Model Selection and Feature Selection

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CS5350/6350: Machine Learning

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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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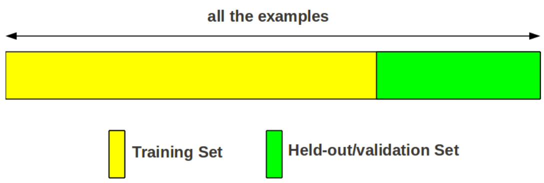

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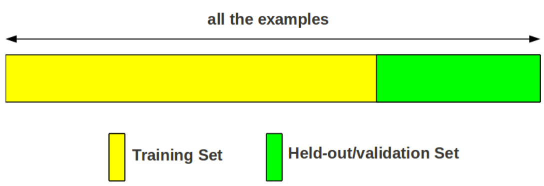

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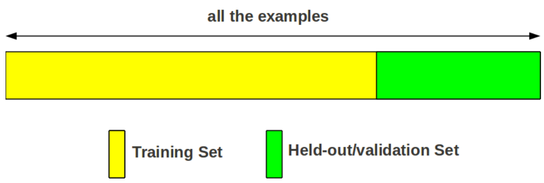

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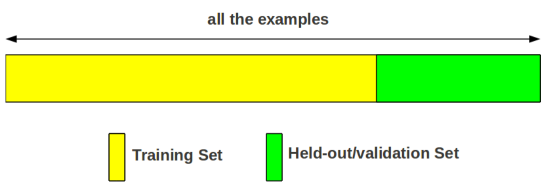

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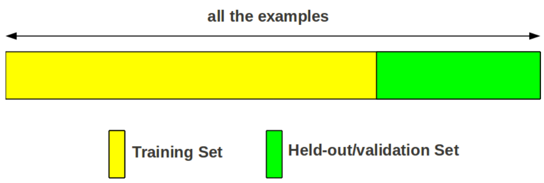

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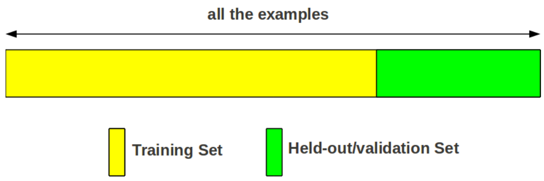

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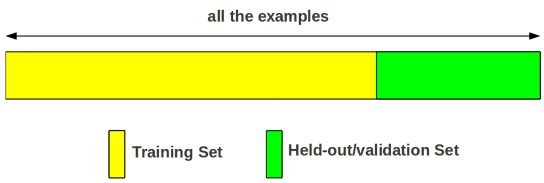

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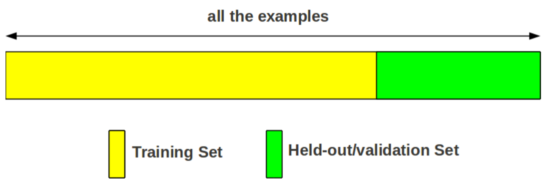

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    - Can ameliorate unfortunate splits by repeated random subsampling

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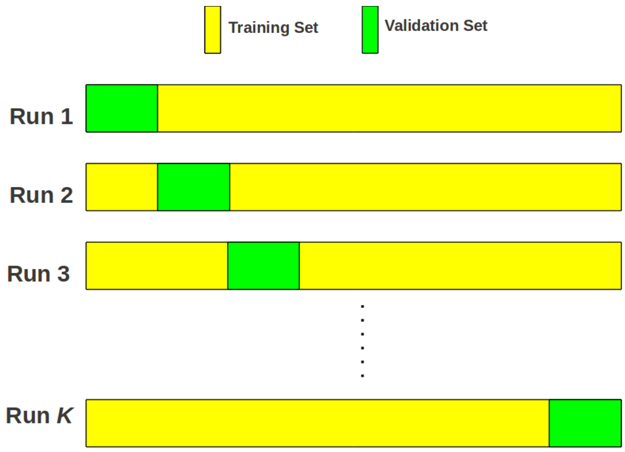

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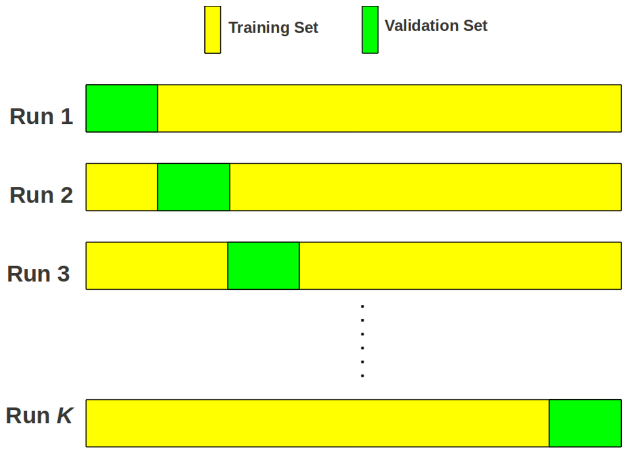

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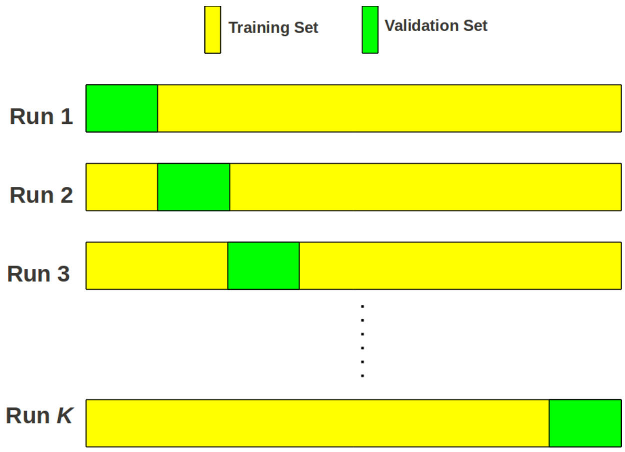

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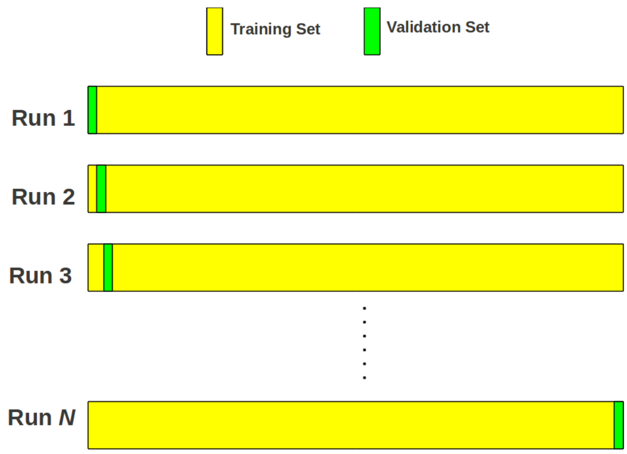

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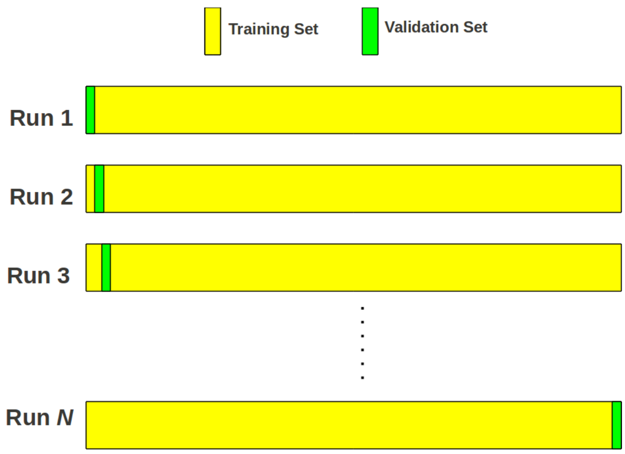

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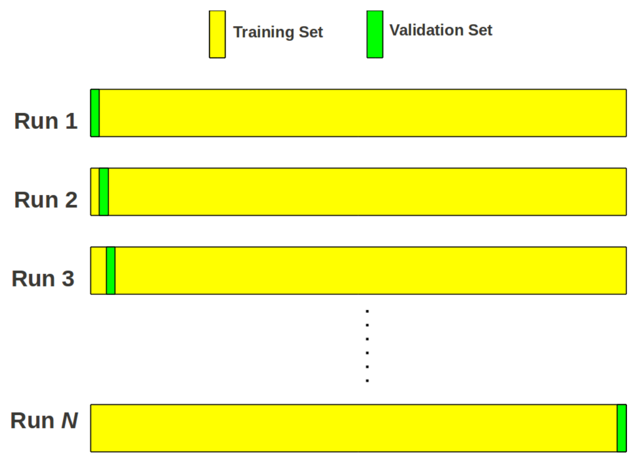

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- Can be expensive for large N. Typically used when N is small

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- **Note:** the above estimate may still be bad if we overfit and have $e_{training-examples} = 0$. Why?

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- Can be used even for model selection in unsupervised learning

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- Note: MDL criteria is kind of equivalent to preferring the best regularized model

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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
  - More on feature extraction when we cover **Dimensionality Reduction**

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  - Requires repeated runs of the learning algorithm with different set of features
  - Can be computationally expensive

Filter Feature Selection

- Uses heuristics but is much faster than wrapper methods

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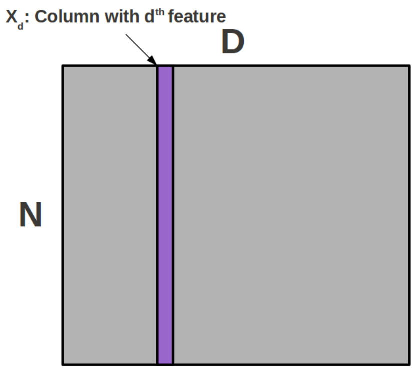

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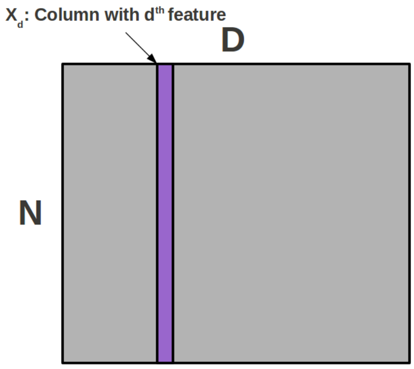

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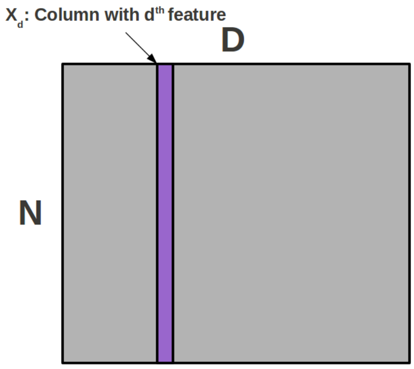

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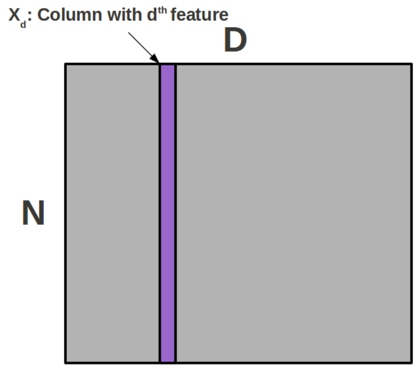

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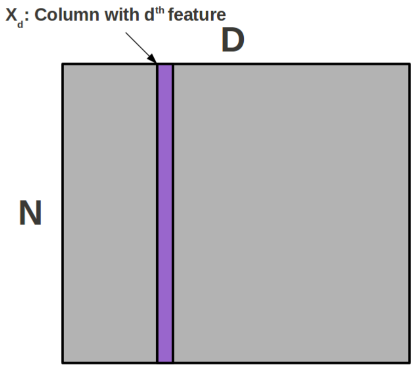

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  - High mutual information mean high relevance of that feature
  - Note: These probabilities can be easily estimated from the data

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- Two types: Forward Search and Backward Search

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  - Inclusion/Removal criteria uses cross-validation

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  - Remove f with lowest error from $\mathcal{F}$

Summary: feature engineering

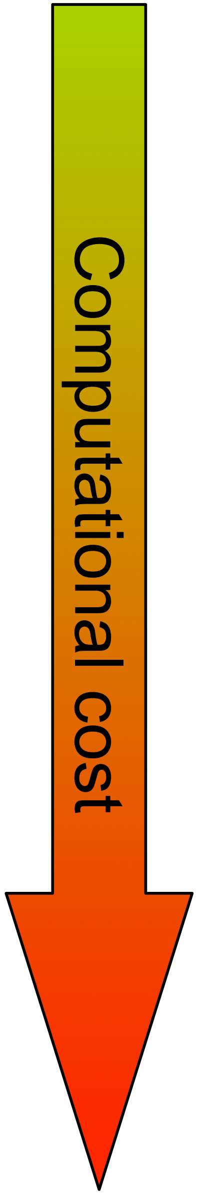
- Feature engineering is often crucial to get good results
- Strategy: overshoot and regularize
  - Come up with lots of features: better to include irrelevant features than to miss important features
  - Use regularization or feature selection to prevent overfitting
  - Evaluate your feature engineering on DEV set. Then, when the feature set is frozen, evaluate on TEST to get a final evaluation (Daniel will say more on evaluation next week)

Summary: feature selection

When should you do it?

- If the only concern is accuracy, and the whole dataset can be processed, feature selection not needed (as long as there is regularization)
- If computational complexity is critical (embedded device, web-scale data, fancy learning algorithm), consider using feature selection
  - But there are alternatives: e.g. the Hash trick, a fast, non-linear dimensionality reduction technique [Weinberger et al. 2009]
- When you care about the feature themselves
  - Keep in mind the correlation/causation issues
  - See [Guyon et al., Causal feature selection, 07]

Summary: how to do feature selection



- Filtering
- L_1 regularization (embedded methods)
- Wrappers
  - Forward selection
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  - Other search
  - Exhaustive

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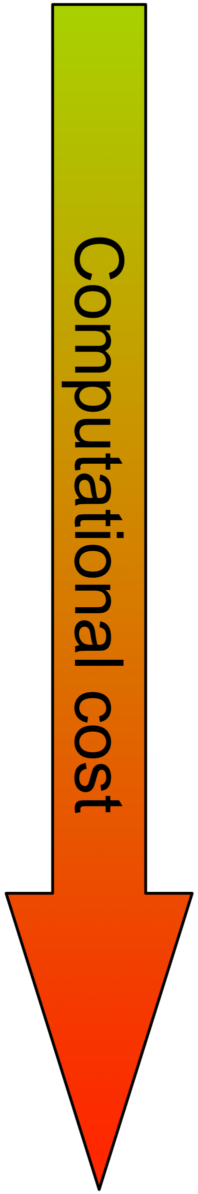

- *Filtering*
- L_1 regularization (embedded methods)
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- Good preprocessing step
- Fails to capture relationship between features

Summary: how to do feature selection

Computational cost

- Filtering
- *L_1 regularization (embedded methods)*
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  - Backward selection
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- Fairly efficient
  - LARS-type algorithms now exist for many linear models.

Summary: how to do feature selection

Computational cost

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  - Forward selection
  - Backward selection
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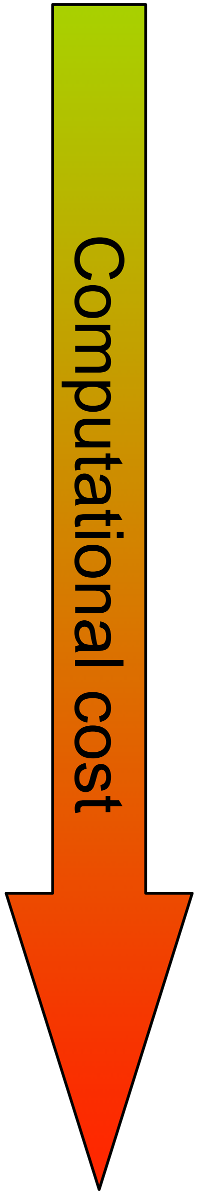
- Most directly optimize prediction performance
- Can be very expensive, even with greedy search methods
- Cross-validation is a good objective function to start with

Summary: how to do feature selection



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- Too greedy—ignore relationships between features
- Easy baseline
- Can be generalized in many interesting ways
  - Stagewise forward selection
  - Forward-backward search
  - Boosting

Summary: how to do feature selection

Computational cost

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- L_1 regularization (embedded methods)
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  - Backward selection
  - *Other search*
  - Exhaustive

- Generally more effective than greedy

Summary: how to do feature selection

Computational cost

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  - Other search
  - *Exhaustive*

- The "ideal"
- Very seldom done in practice
- With cross-validation objective, there's a chance of over-fitting
  - *Some* subset might randomly perform quite well in cross-validation