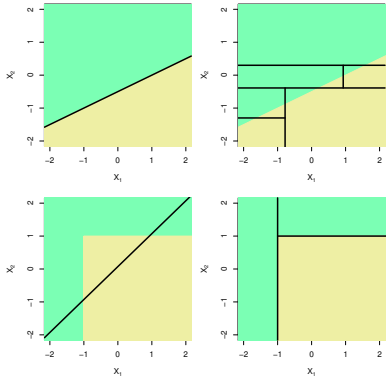


- Trees are easier to visualize and explain than other classifiers (even linear regression)
- Small trees are interpretable – large trees, maybe not so much

Discussion: Trees vs. Linear Models

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



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Decision trees are:

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Additional pros:

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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)

Bagging and Random Forests

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- A statistic $\hat{\theta} = \hat{\theta}(\mathcal{D})$ is a **point estimator** of θ if $\hat{\theta} \approx \theta$

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- Why does variance matter if an estimator is unbiased?
  - $\hat{\theta}(\mathcal{D}) = x_1$ is an unbiased estimator of the mean of a Gaussian, but would be farther away from θ than the sample mean.

Variance of a Mean

- Let $\hat{\theta}(\mathcal{D})$ be an unbiased estimator with variance σ^2: $\mathbb{E}\left[\hat{\theta}\right] = \theta$, $\text{Var}(\hat{\theta}) = \sigma^2$.
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- The average has the same expected value but smaller standard error (recall that $Var(cX) = c^2 Var(X)$, and that the $\hat{\theta}_i$-s are uncorrelated):

$$\mathbb{E}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \theta \qquad \text{Var}\left[\frac{1}{n}\sum_{i=1}^{n}\hat{\theta}_i\right] = \frac{\sigma^2}{n} \tag{26}$$

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- We will define the average prediction function as:

$$\hat{f}_{\text{avg}} \stackrel{\text{def}}{=} \frac{1}{B} \sum_{b=1}^{B} \hat{f}_b \tag{27}$$

Averaging Reduces Variance of Predictions

- The average prediction for x_0 is

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- Problem: in practice we don't have B independent training sets!

The Bootstrap Sample

How do we simulate multiple samples when we only have one?

- A **bootstrap sample** from $\mathcal{D}_n = (x_1, \ldots, x_n)$ is a sample of size n drawn *with replacement* from $\mathcal{D}_n$

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- For large n,

$$\left(1-\frac{1}{n}\right)^n \approx \frac{1}{e} \approx .368. \tag{28}$$

- So we expect ~63.2% of elements of $\mathcal{D}_n$ will show up at least once.

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- Use these values as though $D_n^1, \ldots, D_n^B$ were i.i.d. samples from P.
- This often ends up being very close to what we'd get with independent samples from P!

Independent Samples vs. Bootstrap Samples

- Point estimator $\hat{\alpha} = \hat{\alpha}(\mathcal{D}_{100})$ for samples of size 100, for a synthetic case where the data generating distribution is known
- Histograms of $\hat{\alpha}$ based on
  - 1000 independent samples of size 100 (left), vs.
  - 1000 bootstrap samples of size 100 (right)

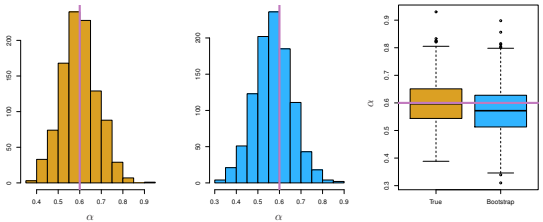

Figure 5.10 from *ISLR* (Springer, 2013) with permission from the authors: G. James, D. Witten, T. Hastie and R. Tibshirani.

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  - We try to find new learners that do well where previous learners fall short

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- The **bagged prediction function** is a *combination* of these:

$$\hat{f}_{\text{avg}}(x) = \text{Combine}\left(\hat{f}_1(x), \hat{f}_2(x), \ldots, \hat{f}_B(x)\right)$$

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- Yes: if we have many trees, the bagged predictor is much less interpretable

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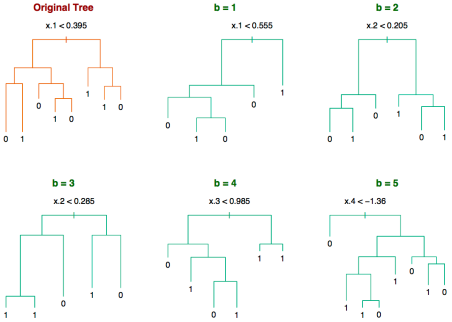
- The OOB error is a good estimate of the test error
- Similar to cross validation error: both are computed on the training set

Applying Bagging to Classification Trees

- Input space $\mathcal{X} = \mathrm{R}^5$ and output space $\mathcal{Y} = \{-1, 1\}$. Sample size $n = 30$.



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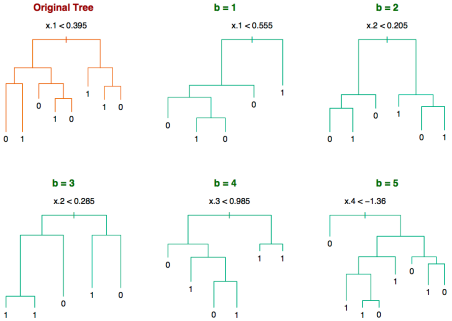

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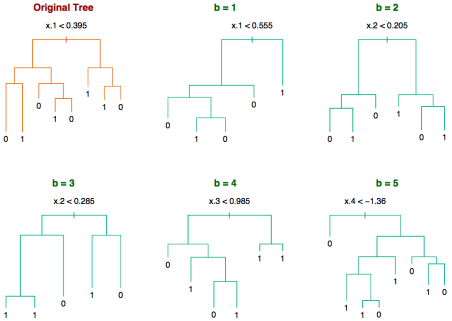

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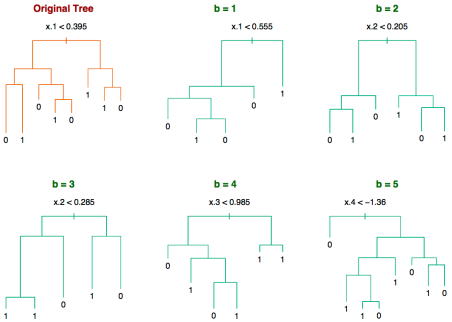

- Each bootstrap tree is quite different: different splitting variable at the root!
- **High variance**: small perturbations of the training data lead to a high degree of model variability
- Bagging helps most when the base learners are relatively unbiased but have high variance (exactly the case for decision trees)

From HTF Figure 8.9

Motivating Random Forests: Correlated Prediction Functions

Recall the motivating principle of bagging:

- For $\hat{\theta}_1, \ldots, \hat{\theta}_n$ *i.i.d.* with $\mathbb{E}\left[\hat{\theta}\right] = \theta$ and $\mathrm{Var}\left[\hat{\theta}\right] = \sigma^2$,

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- Can we reduce the dependence between $\hat{f}_i$'s?

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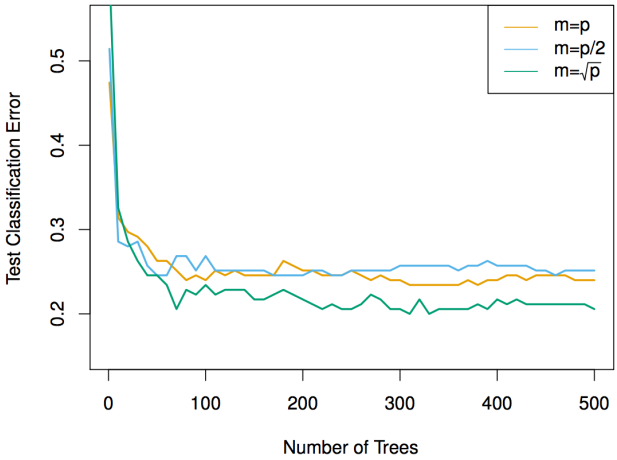
- If $m = p$, this is just bagging

Random Forests: Effect of m



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- But bootstrap samples (and the induced models) are correlated
- Ensembling works better when we combine a diverse set of prediction functions
  - $\Longrightarrow$ Random forests: select a random subset of features for each decision tree