Lecture 3: Model evaluation and bias-variance tradeoff

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MSA220/MVE440 Statistical Learning for Big Data

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Evaluating performance of a statistical method

Goals

- **Model selection:** Choose a hyper-parameter or model structure, e.g. k in kNN regression/classification, or 'Choose between logistic regression, LDA and kNN'
- **Model assessment:** How well did a model do on a data set?

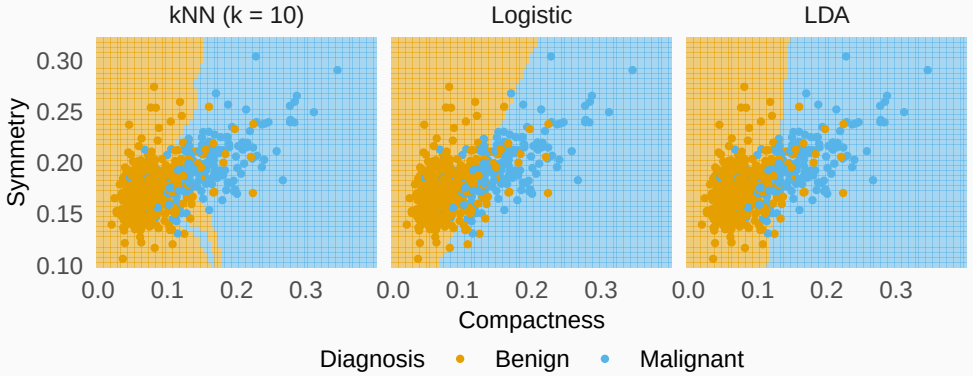
UCI Breast Cancer Wisconsin (Diagnostic) Data Set

UCI Breast Cancer Wisconsin (Diagnostic) Data Set[1]

- Classification data set with binary response (**malignant** or **benign** cancer)
- 569 samples (357 benign, 212 malignant)
- 10 features (given as *mean*, *standard error*, and *worst case*)
  - e.g. radius, symmetry, compactness, fractal dimension, …

[1] https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic)

Choosing the best method for prediction



Which method **generalises best** to new data, i.e. **performs class prediction well**?

Conditional and total expected prediction error

Recall: To determine the optimal regression function or classifier minimize expected prediction error

$$J(f) = \mathbb{E}_{p(\mathbf{x},y)}\left[L(y, f(\mathbf{x}))\right]$$

with respect to arbitrary functions f or a limited sub-class of functions.

- Estimate and fix $\widehat{f}(\mathbf{x}|\mathcal{T})$ from training data $\mathcal{T} = \{(y_l, \mathbf{x}_l) : l = 1, \ldots, n\}$.
- **Conditional expected prediction error** for a fixed training set $\mathcal{T}$

$$R(\mathcal{T}) = \mathbb{E}_{p(\mathbf{x},y)}\left[L(y, \widehat{f}(\mathbf{x}|\mathcal{T})\right]$$

- **Note:** Training data is random too, i.e. $p(\mathcal{T}) = \prod_{l=1}^{n} p(\mathbf{x}_l, y_l)$
- **Total expected prediction error**

$$R = \mathbb{E}_{p(\mathcal{T})}\left[R(\mathcal{T})\right] = \mathbb{E}_{p(\mathcal{T})}\left[\mathbb{E}_{p(\mathbf{x},y)}\left[L(y, \widehat{f}(\mathbf{x}|\mathcal{T}))\right]\right]$$

Common empirical error rates

- **Training error**

$$R^{tr} = \frac{1}{n} \sum_{l=1}^{n} L(y_l, \widehat{f}(\mathbf{x}_l | \mathcal{T}))$$

  where $(y_l, \mathbf{x}_l)$ are the samples in $\mathcal{T}$.

- **Test error**

$$R^{te} = \frac{1}{m} \sum_{l=1}^{m} L(y'_l, \widehat{f}(\mathbf{x}'_l | \mathcal{T}))$$

  where $(y'_l, \mathbf{x}'_l)$ for $1 \leq l \leq m$ are new samples from $p(\mathbf{x}, y)$.

Common empirical error rates (II)

Can these empirical error rates be used to approximate total or conditional expected prediction error?

Observations:

- $\mathcal{T}$ has already been used to determine $\widehat{f}(\cdot|\mathcal{T})$
- Training error is often smaller for more complex models (so-called **optimism of the training error**) since they can adjust better to the available data (**overfitting!**)
- How do we get new samples from the data distribution $p(\mathcal{T})$? What do we do if all we have is one set of training samples?

Splitting up the data

Holdout method

If we have a lot of samples, **randomly split** available data into **training set** and **test set** (e.g. 75% to 25%)

c-fold cross-validation (CV)

If we have few samples

1. **Randomly split** available data into c equally large subsets $\mathcal{F}_1, \ldots, \mathcal{F}_c$, so-called **folds**.
2. For each j
   - Use $c-1$ folds, denoted by $\mathcal{F}_{-j} = \cup_{i \neq j} \mathcal{F}_i$, as the **training set**
   - Use fold $\mathcal{F}_j$ as the **test set**

Note: No training must be done on the test set or outside of CV (see ESL Ch. 7.10.2)

Leave-one-out cross-validation

CV with $c = n$ is called **leave-one-out cross-validation (LOOCV)**.

- Popular because explicit formulas (or approximations) exist for many special cases (see ESL End of Ch. 7.10.1)
- Uses the most data for training possible
- More variable than c-fold CV for $c < n$ since only one data point is used for testing and the training sets are very similar
- In praxis: Try out different values for c. Be cautious if results vary drastically with c.

Approximations of expected prediction error

- Use **test error** for hold-out method, i.e.

$$R^{te} = \frac{1}{m} \sum_{l=1}^{m} L(y'_l, \widehat{f}(\mathbf{x}'_l | \mathcal{T}))$$

  where $(y'_l, \mathbf{x}'_l)$ for $l = 1, \ldots, m$ are the elements in the test set.

- Use **average test error** for c-fold CV, i.e.

$$R^{cv} = \frac{1}{c} \sum_{j=1}^{c} \frac{1}{|\mathcal{F}_j|} \sum_{(y_l, \mathbf{x}_l) \in \mathcal{F}_j} L(y_l, \widehat{f}(\mathbf{x}_l | \mathcal{F}_{-j}))$$

  where $\mathcal{F}_j$ is the j-th fold and $\mathcal{F}_{-j}$ is all data except fold j.

Note: For the approximations to be justifiable, test and training sets need to be identically distributed

Stratification

If data is unbalanced, then **stratification** is necessary.

Examples

- Class imbalance in a classification problem

  Solution: Sample so that each fold has the same class proportions as the original data
- Localised continuous outcome: Outcome is observed more often in some intervals than others (e.g. more high values than low values)

  Solution:
  1. Stratify outcome (divide into intervals)
  2. Sample such that the relative frequency of samples from each strata (interval) in each fold is the same as in the original data

Error estimation and tuning parameters

The holdout method and CV can be used to determine tuning parameters.

1. For a sequence of tuning parameters $\lambda_1, \dots, \lambda_S$ calculate

$$R^{cv}(\lambda_s) = \frac{1}{c} \sum_{j=1}^{c} \frac{1}{|\mathcal{F}_j|} \sum_{(y_l, \mathbf{x}_l) \in \mathcal{F}_j} L(y_l, \widehat{f}(\mathbf{x}_l | \lambda_s, \mathcal{F}_{-j}))$$

2. Choose

$$\hat{\lambda} = \arg\min_{\lambda_s} R^{cv}(\lambda_s)$$

Also works for a sequence of methods $M_1, \dots, M_S$ (e.g. kNN, QDA, Logistic Regression)

Motivating example for method selection

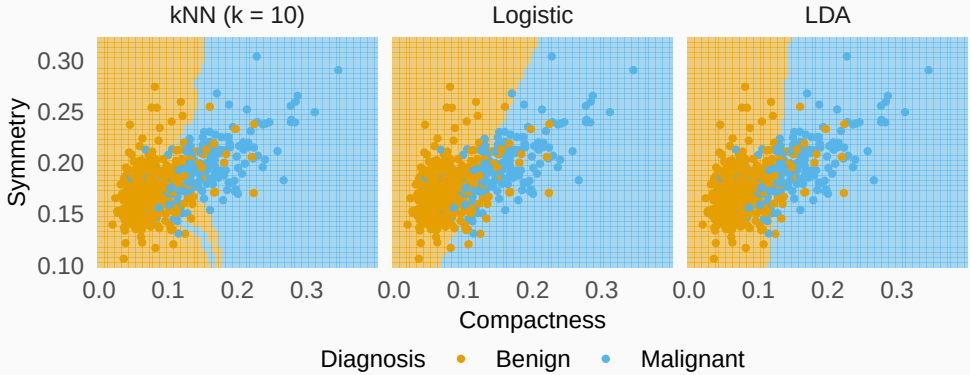
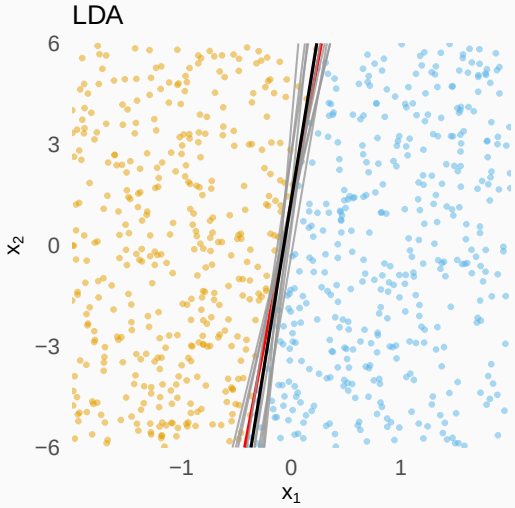


Table 1: Mean test error from 10-fold CV (standard deviation in parantheses)

kNN	Logistic	LDA
0.211 (0.017)	0.211 (0.017)	0.214 (0.017)

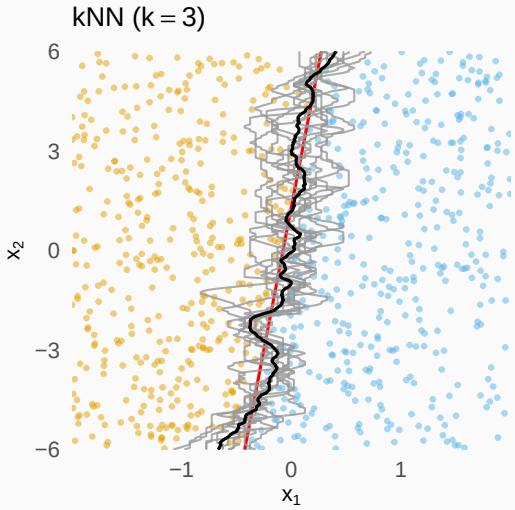
Bias-Variance Tradeoff

Global rule & Simple boundary



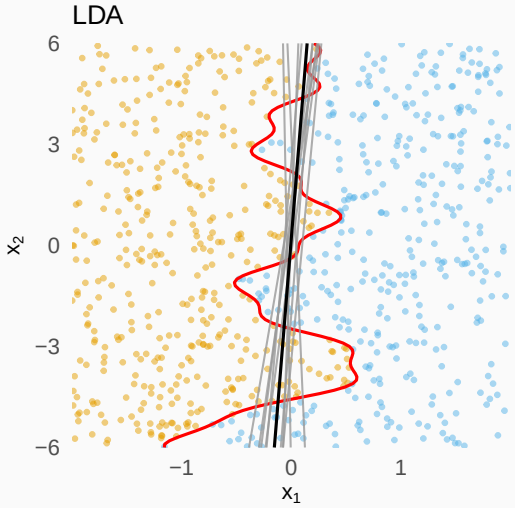
- The red line is the true boundary.
- Each grey line represents a fit to randomly chosen 20% of all data.
- The black line is the average of the grey lines.
- Here: **low variance** and **low bias**

Local rule & Simple boundary



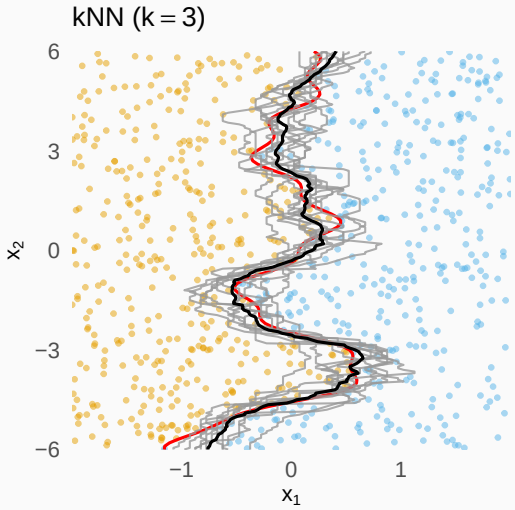
- Here: **high variance** but on average **low bias**

Global rule & Complex boundary



- Here: **low variance** but also **large bias**

Local rule & Complex boundary



- Here: **high variance** but on average **low bias**

Global vs local rules

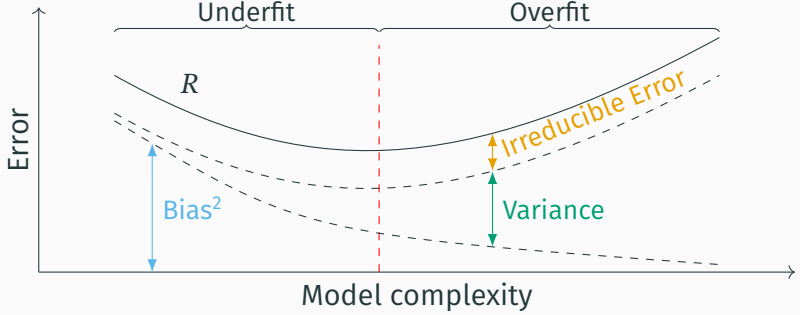
Observations

- **Local rules** are built using data in a local neighbourhood, can capture complex boundaries, but have high variance
- **Global rules** are built using all data, are usually less flexible, but have low variance
- **Bias-Variance Trade-off**: It can be theoretically motivated that bias and variance affect the expected prediction error. **The goal is to find a balance**.

Bias-Variance Tradeoff

If $y = f(\mathbf{x}) + \varepsilon$ where $\varepsilon \sim N(0, \sigma^2)$, then

$$
\begin{aligned}
R &= \mathbb{E}_{p(\mathcal{T},\mathbf{x},y)}\left[(y - \widehat{f}(\mathbf{x}))^2\right] && \text{Total expected prediction error} \\
&= \sigma^2 && \text{Irreducible Error} \\
&+ \mathbb{E}_{p(\mathbf{x})}\left[\left(f(\mathbf{x}) - \mathbb{E}_{p(\mathcal{T})}\left[\widehat{f}(\mathbf{x})\right]\right)^2\right] && \text{Bias}^2 \text{ averaged over } \mathbf{x} \\
&+ \mathbb{E}_{p(\mathbf{x})}\left[\mathrm{Var}_{p(\mathcal{T})}\left[\widehat{f}(\mathbf{x})\right]\right] && \text{Variance of } \widehat{f} \text{ averaged over } \mathbf{x}
\end{aligned}
$$



Observations

- Irreducible error cannot be changed
- Bias and variance of $\widehat{f}$ are sample-size dependent
  - For a consistent estimator $\widehat{f}$

    $$\mathbb{E}_{p(\mathcal{T})}[\widehat{f}(x)] \to f(x)$$

    for increasing sample size
  - In many cases:

    $$\mathrm{Var}_{p(\mathcal{T})}(\widehat{f}(x)) \to 0$$

    for increasing sample size
  - **Caution:** Theoretical guarantees are often dependent on the number of variables p staying fixed and increasing n. Might not be fulfilled in reality.

Performance of LDA vs KNN

Table 2: Mean test error from 10-fold CV (standard deviation in parantheses)

	Boundary	
	simple	complex
LDA	0.013 (0.004)	0.091 (0.01)
kNN ($k = 3$)	0.021 (0.005)	0.023 (0.005)

- LDA estimates have lower variance but higher bias for complex domains
- kNN estimates can adapt locally and have low bias, but are often highly variable

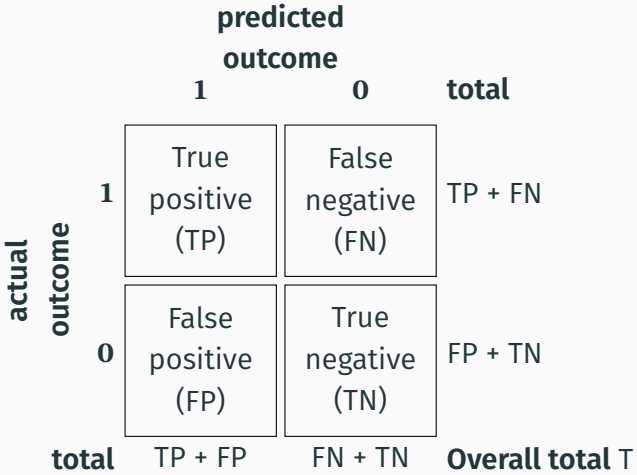
Evaluation metrics for classification

What are evaluation metrics?

So far, we used the loss function to determine the quality of the test result.

- For regression: **Mean squared error (MSE)**
  - Low MSE ensures that the model is correct on average (given that model assumptions are correct)
- For classification: **Rate of misclassification**
  - Penalises wrong predictions across all classes, but problematic for unbalanced datasets

Confusion matrix

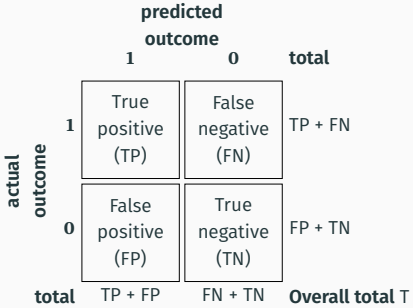


Accuracy

Accuracy is defined as

$$\frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{T}}$$

- Measures fraction of correct predictions
- **Symmetric:** Useful if costs of false negatives and false positives are equally high
- **Weakness:** If one class is highly prevalent (unbalanced dataset), then predicting everything as the majority class can still achieve good accuracy.

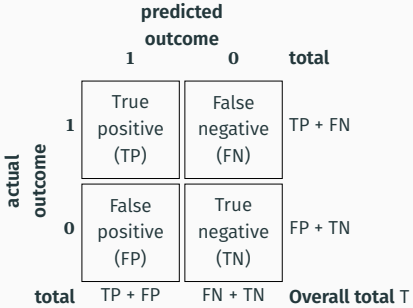


Sensitivity/Recall/True positive rate (TPR)

Sensitivity is defined as

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}}$$

- Measures fraction of correct positive predictions to all actual positive outcomes
- **Strength:** Useful if costs of false negatives are high
- **Be aware:** A predictor trained on sensitivity is likely to overpredict positive cases.
- **Typical example:** Medical test

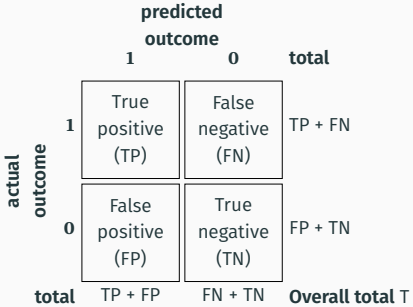


Specificity/True negative rate

Specificity is defined as

$$\frac{\mathrm{TN}}{\mathrm{TN} + \mathrm{FP}}$$

- Measures fraction of correct negative predictions to all actual negative outcomes
- **Strength:** Useful to make classifier recognize negative cases
- **Typical example:** Medical test, in balance with training on sensitivity
- False positive rate (FPR) $= 1 -$ Specificity

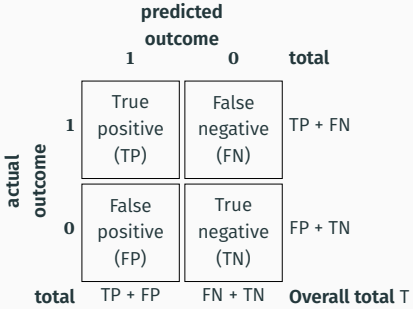


Precision

Precision is defined as

$$\frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FP}}$$

- Measures fraction of correct positive predictions to all positively predicted outcomes
- **Strength:** Useful if costs of false positives are high
- **Be aware:** A predictor trained on precision is likely to overpredict negative cases.
- **Typical example:** Spam filter



Combined measures (I)

- **F_1 score**

$$2 \cdot \frac{\text{Precision} \cdot \text{Recall}}{\text{Precision} + \text{Recall}} \in [0, 1]$$

- **Matthew's correlation coefficient**

$$\text{MCC} = \frac{\text{TP} \cdot \text{TN} - \text{FP} \cdot \text{FN}}{\sqrt{(\text{TP} + \text{FP})(\text{TP} + \text{FN})(\text{TN} + \text{FP})(\text{TN} + \text{FN})}} \in (-1, 1)$$

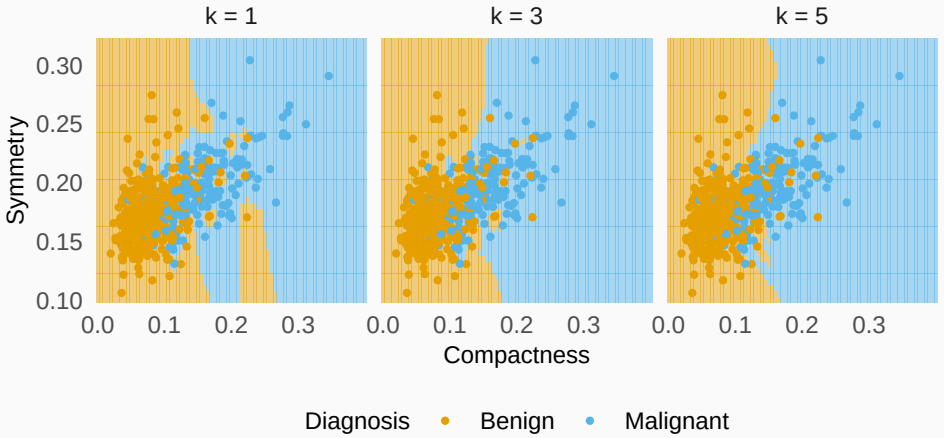
where

  - $\text{MCC} = 0$ for a random classifier
  - $\text{MCC} < 0$ if worse than random and $\text{MCC} > 0$ if better than random.
  - Takes both classes into account.

Combined measures (II)

- **Receiver Operating Characteristic (ROC) curve**
  - Given a test sample and the respective estimated probabilities for the positive class, plot the trade-off between FPR and TPR.
  - Diagonal line from (0, 0) to (1, 1) for a random classifier
  - $\mathrm{TPR} < \mathrm{FPR}$ for a worse than random classifier and $\mathrm{TPR} > \mathrm{FPR}$ if better than random
- **Area under the ROC curve (AUC)**
  - Integral over the ROC curve
  - 0.5 for a random classifier and > 0.5 for better classifiers.
  - $\mathrm{AUC} \in [0, 1]$

Choose k in kNN



Best k for kNN

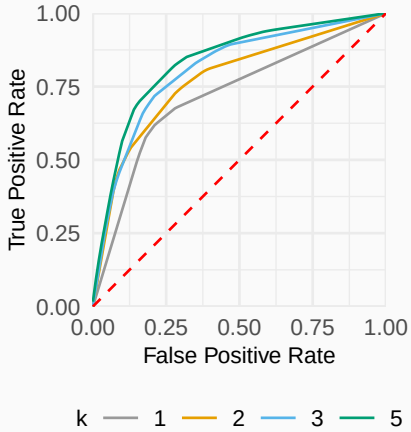


Table 3: Mean training and testing 5-fold CV errors (standard deviation in parantheses)

k	R^{tr}	R^{cv}
1	0 (0)	0.26 (0.018)
2	0.147 (0.007)	0.246 (0.018)
3	0.14 (0.007)	0.23 (0.018)
5	0.163 (0.008)	0.207 (0.017)

Take-home message

- Cross-validation or splitting data into a training and test set are valuable approaches for model selection and model assessment
- Method complexity and global/local rules exhibit a bias-variance trade-off
- There is no single best measurement of classification quality, use multiple!