Practical Issues: Model/Feature Selection and Debugging Learning Algorithms

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Machine Learning (CS771A)

Oct 19, 2016

Model Selection

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Note: Usually considered in supervised learning contexts but unsupervised learning too faces this issue (e.g., "how many clusters" when doing clustering)

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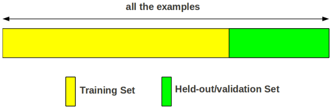
    - Other names: validation/development data.



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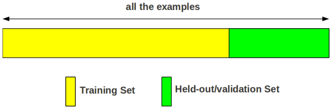

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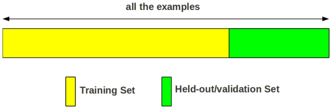

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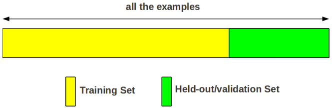

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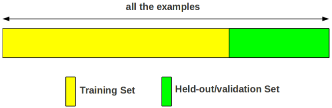

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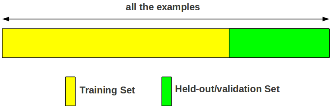

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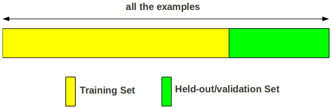

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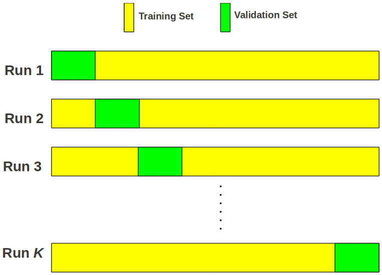
  - What if there was an unfortunate train/held-out split?

K-fold Cross-Validation

- Create K (e.g., 5 or 10) equal sized partitions of the training data
- Each partition has N/K examples
- Train using $K-1$ partitions, validate on the remaining partition
- Repeat this K times, each with a different validation partition



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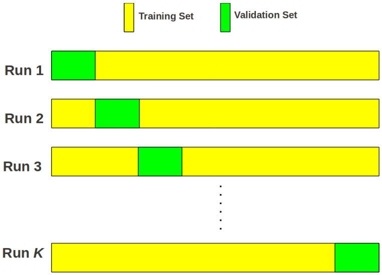

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- Choose the model that gives the smallest average validation error

Leave-One-Out (LOO) Cross-Validation

Special case of K-fold CV when $K = N$

- Each partition is now a single example
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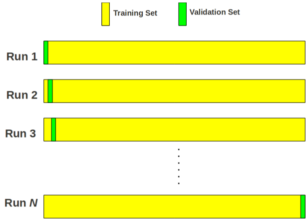

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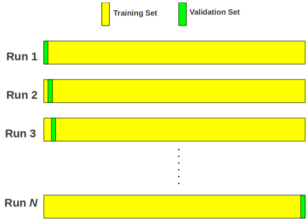

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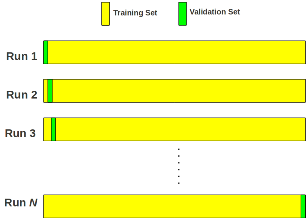

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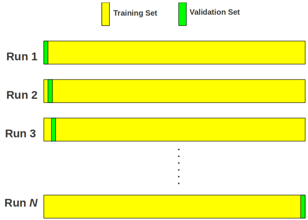

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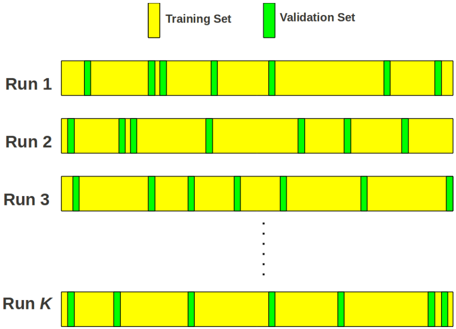

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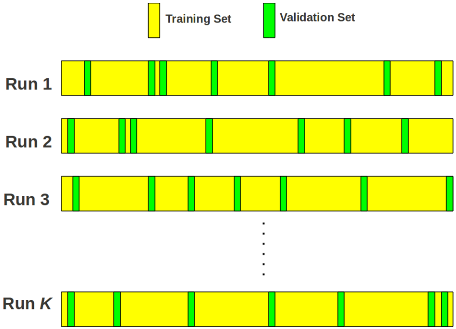

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- Use the following equation to compute the expected model error

$$err = 0.632 \times err_{\text{test-examples}} + 0.368 \times err_{\text{training-examples}}$$

Information Criteria based methods

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$$AIC = 2k - 2\log(\mathcal{L})$$

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- Can be used even for model selection in unsupervised learning

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- **Note:** Feature Selection is different from Feature Extraction
  - The latter transforms original features to get a small set of new features (e.g., PCA or other dimensionality reduction methods)

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(Also see: "An Introduction to Variable and Feature Selection" by Guyon and Elisseeff)

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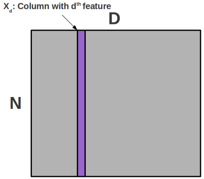

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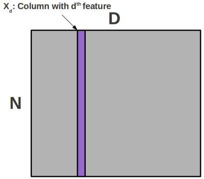

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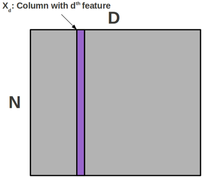

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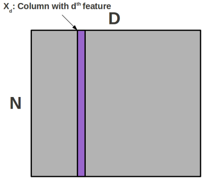

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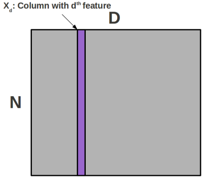

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  - Note: These probabilities can be easily estimated from the data

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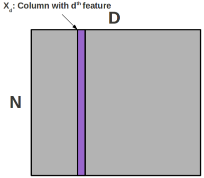

- **Correlation Criteria:** Rank features in order of their correlation with labels

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- **Mutual Information Criteria:**

$$MI(X_d, Y) = \sum_{X_d \in \{0,1\}} \sum_{Y \in \{0,1\}} P(X_d, Y) \frac{\log P(X_d, Y)}{P(X_d)P(Y)}$$

  - High mutual information mean high relevance of that feature
  - Note: These probabilities can be easily estimated from the data

- Various other statistical tests exist, e.g., χ^2 test

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  - Remove f with lowest error from $\mathcal{F}$
- In practice, these methods can be expensive. Also myopic and sub-optimal because the adding/removing of features is greedy

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- How to know what might be going wrong and how to debug?

Bias-Variance Decomposition

- For some model $y = f(\boldsymbol{x}) + \epsilon$ with $\epsilon \sim \mathcal{N}(0, \sigma^2)$, given its estimate $\hat{f}$ learned by a "learner" using a finite training set, the following decomposition holds

$$\mathbb{E}[(y - \hat{f}(\boldsymbol{x}))^2] = \text{Bias}[\hat{f}(\boldsymbol{x})]^2 + \text{Var}[\hat{f}(\boldsymbol{x})] + \sigma^2$$

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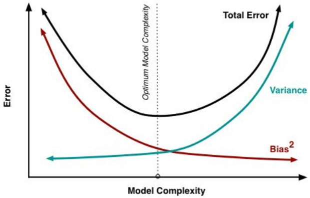
- The proof (note that $\mathbb{E}[y] = f(\boldsymbol{x})$):

$$\begin{aligned}
\mathrm{E}\big[(y-\hat{f})^2\big] &= \mathrm{E}[y^2 + \hat{f}^2 - 2y\hat{f}] \\
&= \mathrm{E}[y^2] + \mathrm{E}[\hat{f}^2] - \mathrm{E}[2y\hat{f}] \\
&= \mathrm{Var}[y] + \mathrm{E}[y]^2 + \mathrm{Var}[\hat{f}] + \mathrm{E}[\hat{f}]^2 - 2f\mathrm{E}[\hat{f}] \\
&= \mathrm{Var}[y] + \mathrm{Var}[\hat{f}] + (f - \mathrm{E}[\hat{f}])^2 \\
&= \mathrm{Var}[y] + \mathrm{Var}[\hat{f}] + \mathrm{E}[f - \hat{f}]^2 \\
&= \sigma^2 + \mathrm{Var}[\hat{f}] + \mathrm{Bias}[\hat{f}]^2
\end{aligned}$$

Bias-Variance Trade-off

- Simple models have high bias and small variance, complex models have small bias and high variance



	Model				
	Bias	Variance	Complexity	Flexibility	Generalizability
Underfitting: you have an overly simple model	High	Low	Low	Low	High
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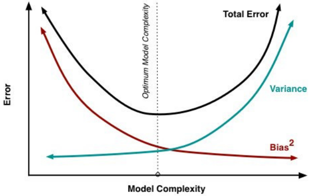

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- If you modified a model to reduce its bias (e.g., by increasing the model's complexity), you are likely to increase its variance, and vice-versa (if both increase then you might be doing it wrong!)

(Pic courtesy: Scott Fortmann-Roe, Latysheva and Ravarani)

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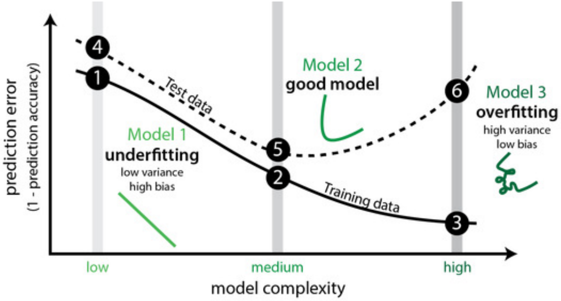

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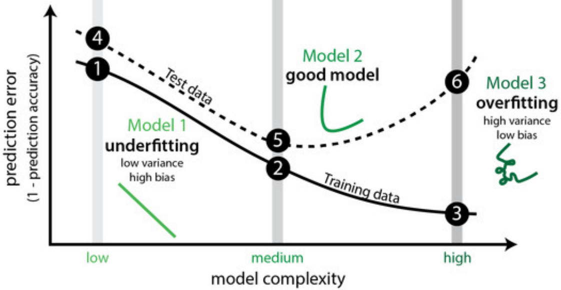

- High Bias: Both training and test errors are large
- High Variance: Small training error, large test error (and huge gap)

(Pic courtesy: Latysheva and Ravarani)

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  - If $\mathcal{L}(\boldsymbol{w}_{LR}) < \mathcal{L}(\boldsymbol{w}_{SVM})$ then LR isn't a good model for this problem

Next Class: Ensemble Methods