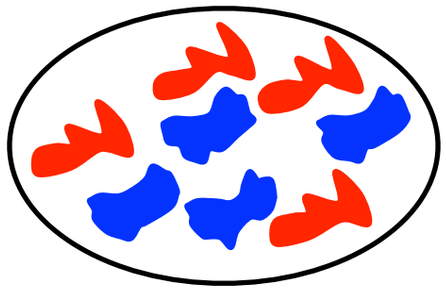
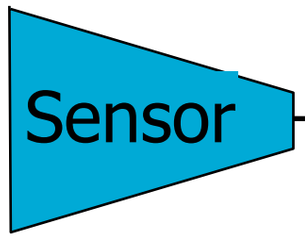
# Classifier evaluation





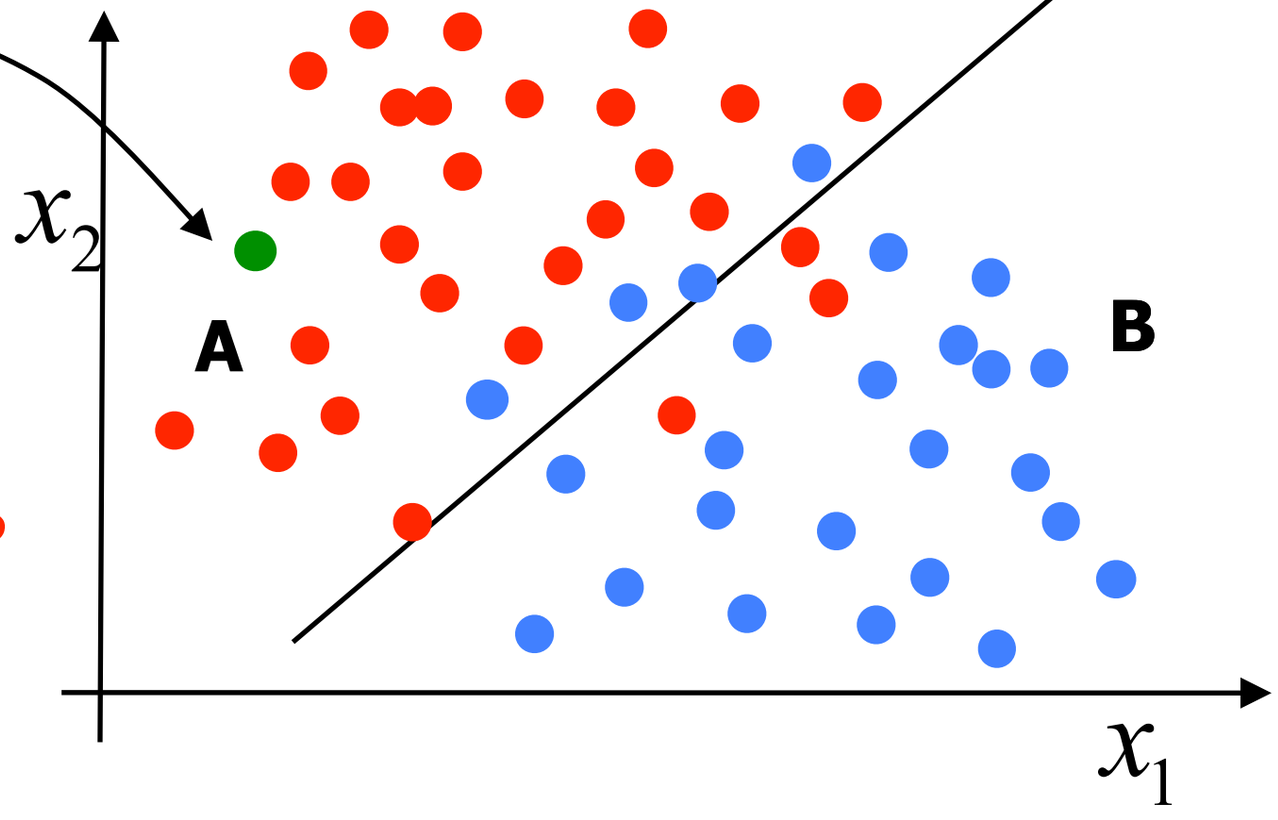

Representation

Generalization

Feature Space

Classification

Test object classified as 'A'




**How to estimate classifier performance?**

**Learning curves**

**Feature curves**



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# Recap classifiers

$$p(y|\mathbf{x})$$

# Recap classifiers

$$p(y|\mathbf{x})$$

generative classifiers:

$$\hat{p}(y|\mathbf{x}) = \frac{\hat{p}(\mathbf{x}|y)\hat{p}(y)}{\hat{p}(\mathbf{x})}$$

maximise the likelihood

$$\max \hat{p}(\mathbf{x}|y)$$

discriminative classifiers:

$$\hat{p}(y|\mathbf{x}) = f(\mathbf{x};\mathbf{w})$$

1. define a model
2. define an error/loss
3. find minimum loss:

- set derivative=0 and solve
- get derivative and do gradient descent

# Recap classifiers

$$p(y|\mathbf{x})$$

generative classifiers:

$$\hat{p}(y|\mathbf{x}) = \frac{\hat{p}(\mathbf{x}|y)\hat{p}(y)}{\hat{p}(\mathbf{x})}$$

parametric densities:
- QDC
- LDC
- Nearest mean

nonparametric densities:
- k-nearest neighbour
- Parzen classifier

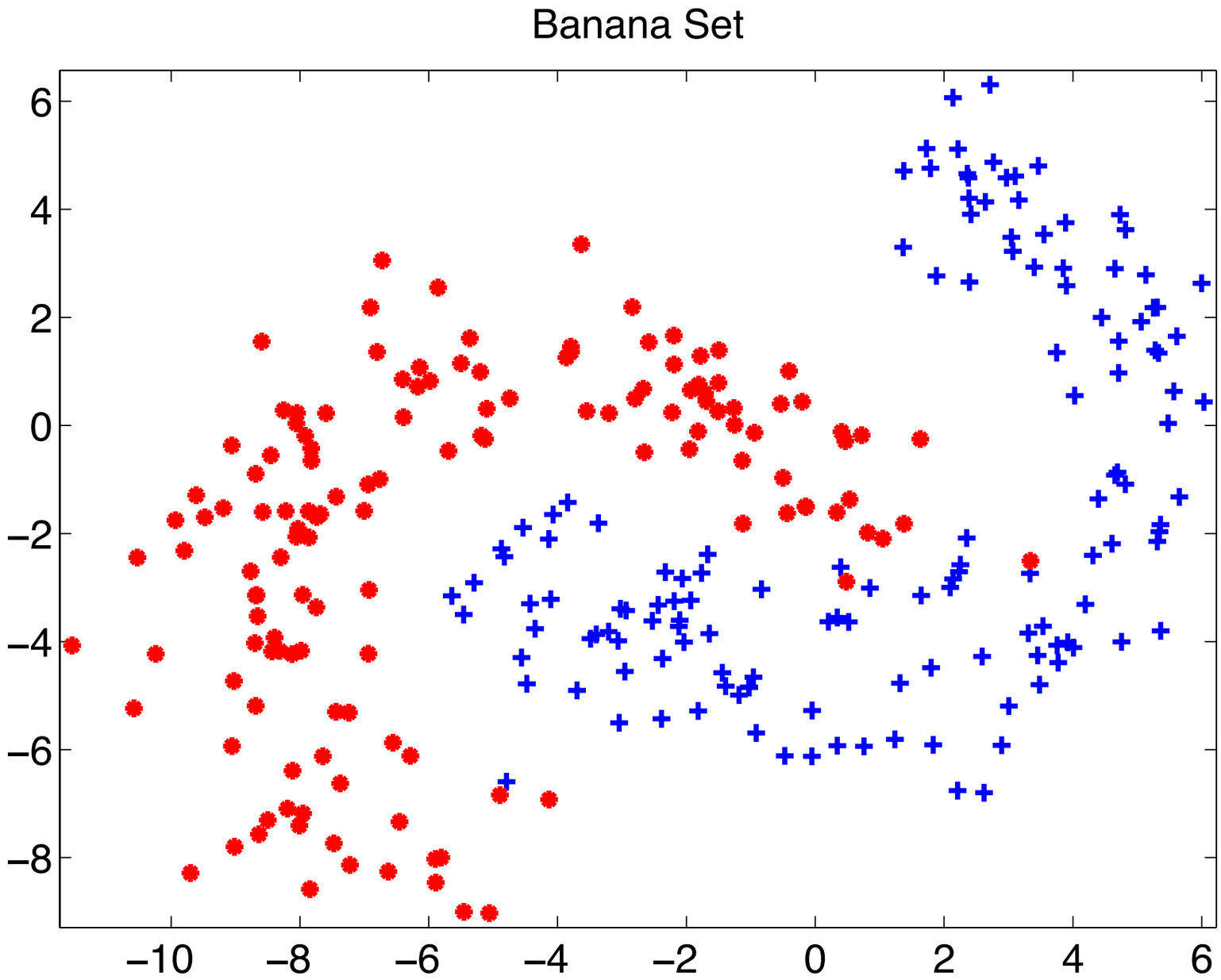
discriminative classifiers:

$$\hat{p}(y|\mathbf{x}) = f(\mathbf{x};\mathbf{w})$$

- logistic classifier
- support vector
- decision trees
- perceptron
- neural networks

# What classifier to use here?

- NMC
- LDC
- QDC
- k-NN
- Parzen classifier
- Logistic
- Support vector
- Decision tree
- Neural network
- …



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# What classifier to use here?

- NMC
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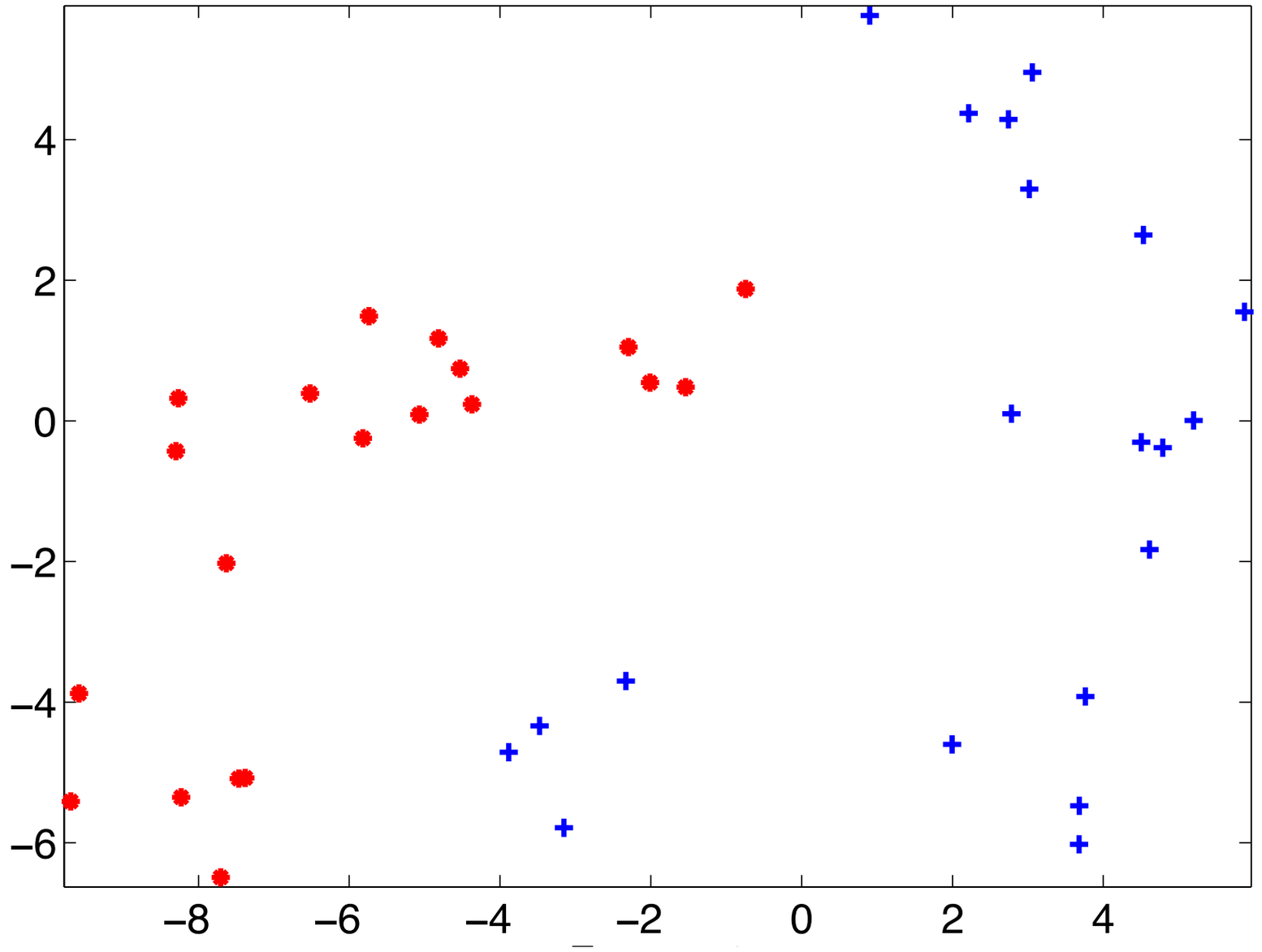

# What classifier to use here?

- NMC
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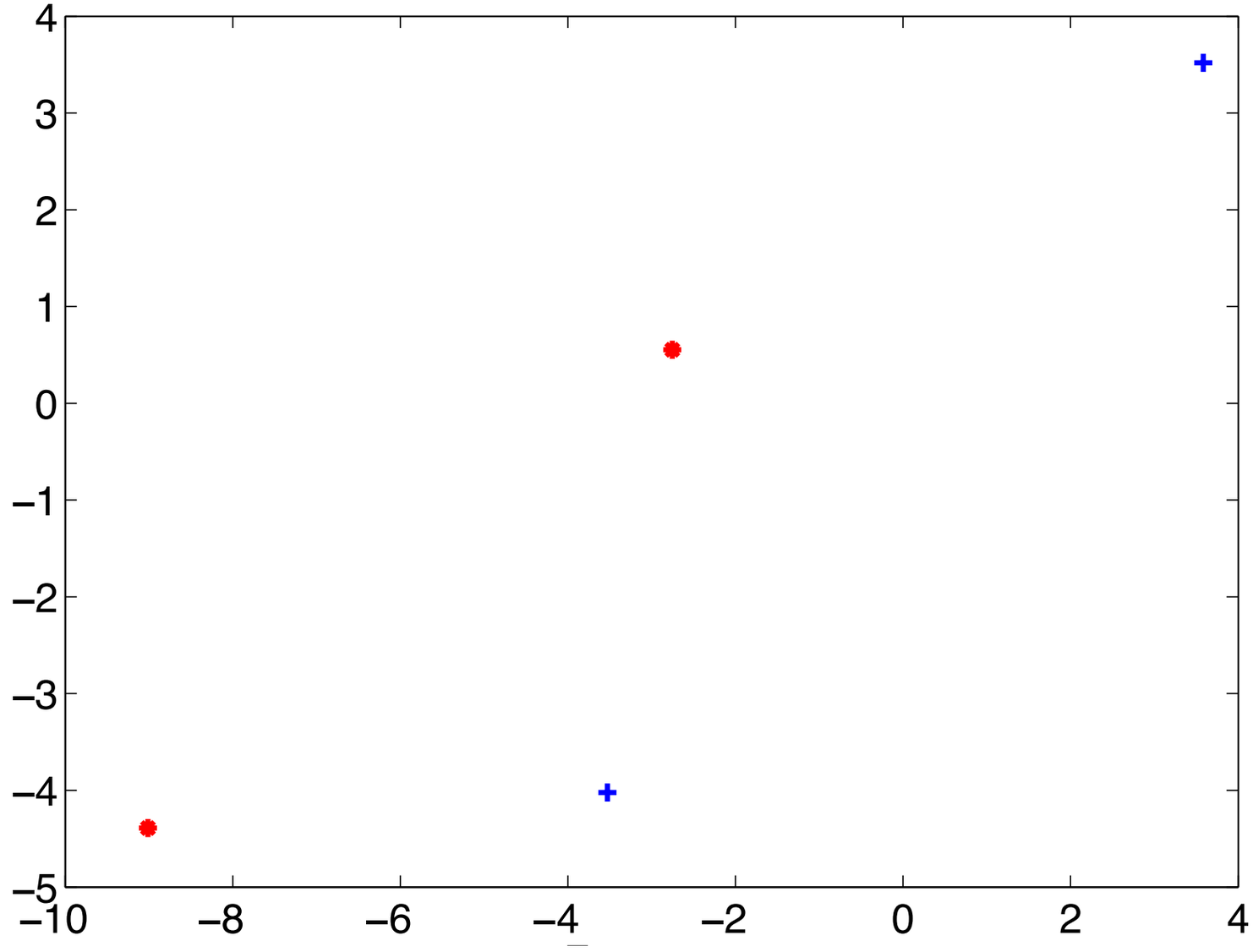
- …



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# What classifier to use here?

- Loaded our famous Iris dataset
- 150 objects in 4D

- What now?

**iris =**

| | sepal l. | sepal w. | petal l. | petal |
|---|---|---|---|---|
| | 5.1000 | 3.5000 | 1.4000 | 0.2000 |
| | 4.9000 | 3.0000 | 1.4000 | 0.2000 |
| | 4.7000 | 3.2000 | 1.3000 | 0.2000 |
| | 4.6000 | 3.1000 | 1.5000 | 0.2000 |
| | 5.0000 | 3.6000 | 1.4000 | 0.2000 |
| | 5.4000 | 3.9000 | 1.7000 | 0.4000 |
| | 4.6000 | 3.4000 | 1.4000 | 0.3000 |
| | 5.0000 | 3.4000 | 1.5000 | 0.2000 |
| | 4.4000 | 2.9000 | 1.4000 | 0.2000 |
| | 4.9000 | 3.1000 | 1.5000 | 0.1000 |
| | 5.4000 | 3.7000 | 1.5000 | 0.2000 |
| | 4.8000 | 3.4000 | 1.6000 | 0.2000 |
| | 4.8000 | 3.0000 | 1.4000 | 0.1000 |
| | 4.3000 | 3.0000 | 1.1000 | 0.1000 |
| | 5.8000 | 4.0000 | 1.2000 | 0.2000 |
| | 5.7000 | 4.4000 | 1.5000 | 0.4000 |
| | 5.4000 | 3.9000 | 1.3000 | 0.4000 |

# What classifier to use?

- If cannot visualise high-dimensional data: how to choose?

- Need some criterion!
- Typically: classification performance/error

- (1) Test it on independent data
- (2) What if we still get the same error?

# True or false?

- The classification error of the training set is a good measure of the true classification error

TRUE? FALSE?

- A good estimate of the actual, true, error is all we are after

TRUE? FALSE?

# What classifier to use?

- If cannot visualise high-dimensional data: how to choose?

- Need some criterion!
- Typically: classification performance/error

- Test it on independent data

- For simplicity we assume now that classification error is good enough

# Material/literature

- Chapter 19 “Design and Analysis of Machine Learning experiments” in ‘Introduction to Machine Learning’ by E. Alpaydin
- Ebook available at library.tudelft.nl

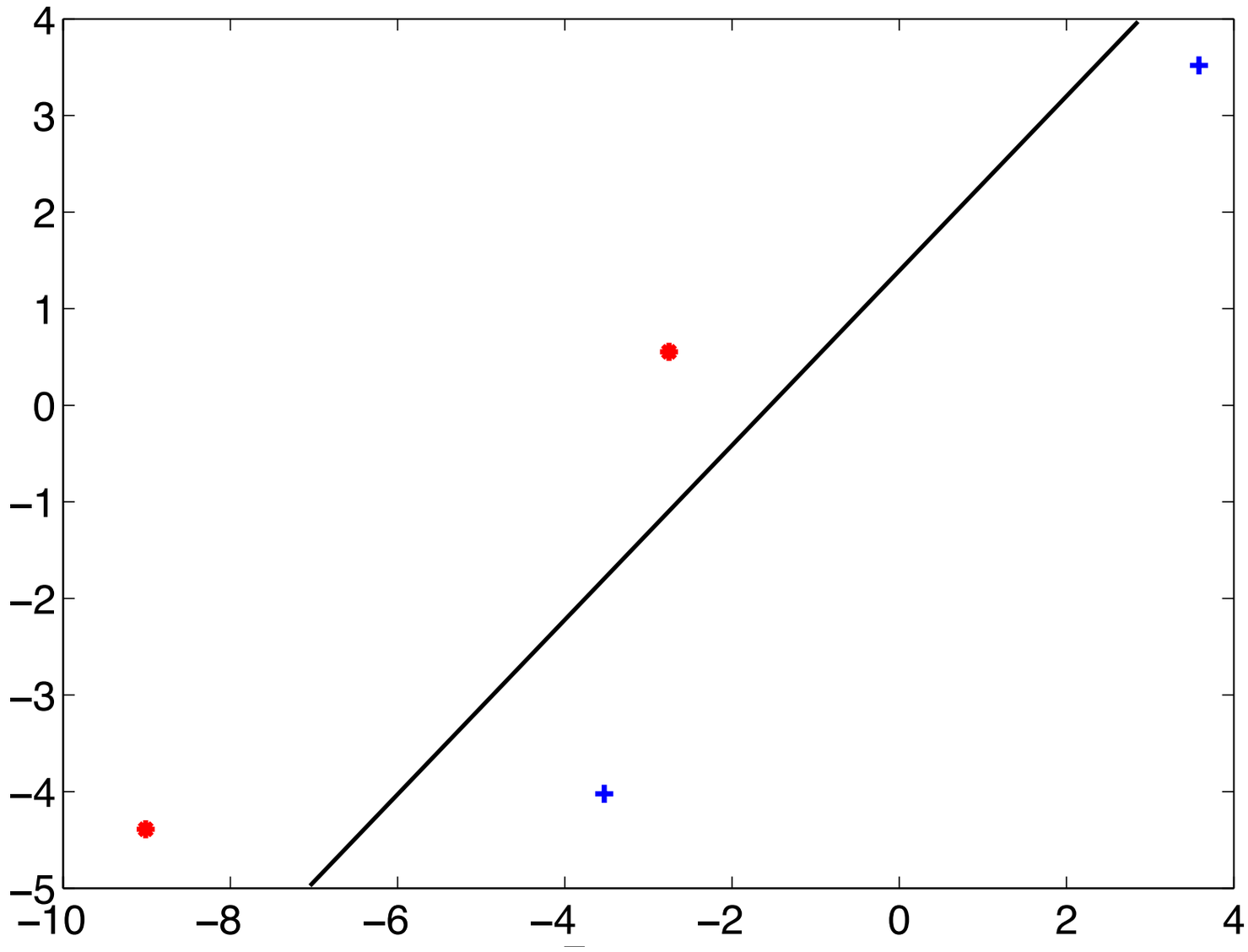
- Some sections are not discussed (19.8 and further)

- ‘Reject option’ is (unfortunately) not in the book: get it from the slides.

# Classifier evaluation

- This lecture:
  - Train and test set
  - Bootstrapping, cross-validation, leave-one-out
  - Learning curve
  - Classifier complexity
  - Bias-variance tradeoff
- Second lecture:
  - Confusion matrices
  - Reject curve
  - ROC curve
- Question hour

# How good is this classifier?



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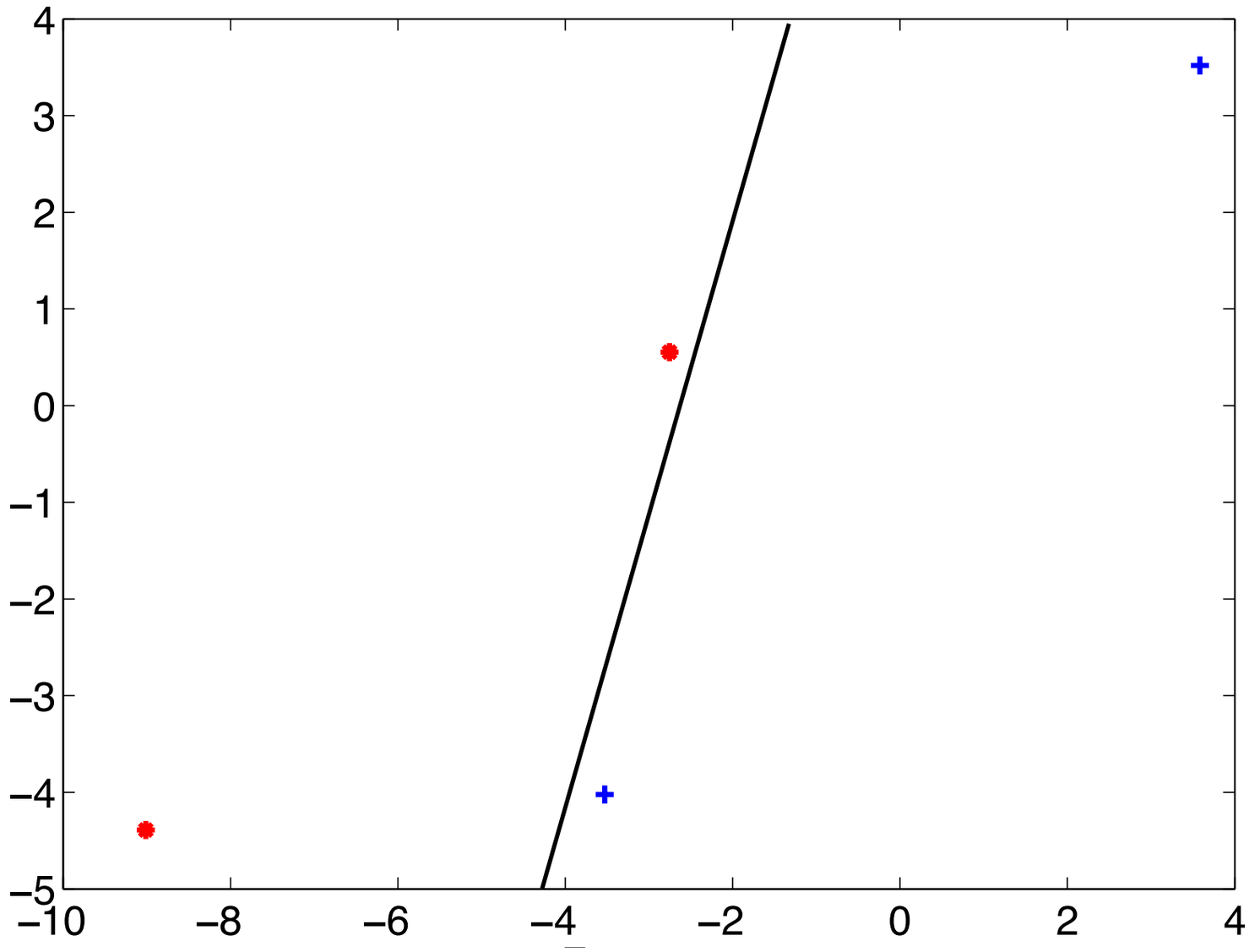
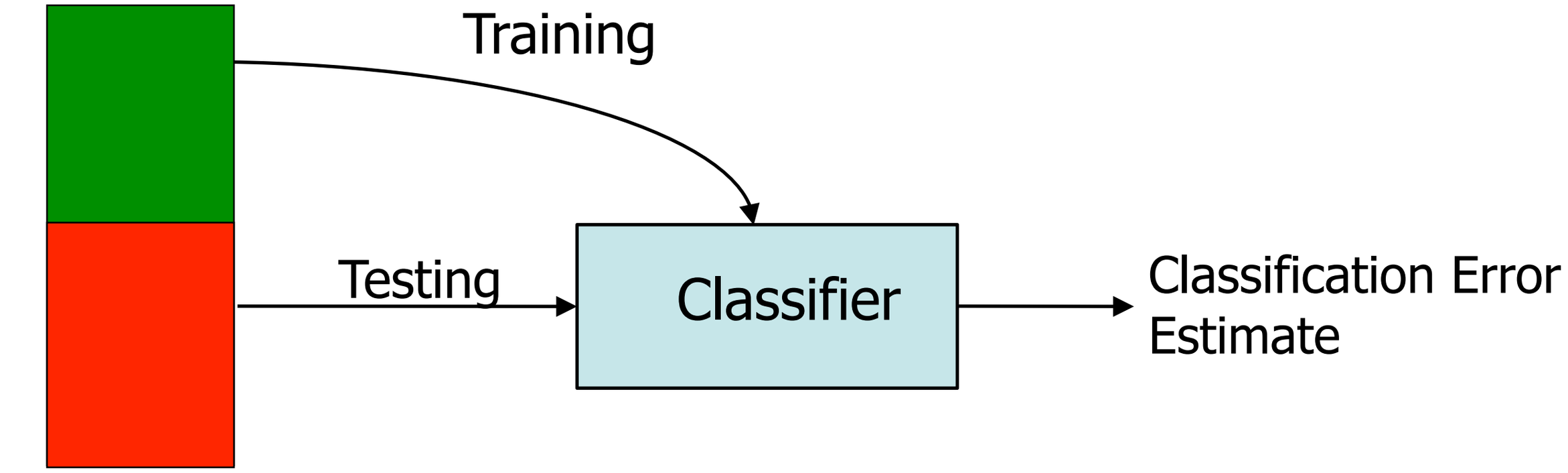
# And this one?



# Error Estimation by Test Set




Design Set

Other training set → other classifier
Other test set → other error estimate $\hat{\varepsilon}$

# Some Error Estimate Variability

- Error is a sum of Bernoulli random variables:

$$\hat{\varepsilon} = \frac{1}{N}\sum_{i=1}^{N} Z_i$$

where

$$Z_i = \begin{cases} 0 & \text{if } \mathbf{x}_i \text{ is correctly classified} \\ 1 & \text{if } \mathbf{x}_i \text{ is incorrectly classified} \end{cases}$$

- You can show that the variance is:

$$\sigma^2_{\hat{\varepsilon}} = \mathrm{Var}(\hat{\varepsilon} \mid \text{test set size } N) = \frac{\varepsilon(1-\varepsilon)}{N}$$

# Some Error Estimate Variability

- Error is a sum of Bernoulli random variables:

$$\hat{\varepsilon} = \frac{1}{N}\sum_{i=1}^{N} Z_i$$

- When: $\sigma^2_{\hat{\varepsilon}} = \mathrm{Var}(\hat{\varepsilon} \mid \text{test set size } N) = \dfrac{\varepsilon(1-\varepsilon)}{N}$

you can compute the standard deviation for different sample sizes and errors:

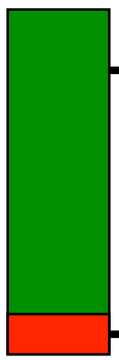
$$\sigma_{\hat{\varepsilon}} = \sqrt{\frac{\varepsilon(1-\varepsilon)}{N}}$$

| $N$ \ $\varepsilon$ | 0.01 | 0.03 | 0.1 |
|---|---|---|---|
| 10 | 0.031 | 0.054 | 0.095 |
| 100 | 0.010 | 0.017 | 0,030 |
| 1000 | 0.003 | 0.005 | 0.0095 |

# Training Set Size vs. Test Set Size

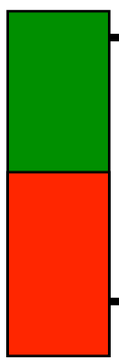
- Large training set -> good classifiers
- Large test set -> reliable, unbiased error estimate
- In practice often just a single design set is given

Same set for training and testing may give a good classifier, but will definitely yield an optimistically biased error estimate



A small, independent test set yields an unbiased, but unreliable [large variance] error estimate for a well trained classifier

A large, independent test set yields an unbiased and reliable [small variance] error estimate for a badly trained classifier

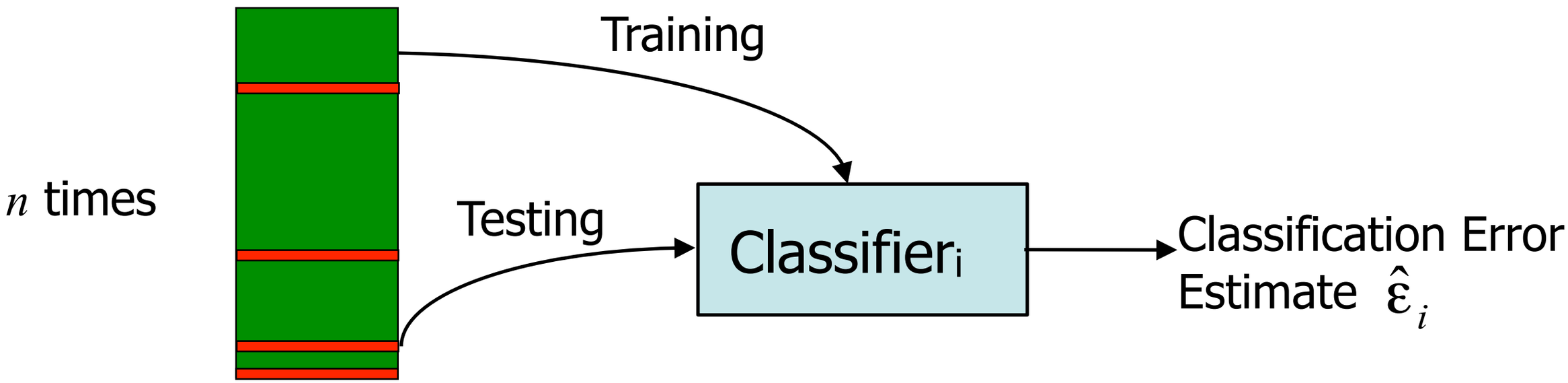


50-50 is an often used standard solution for the sizes for training and testing

But is it really good?

# Bootstrapping

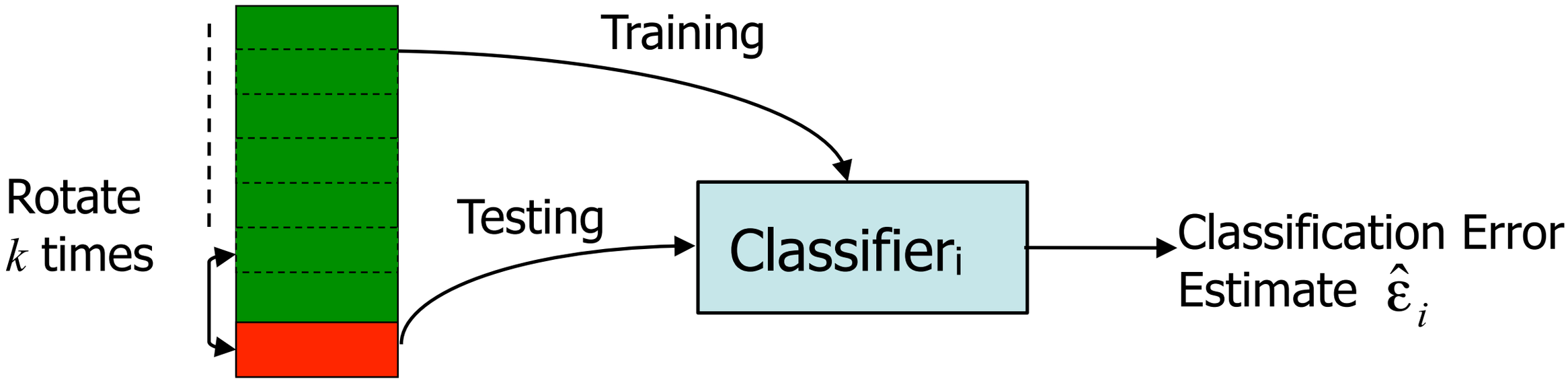
- Randomly draw N objects from N objects (**with** replacement)




$$\hat{\varepsilon} = \frac{1}{m} \sum_i \hat{\varepsilon}_i$$

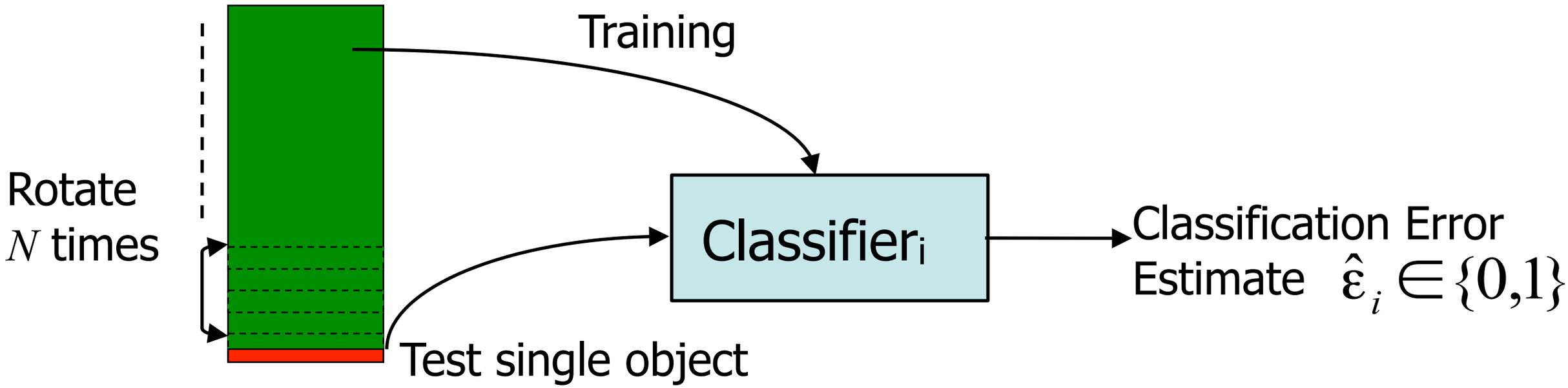
- Left-over objects are used for testing
- Repeat m times

# k-fold cross validation




$$\hat{\varepsilon} = \frac{1}{k} \sum_i \hat{\varepsilon}_i$$

# Leave-one-out Procedure




$$\hat{\varepsilon} = \frac{1}{N} \sum_i \hat{\varepsilon}_i$$

# Optimising 'hyperparameters'

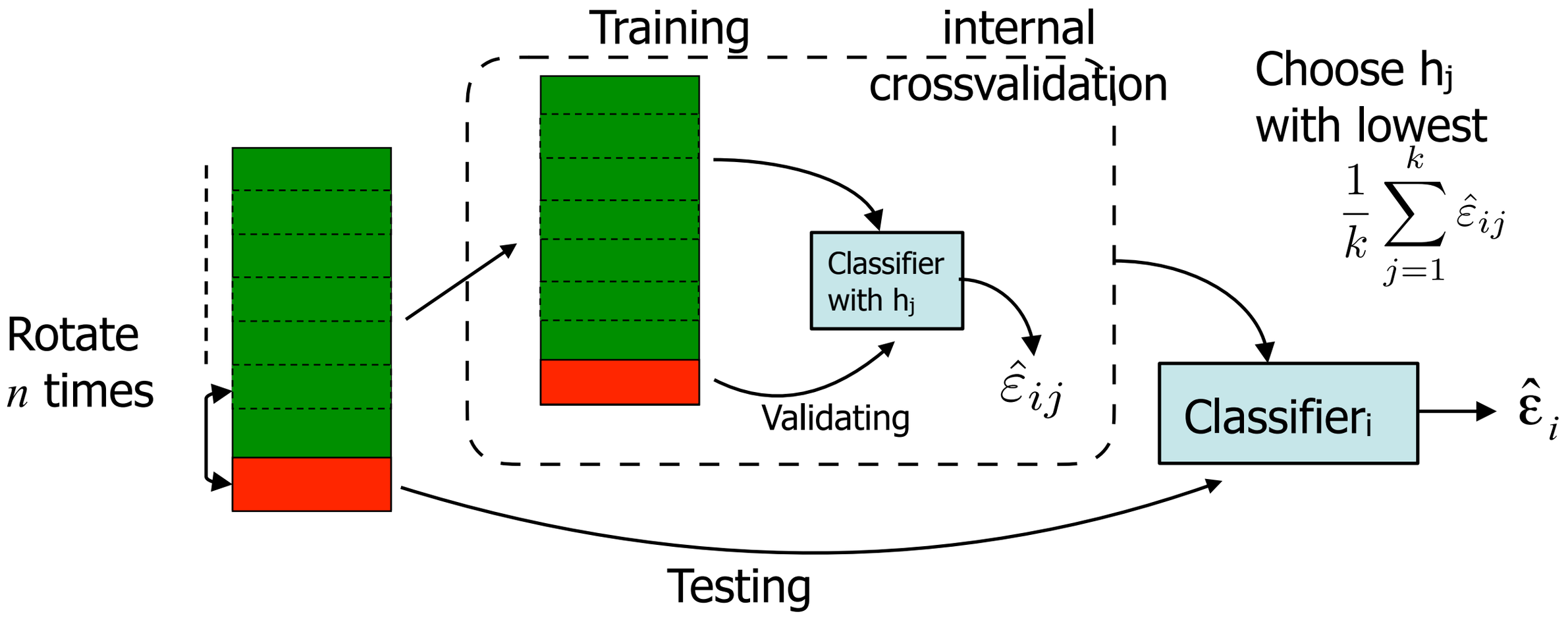
- Machine learning methods often have 'hyperparameters'

- Parzen density estimator: width parameter h
- k-nearest neighbour: number of neighbours k
- Decision trees: pruning method, stopping criterion
- Neural networks: architecture, learning rate, …

- DON'T optimise these numbers by looking at the test set!
  Then you're **CHEATING**!

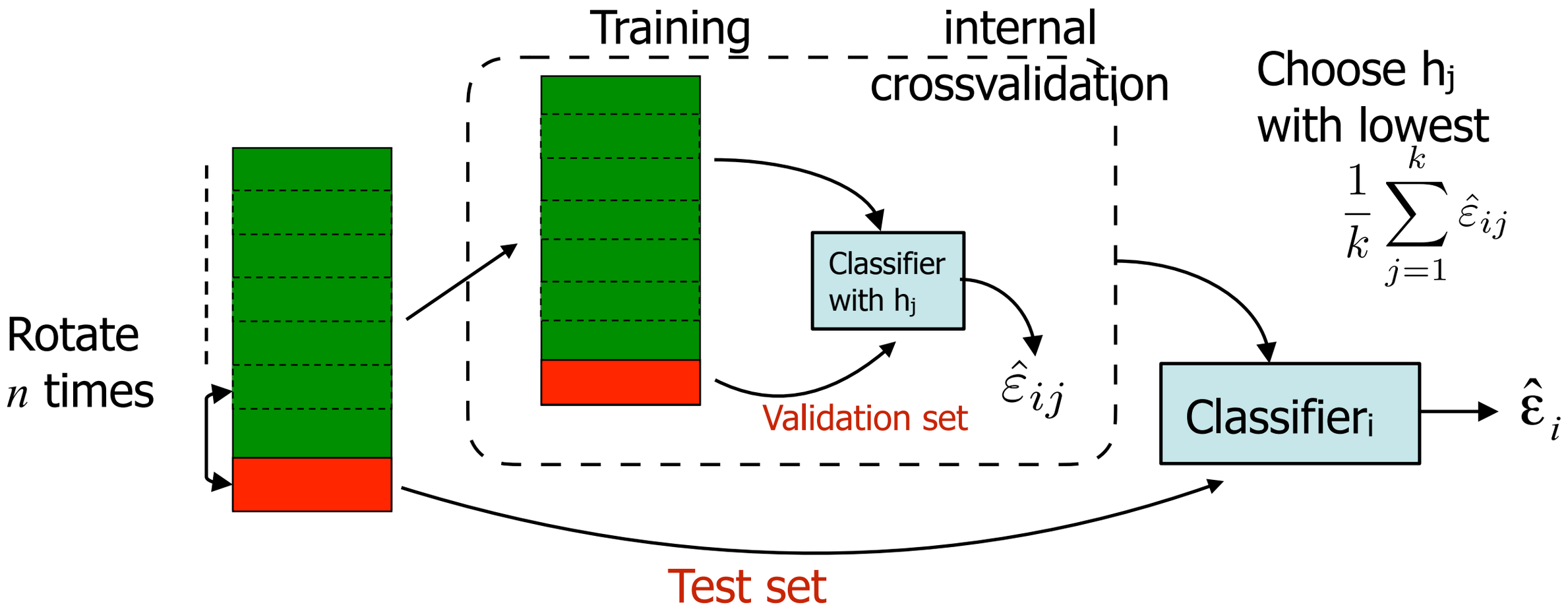
# Double cross-validation

- To optimise hyperparameters, do cross-validation **inside** another cross-validation:



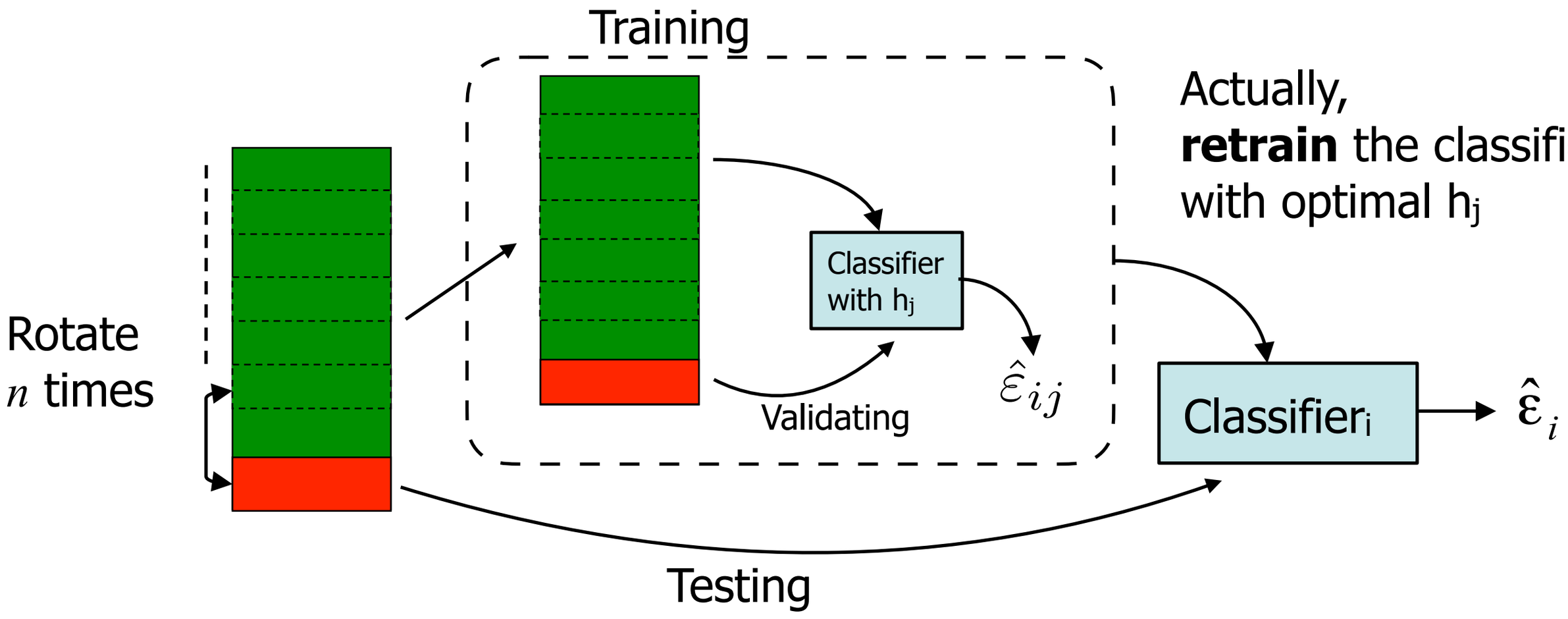
# Double cross-validation

- To optimise hyperparameters, do cross-validation **inside** another cross-validation:



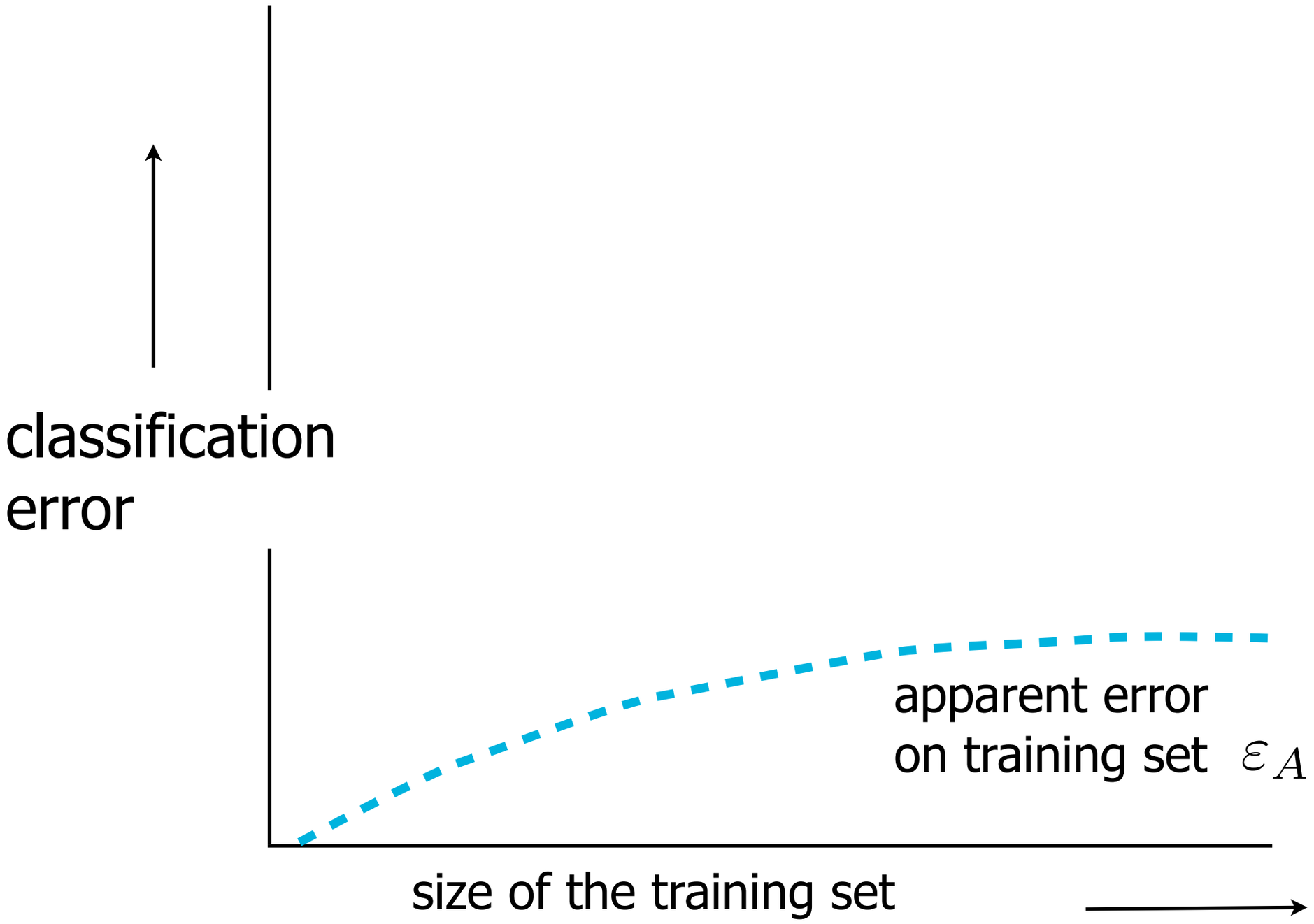
# Double cross-validation

- To optimise hyperparameters, do cross-validation **inside** another cross-validation:

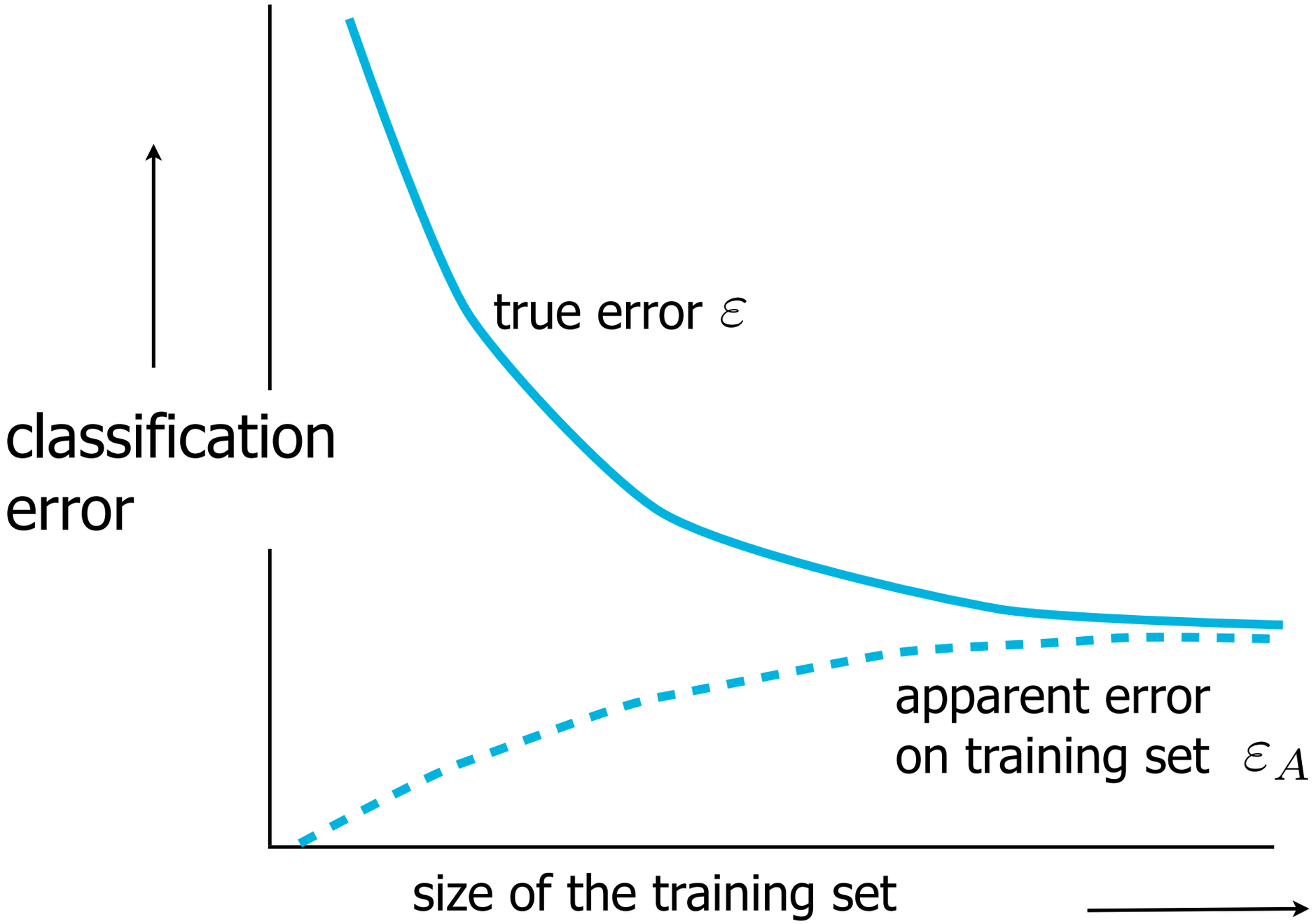



Actually,
**retrain** the classifier
with optimal $h_j$

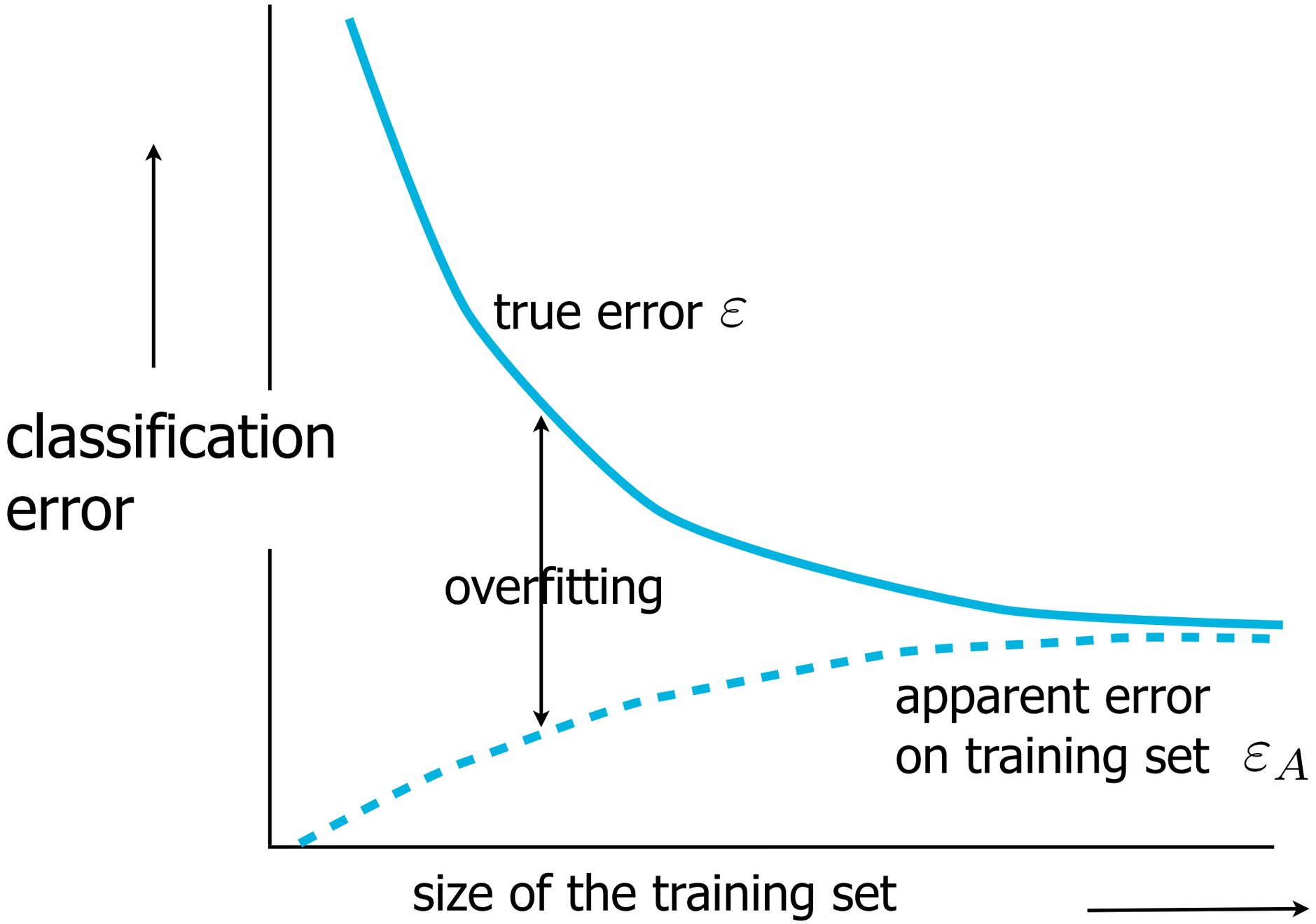
# Apparent Classification error



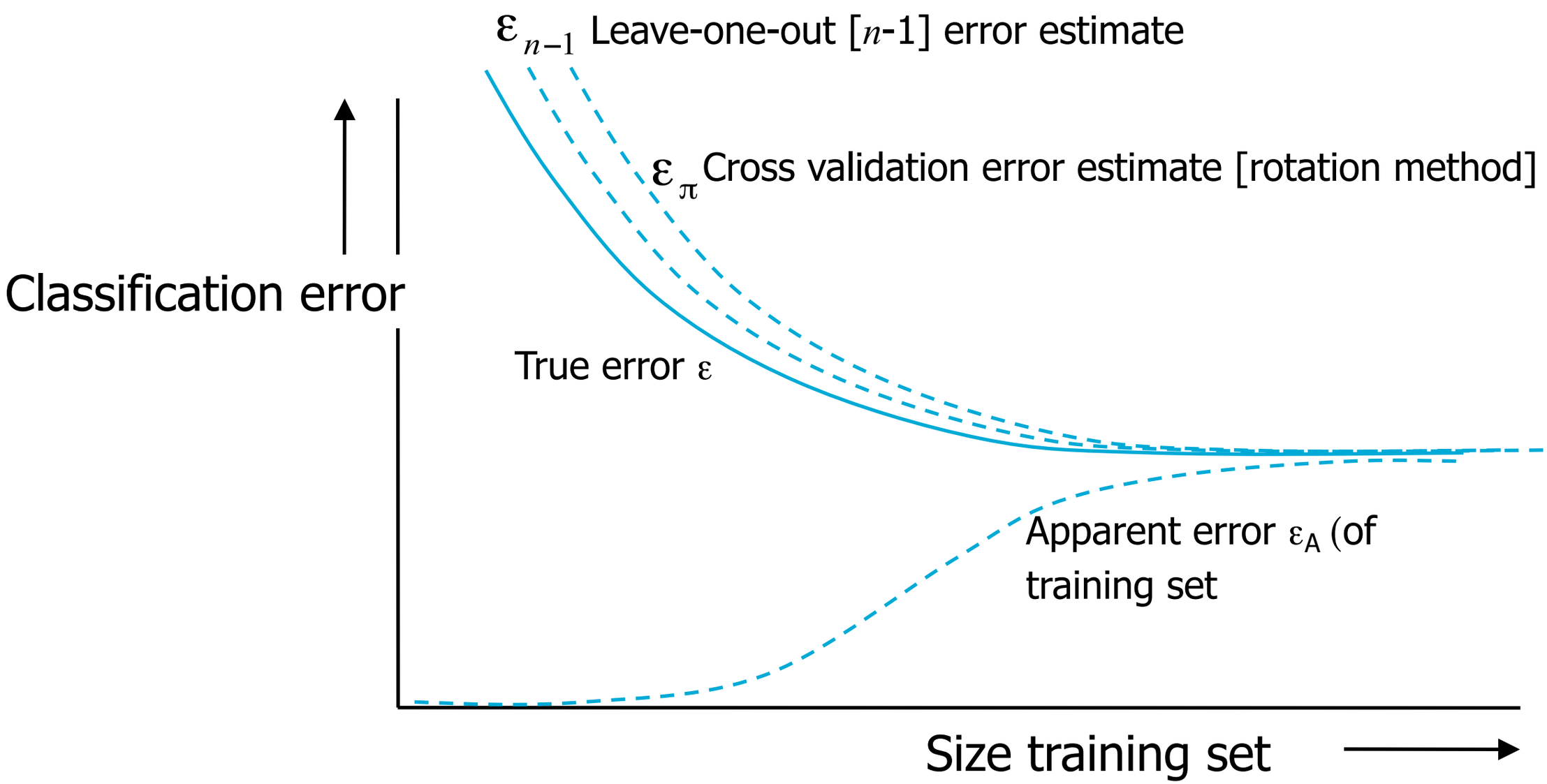
# Classification error



# Apparent Classification error



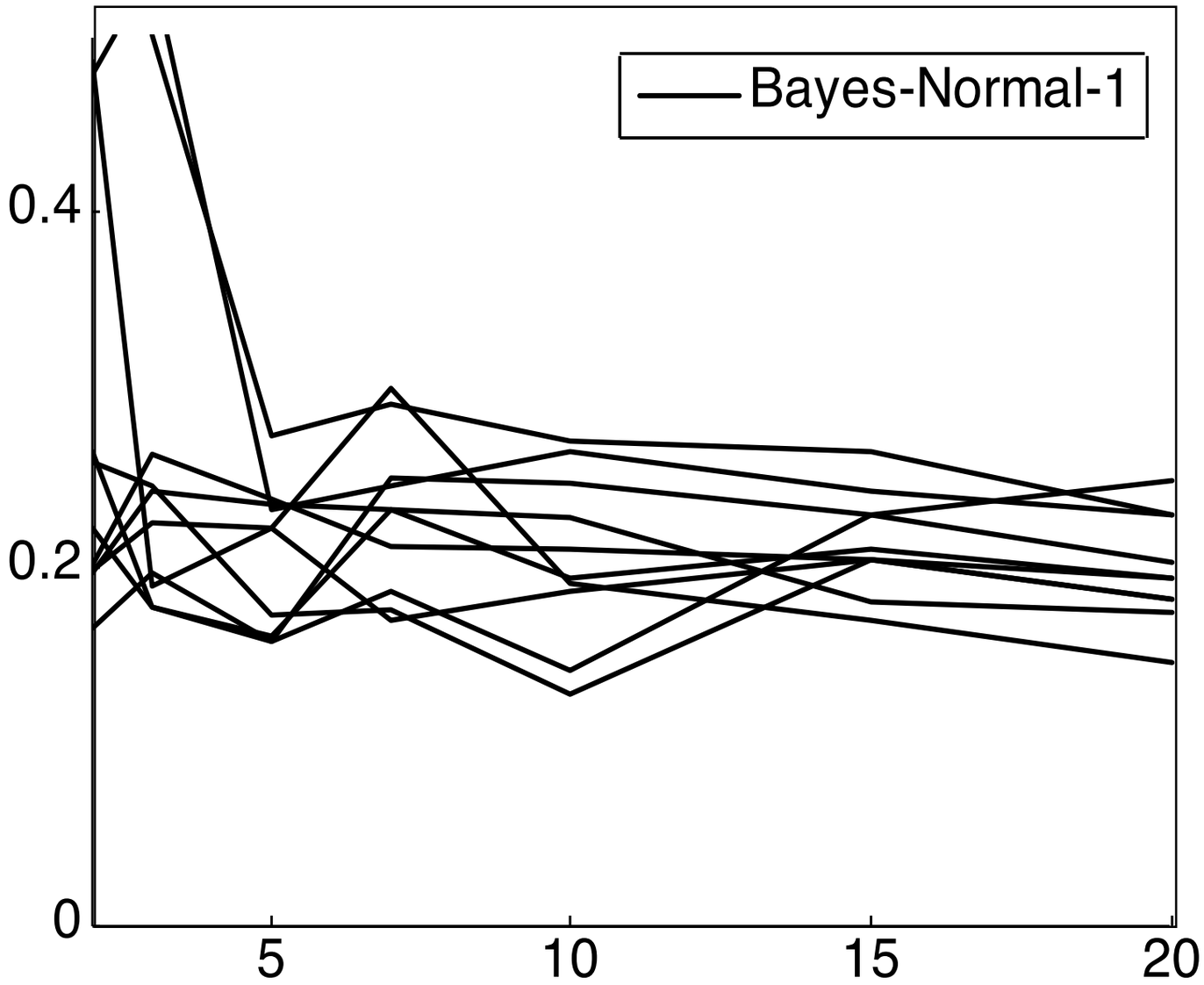
# Cross Validation Curves [and Related]



# Learning Curves

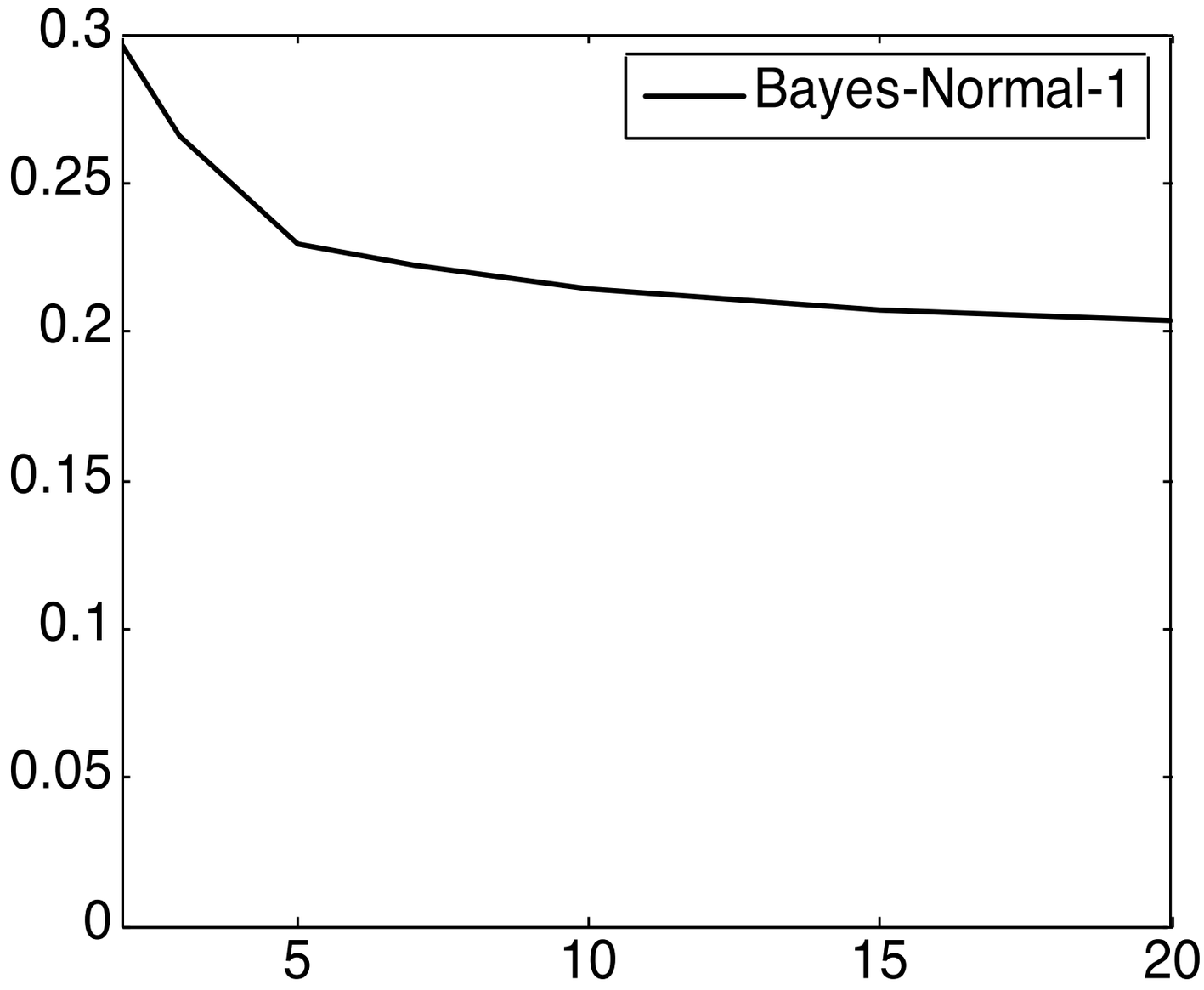
- Curves that plot [estimated] classification errors against the number of samples in training set
  - Usually plot error both on training and on test set
- Gives insight in, e.g.
  - Amount of overtraining
  - Usefulness of additional data
  - How different classifiers compare
  - Stability of training
  - …

# Repeated Learning Curves



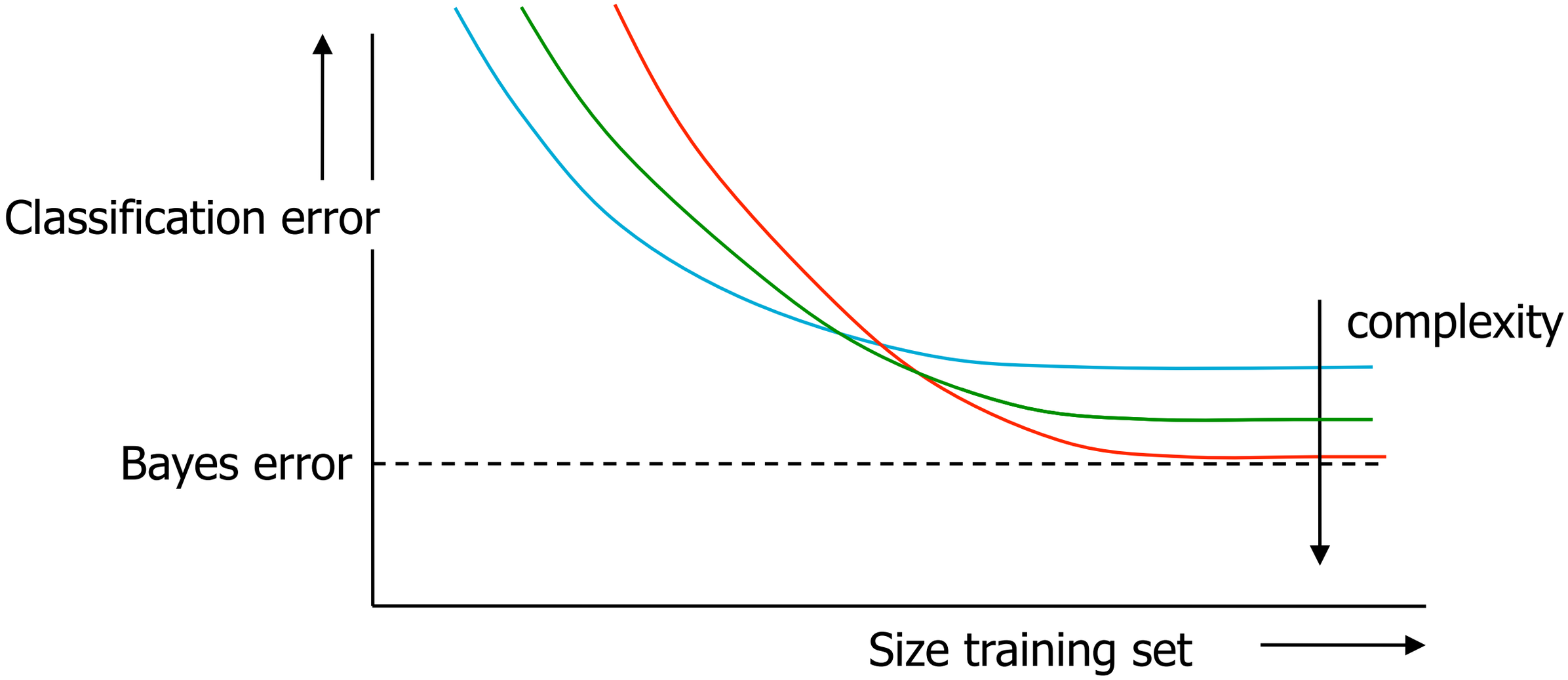

Small sample sizes have a very large variability

# Averaged Learning Curve



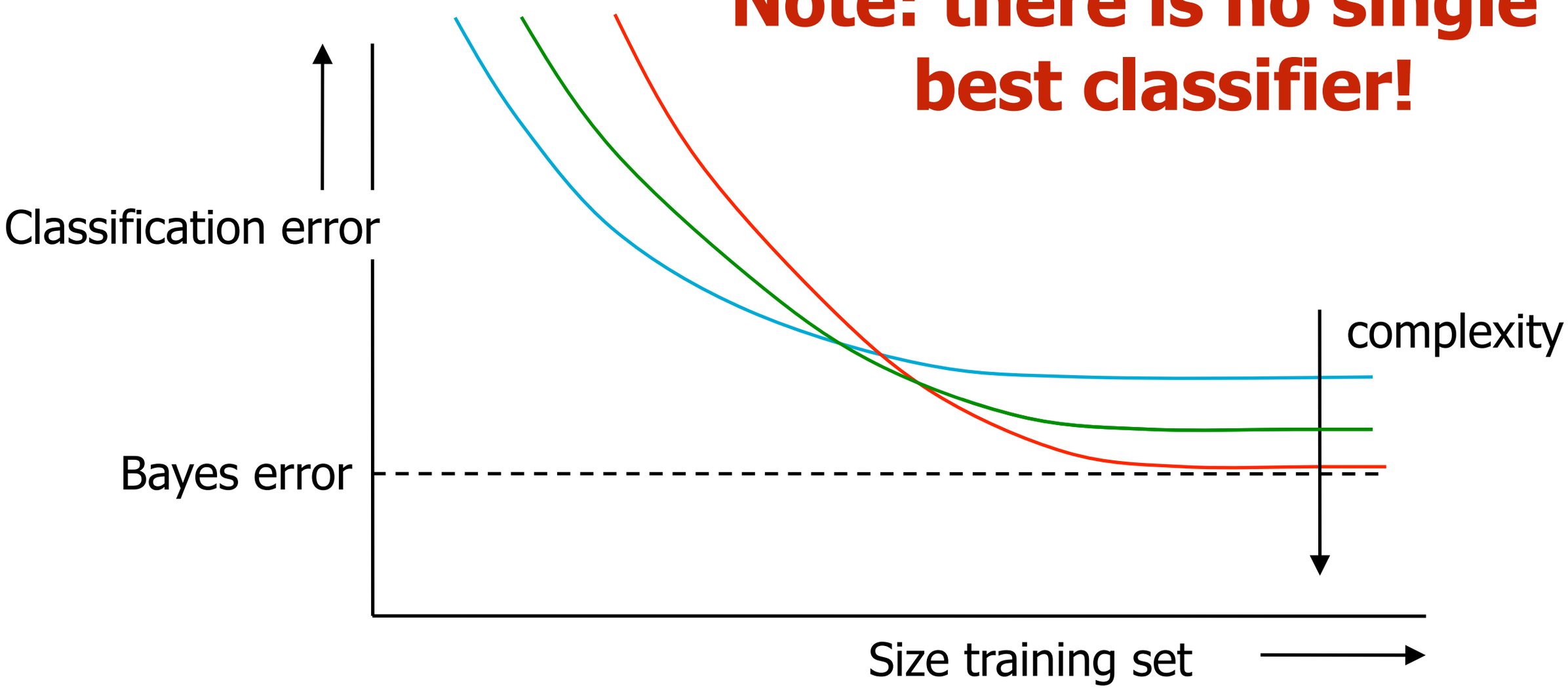

Average a few times

# Different Classifier Complexity

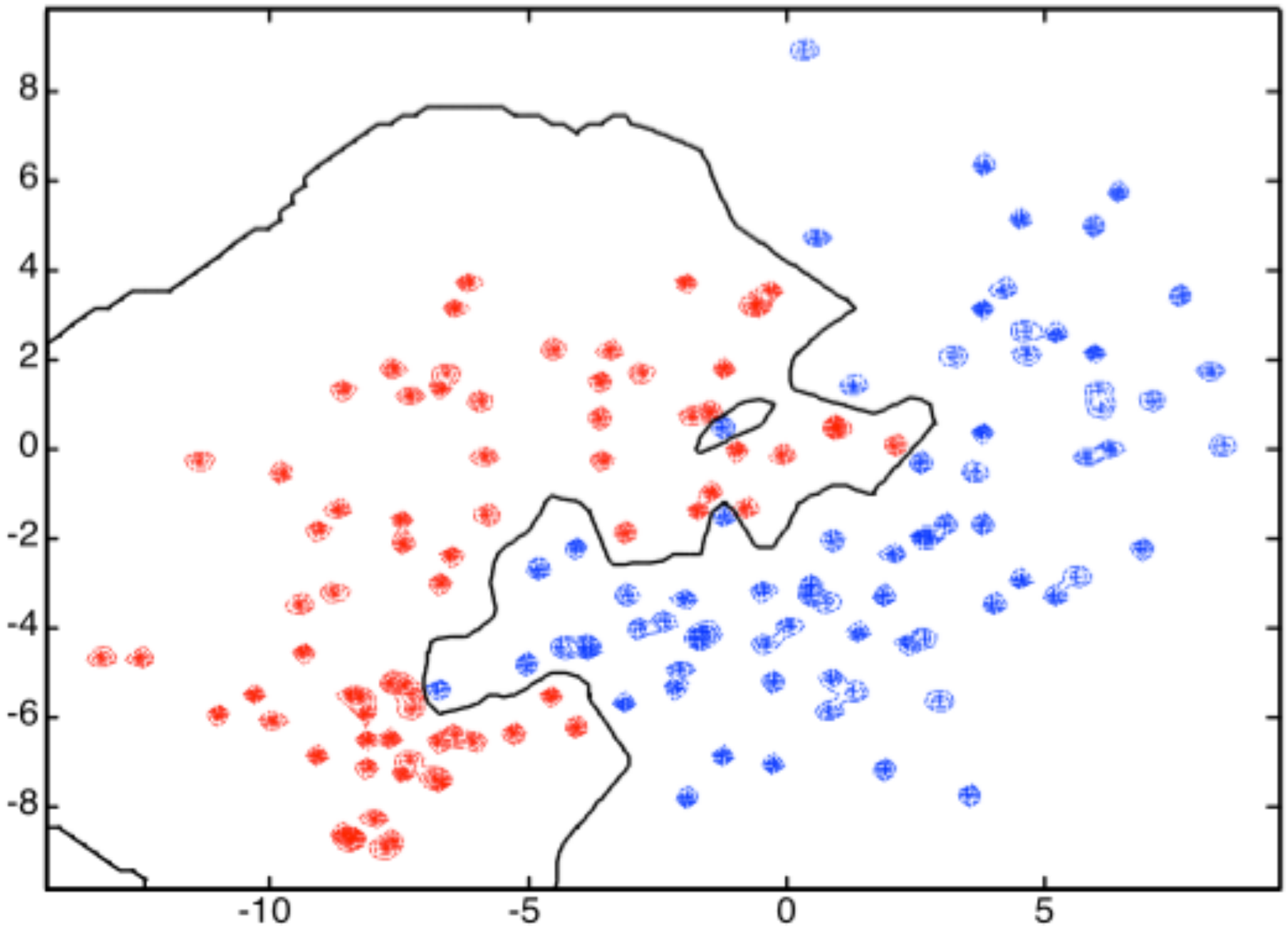


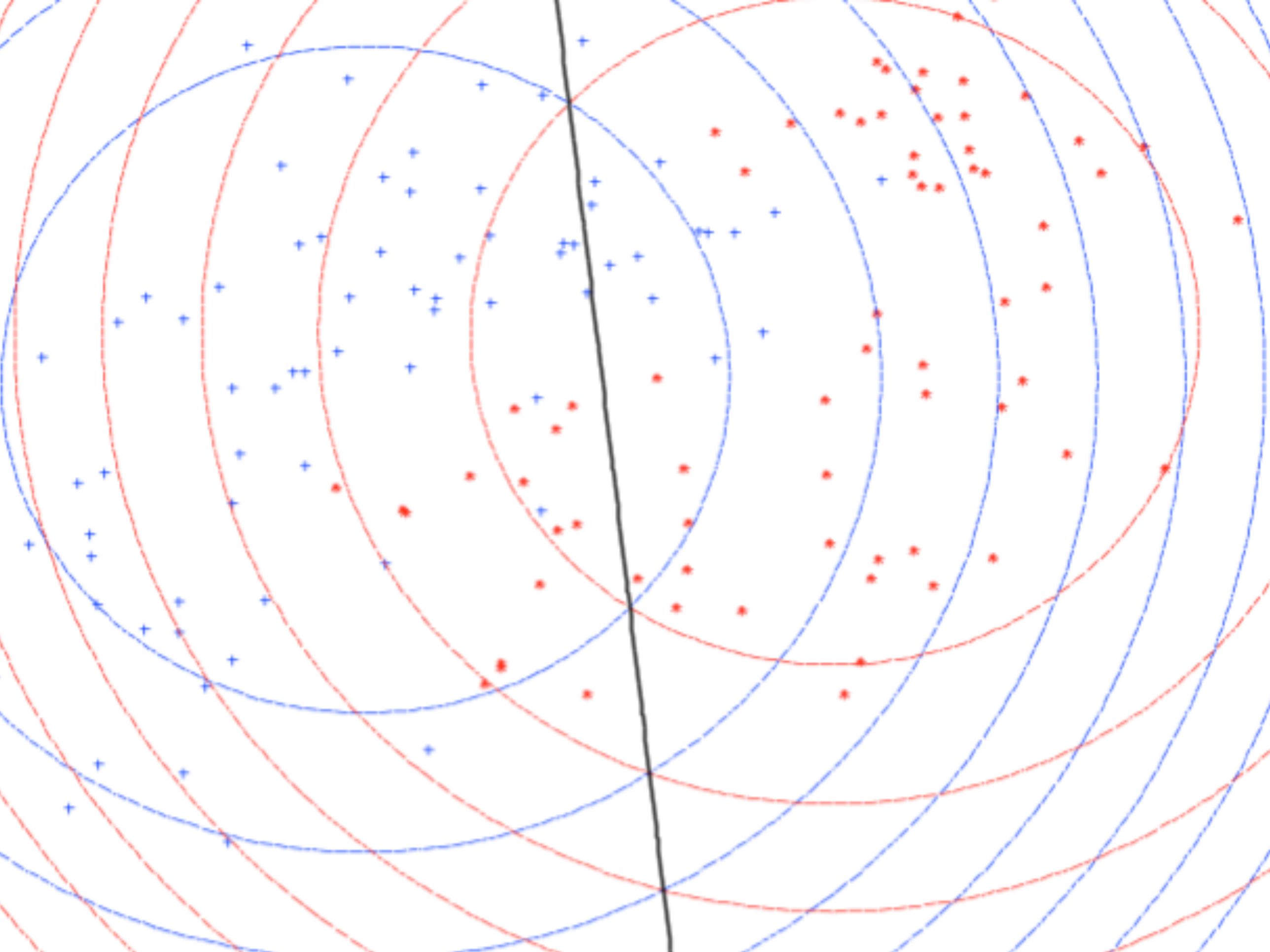
# Different Classifier Complexity

**Note: there is no single best classifier!**

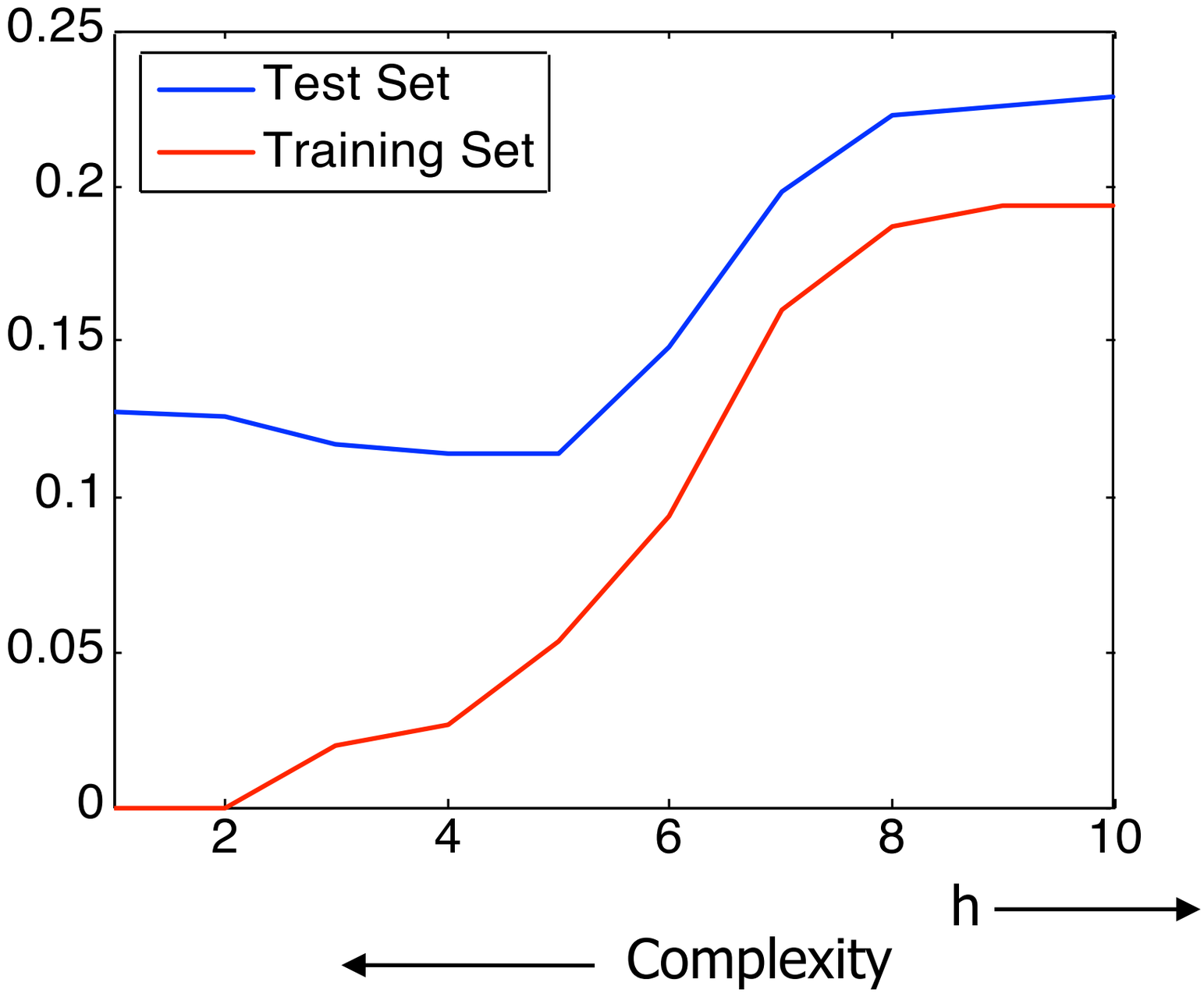


# `Parzenc` Complexity Example

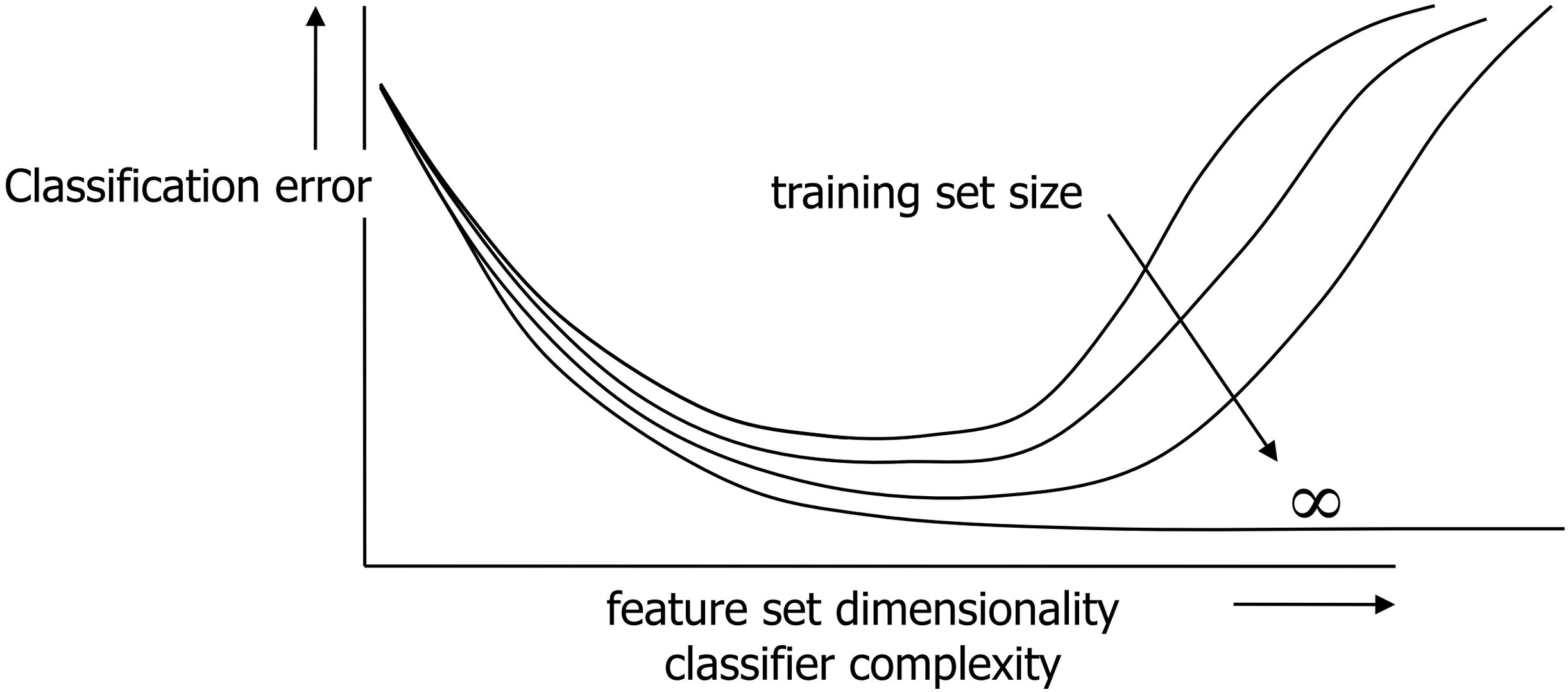




# `Parzenc` Complexity Example



# Feature Curves



# Some intermediate conclusions…

- Larger training sets yield better classifiers
- Independent test sets needed for unbiased error estimates
- Larger test sets yield more accurate error estimates
- LOO cross validation "optimal", but might be infeasible
- 10-fold crossvalidation is often used
- More complex classifiers need larger training sets
  - Same holds for larger feature set sizes
- Small training sets need simpler classifiers or smaller feature sets

# Squared Error

- When we have the error

$$L(\mathbf{w}) = E[\|g(\mathbf{x}) - y\|^2]$$

  we can actually derive something more general...

- In general?!

- Unfortunately, theory in Pattern Recognition is tough… how to deal with **all** possible datasets?

# Bias-variance dilemma

- When we are given some data, we may get lucky, or unlucky:
  sometimes we get very a-typical data:-(

- To say something general, we need to **average** over different (training-) sets

$$\mathcal{D} = \{(y_i, \mathbf{x}_i); i = 1, .., N\}$$

- The classifier is now also a function of the training set:

$$g(\mathbf{x}; \mathcal{D})$$

# Bias-variance dilemma

- Consider the squared error:

$$E_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - E[y|\mathbf{x}])^2\right]$$

- $E[y|\mathbf{x}]$ is the optimal mean-squared regressor (not proven now; see book)
- Now we do a trick:

$$= E_{\mathcal{D}}\Big[(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] + E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])^2\Big]$$

# Bias-variance dilemma

- Now working out the square:

$$= E_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])^2 \right.$$
$$+ 2(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])(E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])$$
$$\left. + (E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])^2\right]$$

# Bias-variance dilemma

- Now working out the square:

$$= E_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])^2 + 2(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])(E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}]) + (E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])^2\right]$$

$$= E_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])^2\right] \quad \text{(variance)}$$

$$+ E_{\mathcal{D}}\left[2(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])(E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])\right] = 0$$

$$+ E_{\mathcal{D}}\left[(E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])^2\right] \quad \text{(bias}^2\text{)}$$

# Bias-variance dilemma

(variance)

$$MSE = E_{\mathcal{D}}\left[(g(\mathbf{x};\mathcal{D}) - E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})])^2\right]$$
$$+ E_{\mathcal{D}}\left[(E_{\mathcal{D}}[g(\mathbf{x};\mathcal{D})] - E[y|\mathbf{x}])^2\right]$$

(bias$^2$)

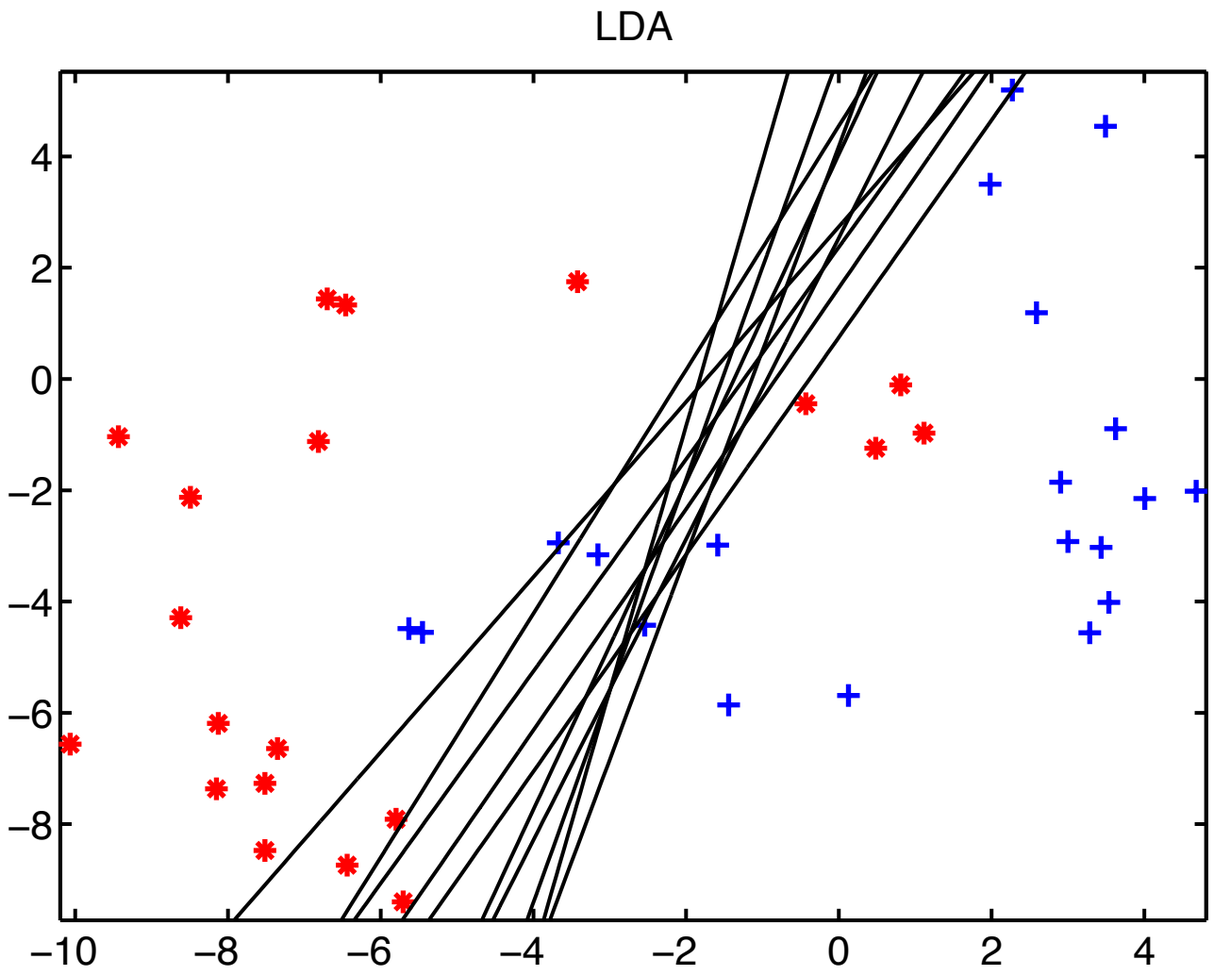
- variance: how much does classifier g vary over different training sets

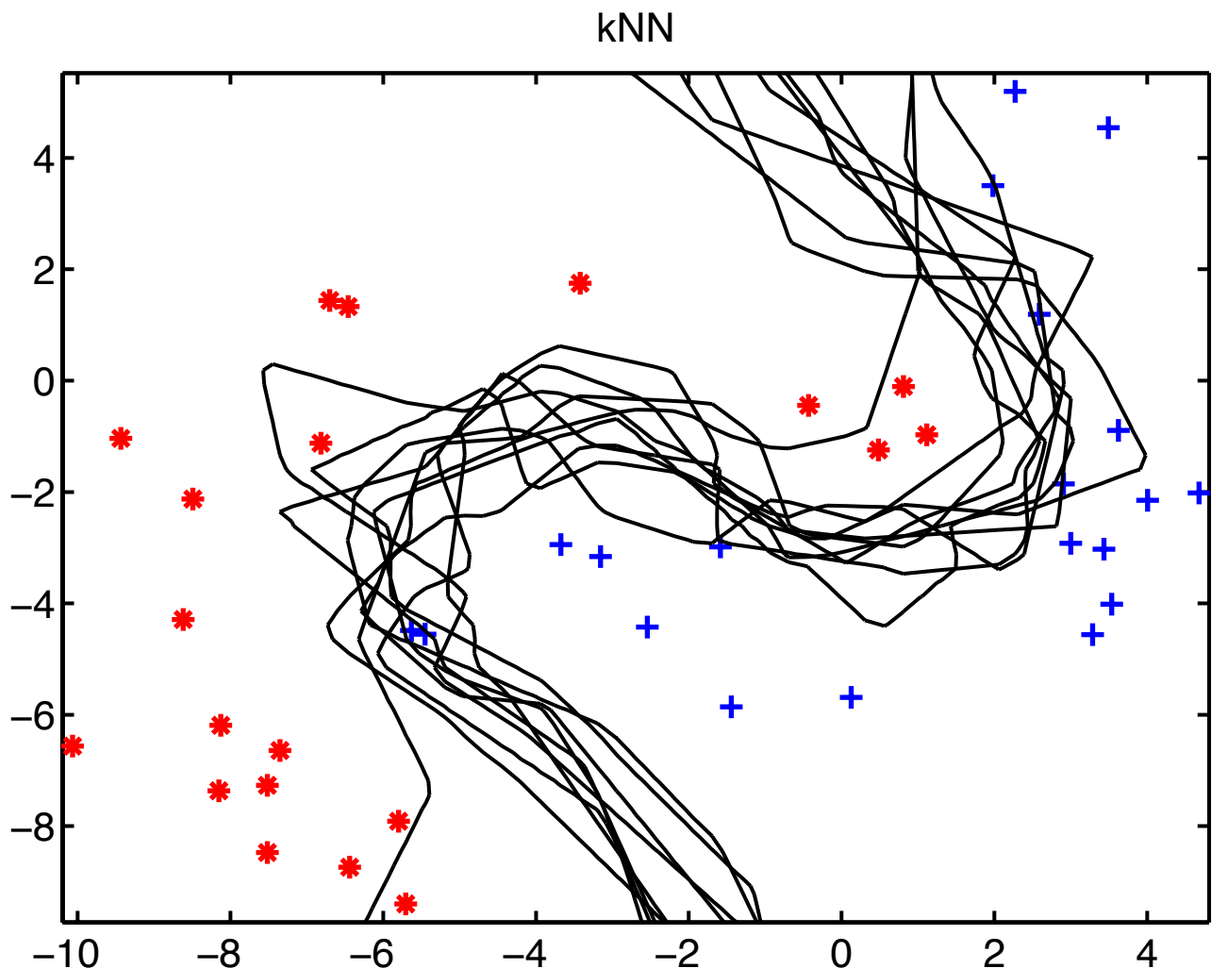
- bias: how much does the average classifier g differ from the true output

# Bias-variance dilemma

- Compare LDA with kNN:

low variance, high bias



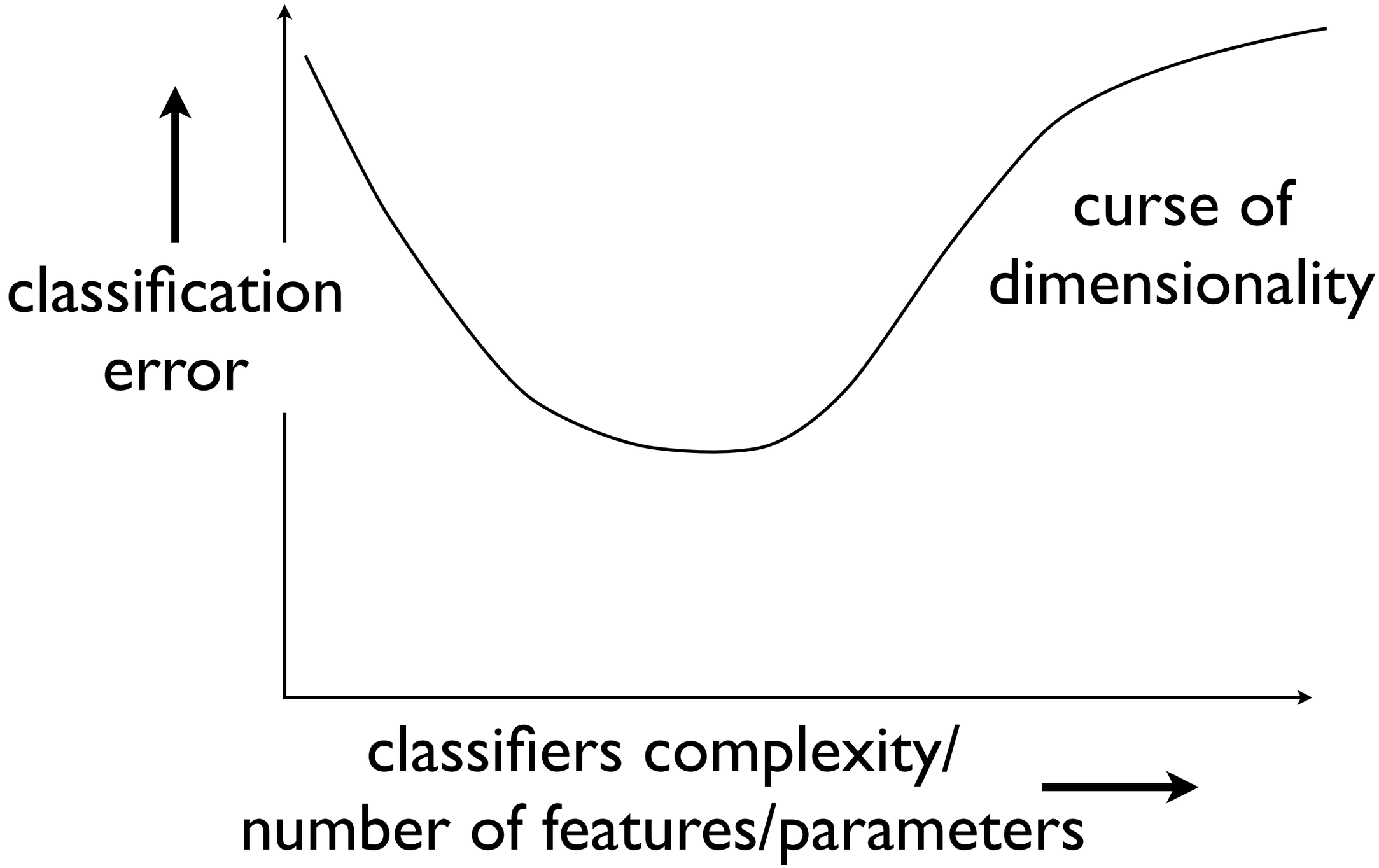




high variance, low bias

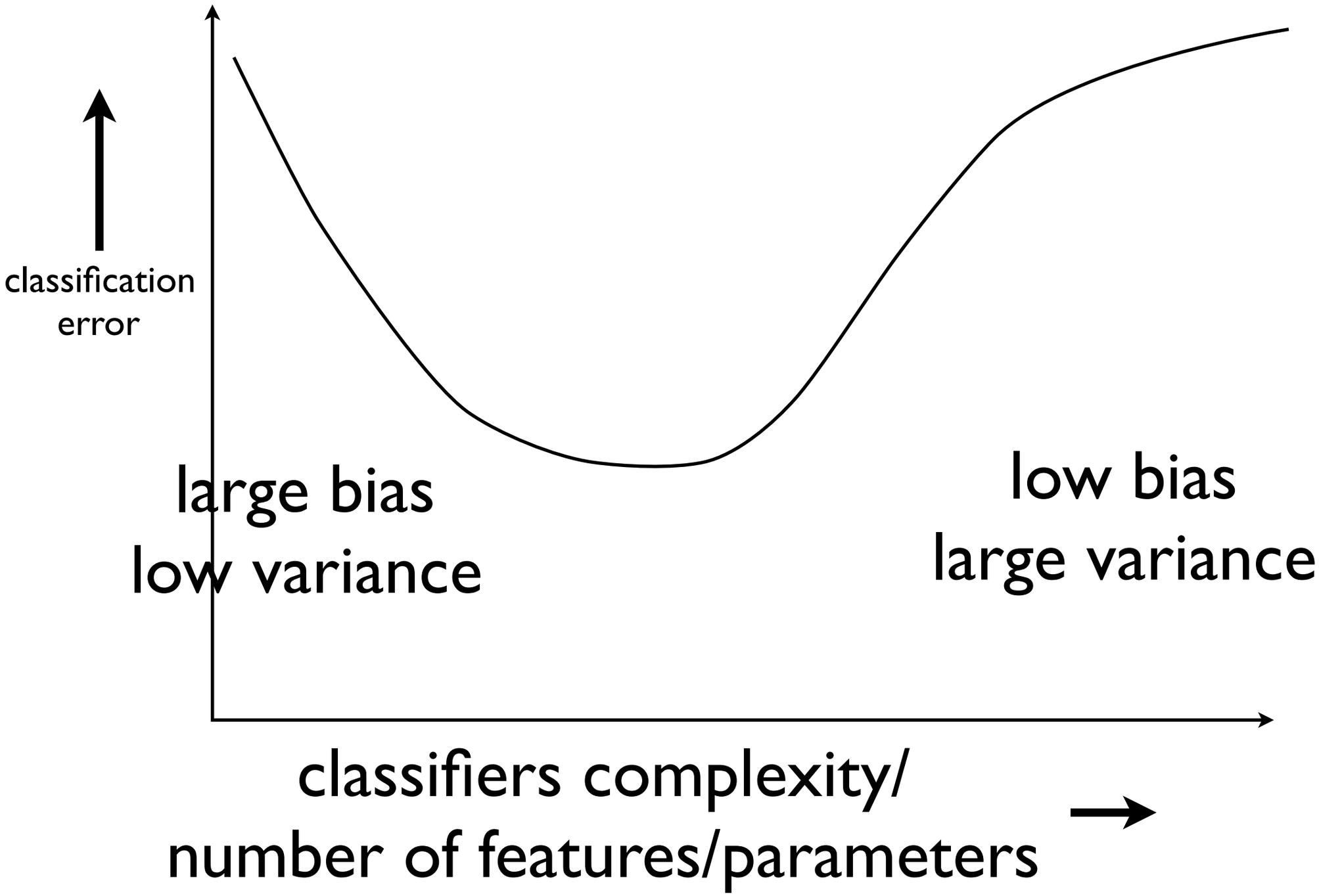
# Bias-variance tradeoff

- Originally derived for neural networks
- It is a very general phenomenon: we encounter it more often in pattern recognition
- More simple classifier is more stable (and need less data to train)
- More complex classifier only works when you have sufficient number of training data

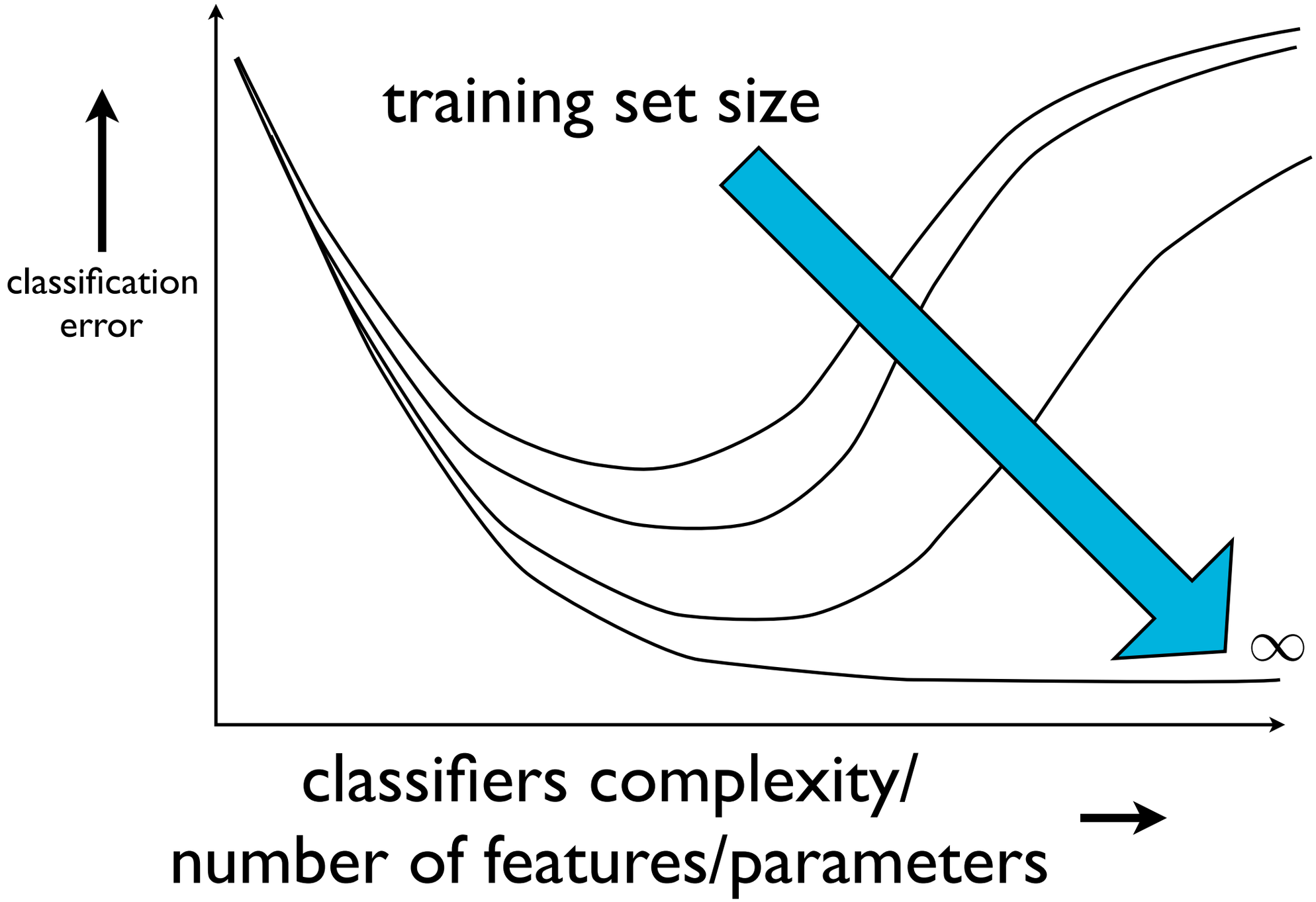
# Feature curve



# Feature curve



# Feature curve



# Regularisation

- (Almost) all machine learning methods optimise a loss/ cost function like:

$$L = \frac{1}{N} \sum_{i=1}^{N} l(f(\mathbf{x}_i; \mathbf{w}), y_i)$$

- This holds for NMC, LDA, QD, logistic classifier, perceptron, MLP, SVM, decision tree

- Sometimes people add an additional regulariser $\Omega(\mathbf{w})$:

$$L = \frac{1}{N} \sum_{i=1}^{N} l(f(\mathbf{x}_i; \mathbf{w}), y_i) + \lambda \Omega(\mathbf{w})$$

regularisation parameter  regulariser

# Regularisation

- Want to know more about

$$L = \frac{1}{N}\sum_{i=1}^{N} l(f(\mathbf{x}_i; \mathbf{w}), y_i) + \lambda\Omega(\mathbf{w}) \quad ?$$

wait for the Master course:

CS4220 Machine Learning 1

# Conclusions

- There is no best classifier
- There are alternative principles to find a good classifier:
  - maximising the likelihood
  - minimising the classification error
  - minimising the mean squared error
  - ...

- There is a fundamental tradeoff between the bias and variance of a classifier (depending on how flexible/ complex a classifier is)
- Finding the correct regulariser is a ‘black art’ of ML