COMPSCI 389
Introduction to Machine Learning

Validation Sets (and Review of NN Variants and Model Evaluation)

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Nearest Neighbors (NN)

- Given a query, find the label associated with the closest point in the training data.
- "Closest" is determined using Euclidean distance:

$$\text{dist}(x, x') = \sqrt{\sum_{i=1}^{n} \left(x_i - x_i'\right)^2}$$

- If multiple points equally near, break ties arbitrarily.
  - For example, return the label of just one of the nearest neighbors.

K-Nearest Neighbors (k-NN)

- NN was unreasonable when many points are equally close but have different labels.
- NN is also unreasonable when many points are close to the query (but not precisely equal in distance).
- k-NN improves upon NN by returning the average of the labels of the k nearest neighbors.
    - Data structures like KD-Trees and Ball-Trees can be used to efficiently find the k nearest neighbors to a query point.

Weighted k-Nearest Neighbors (Weighted k-NN)

- The k-NN algorithm does not distinguish between the cases:
  - All k neighbors are roughly the same distance from the query.
  - Some of the k neighbors are much closer than others.
- Instead, it gives the same weight to all k neighbors.
- Weighted k-NN weights each of the k points based on their distance:

$$\hat{y} = \sum_{i=1}^{k} \frac{w_i}{\sum_{j=1}^{k} w_j} y_i^{NN}$$

i^{th} nearest neighbor's label

Weighted k-NN (cont.)

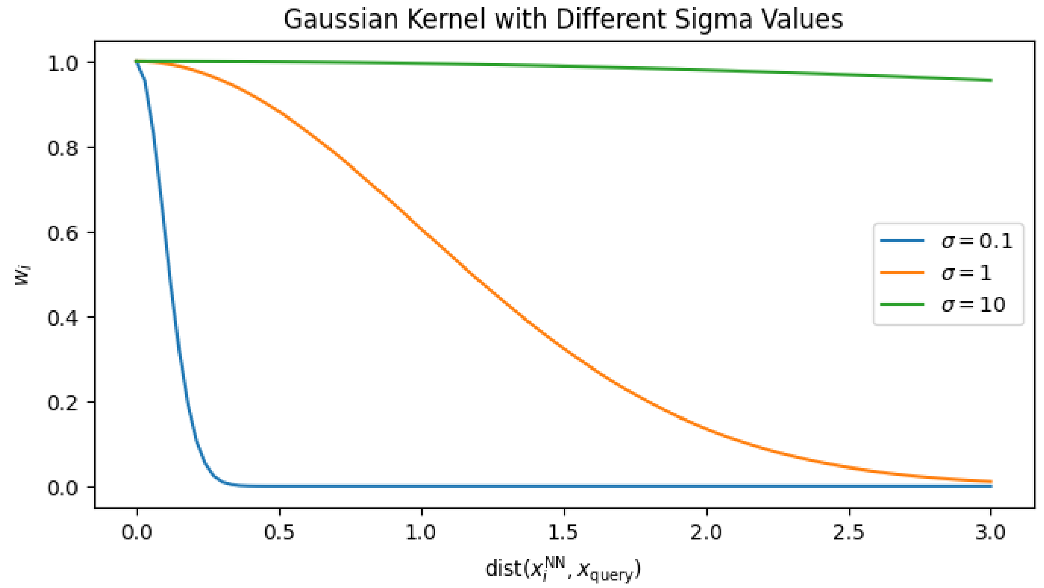
i^{th} nearest neighbor's features

Query features

- Many choices of weighting functions.
- One common choice is the Gaussian kernel:

$$w_i = e^{-\frac{\text{dist}\left(x_i^{NN},\, x_{\text{query}}\right)^2}{2\sigma^2}}$$

- Sigma scales how quickly weights decrease with distance.



Tuning Hyperparameters

- **Hyperparameter**: a variable, like *k*, that changes the behavior of the algorithm, and which is often set by the data scientist applying the algorithm.
- **Grid Search**: Specify possible values for each hyperparameter (often equally spaced), train models using all possible combinations of hyperparameter settings, and select the ones that result in the best fit.

Classification with NN-Variants

- NN: No changes needed!
- k-NN: The predicted label comes from a majority vote of the k nearest neighbors.
- Weighted k-NN: Each neighbor’s vote is weighted in the vote.

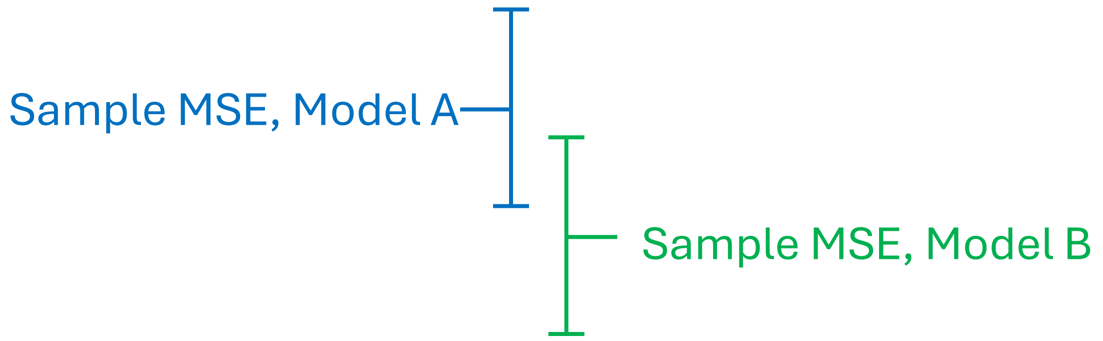
- **Note**: We will focus on regression for a while and will then return to classification after a few lectures.

Confidence Intervals

- We shouldn't always trust the sample performance metrics.
  - Sample MSE: $\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2$
    - This is a statistic or sample statistic.
  - It could be quite different from the true MSE: $\mathbf{E}\left[\left(Y - \hat{Y}\right)^2\right]$.
    - This is a parameter or population statistic.
- We can compute *confidence intervals* for sample statistics.
  - If the sample statistic is an average (of normally distributed values) then $\pm\, 1.96 \times SE$ is a 95% confidence interval.
    - SE is the *standard error*: $SE = \frac{\sigma}{\sqrt{n}}$, where σ is the sample standard deviation with Bessel's correction.
- We often report performance metrics with $\pm X$, where X is standard error, 1.96 times standard error, a 95% or 90% confidence interval, or standard deviation.

Model Evaluation

- We can evaluate models trained on the training data by:
  - Compute the sample MSE (or metric of interest) on the test set.
  - Compute a confidence interval (or related quantity) for the sample MSE.
  - Check whether one model's high-confidence lower-bound is larger than another model's high-confidence upper bound.



Cannot conclude that Model A is better than Model B with sufficient confidence.

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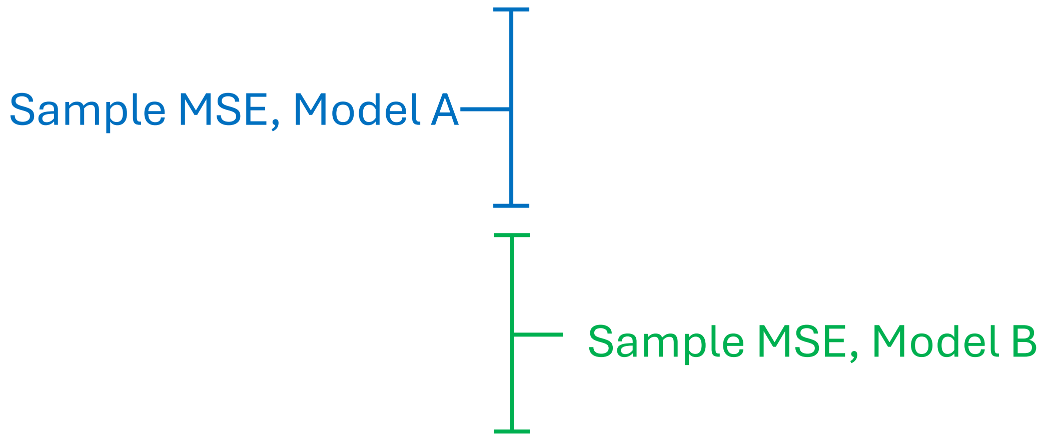

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Algorithm Evaluation

- Consider the following:
  - Train model A using one algorithm.
  - Train model B using another algorithm.
  - Evaluate models A and B using confidence intervals.
- This does **not** fully evaluate the two algorithms.
- It fails to capture how much the learned models vary with different training sets.

K-Fold Cross-Validation

- Split data D into k equal-sized subsets (folds), F1, F2, ..., Fk
- For i from 1 to k:
    - Set aside fold Fi as the validation set, and combine the remaining k-1 folds to form a training set.
    - Train the model M on the k-1 training folds using the ML algorithm being evaluated.
    - Evaluate the performance of model M on the validation fold Fi. Store the performance metric Pi
- Calculate the average performance metric: mean(P1,P2, ..., Pk).
- Optionally, calculate other statistics (like standard error) of the performance metrics across the folds.

Train/Validation/Test Sets (**New Material**!)

- Validation sets are often used to automatically tune hyperparameters.
- The data is split into three sets: train, validation, and test. The following procedure is then used:
  - For each hyperparameter setting:
    - Train a model using the training data.
    - Evaluate the model using the validation data.
  - Select the hyperparameter settings that achieve the best evaluation on the validation set.
  - Train a model using all the training and validation data and the hyperparameters that achieved the best evaluation.
  - Evaluate the model using the testing set.

Nested Cross-Validation: Train/Test/Validation + k-Fold Cross-Validation

- Train/Test/Validation does not account for the variance that results from the selection of the training and validation sets.
  - It evaluates the performance of the one model learned from a specific pair of training and validation sets.
- The use of train/validation/test sets can be combined with k-fold cross-validation to account for this additional variance.
  - This method is called **nested cross-validation**.
    - Use cross-validation to evaluate the performance of an *algorithm*.
    - Within the algorithm, use cross-validation to optimize hyperparameters.
  - While principled, this method is computationally intensive.
  - For this introductory course you should understand the general idea behind nested cross-validation, but need not study the algorithmic details.

End