Model Selection and Optimization

Outline

I. Overfitting and pruning of decision trees

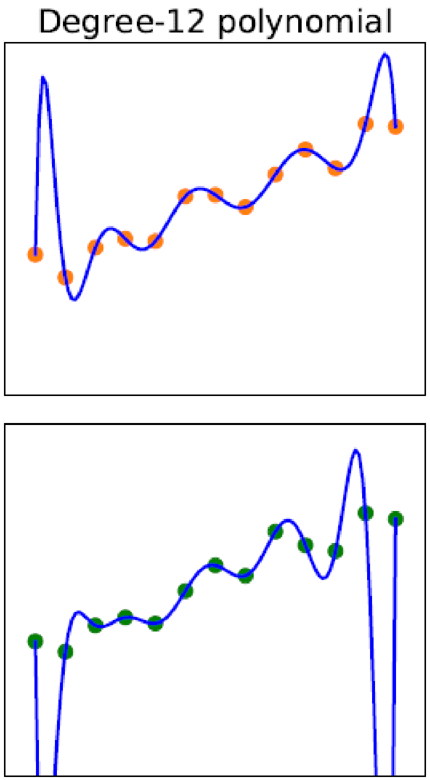
II. Model selection

III. Loss function

IV. Regularization and tuning

* Figures are from the textbook site or plotted by the instructor.

I. Issue of Overfitting



Overfitting

- ♦ Too much attention paid to the training set, and performs poorly on unseen data.
- ♦ More likely to happen as #attributes increases.
- ♦ Less likely with more training examples.

- ♠ Polynomials with higher degrees are more likely to overfit.
- ♠ Decision trees with more nodes have more capacity to overfit.

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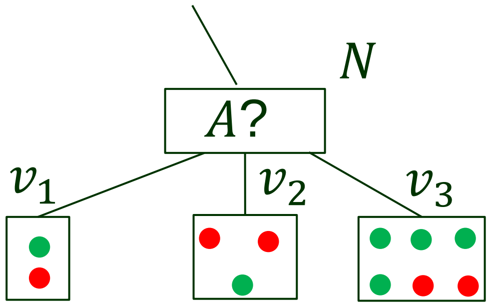

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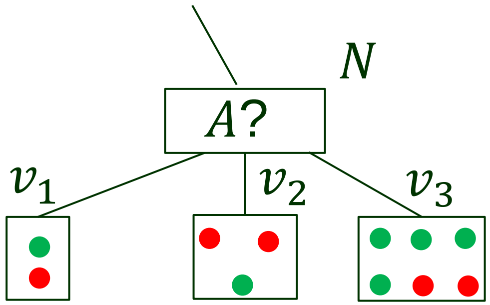

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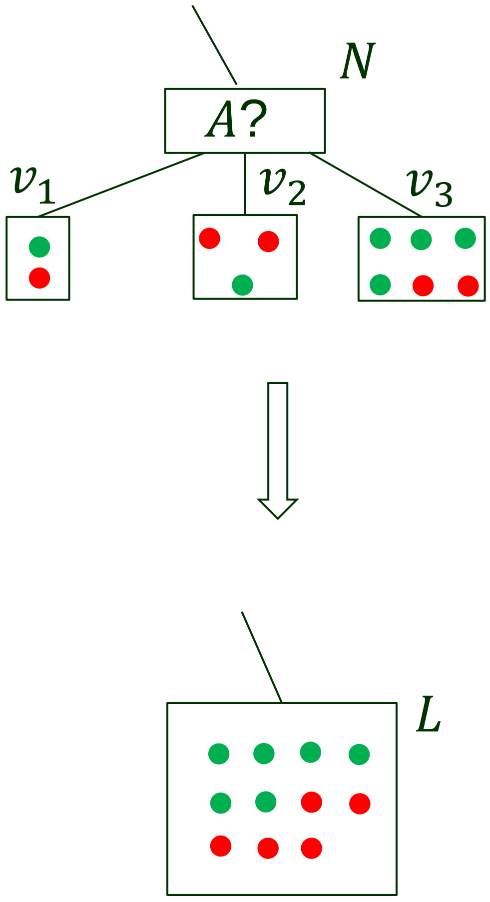

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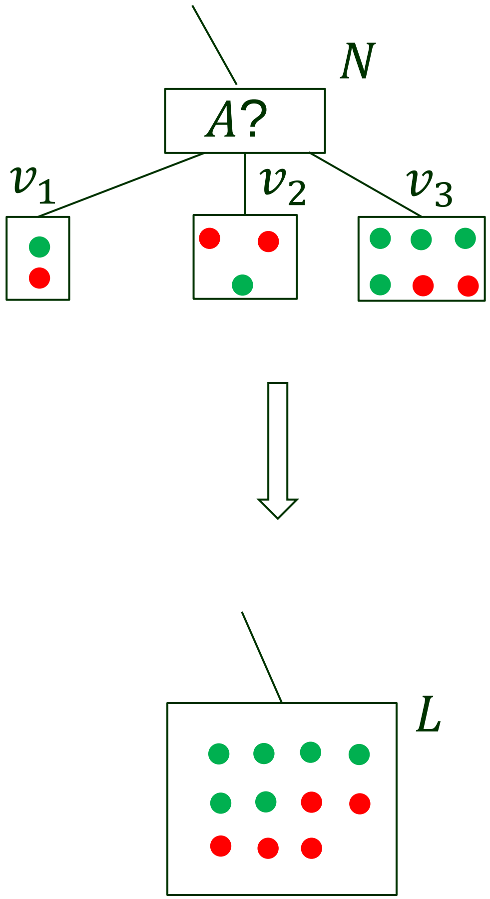

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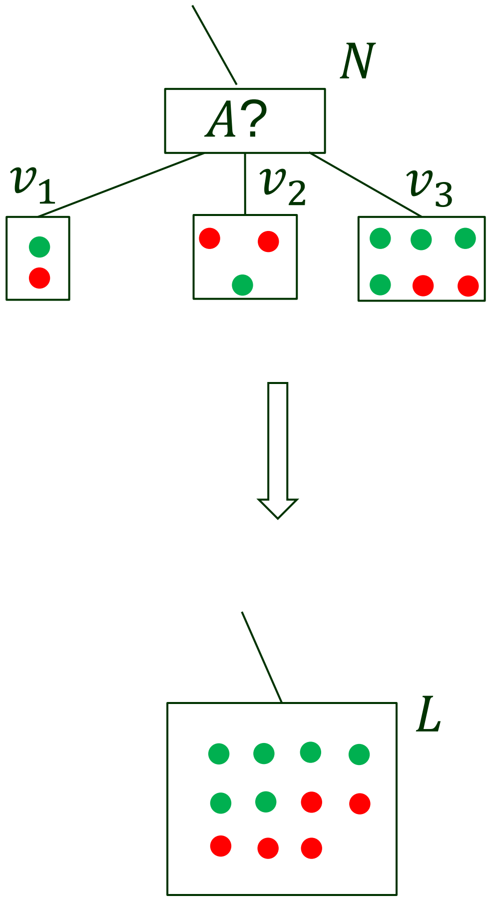

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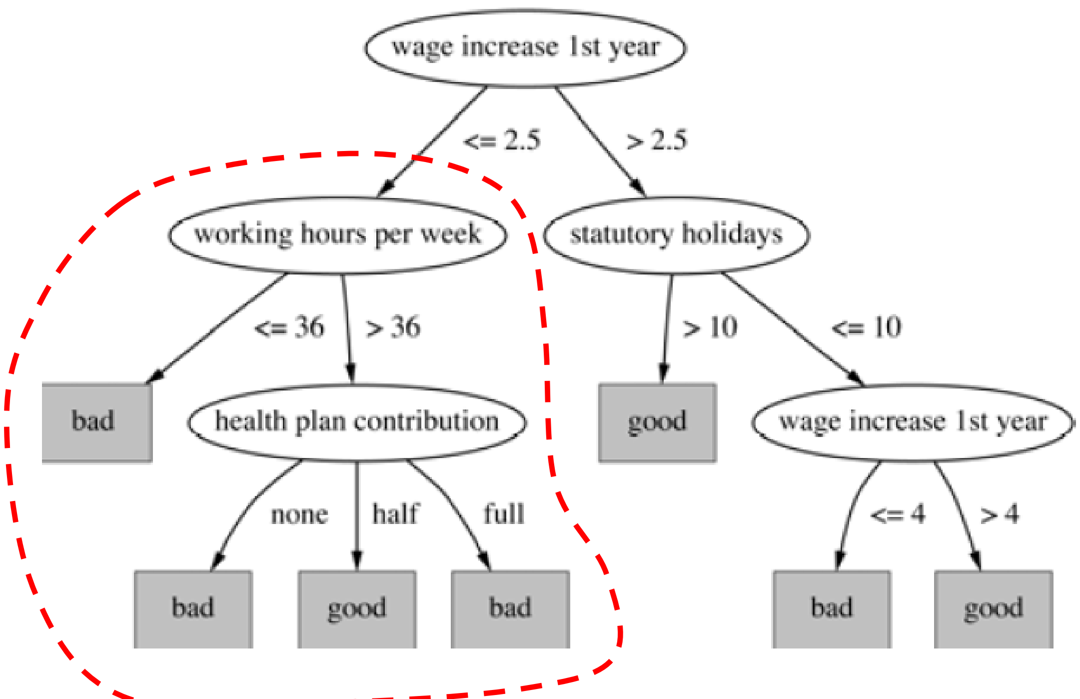
Low information gain.

$$Gain(A) = B\left(\frac{p}{p+n}\right) - \sum_{k=1}^{d} \frac{p_k+n_k}{p+n} B\left(\frac{p_k}{p_k+n_k}\right)$$

Example of Pruning



* Example from Dr. Jin Tian's notes.

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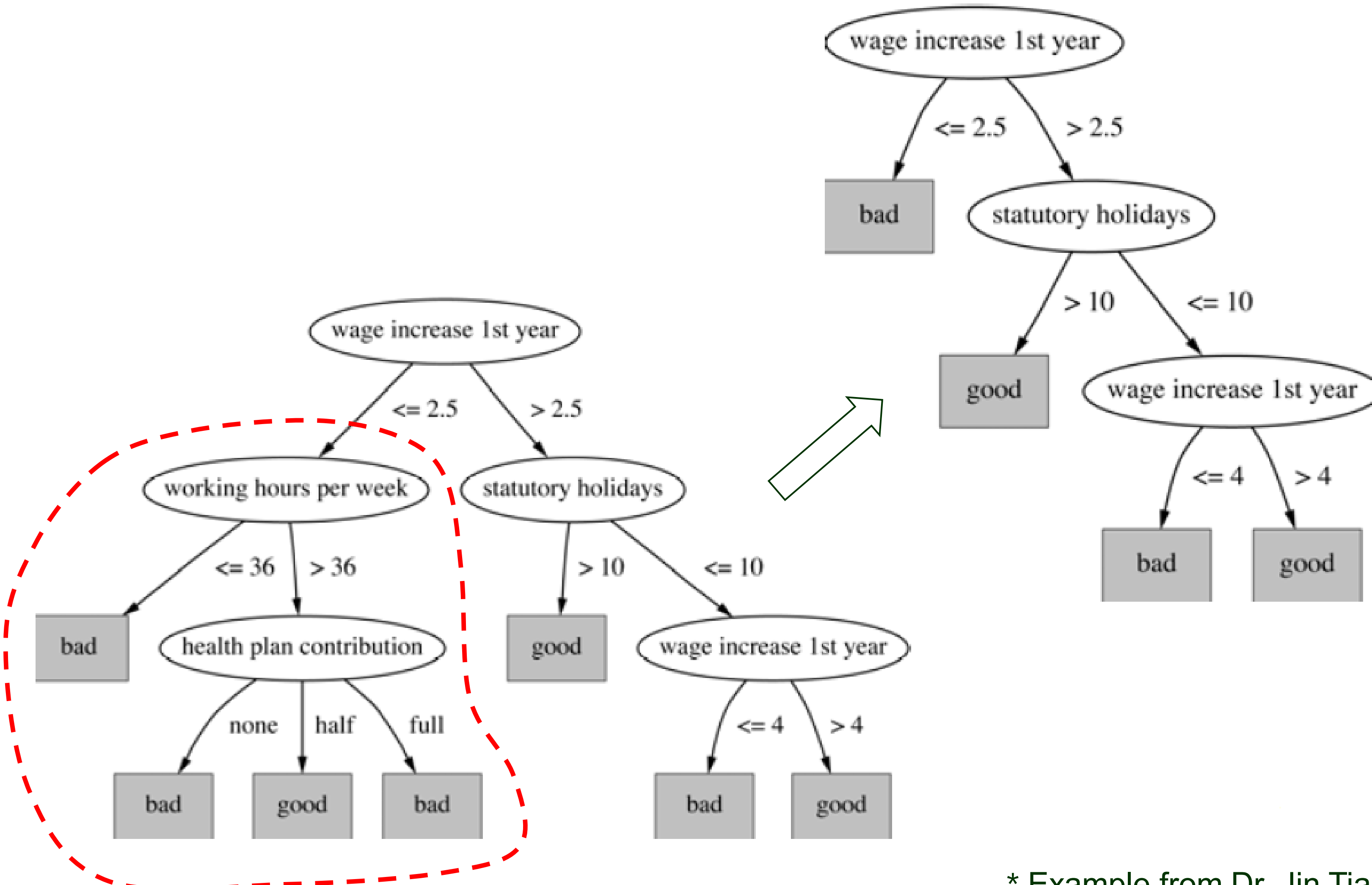

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Significance Test

- The node N has p positive and n negative examples.
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- Measure of the total deviation is given by

$$\Delta = \sum_{k=1}^{d} \left(\frac{(p_k - \hat{p}_k)^2}{\hat{p}_k} + \frac{(n_k - \hat{n}_k)^2}{\hat{n}_k} \right)$$

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χ^2 distribution with $d - 1$ degrees of freedom

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Apply χ^2 pruning:

$\Delta = 7.82$ would mean the attribute is irrelevant at the 5% level. (The higher the value of Δ, the more significant the attribute is.)

II. Model Selection

Goal: Select a hypothesis that will *optimally fit* *future examples*.

- ♦ Future examples are assumed to be like the past.

Stationarity:

$$\boldsymbol{P}(E_j) = \boldsymbol{P}(E_{j+1}) = \boldsymbol{P}(E_{j+2}) = \cdots$$

// every example has the
// the same prior probability.

$$\boldsymbol{P}(E_j) = \boldsymbol{P}(E_j \mid E_{j-1}, E_{j-2}, \ldots)$$

// every example is independent
// of the previous examples.

Optimal Fit

Split the examples into three sets:

- a *training set* to train candidate models (hypotheses)
- a *validation set* to evaluate the candidate models and choose the best one
- a *test set* to do a final unbiased evaluation of the best model

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Two tasks:

- *Model selection* chooses a good hypothesis space.
- *Optimization* (aka *training*) finds the best hypothesis within that space.

Model Selection via Cross Validation

function MODEL-SELECTION($Learner$, $examples$, k) **returns** a (hypothesis, error rate) pair

$err \leftarrow$ an array, indexed by $size$, storing validation-set error rates
$training\_set$, $test\_set \leftarrow$ a partition of $examples$ into two sets
for $size$ = 1 **to** ∞ **do**
  $err[size] \leftarrow$ CROSS-VALIDATION($Learner$, $size$, $training\_set$, k)
  if err is starting to increase significantly **then**
    $best\_size \leftarrow$ the value of $size$ with minimum $err[size]$
    $h \leftarrow Learner(best\_size, training\_set)$
    return h, ERROR-RATE(h, $test\_set$)

function CROSS-VALIDATION($Learner$, $size$, $examples$, k) **returns** error rate

$N \leftarrow$ the number of $examples$
$errs \leftarrow 0$
for i = 1 **to** k **do**
  $validation\_set \leftarrow examples[(i - 1) \times N/k{:}i \times N/k]$
  $training\_set \leftarrow examples - validation\_set$
  $h \leftarrow Learner(size, training\_set)$
  $errs \leftarrow errs$ + ERROR-RATE(h, $validation\_set$)
return $errs$ / k // *average error rate on validation sets, across k-fold cross-validation*

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  for size = 1 to ∞ do                                              // size is a hyperparameter
     err[size] ← CROSS-VALIDATION(Learner, size, training_set, k)   // of the model class, e.g.,
     if err is starting to increase significantly then              // #nodes in a decision tree
        best_size ← the value of size with minimum err[size]       // degree of polynomials.
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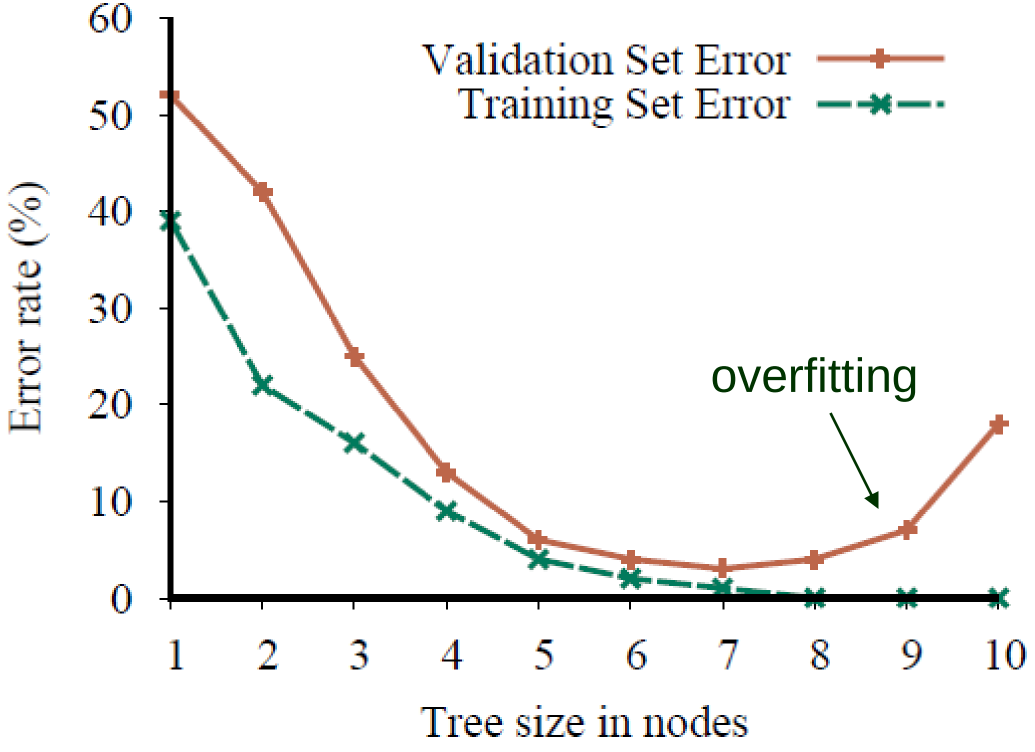
// validation set rotates among
// k equally partitioned subsets
// of examples. A large error due
// to overfitting is expected for
// a large k value.

Training and Validation Errors (1)



Data: obtained from a version of the restaurant problem

Model class: decision trees

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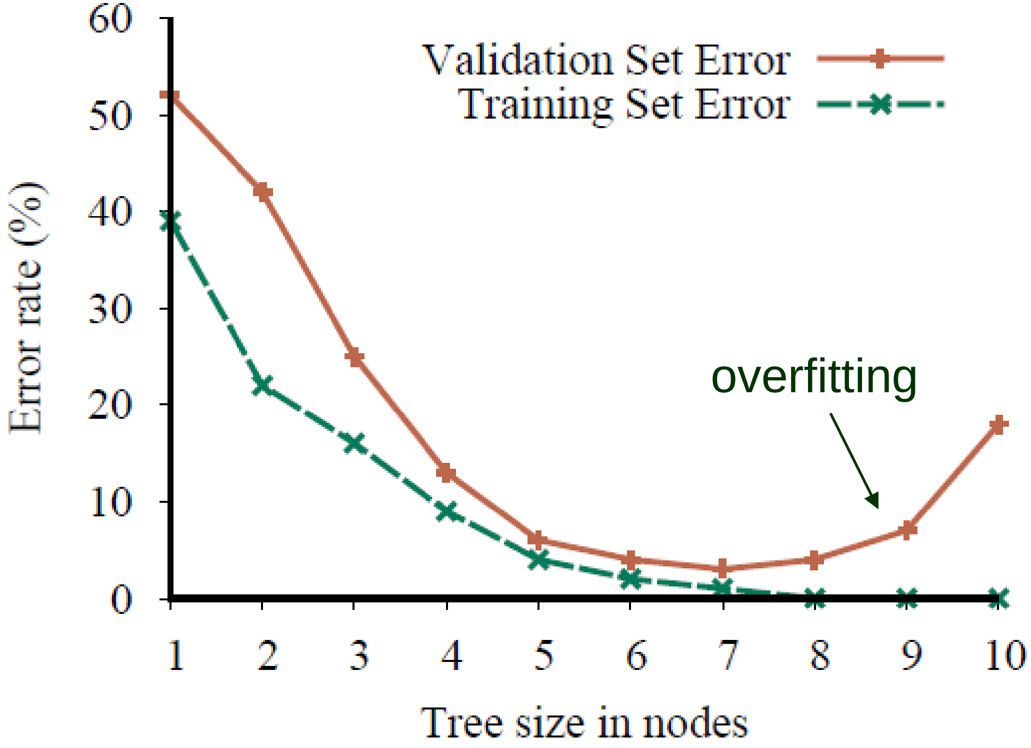

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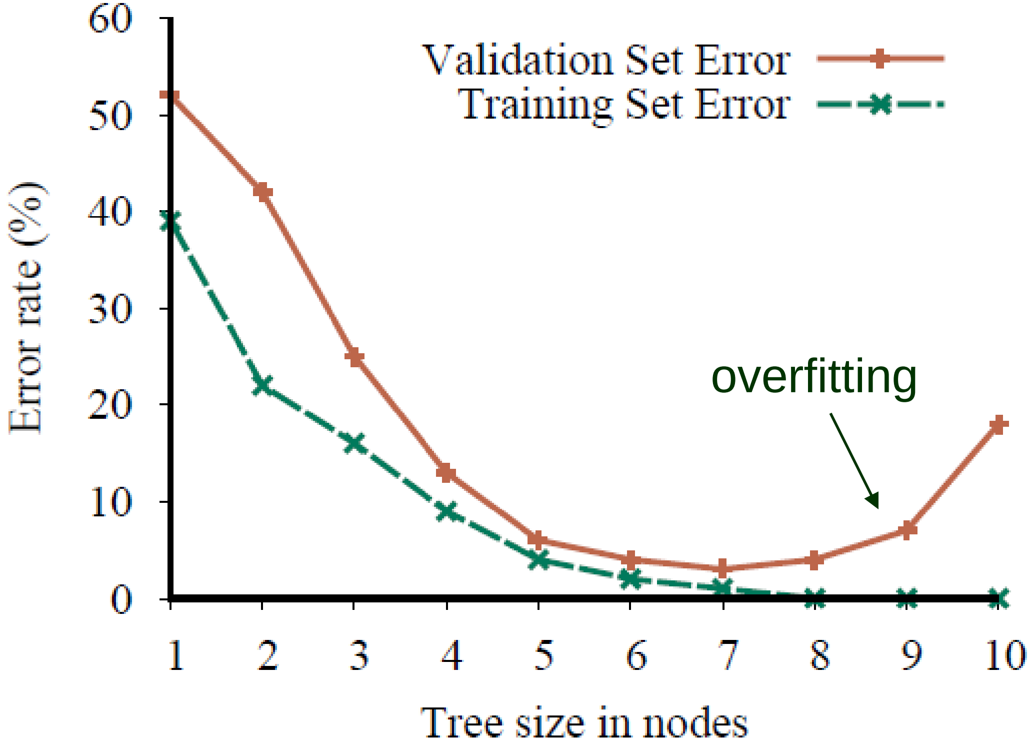

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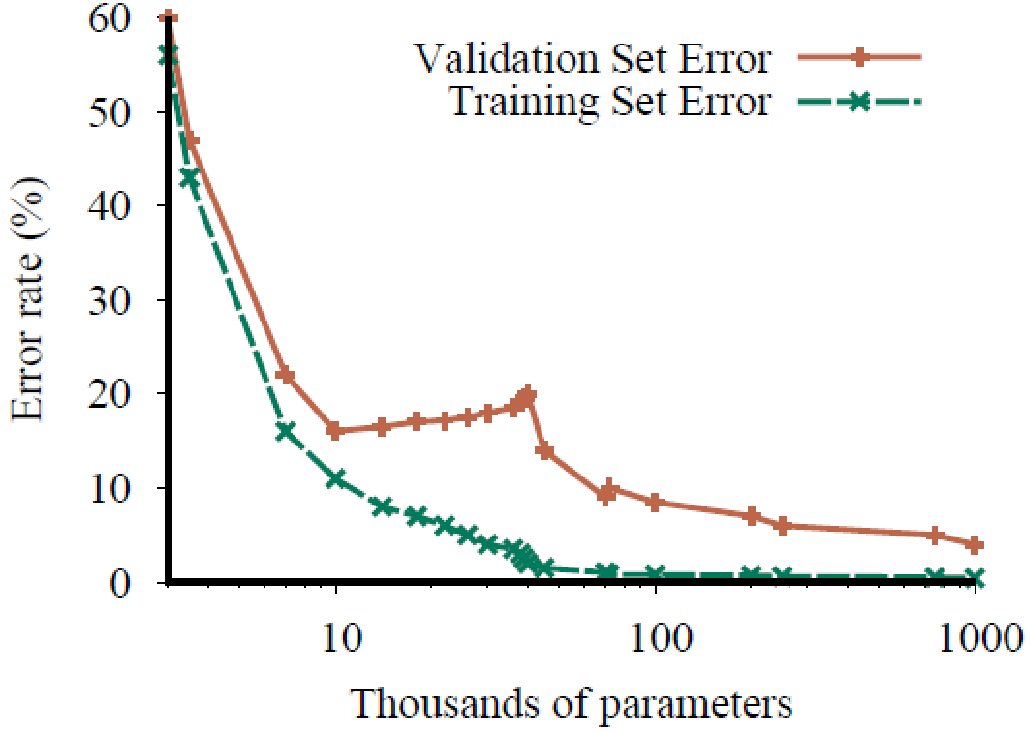
- ♦ The training set error decreases monotonically as the model complexity (tree size) increases.
- ♠ As the decision tree's size increases, the validation error initially decreases (until tree size = 7), and later increases since the model starts to overfit.

Training and Validation Errors (2)



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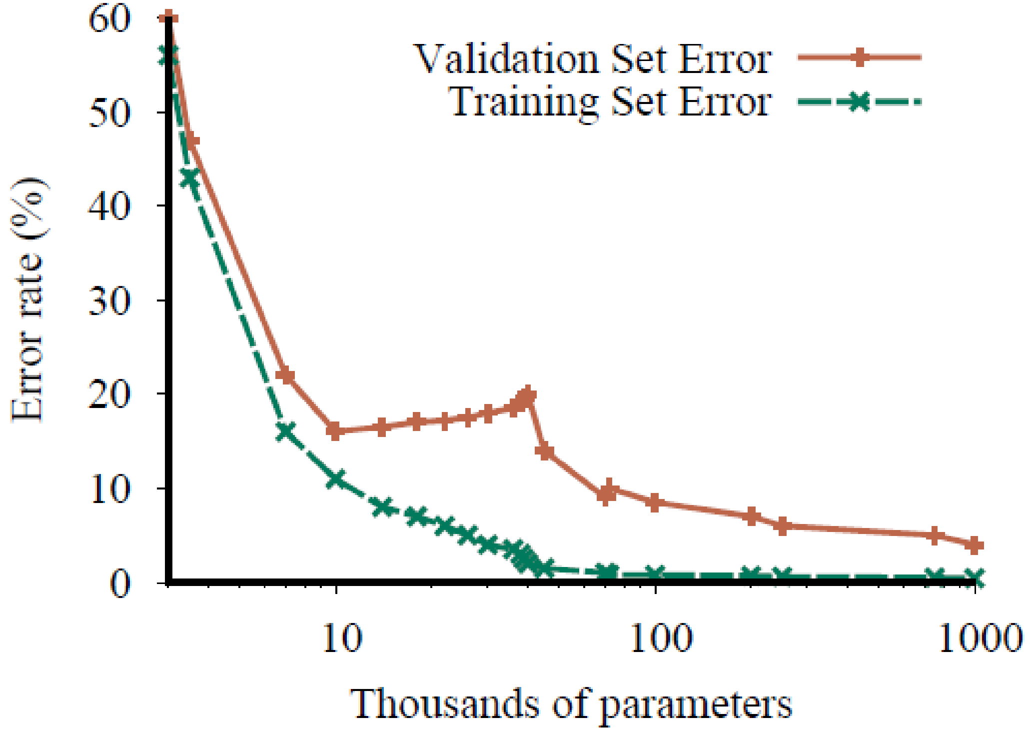

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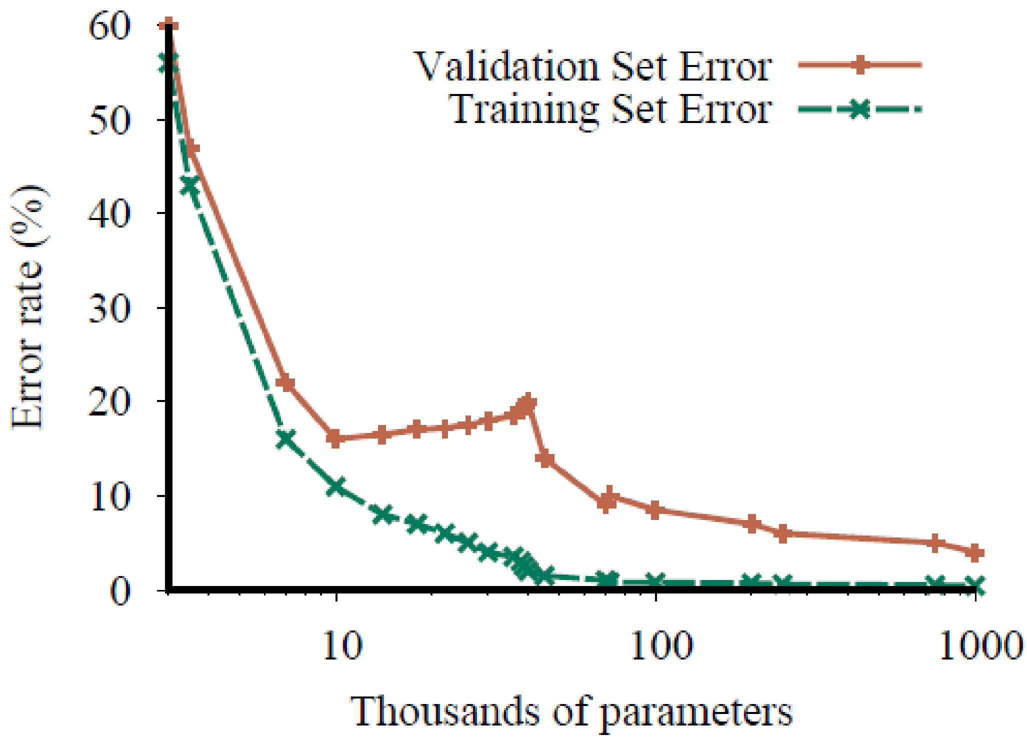

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- The training set error decreases monotonically.
- The validation error shows an initial U-shaped curve and then starts to decrease again, reaching the lowest value at the max number (1,000,000) of parameters.

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Generalization Loss

Absolute-value loss: $L_1(y, \hat{y}) = |y - \hat{y}|$

Squared-error loss: $L_2(y, \hat{y}) = (y - \hat{y})^2$

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Best hypothesis is chosen as

$$h^* = \operatorname*{argmin}_{h\in\mathcal{H}} \mathit{GenLoss}_L(h)$$

Empirical Loss

- $GenLoss_L(h)$ can only be estimated since $P(x, y)$ is often unknown.

Empirical loss on a set of examples E of size N:

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This defines an estimated best hypothesis:

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- ♠ Noise. f may be nondeterministic or noisy, returning different values $f(x)$ for the same x (e.g., measurements of a person's height).
- ♠ Computational complexity. Searching large hypothesis space $\mathcal{H}$ systematically can be computationally intractable. Often, a subspace search is conducted to return a reasonably good (but not optimal) hypothesis.

IV. Regularization

Model selection as a minimization:

$$\hat{h}^* = \operatorname*{argmin}_{h \in \mathcal{H}} \mathit{Cost}(h)$$

where

$$\mathit{Cost}(h) = \mathit{EmpLoss}(h) + \lambda \mathit{Complexity}(h)$$

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Regularization refers to the process of explicitly penalizing complex hypotheses to favor functions that are more regular.

- Choice of regularization function depends on the hypothesis space.

  For polynomials, we could use the sum of the squares of the coefficients, of which a small value would prevent a wiggling behavior.

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  Task: find a function $h(\boldsymbol{x})$ to minimize y over the N pairs $(y_i, h(\boldsymbol{x_i}))$