Recap

- 90% of ML:
  - Dataset D
    - e.g., D = $\{(x_1, y_1), \ldots, (x_m, y_m)\}$
  - Hypothesis class: H = $\{h_1, \ldots, h_n\}$
  - Learning algorithm A_H
    - $A_H(D) = \arg\min_{h \in H} f(D, h)$

Supervised Classification

- Classifier: h(x) -> y
- Training data: D = {(x_1, y_1), …, (x_m, y_m)}
  - Examples come from “real world.”
- Learning algorithm: A(D) -> h
  - h should do well on real world. Training data is just a proxy

Nearest Neighbor Classification

- $D = \{(x_1, y_1), \ldots, (x_m, y_m)\}$
- $h(x) = y_k$, where $k = \text{argmin}_i\ d(x, x_i)$
- How much does this cost?
  - How to make it cheaper?
- How to improve this to avoid mistakes?

Today's Plan

- First (second) machine learning algorithm: decision tree learning
  - Another example of supervised classification

Decision Trees

Machine Learning
CS4824/ECE4424
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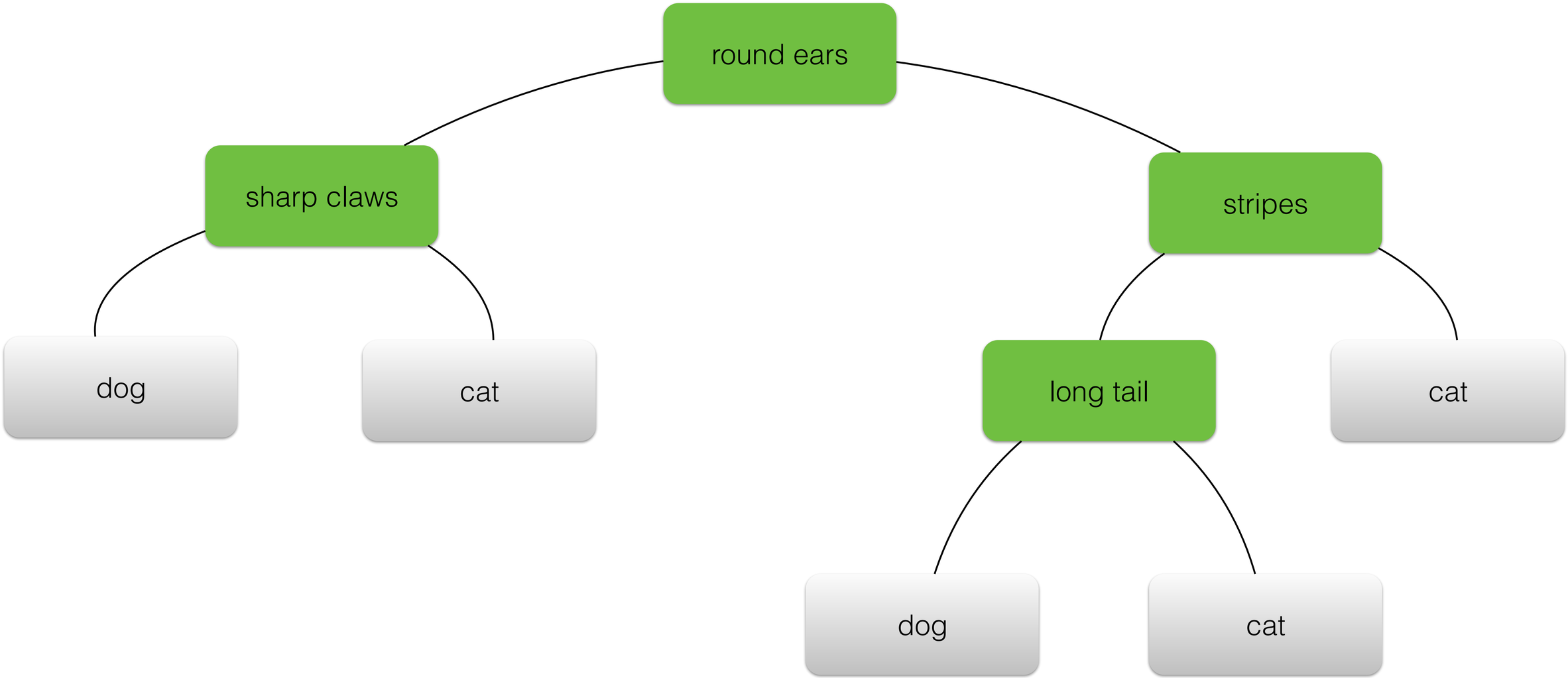
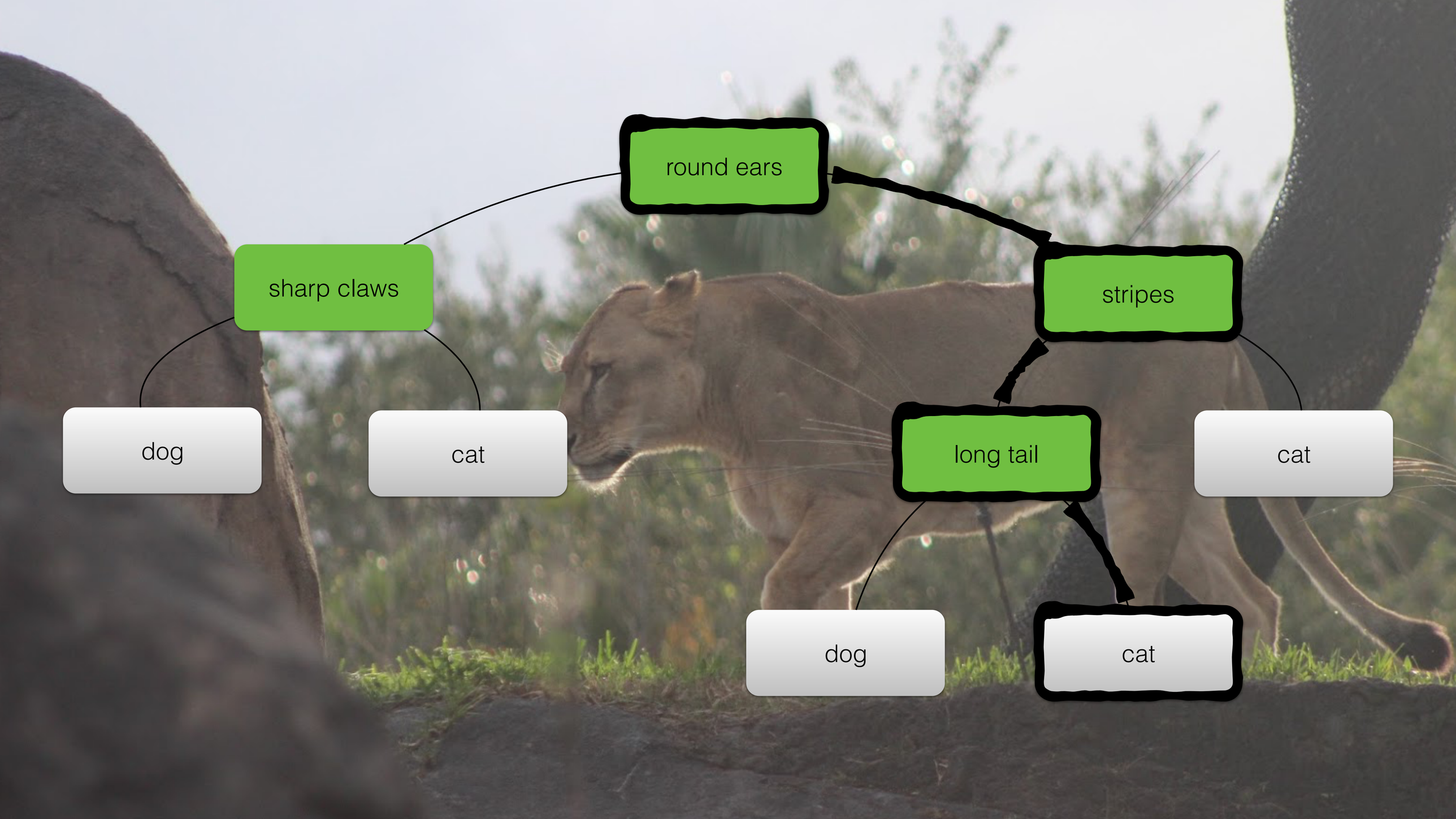
Outline

- Learning decision trees
- Extensions: random forests


round ears
sharp claws
stripes
dog
cat
long tail
cat
dog
cat


round ears
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cat

Decision Tree Learning

- Greedily choose best decision rule
- Recursively train decision tree for each resulting subset

```
function fitTree(D, depth)
  if D is all one class or depth >= maxDepth
    node.prediction = most common class in D
    return node
  rule = BestDecisionRule(D)
  dataLeft = {(x, y) from D where rule(D) is true}
  dataRight = {(x, y) from D where rule(D) is false)}
  node.left = fitTree(dataLeft, depth+1)
  node.right = fitTree(dataRight, depth+1)
  return node
```

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```

Choosing Decision Rules

- Define a cost function **cost(D)**
  - Misclassification rate (training error)
  - Entropy or information gain
  - Gini index (smoothed training error)

Misclassification Rate

$$\hat{\pi}_c := \frac{1}{|\mathcal{D}|} \sum_{i \in \mathcal{D}} \mathbb{I}(y_i = c)$$

class proportion
(estimated probability)

$$\hat{y} := \operatorname*{argmax}_c \ \hat{\pi}_c$$

best prediction

$$\text{cost}(\mathcal{D}) := \frac{1}{|\mathcal{D}|} \sum_{i \in \mathcal{D}} \mathbb{I}(y_i \neq \hat{y}) = 1 - \hat{\pi}_{\hat{y}}$$

error rate

$$\text{cost}(\mathcal{D}) - \left(\frac{|\mathcal{D}_L|}{|\mathcal{D}|} \text{cost}(\mathcal{D}_L) + \frac{|\mathcal{D}_R|}{|\mathcal{D}|} \text{cost}(\mathcal{D}_R) \right)$$

cost reduction

Entropy and Information Gain

$$\hat{\pi}_c := \frac{1}{|\mathcal{D}|} \sum_{i \in \mathcal{D}} \mathbb{I}(y_i = c)$$

$$H(\hat{\boldsymbol{\pi}}) := -\sum_{c=1}^{C} \hat{\pi}_c \log \hat{\pi}_c$$

$$\text{cost}(\mathcal{D}) - \left(\frac{|\mathcal{D}_L|}{|\mathcal{D}|} \text{cost}(\mathcal{D}_L) + \frac{|\mathcal{D}_R|}{|\mathcal{D}|} \text{cost}(\mathcal{D}_R) \right)$$

$$\begin{aligned}
\text{infoGain}(j) &= H(Y) - H(Y|X_j) \\
&= -\sum_y \Pr(Y = y) \log \Pr(Y = y) + \\
&\quad \sum_{x_j} \Pr(X_j = x_j) \sum_y \Pr(Y = y|X_j = x_j) \log \Pr(Y = y|X_j = x_j).
\end{aligned}$$

Information Gain

$$\begin{aligned}\text{infoGain}(j) &= H(Y) - H(Y|X_j) \\ &= -\sum_y \Pr(Y = y) \log \Pr(Y = y) + \\ &\quad \sum_{x_j} \Pr(X_j = x_j) \sum_y \Pr(Y = y|X_j = x_j) \log \Pr(Y = y|X_j = x_j).\end{aligned}$$

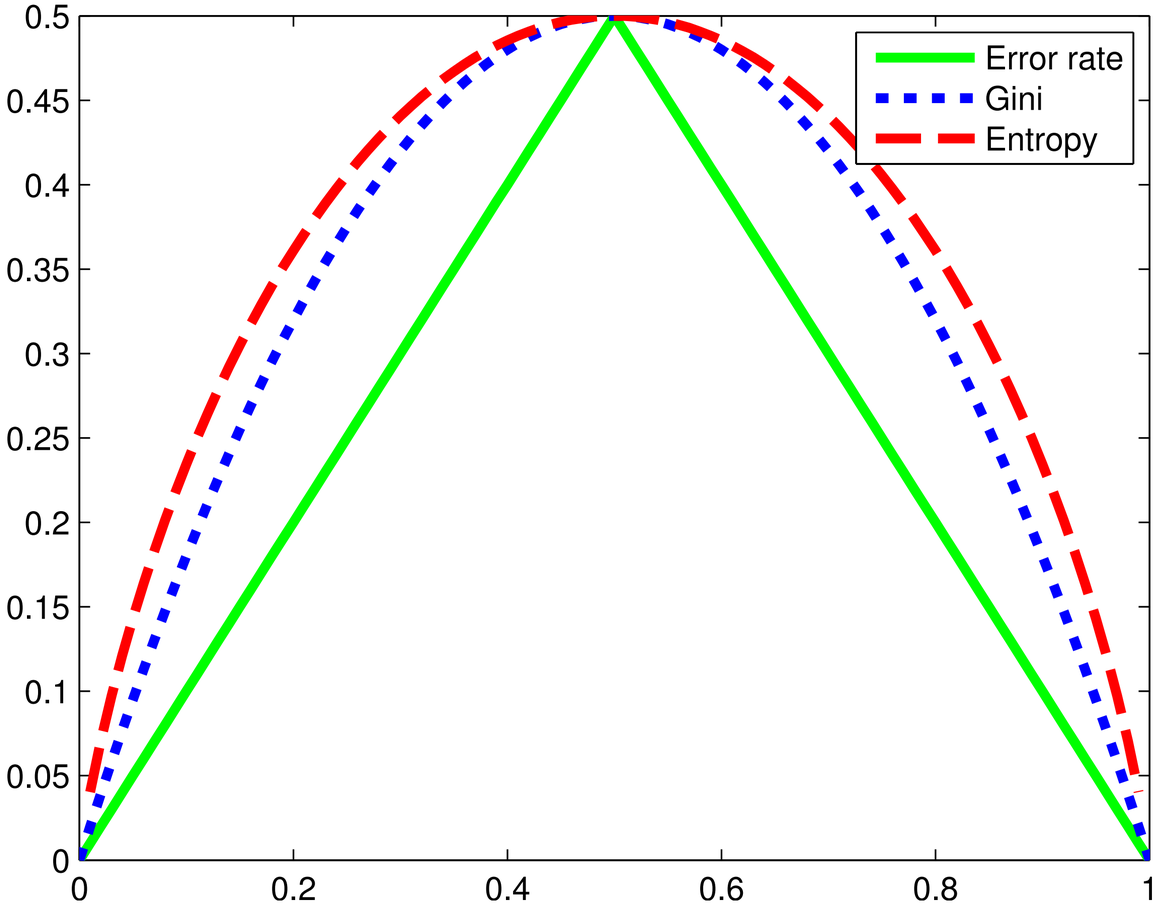
$X_j = Y$ $X_j \perp Y$

Gini Index

$$\sum_{c=1}^{C} \hat{\pi}_c(1 - \hat{\pi}_c) = \sum_c \hat{\pi}_c - \sum_c \hat{\pi}_c^2 = 1 - \sum_c \hat{\pi}_c^2$$

like misclassification rate, but accounts for uncertainty

Comparing the Metrics



probability of class 1

```
% Fig 9.3 from Hastie book

p=0:0.01:1;
gini = 2*p.*(1-p);
entropy = -p.*log(p) - (1-p).*log(1-p);
err = 1-max(p,1-p);


% scale to pass through (0.5, 0.5)
entropy = entropy./max(entropy) * 0.5;


figure;
plot(p, err, 'g-', p, gini, 'b:', p, …
       entropy, 'r--', 'linewidth', 3);
legend('Error rate', 'Gini', 'Entropy')
```

Overfitting

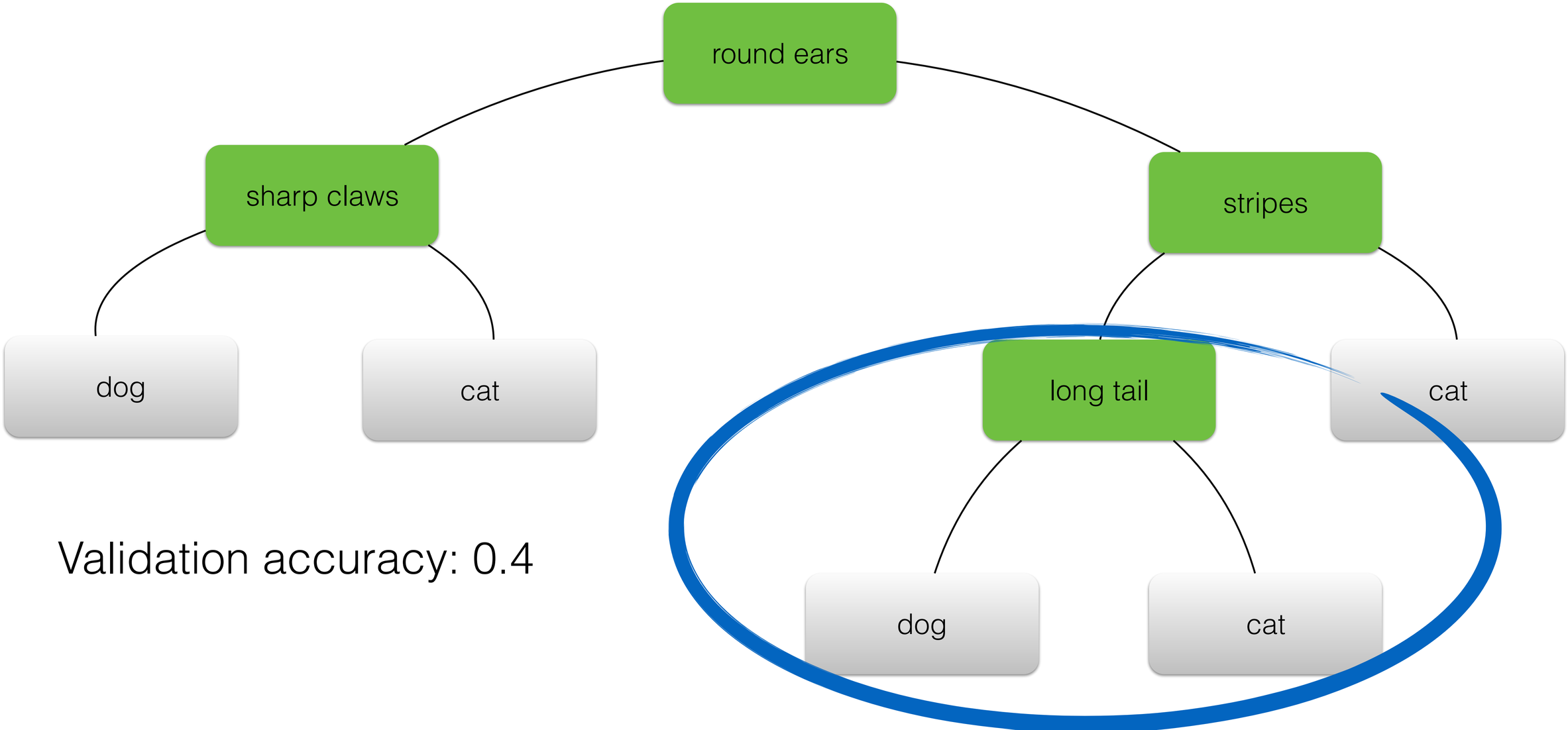
- A decision tree can achieve 100% training accuracy when each example is unique
- Limit depth of tree
- Strategy: train very deep tree
  - Adaptively prune

Validation

- Take training data and split into **training set** and **validation set**
- $D = \{(x_1, y_1), \ldots, (x_n, y_n)\}$

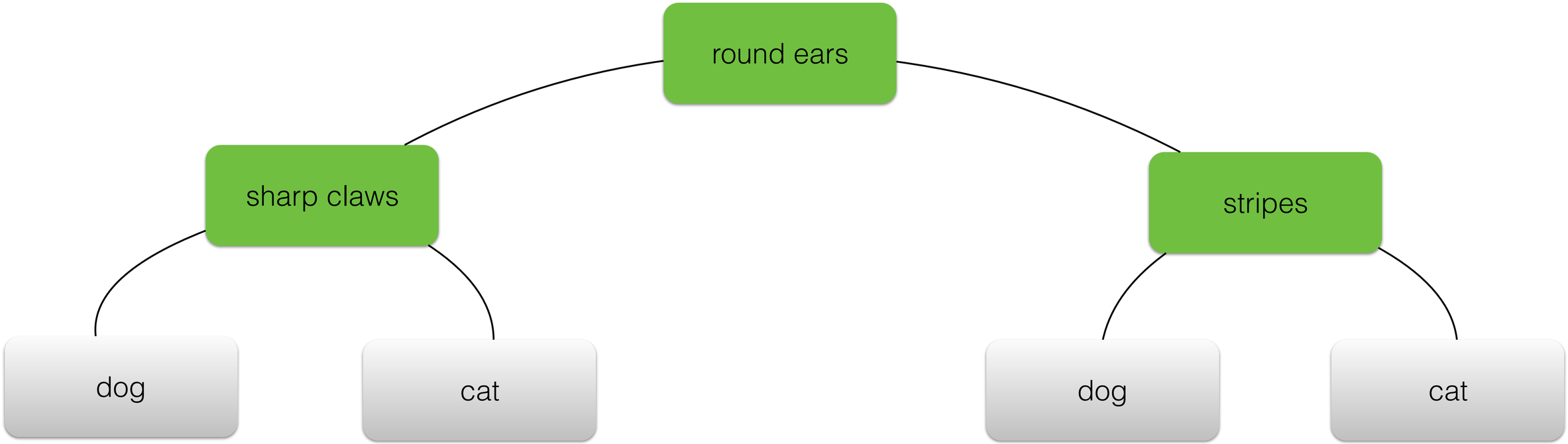
  $D_t = \{(x_1, y_1), \ldots, (x_m, y_m)\}$ $D_v = \{(x_{m+1}, y_{m+1}), \ldots, (x_n, y_n)\}$
- Only allow learning algorithm to look at D_t

Pruning with Validation Set



Validation accuracy: 0.4

Pruning with Validation Set

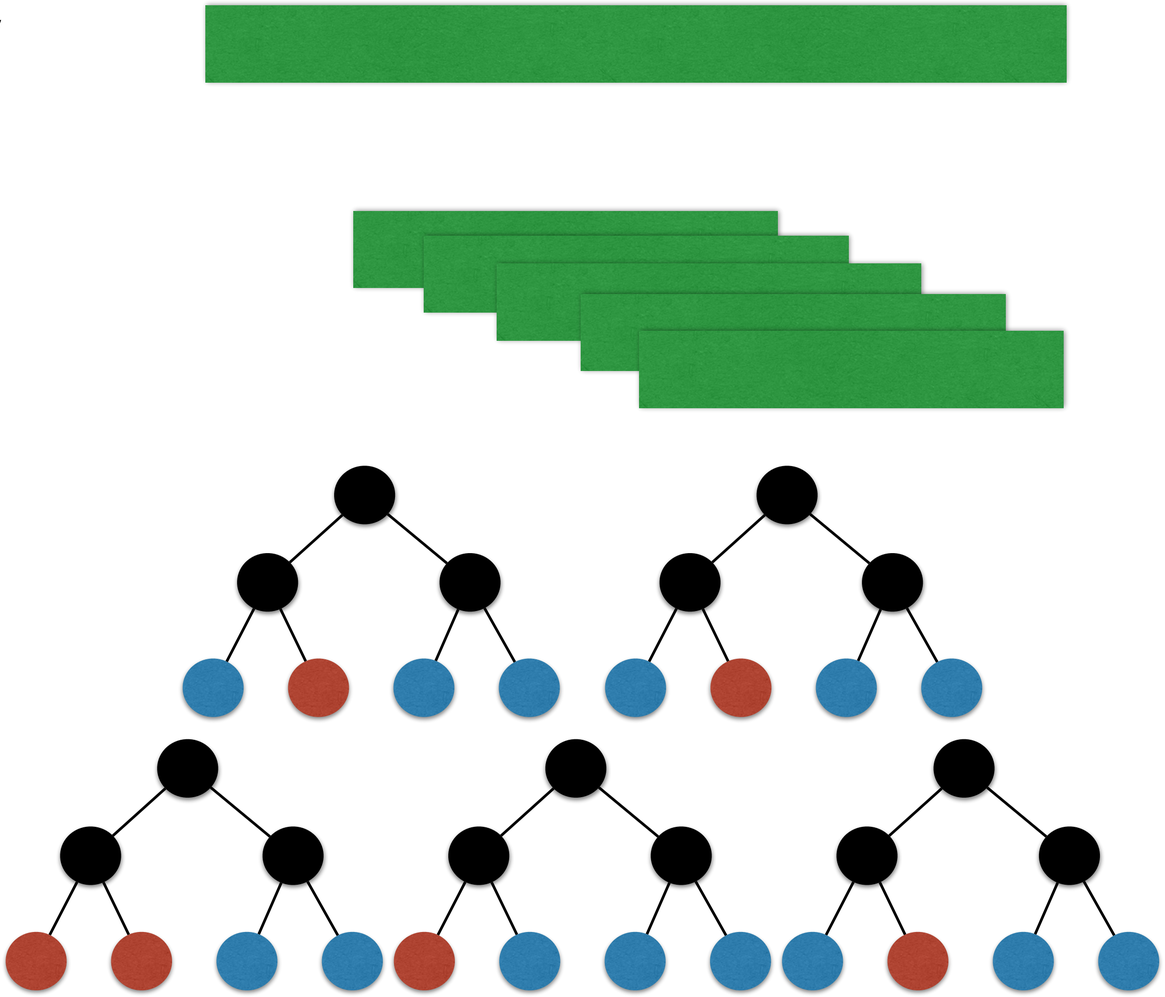


Validation accuracy: 0.4

new validation accuracy: 0.41

Random Forests

- Use **bootstrap aggregation** to train many decision trees
  - Randomly subsample **n** examples
  - Train decision tree on subsample
  - Use average or majority vote among learned trees as prediction
- Also randomly subsample features
- Reduces *variance* without changing *bias*



Summary

- Training decision trees
- Cost functions
  - Misclassification
  - Entropy and information gain
  - Gini index (expected error)
- Pruning
- Random forests (bagging)