# CS-E4710 Machine Learning: Supervised Methods

## Lecture 4: Model selection

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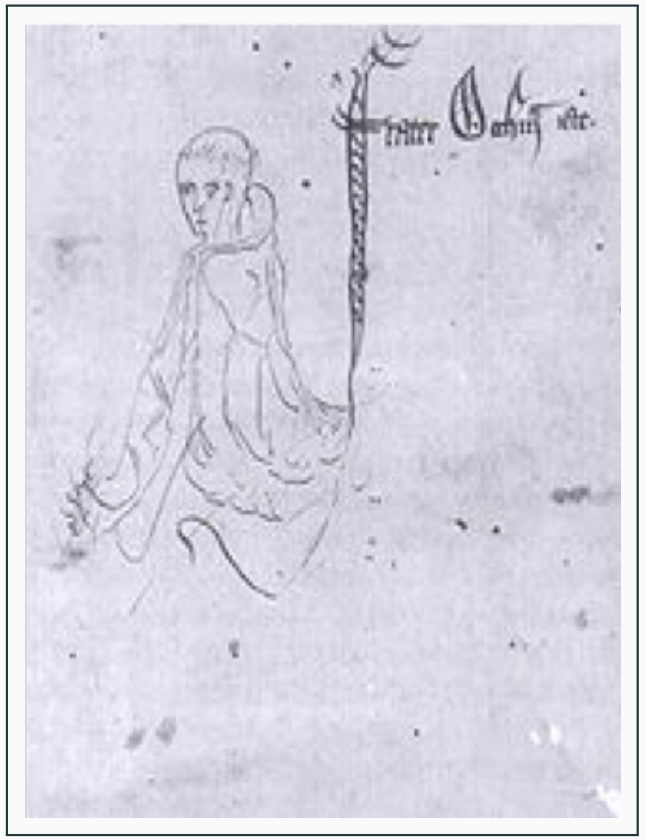
# Model selection and Occam's Razor

- Occam's razor principle "Entities should not be multiplied unnecessarily" captures the trade-off between generalization error and complexity
- Model selection in machine learning can be seen to implement Occam's razor



William of Ockham (1285–1347) "Pluralitas non est ponenda sine neccesitate"

# Stochastic scenario

- The analysis so far assumed that the labels are deterministic functions of the input
- Stochastic scenario relaxes this assumption by assuming the output is a probabilistic function of the input
- The input and output is generated by a joint probability distribution $D$ or $X \times \mathcal{Y}$.
- This setup covers different cases when the same input $x$ can have different labels $y$
- In the stochastic scenario, there **may not always exist** a target concept $f$ that has zero generalization error $R(f) = 0$

# Sources of stochasticity

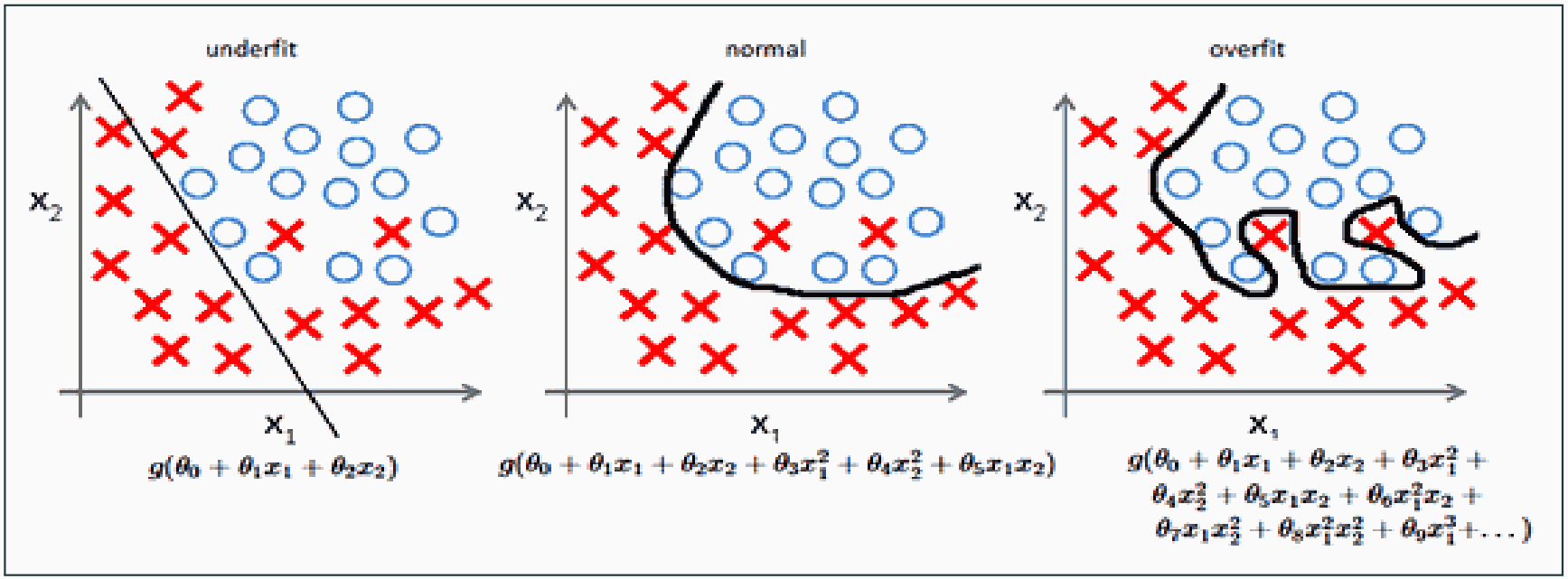
The stochastic dependency between input and output can arise from various sources

- Imprecision in recording the input data (e.g. measurement error), shifting our examples
- Errors in the labeling of the training data (e.g. human annotation errors), flipping the labels some examples
- There may be additional variables that affect the labels that are not part of our input data

All of these sources could be characterized as adding noise (or hiding signal)

# Noise and complexity

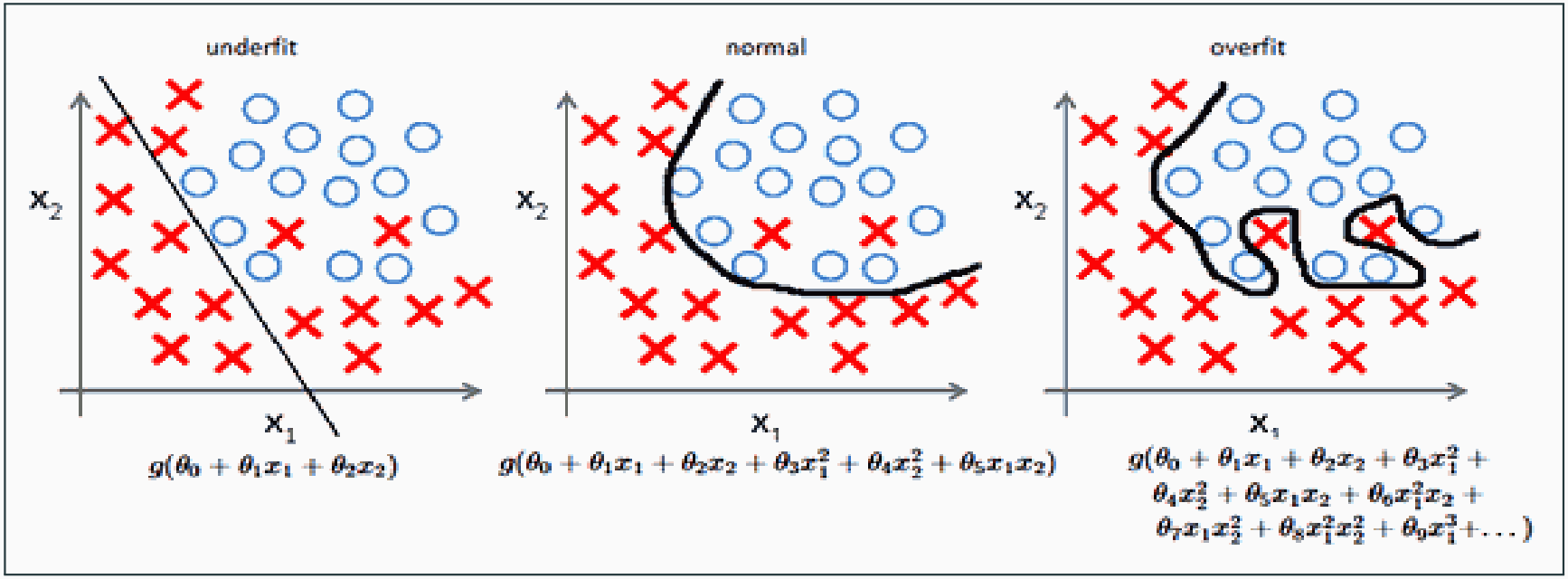
- The effect of noise is typically to make the decision boundary more complex
- To obtain a consistent hypothesis on noisy data, we can use a more complex model e.g. a spline curve instead of a hyperplane
- But this may not give a better generalization error, if we end up merely re-classifying points corrupted by noise



# Noise and complexity

In practice, we need to balance the complexity of the hypothesis and the empirical error carefully

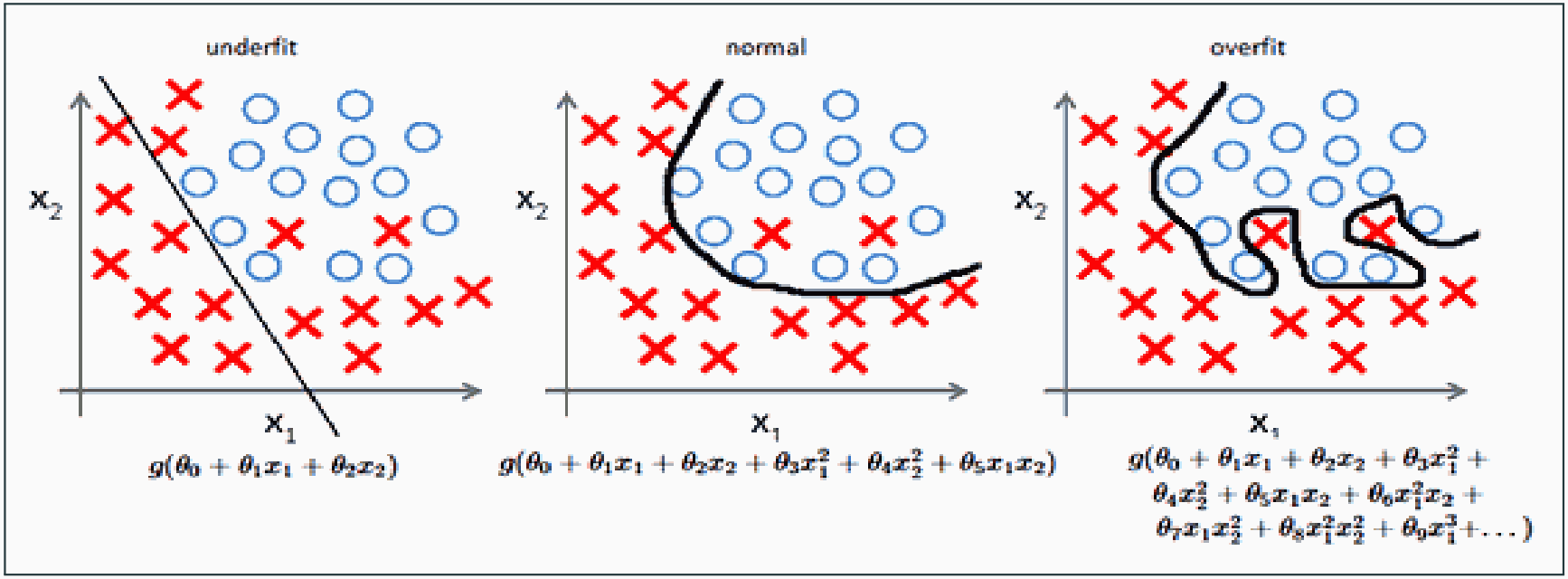
- A too simple model does not allow optimal empirical error to obtained, this is called underfitting
- A too complex model may obtain zero empirical error, but have worse than optimal generalization error, this is called overfitting



# Controlling complexity

Two general approaches to control the complexity

- Selecting a hypothesis class, e.g. the maximum degree of polynomial to fit the regression model
- Regularization: penalizing the use of too many parameters, e.g. by bounding the norm of the weights (used in SVMs and neural networks)



# Measuring complexity

What is a good measure of complexity of a hypothesis class?

We have already looked at some measures:

- Number of distinct hypotheses $|\mathcal{H}|$: works for finite $\mathcal{H}$ (e.g. models build form binary data), but not for infinite classes (e.g. geometric hypotheses such as polygons, hyperplanes, ellipsoids)
- Vapnik-Chervonenkis dimension (VCdim): the maximum number of examples that can be classified in all possible ways by choosing different hypotheses $h \in \mathcal{H}$
- Rademacher complexity: measures the capability to classify after randomizing the labels

Lots of other complexity measures and model selection methods exist c.f. `https://en.wikipedia.org/wiki/Model_selection` (these are not in the scope of this course)

# Bayes error

# Bayes error

- In the stochastic scenario, there is a minimal non-zero error for any hypothesis, called the **Bayes error**
- Bayes error is the minimum achievable error, given a distribution $D$ over $X \times \mathcal{Y}$, by measurable functions $h : X \mapsto \mathcal{Y}$

$$R^* = \inf_{\{h | h \text{ measurable } \}} R(h)$$

- Note that we cannot actually compute $R^*$:
  - We cannot compute the generalization error $R(h)$ exactly (c.f. PAC learning)
  - We cannot evaluate all measurable functions (intuitively: hypothesis class that contains all functions that are mathematically well-behaved enough to allow us to define probabilities on them)
- Bayes error serves us a a theoretical measure of best possible performance

# Bayes error and noise

- A hypothesis with $R(h) = R^*$ is called the **Bayes classifier**
- The Bayes classifier can be defined in terms of conditional probabilities as

$$h_{Bayes}(x) = \text{argmax}_{y \in \{0,1\}} Pr(y|x)$$

- The average error made by the Bayes classifer at $x \in X$ is called the **noise**

$$noise(x) = \min(Pr(1|x), Pr(0|x))$$

- Its expectation $E(noise(x)) = R^*$ is the Bayes error
- Similarly to the Bayer error, Bayes classifier is a theoretical tool, not something we can compute in practice

# Decomposing the error of a hypothesis

The **excess error** of a hypothesis compared to the Bayes error $R^*$ can be decomposed as:

$$R(h) - R^* = \epsilon_{estimation} + \epsilon_{approximation}$$

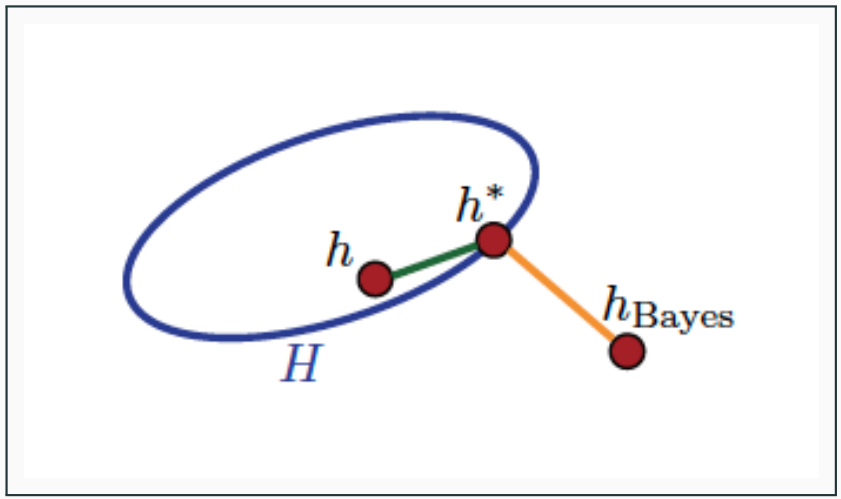
- $\epsilon_{estimation} = R(h) - R(h^*)$ is the excess generalization error $h$ has over the optimal hypothesis $h^* = \operatorname{argmin}_{h' \in \mathcal{H}} R(h')$ in the hypothesis class $\mathcal{H}$
- $\epsilon_{approximation} = R(h^*) - R^*$ is the approximation error due to selecting the hypothesis class $\mathcal{H}$ instead of the best possible hypothesis class (which is generally unknown to us)

Note: The approximation error is sometimes called the **bias** and the estimation error the **variance**, and the decomposition **bias-variance decomposition**

# Decomposing the error of a hypothesis

Figure on the right depicts the concepts:

- $h_{Bayes}$ is the Bayes classifier, with $R(h_{Bayes}) = R^*$
- $h* = \inf_{h \in \mathcal{H}} R(h)$ is the hypothesis with the lowest generalization error in the hypothesis class $\mathcal{H}$
- $R(h)$ has both non-zero estimation error $R(h) - R(h^*)$ and approximation error $R(h^*) - R(h_{Bayes})$

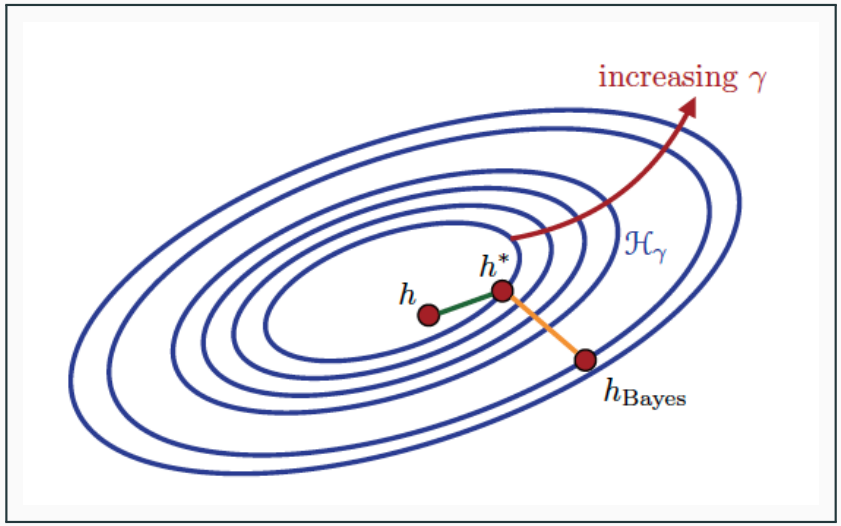



Challenge for model selection: We can bound the estimation error by generalization bounds but we cannot do the same for the approximation error as $R^*$ remains unknown to us.

# Learning with complex hypothesis classes

- One strategy for model selection to initially choose a very complex hypothesis class with zero or very low empirical risk $\mathcal{H}$
- Assume in addition the class can be decomposed into a union of increasingly complex hypothesis classes $\mathcal{H} = \bigcup_{\gamma \in \Gamma} \mathcal{H}_\gamma$

- The complexity increases by parameter $\gamma$ e.g.
  - $\gamma =$ degree of a polynomial function
  - $\gamma =$ size of a neural network
  - $\gamma =$ norm of weights of a linear regression model

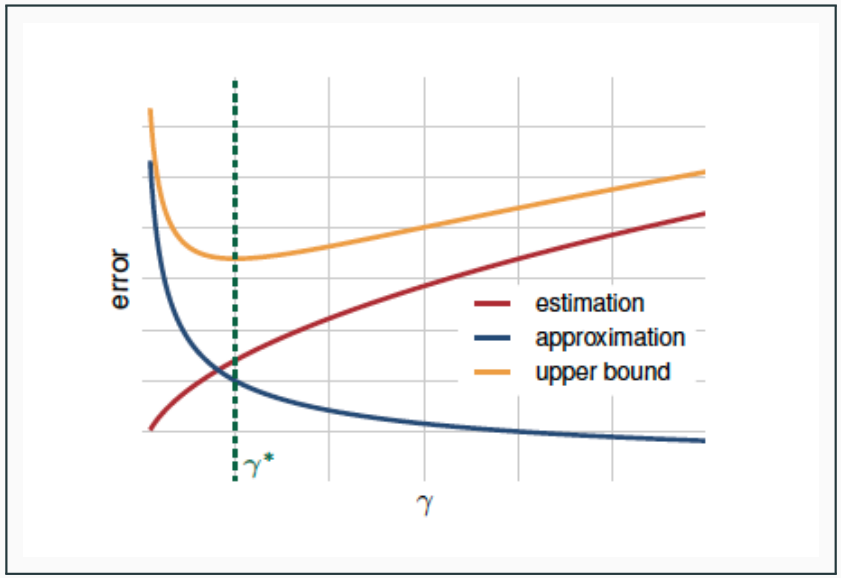



The model selection problem then entails choosing a parameter value $\lambda^*$ that gives the best generalization performance

# Learning with complex hypothesis classes

We have a trade-off: increasing the complexity of the hypothesis class

- decreases the approximation error as the class is more **likely to contain** a hypothesis with error close to the Bayes error
- increases the estimation error as **finding the good hypothesis** becomes more hard and the generalization bounds become looser(due to increasing $\log |\mathcal{H}_\gamma|$ or the VC dimension)

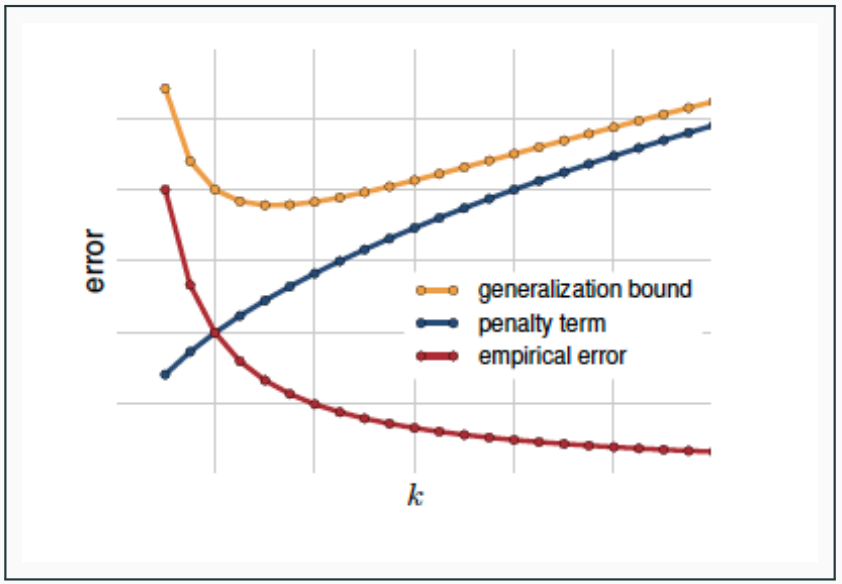



To minimize the generalization error over all hypothesis classes, we should find a balance between the two terms

# Structural risk minimization

Structural risk minimization (SRM) assumes a countable union of hypothesis classes $\mathcal{H} = \bigcup_{k \geq 1} \mathcal{H}_k$, indexed by complexity parameter $k$:

- SRM aims to minimize the excess risk $R(h) - R(h_{Bayes})$ by bounding $R(h)$
- The bound takes both the empirical error and the complexity of the hypothesis class into account (through a penalty term)




The model selection task is to select the optimal index $k^*$ and the hypothesis $h \in \mathcal{H}_{k^*}$ that gives the best generalization bound

# Structural risk minimization

Generalization bound for SRM (Mohri et al. 2018): for any $\delta > 0$ with probability at least $1 - \delta$ over the draw of a sample S of size m, we have for all $k \geq 1$ and $h \in \mathcal{H}_k$

$$R(h) \leq \hat{R}_S(h) + \mathcal{R}_m(\mathcal{H}_k(h)) + \sqrt{\frac{\log k}{m}} + \sqrt{\frac{\log \frac{2}{\delta}}{2m}}$$

- $\hat{R}_S(h)$ - empirical error on the training set
- $\mathcal{R}_m(\mathcal{H}_k(h))$ - Rademacher complexity of the least complex hypothesis class where $h$ belongs
- The term $\sqrt{\frac{\log k}{m}}$ is essentially the only difference to the bound that we have for the case where assume a fixed hypothesis class (Lecture 3, slide 27)!

# Structural risk minimization

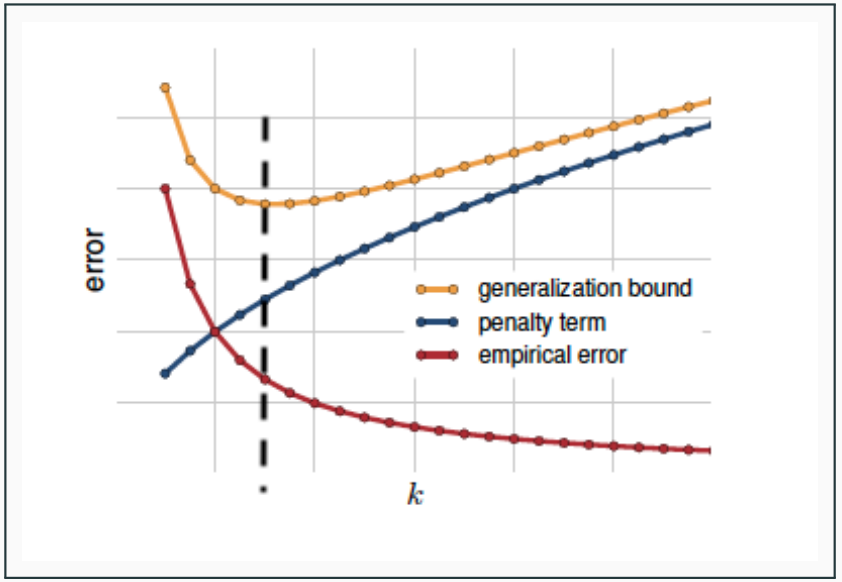
- Given a training sample $S$, the SRM model selection algorithm picks the index $k$ and $h_S^{SRM} \in \mathcal{H}_k$ that minimizes

$$h_S^{SRM} = \operatorname{argmin}_{k \geq 1, h \in \mathcal{H}_k} \hat{R}_S(h) + \mathcal{R}_m(\mathcal{H}_k) + \sqrt{\frac{\log k}{m}}$$

- Note that this may be a computationally difficult task:
  - Requires finding the hypothesis that minimizes training error for each hypothesis class separately
  - Obtaining the empirical Rademacher complexity generally requires simulation with multiple datasets with randomized labels for each hypothesis class

# SRM model selection: pros and cons

- Structural risk minimization benefits from strong learning guarantees
- However, the assumption of a countable decomposition of the hypothesis class is a restrictive one
- The computational price to pay is large, especially when a large number of hypothesis classes $\mathcal{H}_k$ has to be processed



# Regularization-based algorithms

# Regularization-based algorithms

- Regularization is an alternative model selection approach to SRM
- The methods rely on a very complex family $\mathcal{H} = \bigcup_{\gamma \geq 0} \mathcal{H}_\gamma$ of **uncountable union** of nested hypothesis classes $\mathcal{H}_\gamma$
- This extension to the SRM method would then ask to minimize

$$\operatorname{argmin}_{\gamma > 0, h \in \mathcal{H}_\gamma} \hat{R}_S(h) + \mathcal{R}_m(\mathcal{H}_\gamma) + \sqrt{\frac{\log \gamma}{m}}$$

- This problem seems to require evaluating the Rademacher complexity of an uncountably infinite number of hypothesis classes $\mathcal{H}_\gamma$!
- Need efficient algorithms to do this

# Regularization-based algorithms

- An example where efficient model selection becomes possible is the class of linear functions $\mathbf{x} \mapsto \mathbf{w}^T\mathbf{x}$
- The classes as parametrized by the norm $\|\mathbf{w}\|$ of the weight vector bounded by $\gamma$:

$$\mathcal{H}_\gamma = \{\mathbf{x} \mapsto \mathbf{w}^T\mathbf{x} : \|\mathbf{w}\| \leq \gamma\}$$

- The norm is typically either
  - $L^2$ norm (Also called Euclidean norm or 2-norm): $\|\mathbf{w}\|_2 = \sqrt{\sum_{j=1}^n w_j^2}$: used e.g. in support vector machines and ridge regression
  - $L^1$ norm (Also called Manhattan norm or 1-norm): $\|\mathbf{w}\|_1 = \sum_{j=1}^n |w_j|$: used e.g. in LASSO regression

# Regularization-based algorithms

- For the $L^2$-norm case, we have an important computational shortcut: the empirical Rademacher complexity of this class can be bounded analytically!
- Let $S \subset \{\mathbf{x} | \|\mathbf{x}\| \leq r\}$ be a sample of size $m$ and let $\mathcal{H}_\gamma = \{\mathbf{x} \mapsto \mathbf{w}^T\mathbf{x} : \|\mathbf{w}\|_2 \leq \gamma\}$ .Then

$$\hat{\mathcal{R}}_S(\mathcal{H}_\gamma) \leq \sqrt{\frac{r^2\gamma^2}{m}} = \frac{r\gamma}{\sqrt{m}}$$

- Thus the Rademacher complexity depends linearly on the upper bound $\gamma$ norm of the weight vector, as $r$ and $m$ are constant for any fixed training set
- We can use $\|\mathbf{w}\|$ as a efficiently computable upper bound of $\hat{\mathcal{R}}_m(\mathcal{H}_\gamma)$

# Regularization-based algorithms

- A regularized learning problem is to minimize

$$\text{argmin}_{h \in \mathcal{H}} \hat{R}_S(h) + \lambda \Omega(h)$$

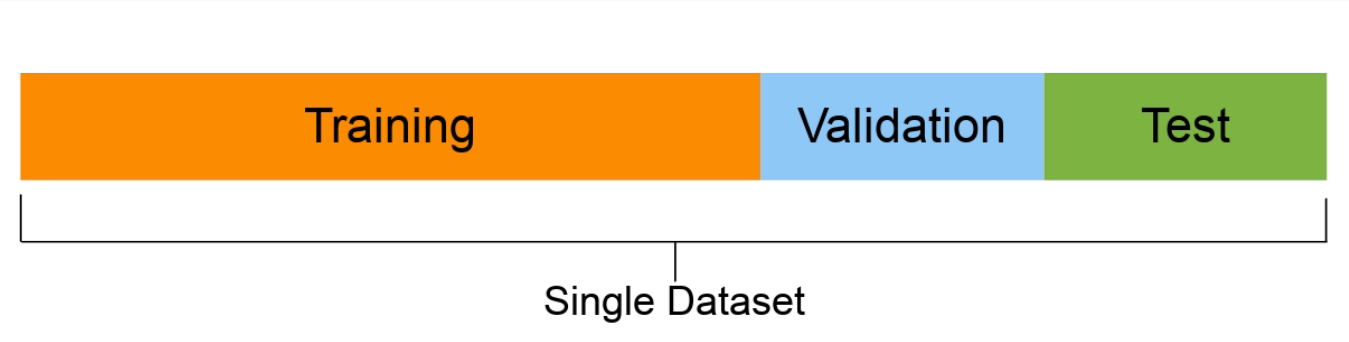
  - $\hat{R}_S(h)$ is the empirical error
  - $\Omega(h)$ is the regularization term which increases when the complexity of the hypothesis class increases
  - $\lambda$ is a regularization parameter, which is usually set by cross-validation
- For the linear functions $h : \mathbf{x} \mapsto \mathbf{w}^T \mathbf{x}$, usually $\Omega(h) = \|\mathbf{w}\|_2^2$ or $\Omega(h) = \|\mathbf{w}\|_1$
- We will study regularization-based algorithms during the next part of the course

# Model selection using a validation set

# Model selection by using a validation set

We can use the given dataset for empirical model selection, if the algorihm has input parameters (hyperparameters) that define/affect the model complexity

- Split the data into training, validation and test sets
- For the hyperparameters, use **grid search** to find the parameter combination that gives the best performance on the validation set
- Retrain a final model using the optimal parameter combination, use both the training and validation data for training
- Evaluate the performance of the final model **on the test set**



# Grid search

- Grid search is an technique frequently used to optimize hyperparameters, including those that define the complexity of the models
- In its basic form it goes through all combinations of parameter values, given a set of candidate values for each parameter

- For two parameters, taking of value combinations $(v, u) \in V \times U$, where $V$ and $U$ are the sets of values for the two parameters, defines a two-dimensional **grid** to be searched
- Even more parameters can be optimized but the exhaustive search becomes computationally hard due to exponentially exploding search space

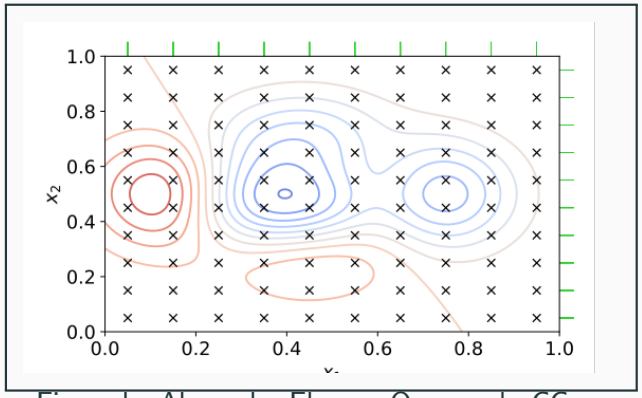
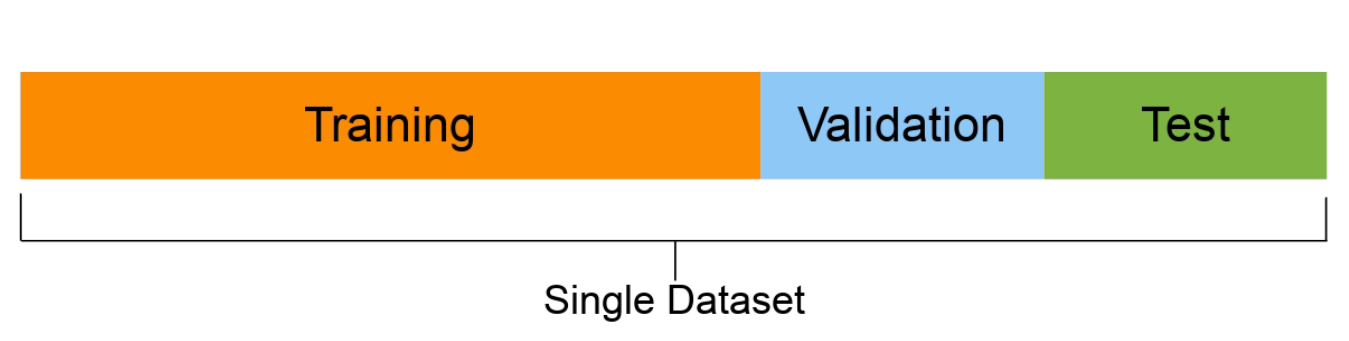



Figure by Alexander Elvers - Own work, CC BY-SA 4.0, https://commons.wikimedia.org/w/index.php?curid=842554

# Model selection by using a validation set

- The need for the validation set comes from the need to avoid overfitting
- If we only use a simple training/test split and selected the hyperparameter values by repeated evaluation on the test set, the performance estimate will be optimistic
- A reliable performance estimate can only be obtained form the test set



# How large should the training set be in comparison of the validation set?

- The larger the training set, the better the generalization error will be (e.g. by PAC theory)
- The larger the validation set, the less variance there is in the test error estimate.
- When the dataset is small generally the training set is taken to be as large as possible, typically 90% or more of the total
- When the dataset is large, training set size is often taken as big as the computational resources allow

# Stratification

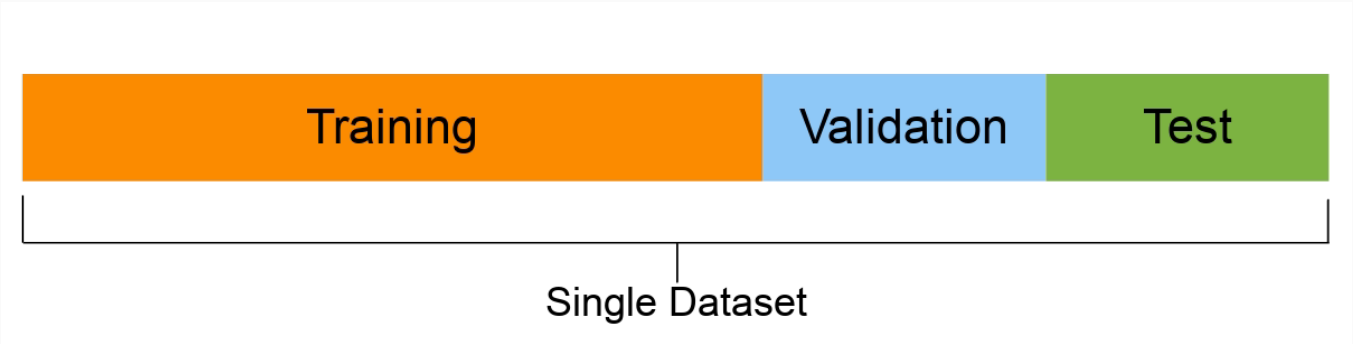
- Class distributions of the training and validation sets should be as similar to each another as possible, otherwise there will be extra unwanted variance
  - when the data contains classes with very low number of examples, random splitting might result in no examples in the class in the validation set
- Stratification is a process that tries to ensure similar class distributions across the different sets
- Simple stratification approach is to divide all classes separately into the training and validation sets and the merge the class-specific training sets into global training set and class-specific validation sets into a global validation set.

# Cross-validation

# The need of multiple data splits

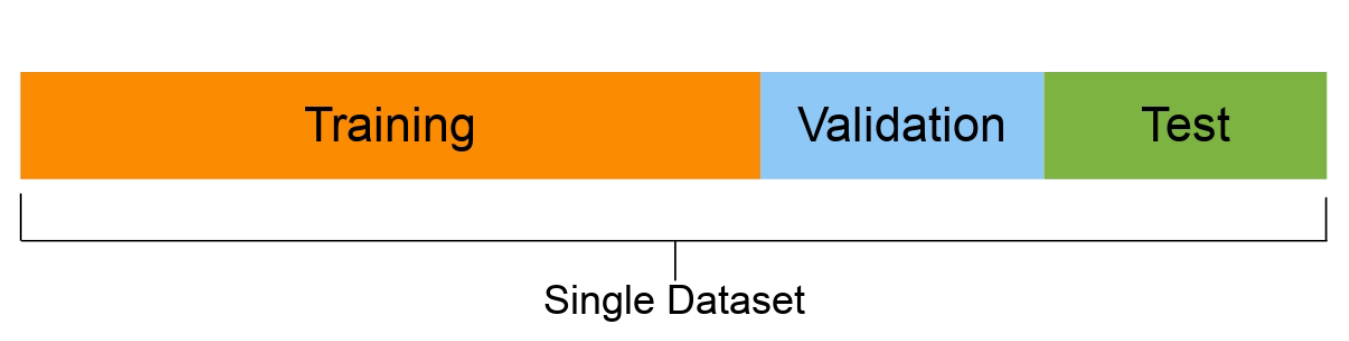
One split of data into training, validation and test sets may not be enough, due to randomness:

- The training and validation sets might be small and contain noise or outliers
- There might be some randomness in the training procedure (e.g. initialization)
- We need to fight the randomness by averaging the evaluation measure over multiple (training, validation) splits
  - The best hyperparameter values are chosen as those that have the best average performance over the $n$ validation sets.



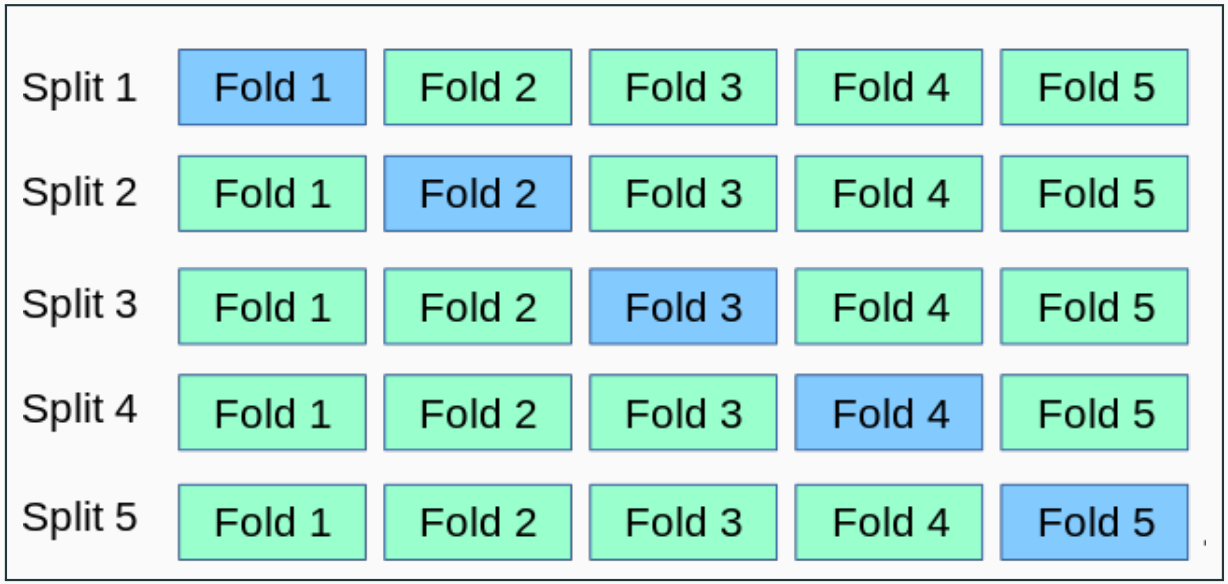
# Generating multiple data splits

- Let us first consider generating a number of training and validation set pairs, after first setting a side a separate test set
- Given a dataset $S$, we would like to generate $n$ random splits into training and validation set
- Two general approaches:
  - Repeated random splitting
  - $n$-fold cross-validation



# $n$-Fold Cross-Validation

- The dataset $S$ is split randomly into $n$ equal-sized parts (or folds)
- We keep one of the $n$ folds as the validation set (light blue in the Figure) and combine the remaining $n - 1$ folds to form the training set for the split




- $n = 5$ or $n = 10$ are typical numbers used in practice

# Leave-one-out cross-validation (LOO)

- Extreme case of cross-validation is leave-one-out (LOO) : given a dataset of $m$ examples, only one example is left out as the validation set and training uses the $m-1$ examples.
- This gives an unbiased estimate of the average generalization error over samples of size $m-1$ (Mohri, et al. 2018, Theorem 5.4.)
- However, it is comptationally demanding to compute if $m$ is large

# Nested cross-validation

- *n*-fold cross-validation gives us a well-founded way for model selection
- However, only using a single test set may result in unwanted variation
- Nested cross-validation solves this problem by using two cross-validation loops

# Nested cross-validation

The dataset is initially divided into $n$ outer folds ($n = 5$ in the figure)

- Outer loop uses 1 fold at a time as a test set, and the rest of the data is used in the inner fold
- Inner loop splits the remaining exampls into $k$ folds, 1 fold for validation, $k - 1$ for training ($k = 2$ in the figure)


The average performance over the $n$ test sets is computed as the final performance estimate

# Summary

- Model selection concerns the trade-off between model complexity and empirical error on training data
- Structural risk minimization gives strong guarantees for generalization error but is computationally expensive to use
- Regularization-based methods are based on continuous parametrization the complexity of the hypothesis classes
- Empirical model selection can be achieved by grid search on a validation dataset
- Various cross-validation schemes can be used to tackle the variance of the performance estimates