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Query Selection

- Key Question: Given a partial tree down to node N, what feature s should we choose for the property test T?
- The obvious heuristic is to choose the feature that yields as big a decrease in the impurity as possible.
- The impurity gradient is $\Delta i(N) = (i(N) + P_L i(N_L) + (1 - P_L i(N_R)), \quad (5)$

where N_L and N_R are the left and right descendants, respectively, P_L is the fraction of data that will go to the left sub-tree when property T is used.

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- If the entropy impurity is used, this corresponds to choosing the feature that yields the highest information gain.

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• For the binary-case, it yields one-dimensional optimization problem (which may have non-unique optima).

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- For the binary-case, it yields one-dimensional optimization problem (which may have non-unique optima).
- In the higher branching factor case, it would yield a higher-dimensional optimization problem.
 - In multi-class binary tree creation, we would want to use the **twoing criterion**. The goal is to find the split that best separates groups of the c categories. A candidate "supercategory" C_1 consists of all patterns in some subset of the categories and C_2 has the remainder. When searching for the feature s, we also need to search over possible category groupings.

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- This is a local, greedy optimization strategy.
- Hence, there is no guarantee that we have either the global optimum (in classification accuracy) or the smallest tree.
- In practice, it has been observed that the particular choice of impurity function rarely affects the final classifier and its accuracy.

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A Note About Multiway Splits

• In the case of selecting a multiway split with branching factor *B*, the following is the direct generalization of the impurity gradient function:

$$\Delta i(s) = i(N) - \sum_{k=1}^{B} P_k i(N_k)$$
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- So, we need to normalize each:

$$\Delta i_B(s) = \frac{\Delta i(s)}{-\sum_{k=1}^B P_k \log P_k} \quad . \tag{7}$$

And then we can again choose the feature that maximizes this normalized criterion.

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- So, how to stop splitting?
- 1 Cross-validation...
- 2 Threshold on the impurity gradient.
- 3 Incorporate a tree-complexity term and minimize.
- 4 Statistical significance of the impurity gradient.

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- Drawback: But, how do we set the value of the threshold β ?



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• Define a new global criterion function

$$\alpha \cdot \text{size} + \sum_{\text{leaf nodes}} i(N)$$
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which trades complexity for accuracy. Here, size could represent the number of nodes or links and α is some positive constant.

• The strategy is then to split until a minimum of this global criterion function has been reached.

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- Given the entropy impurity, this global measure is related to the minimum description length principle.
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- But, again, how do we set the constant α ?

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- More generally, we can consider a hypothesis testing approach to stopping: we seek to determine whether a candidate split differs significantly from a random split.
- Suppose we have n samples at node N. A particular split s sends Pn patterns to the left branch and (1 P)n patterns to the right branch. A random split would place P_{n1} of the ω1 samples to the left, P_{n2} of the ω2 samples to the left and corresponding amounts to the right.

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 The chi-squared statistic calculates the deviation of a particular split s from this random one:

$$\mathbf{S} \quad \chi^2 = \sum_{i=1}^2 \frac{(n_{iL} - n_{ie})^2}{n_{ie}} \tag{10}$$

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- When it is greater than a critical value (based on desired significance bounds), we reject the null hypothesis (the random split) and proceed with s.

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- Pruning avoids the "local"-ness of the earlier methods and uses all of the training data, but it does so at added computational cost during the tree construction.

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Assignment of Leaf Node Labels

- This part is easy...a particular leaf node should make the label assignment based on the distribution of samples in it during training. Take the label of the maximally represented class.
- We will see clear justification for this in the next chapter on Decision

Theory.

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Decision Trees CART

Instability of the Tree Construction



Importance of Feature Choice

- The selection of features will ultimately play a major role in accuracy, generalization, and complexity.
- This is an instance of the Ugly Duckling principle.



• Furthermore, the use of multiple variables in selecting a decision rule may greatly improve the accuracy and generalization.





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- One can follow this by pruning.

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C4.5

C4.5 Method (in brief)

• This is a successor to the ID3 method.

J. Corso (SUNY at Buffalo)

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C4.5 Method (in brief)

- This is a successor to the ID3 method.
- It handles real valued variables like CART and uses the ID3 multiway splits for nominal data.

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C4.5 Method (in brief)

- This is a successor to the ID3 method.
- It handles real valued variables like CART and uses the ID3 multiway splits for nominal data.
- Pruning is performed based on statistical significance tests.

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Decision Trees

Example

Example from T. Mitchell Book: PlayTennis

Day	Outlook	Temperature	Humidity	Wind	PlayTennis
D1	Sunny	Hot	High	Weak	No
D2	Sunny	Hot	High	Strong	No
D3	Overcast	Hot	High	Weak	Yes
D4	Rain	Mild	High	Weak	Yes
D5	Rain	Cool	Normal	Weak	Yes
D6	Rain	Cool	Normal	Strong	No
D7	Overcast	Cool	Normal	Strong	Yes
D8	Sunny	Mild	High	Weak	No
D9	Sunny	Cool	Normal	Weak	Yes
D10	Rain	Mild	Normal	Weak	Yes
D11	Sunny	Mild	Normal	Strong	Yes
D12	Overcast	Mild	High	Strong	Yes
D13	Overcast	Hot	Normal	Weak	Yes
D14	Rain	Mild	High	Strong	No

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Which attribute is the best classifier?



Gain (S, Humidity)



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Which attribute should be tested here?

 $S_{sunny} = \{D1, D2, D8, D9, D11\}$

 $Gain(S_{sunny}, Humidity) = .970 - (3/5) 0.0 - (2/5) 0.0 = .970$ $Gain(S_{sunny}, Temperature) = .970 - (2/5) 0.0 - (2/5) 1.0 - (1/5) 0.0 = .570$ $Gain(S_{sunny}, Wind) = .970 - (2/5) 1.0 - (3/5) .918 = .019$

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Learned Tree



Overfitting Instance

• Consider adding a new, noisy training example #15:

Sunny, Hot, Normal, Strong, PlayTennis = No

• What effect would it have on the earlier tree?

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Overfitting Instance

• Consider adding a new, noisy training example #15:

 $Sunny, \ Hot, \ Normal, \ Strong, \ PlayTennis = No$

What effect would it have on the earlier tree?



535 2012 Rondom Forest Classifiers Part I 1 Ricap Decision Trus Input $D = \frac{1}{2} (X_{ij}, y_{i}), (X_{2}, y_{2}), \dots, (X_{p}, y_{p})^{2}$ [ask the contracted disk) Assume $X_{i} \in \mathcal{K}_{0}^{2}$, $y_{i} \in \mathcal{L} = \frac{1}{2} (1, 2, \dots, K_{s}^{2})$ note extension to \mathbb{R}^{d} gin example of $\frac{1}{2}$ and $Output : f(X) := \mathcal{L}$ some classifier. Lesin Decision True (D, TEU, p= p) 1. If T>= MAXDEPTH or pure (D) DFS 2 return ϕ $(Di(D,q)=i(D),-P_{L}^{(D)}(D_{L}) 3 q^{*} = crg \max_{q \in X} X_{i}(D, q)$ (1-P₁(2)) i(D_R) $4 \quad v = p:new Child (5) \quad i(0) = -2 P(y_1) \log P(y_1)$ $5 \quad (L_1 R) = split (D, 5) \quad enpirited propositions$ $6 \quad Learn DT(L, T+1, v) \quad from p$ 6 Lear DT(L, T+1, V) 2 Learn DT(R, TH, W) Limitations of Decision Trees (a) "Estimation Error" of d 13 big need a lof of data (b) What A dis bige or the dynamice? Canot evaluate Step 3 () leaving is greatly be of NP completies of global leaving (d) overfitting / reduce height

555 2012 12 Random Forrest Classifiers Part 1 Huge Fraging Either die rickly big web as patravise relation of pixels the an image or genes a biosofemations or for date * then is a function G(X) -> 2913 generating som frattike subset. (not even contrible) it aftism Note relation These (mathingthing) RandsmithTree Construction -> I die is lasy wither the consider all features when selecting 9 guerry at node V, consider only a smel subset X's * there are principled methemators from Bagesian Decession Theory I internation theory that adaly there choises 3a X5 = Select Random Subset $35 \quad g^{\pm} = arg \max_{g \in X_S} \Delta_i(\mathcal{D}, g)$ Proceed with the rest of the tree as before Randomization avocances featin problem and we can expert a lage enough rendom free to capture some discommative information but doubterat to - ful dasstaction 5-

555 2012 p3 Rendom Forest Classifiers Part I Raiden Forests So, we can expect aggregating hultiple tree reponses into one classifiers Suppose we have a family of true T, ..., TN f(X/T, TN) -> L Nied a bit of probability here draw or port P(y=c|T;(v),x) postero- at that adde v of T; poarpes Denote A ut Aggregate $\overline{\mu}(x) = \overline{h} \stackrel{X}{\simeq} \mu_{T}(x)$ \$5- big I, one may enforce sparsity in MR y = ag may In (K) max mad

535 202 1/24 Kandom Tree Classifiers 1) Y Amit, D Genan "Shape Granfizefor and Recognition Sources: with Randomized Trees" Neural Computation 9,7 1345-1588, 2997 Limitations of Accision Trees O Explore fill future grace, but at prained when the space is too big - infinite dimensional X : space of digital inages C: set of shipe classes Each image XEX have a true cleans label Y(x) E = 21, 2, ..., K3 Roma a probability dost of X P(X) Goal is to construct a classifier Y: X -> C st. P(Y+Y), 3 may Restrict to queries QA with banded complexity. A with trust 20 tags and hardapore. So Q = EQ, , , QAB be as feature veter QE 20,13M Training Set L= Z(x, Y(x,)), ..., (Xm, Y(Xm))3