COMPSCI 589
Lecture 4: Overfitting, Regularization, and Crossvalidation

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Outline

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- In the case of logistic regression, we saw that $P_{\mathbf{w}}(y|\mathbf{x})$ is sensitive to the magnitude of the weights $\mathbf{w}$.
- In this lecture, we'll discuss what changes in these models as we vary these parameters and introduce methodology for selecting optimal values for them.

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- **Question:** How would you rank the capacity of the classifiers we've seen so far?

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- **Capacity Control:** To achieve optimal generalization performance for a given training set, we often need to control model capacity carefully.

Overfitting and Underfitting

- **Overfitting:** The generalization error for a classifier is much worse than the training error. This usually results from choosing a classifier with too much capacity so that it models the noise in the training data.

- **Underfitting:** Occurs when the capacity of the classifier is too low to capture the actual structure in the training data, leading to both high training error and high generalization error.

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- **Bias-Variance and Capacity:** On complex data, models with low capacity have low variance, but high bias; while models with high capacity have low bias, but high variance.

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- **Question:** What are the capacity control parameters for KNN and decision trees?
- **Question:** What are the capacity control parameters for naive Bayes and logistic regression?

Capacity, Smoothness and Regularization

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- **Laplace Smoothing:** Laplace smoothing is a simple method for smoothing the parameter estimates of a categorical distribution:

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- As the regularization hyperparameter α increases, our estimate of the distribution smooths out toward being uniform. This provides capacity control for NB with binary or categorical features.

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- Some formulations of this problem up-weight the contribution from the data instead:

$$\theta_* = \arg\max_{\theta} C\sum_{i=1}^{n} \log P(Y = y_i|\mathbf{X} = \mathbf{x}_i) - ||\mathbf{w}||_2^2$$

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- The regularization hyperparameters are either λ or C. As λ increases, the learned $P(Y|X)$ will smooth out. As C decreases, the learned $P(Y|X)$ will smooth out.

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- In addition, we will want an estimate of the generalization error that the selected parameters achieve.
- To obtain, valid results, we need to use appropriate methodology and construct learning experiments carefully.
- **Guiding Principle:** Data used to estimate generalization error can not be used for any other purpose (ie: model training, hyperparameter selection, feature selection, etc.) or the results of the evaluation will be **biased**.

Recipe 1: Train-Validation-Test

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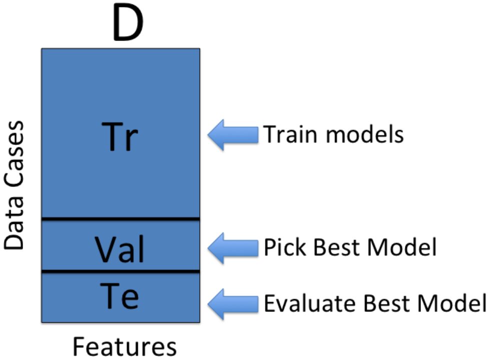
- Generalization performance is estimated by evaluating error/accuracy of M_* on the test data Te.

Example: Train-Validation-Test



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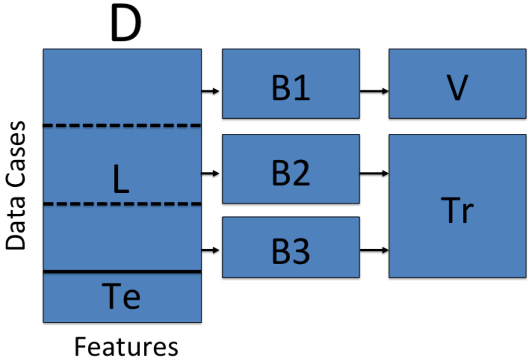
- Estimate generalization performance by evaluating error/accuracy of M_* on Te.

Example: 3-Fold Cross Validation and Test

First Cross Validation Fold



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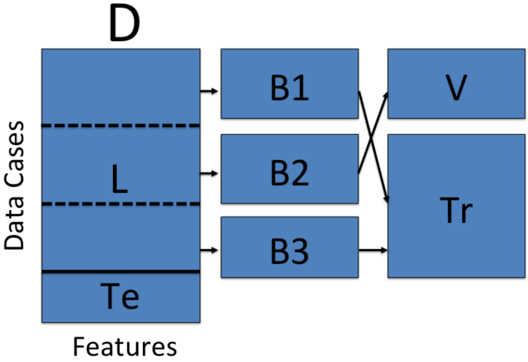

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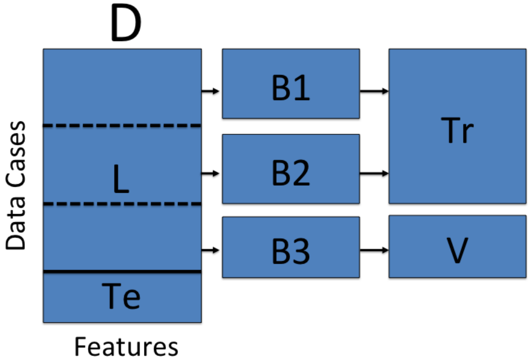

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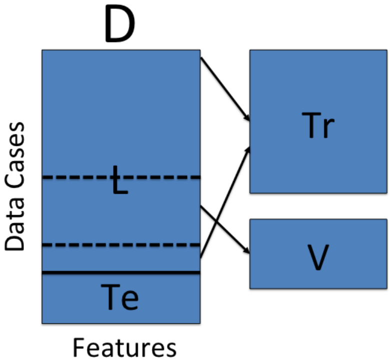

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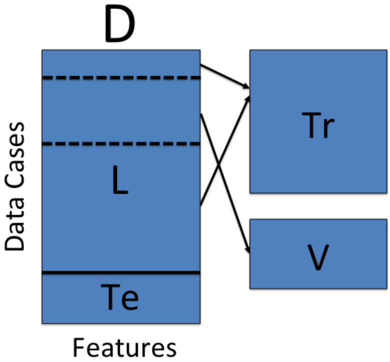

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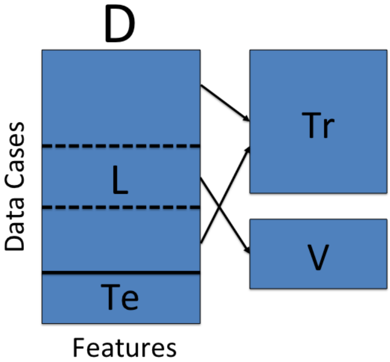

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  - Compute Err_j by evaluating M_{*j} on Te_j.

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  - Partition L_j into a set of K blocks $B_1, ..., B_K$.
  - For $k = 1, ..., K$:
    - Let $V = B_k$ and $Tr = L_j/B_k$.
    - Learn M_{ik} on Tr for each choice of hyperparameters H_i.
    - Compute error Val_{ik} of M_{ik} on V.
  - Select hyperparameters H_* minimizing $\frac{1}{K}\sum_{k=1}^{K} Val_{ik}$ and re-train model on L_j using these hyperparameters, yielding model M_{*j}.
  - Compute Err_j by evaluating M_{*j} on Te_j.
- Estimate generalization error using $\frac{1}{J}\sum_{j=1}^{J} Err_j$

Recipe 4: Crossvalidation-Crossvalidation

- Randomly partition data set D into a set of J blocks $C_1, \ldots, C_J$.
- For $j = 1, \ldots, J$:
  - Let $Te_j = C_j$ and $L_j = D/C_j$
  - Partition L_j into a set of K blocks $B_1, \ldots, B_K$.
  - For $k = 1, \ldots, K$:
    - Let $V = B_k$ and $Tr = L_j/B_k$.
    - Learn M_{ik} on Tr for each choice of hyperparameters H_i.
    - Compute error Val_{ik} of M_{ik} on V.
  - Select hyperparameters H_* minimizing $\frac{1}{K}\sum_{k=1}^{K} Val_{ik}$ and re-train model on L_j using these hyperparameters, yielding model M_{*j}.
  - Compute Err_j by evaluating M_{*j} on Te_j.
- Estimate generalization error using $\frac{1}{J}\sum_{j=1}^{J} Err_j$
- We can define a similar nested random resampling validation procedure.

Trade-Offs

- In cases where the data has a benchmark split into a training set and a test set, we can use Recipes 1-3 by preserving the given test set and splitting the given training set into train and validation sets as needed.

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- In cases where there is relatively little data, using a single held out test set will have high bias. In these cases, Recipe 4 often provides a better estimate of generalization error, but has much higher computational cost.
- Choosing larger K in cross validation will reduce bias. Choosing larger S in random re-sampling validation will reduce variance and bias. However, both increase computational costs. $K = 3, 5, 10$ are common choices for cross validation. $K = N$, also known as Leave-one-out cross validation is also popular when feasible.