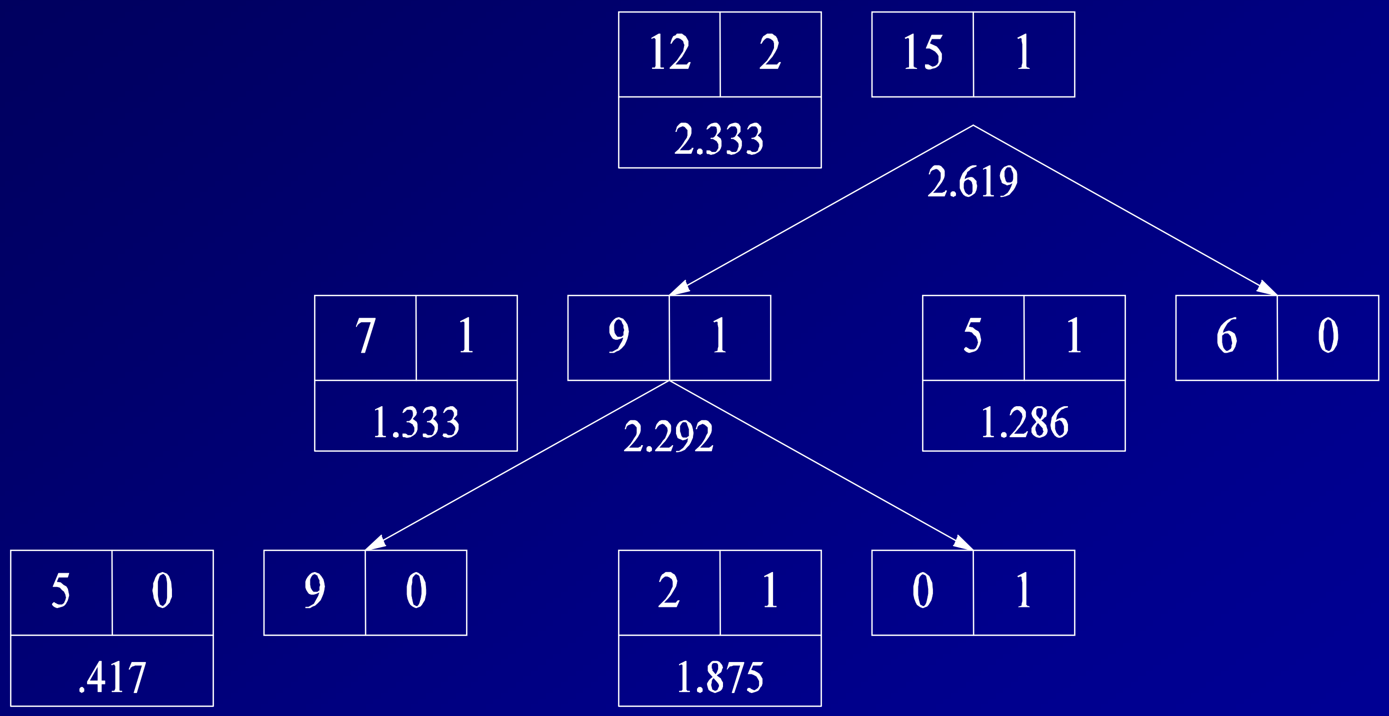
Holdout and Cross-Validation Methods Overfitting Avoidance

- Decision Trees
  - Reduce error pruning
  - Cost-complexity pruning
- Neural Networks
  - Early stopping
  - Adjusting Regularizers via Cross-Validation
- Nearest Neighbor
  - Choose number of neighbors
- Support Vector Machines
  - Choose C
  - Choose σ for Gaussian Kernels

Reduce Error Pruning

- Given a data sets S
  - Subdivide S into S_{train} and S_{dev}
  - Build tree using S_{train}
  - Pass all of the S_{dev} training examples through the tree and estimate the error rate of each node using S_{dev}
  - Convert a node to a leaf if it would have lower estimated error than the sum of the errors of its children

Reduce Error Pruning Example



Cost-Complexity Pruning

- The CART system (Breiman et al, 1984), employs cost-complexity pruning:

  $$J(Tree,S) = ErrorRate(Tree,S) + \alpha\,|Tree|$$

  where |Tree| is the number of nodes in the tree and α is a parameter that controls the tradeoff between the error rate and the penalty
- α is set by cross-validation

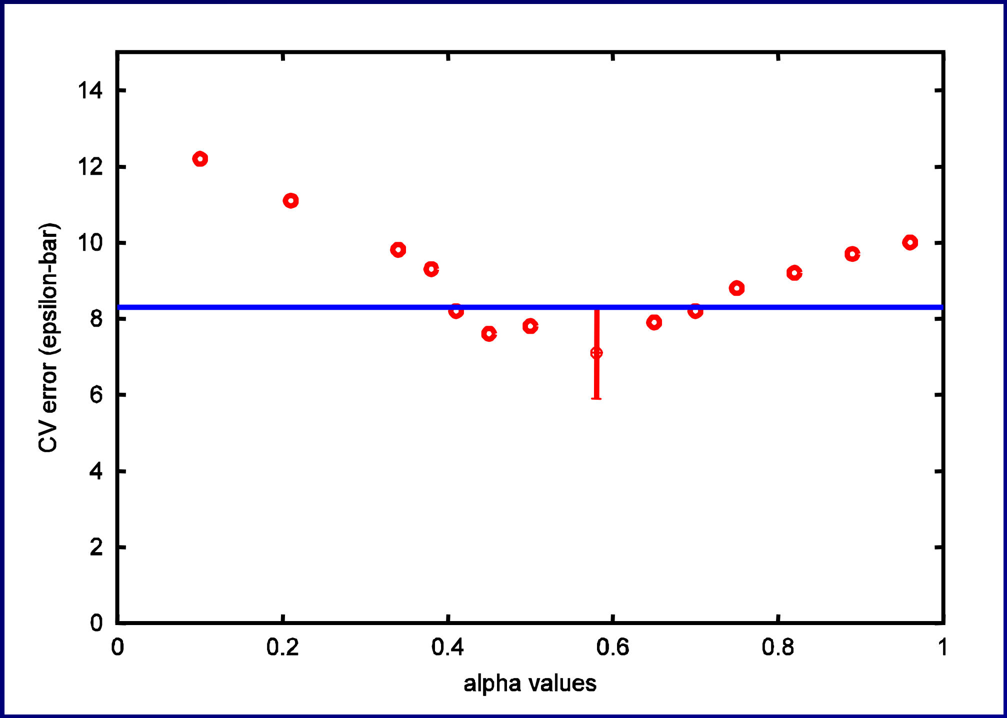
Determining Important Values of α

- Goal: Identify a finite set of candidate values for α. Then evaluate them via cross-validation
- Set $\alpha = \alpha_0 = 0$; $t = 0$
- Train S to produce tree T
- Repeat until T is completely pruned
  – determine next larger value of $\alpha = \alpha_{k+1}$ that would cause a node to be pruned from T
  – prune this node
  – $t := t + 1$
- This can be done efficiently

Choosing an α by Cross-Validation

- Divide S into 10 subsets $S_0, \ldots, S_9$
- In fold v
  - – Train a tree on $\cup_{i \neq v} S_i$
  - – For each α_k, prune the tree to that level and measure the error rate on S_v
  - – Compute $\underline{\varepsilon}_k$ to be the average error rate over the 10 folds when $\alpha = \alpha_k$
  - – Choose the α_k that minimizes $\underline{\varepsilon}_k$. Call it α_* and let ε_* be the corresponding error rate
- Prune the original tree according to α_*

The 1-SE Rule for Setting α



- Compute a confidence interval on $\underline{\varepsilon}_*$ and let U be the upper bound of this interval
- Compute the smallest α_k whose $\varepsilon_k \leq U$. If we use Z=1 for the confidence interval computation, this is called the 1-SE rule, because the bound is one "standard error" above $\underline{\varepsilon}_*$

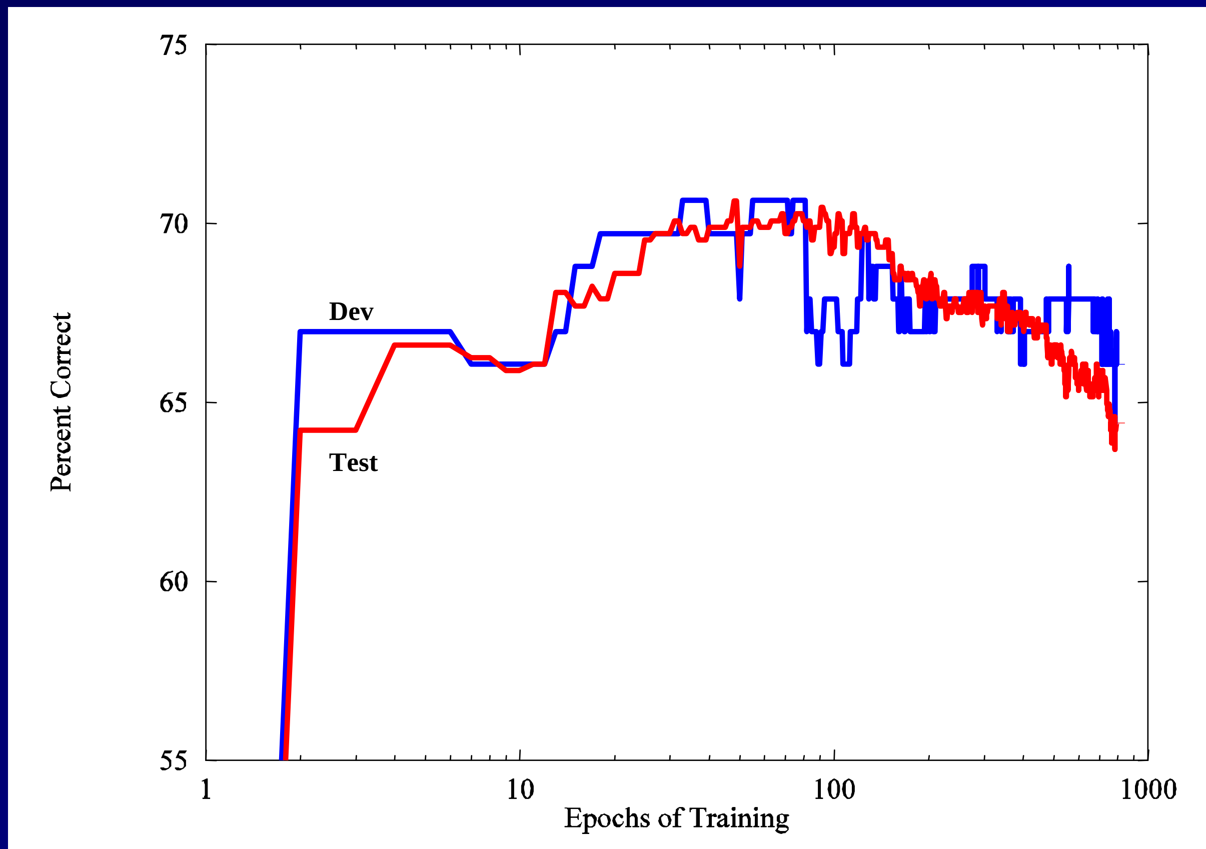
Notes on Decision Tree Pruning

- Cost-complexity pruning usually gives best results in experimental studies
- Pessimistic pruning is the most efficient (does not require holdout or cross-validation) and it is quite robust
- Reduce-error pruning is rarely used, because it consumes training data
- Pruning is more important for regression trees than for classification trees
- Pruning has relatively little effect for classification trees. There are only a small number of possible prunings of a tree, and usually the serious errors made by the tree-growing process (i.e., splitting on the wrong features) cannot be repaired by pruning.
  – Ensemble methods work much better than pruning

Holdout Methods for Neural Networks

- Early Stopping using a development set
- Adjusting Regularizers using a development set or via cross-validation
  - amount of weight decay
  - number of hidden units
  - learning rate
  - number of epochs

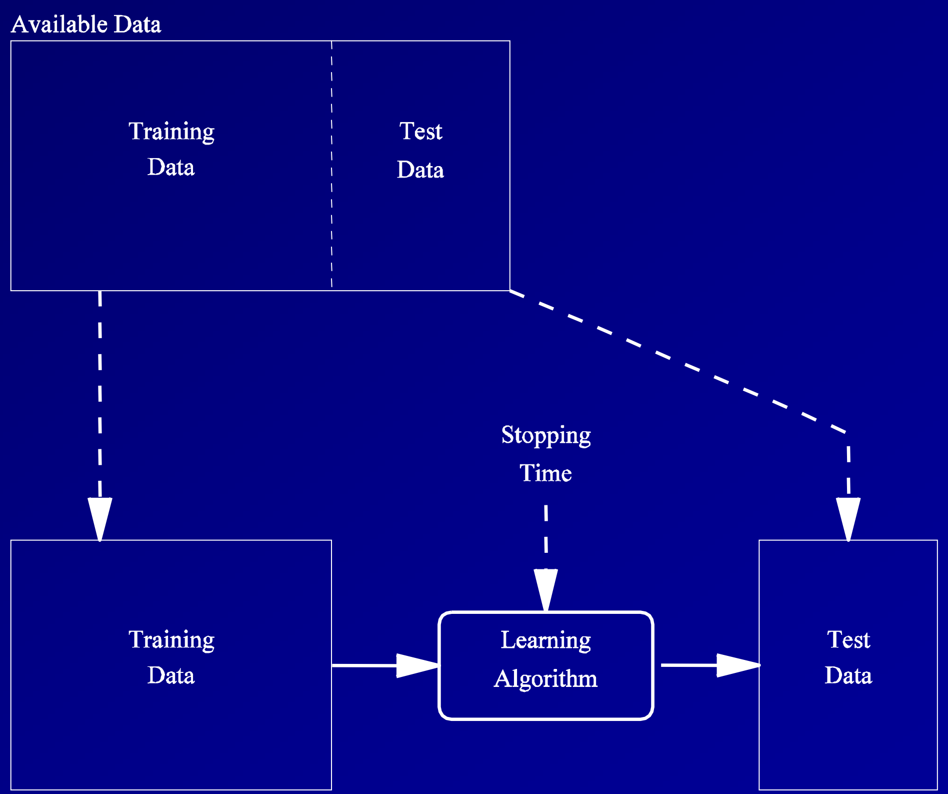
Early Stopping using an Evaluation Set



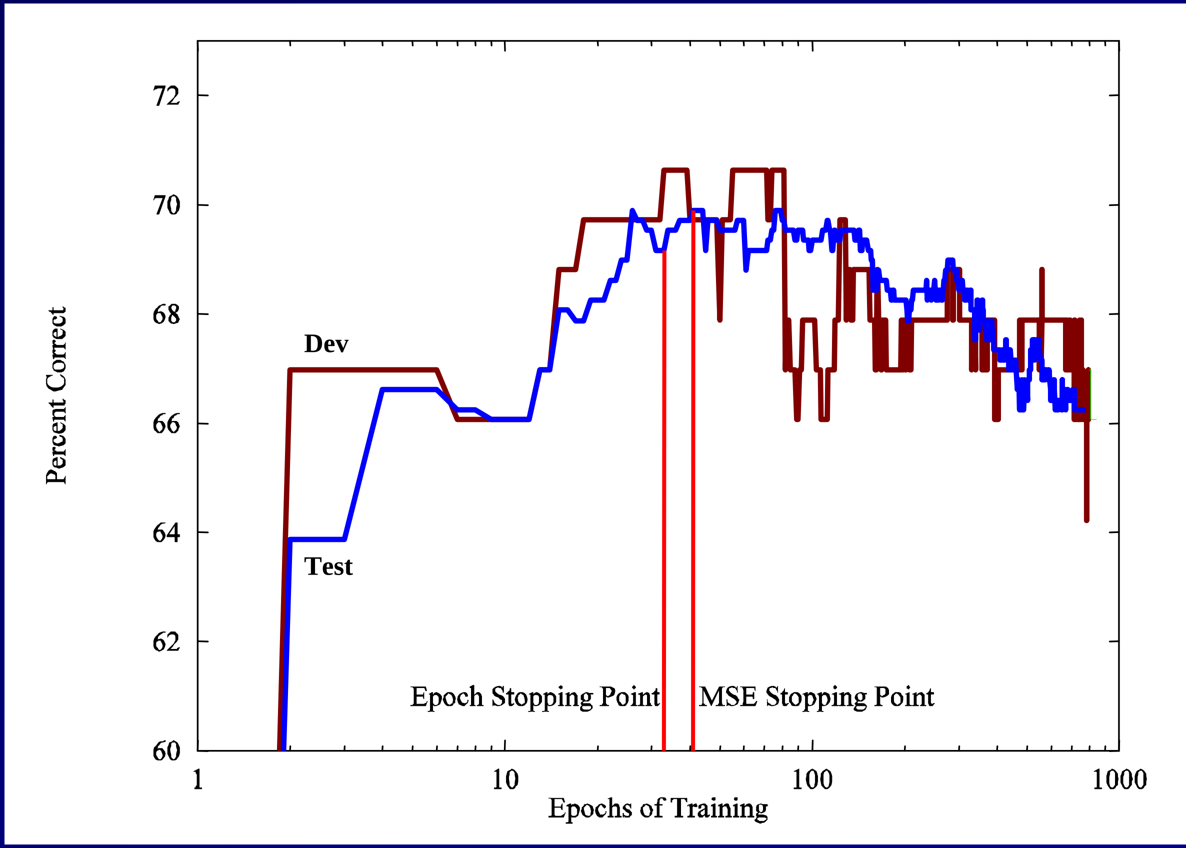
- Split S into S_{train} and S_{dev}
- Train on S_{train}, after every epoch, evaluate on S_{dev}. If error rate is best observed, save the weights

Reconstituted Early Stopping

- Recombine S_{train} and S_{dev} to produce S
- Train on S and stop at the point (# of epochs or mean squared error) identified using S_{dev}

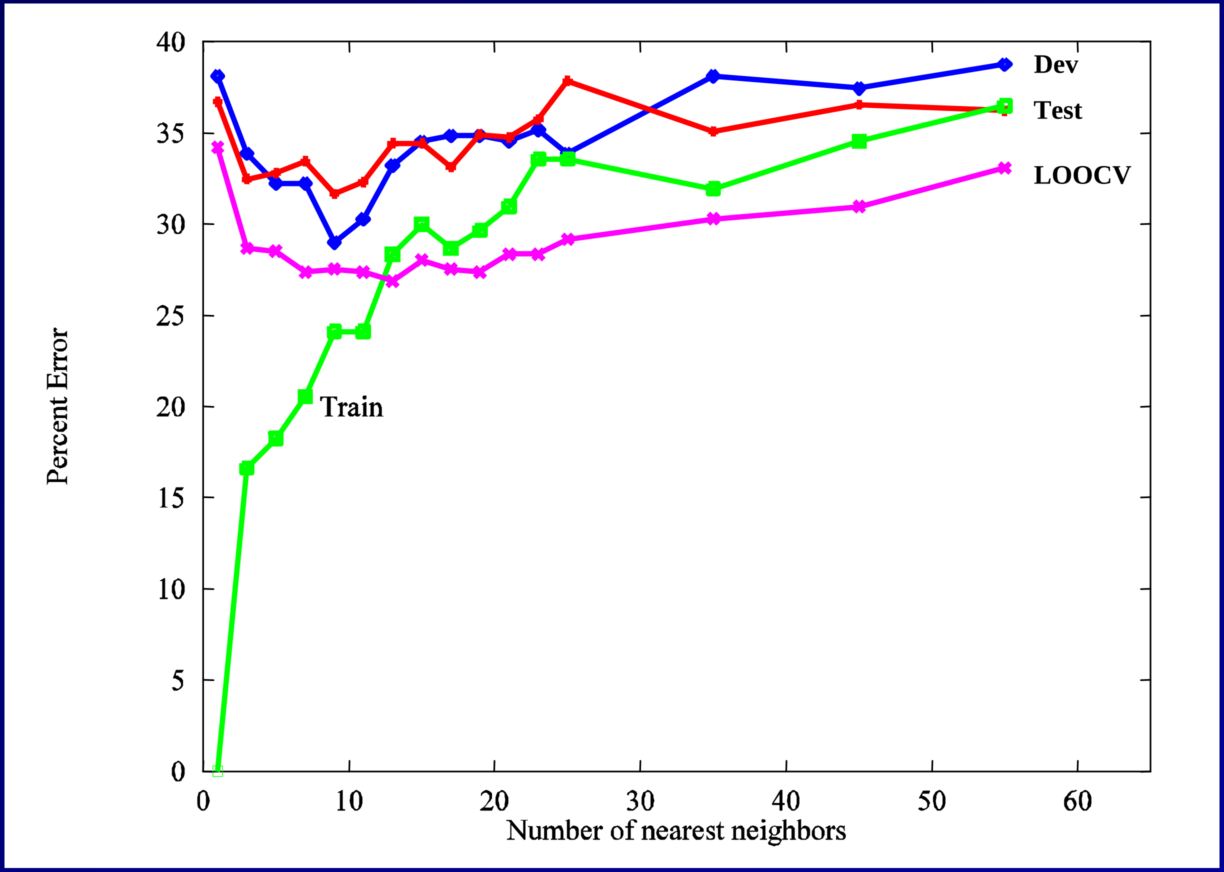


Reconstituted Early Stopping



- We can stop either when MSE on the training set matches the predicted optimal MSE or when the number of epochs matches the predicted optimal number of epochs
- Experimental studies show little or no advantage for reconstituted early stopping. Most people just use simple holdout

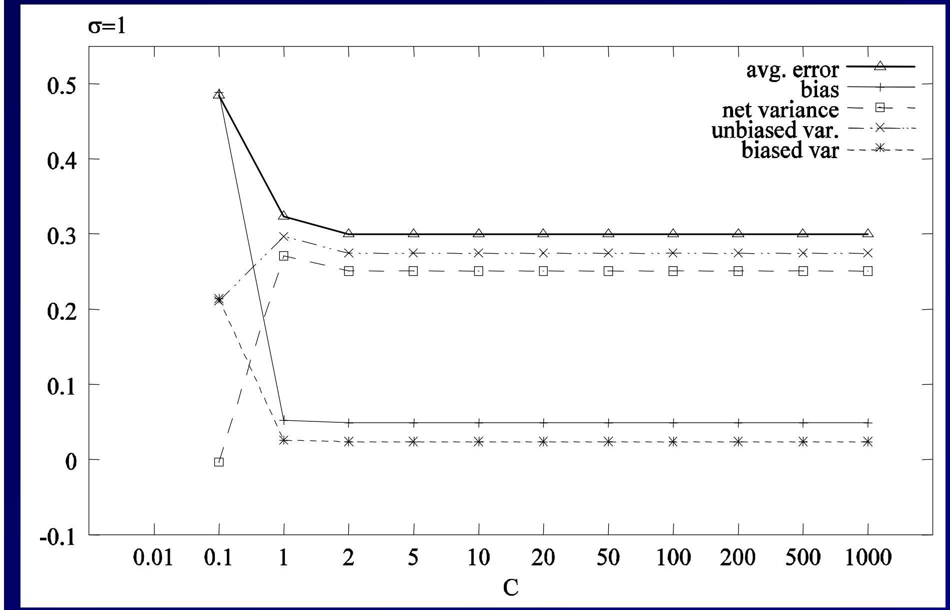
Nearest Neighbor: Choosing k

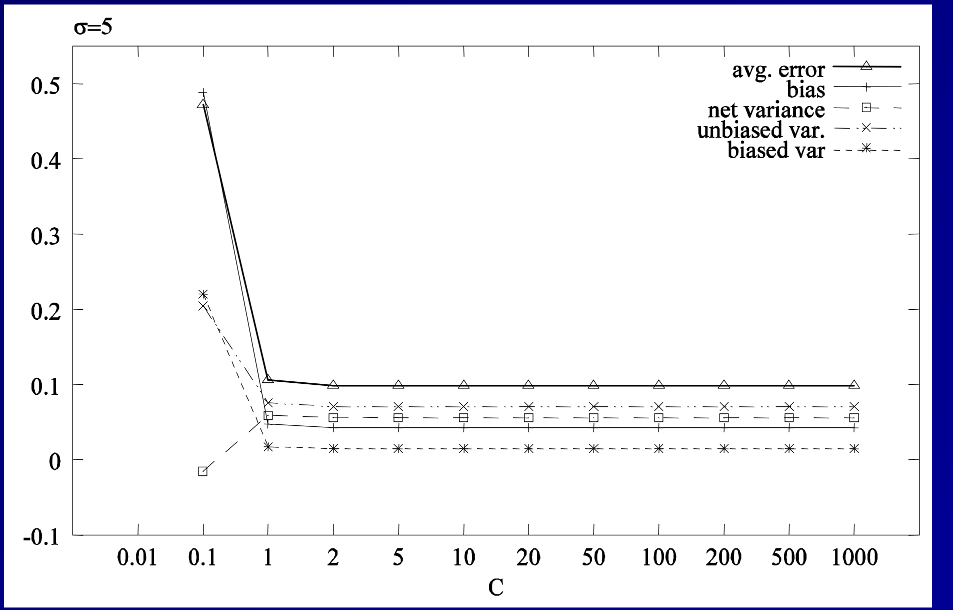


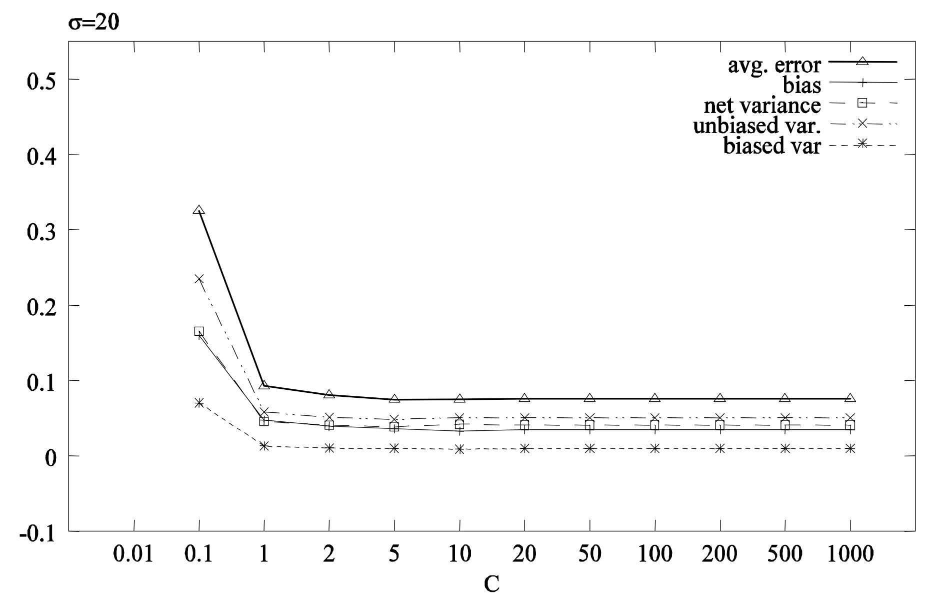
- k=9 gives best performance on development set and on test set. k=13 gives best performance based on leave-one-out cross-validation

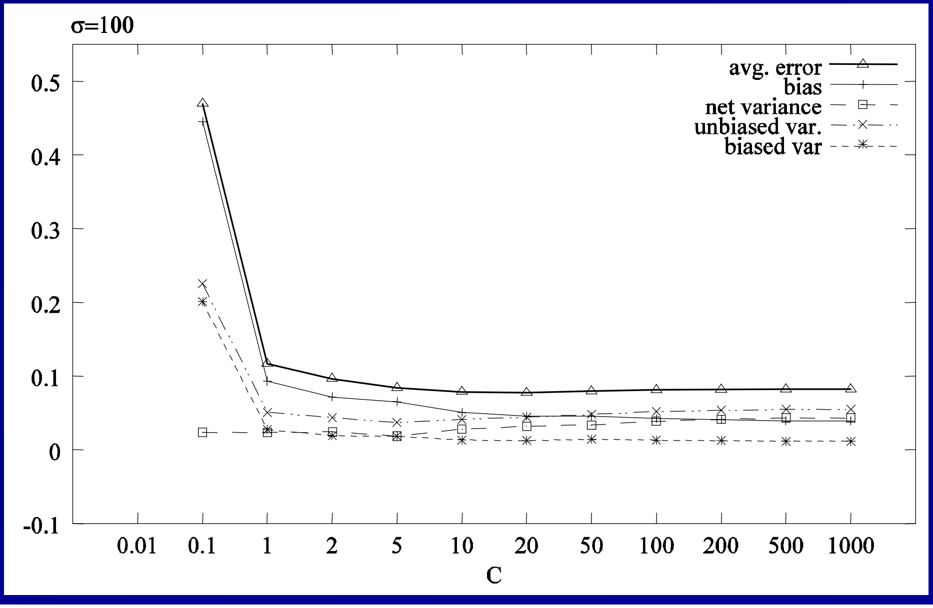
SVM Choosing C and σ

(BR Data Set; 100 examples; Valentini 2003)

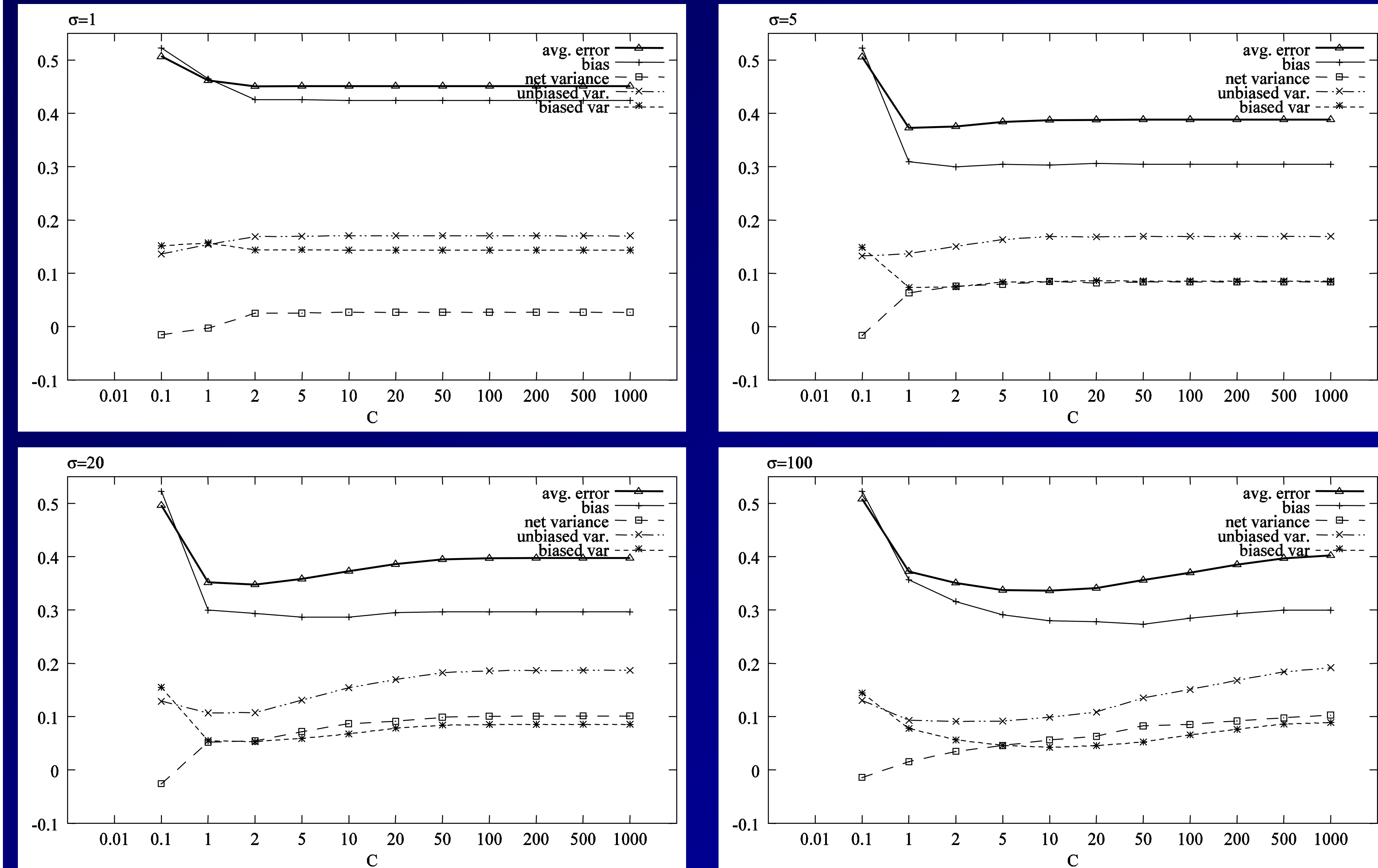




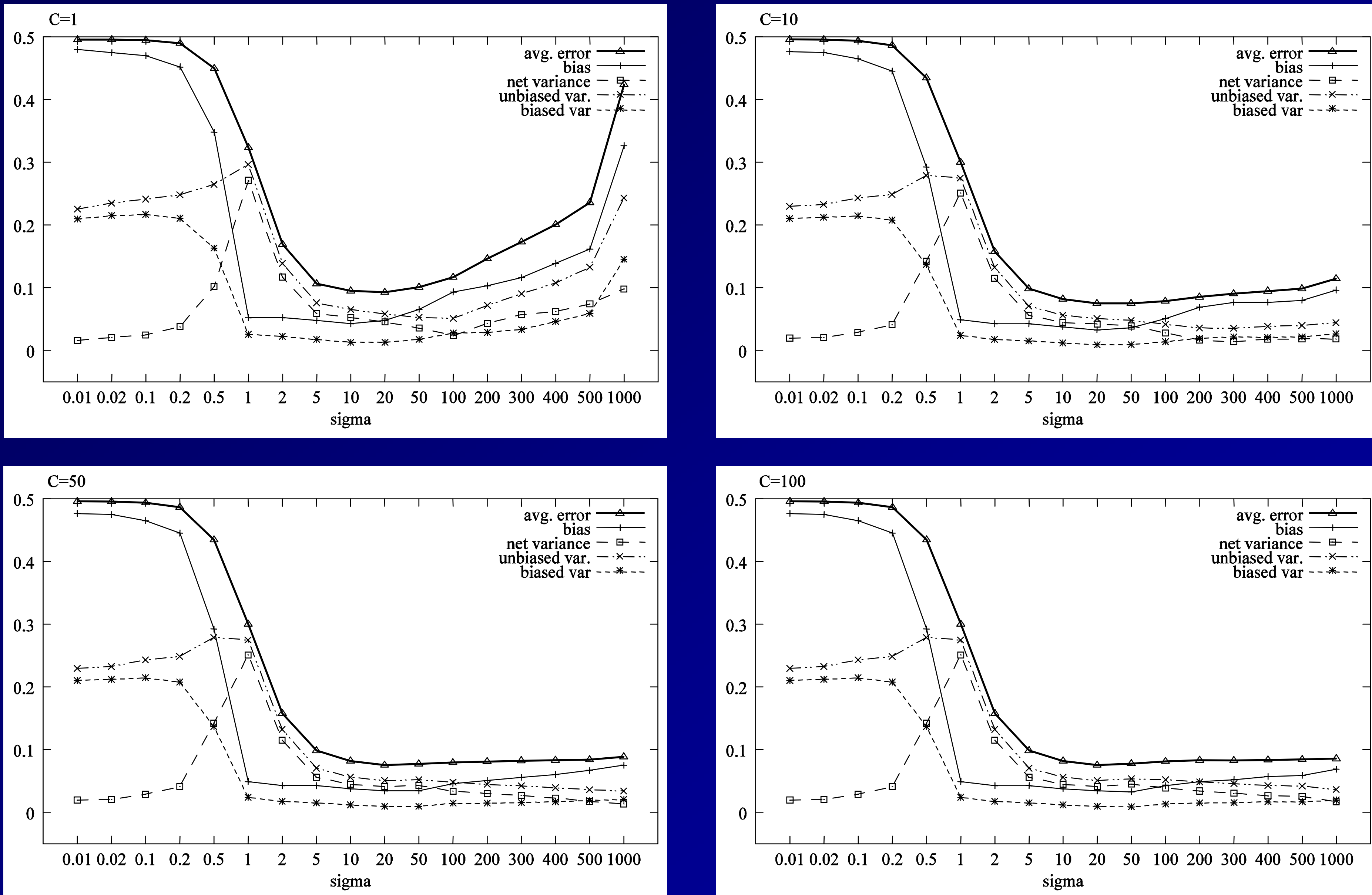




20% label noise



BR Data Set: Varying σ for fixed C



Summary

- Holdout methods are the best way to choose a <u>classifier</u>
  - Reduce error pruning for trees
  - Early stopping for neural networks
- Cross-validation methods are the best way to set a <u>regularization parameter</u>
  - Cost-complexity pruning parameter α
  - Neural network weight decay setting
  - Number k of nearest neighbors in k-NN
  - C and σ for SVMs