Cross-validation

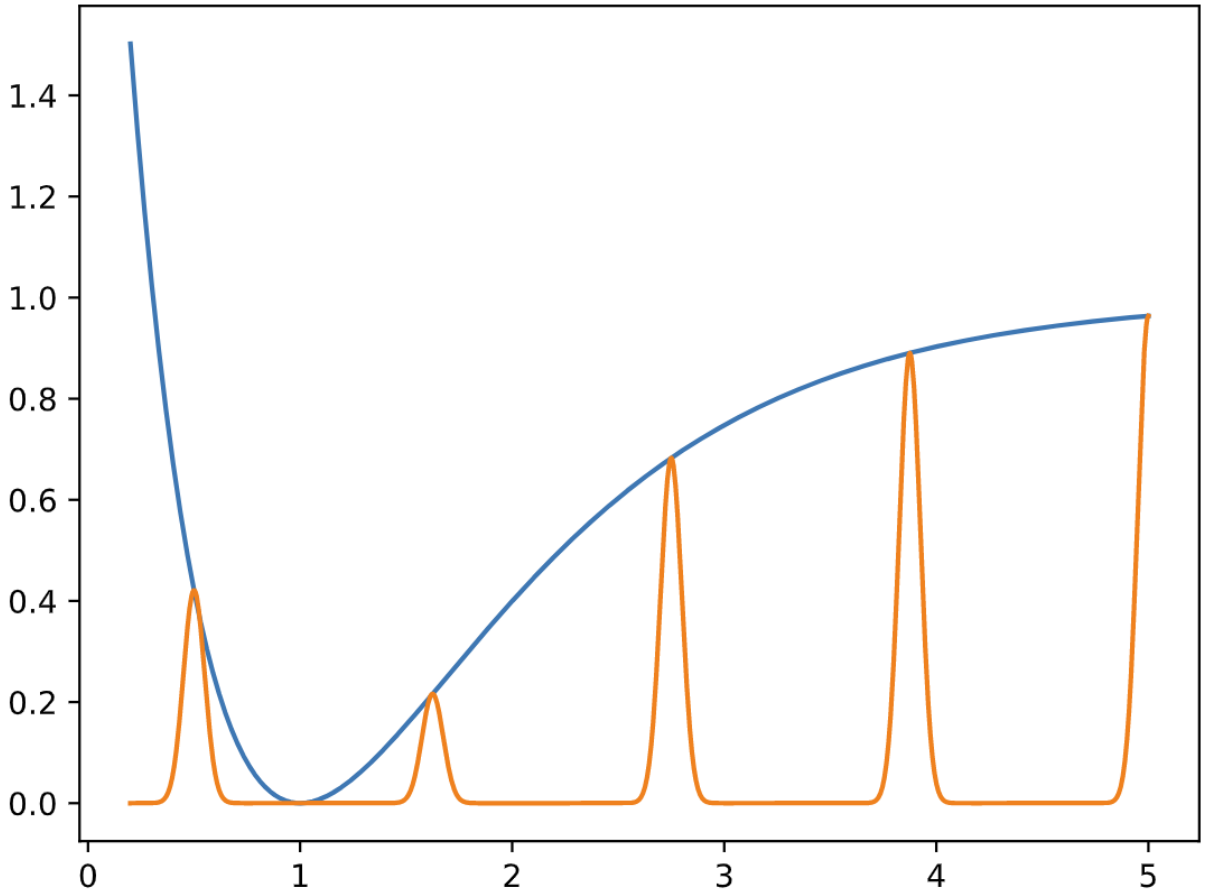
Generalisation error

Challenge

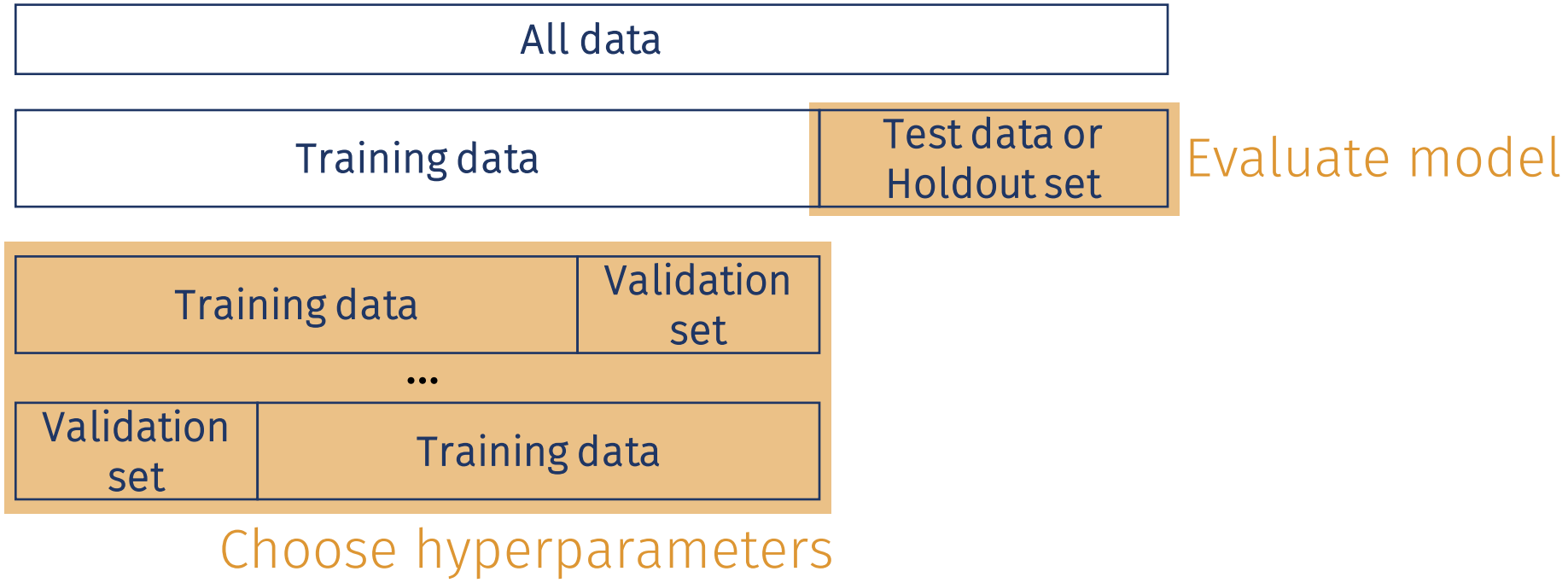
- Need quality assessment
  - Cannot use training data
- Hyperparameters
  - Require unseen data

Solution

- Cross-validation: estimate the expected error if applied to unseen data (generalisation error)



Terminology



Generalisation error

Training points are independent and identically distributed (i.i.d.):

- k-fold — most common: k=5 or 10
- Leave-p-out — most common: p=1
- Shuffle split / Monte Carlo

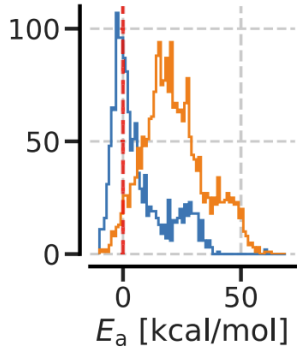
Otherwise:

- Data specific
- Often: stratification first, then one of the above
- Generally: think about what constitutes unseen data and where information could leak into the model

Note on i.i.d.

Is it valid?

- Labels often not identically distributed
- Reference data not independent
  - Converged?
  - Fast enough?
  - Method worked?
  - Generated using assumptions



GFvR, SN Heinen, M Bragato, Anatole von Lilienfeld, *Mach. Learn.: Sci. Technol.* 2020.

K-fold

Method

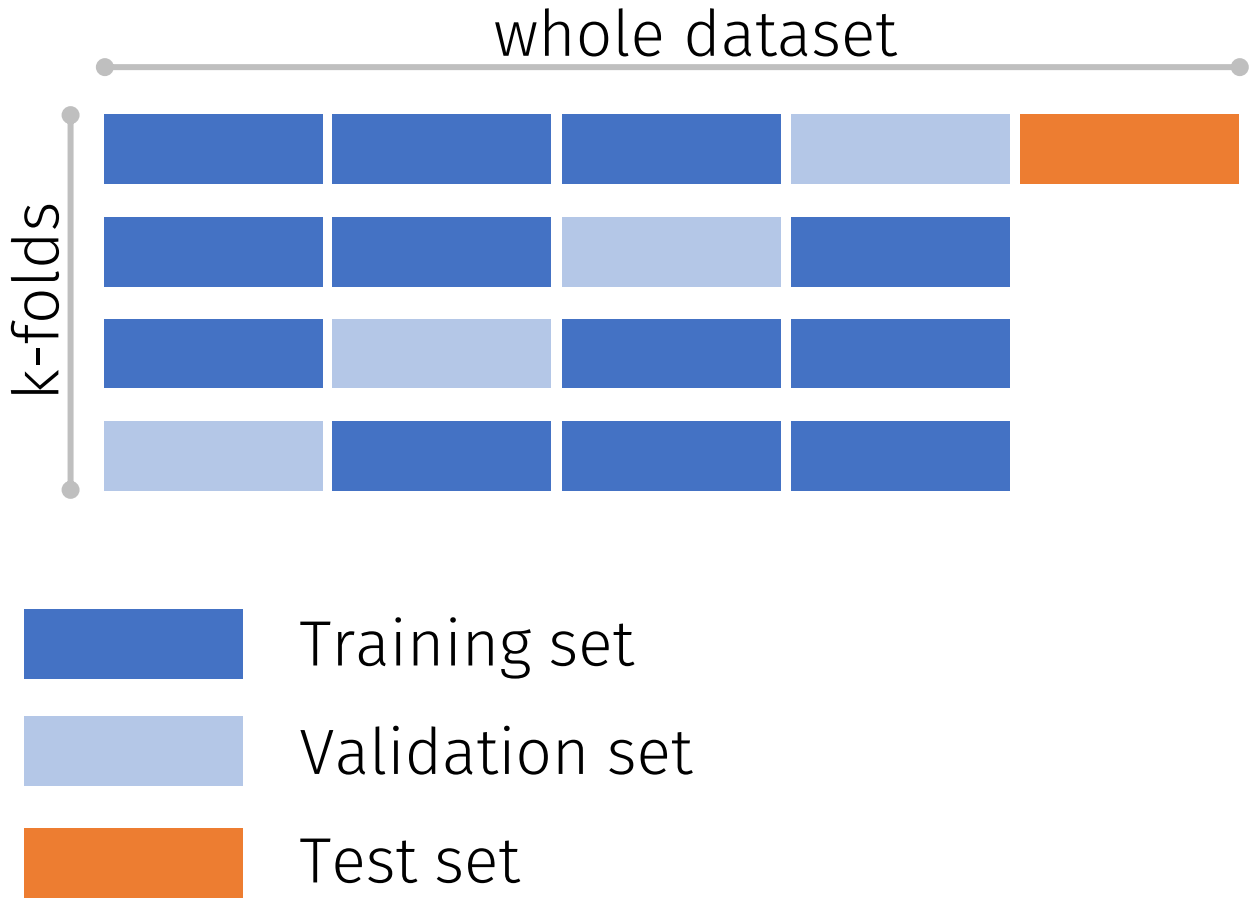
- Build n disjoint blocks
- Choose each block once as validation, train on rest
- Report metric on test set

Advantages

- Chooses all data points equally
- Converges quickly

Disadvantages

- Need to choose k
- Imbalanced blocks for most data sets
- Cannot reduce noise further



Leave-p-out

Method

- Use all but p entries for training, rest validation
- Do all combinations (expensive!)

Advantages

- Low noise, since exhaustive
- Chooses all data points equally

Disadvantages

- Quite expensive, quickly becomes infeasible

Shuffle split

Method

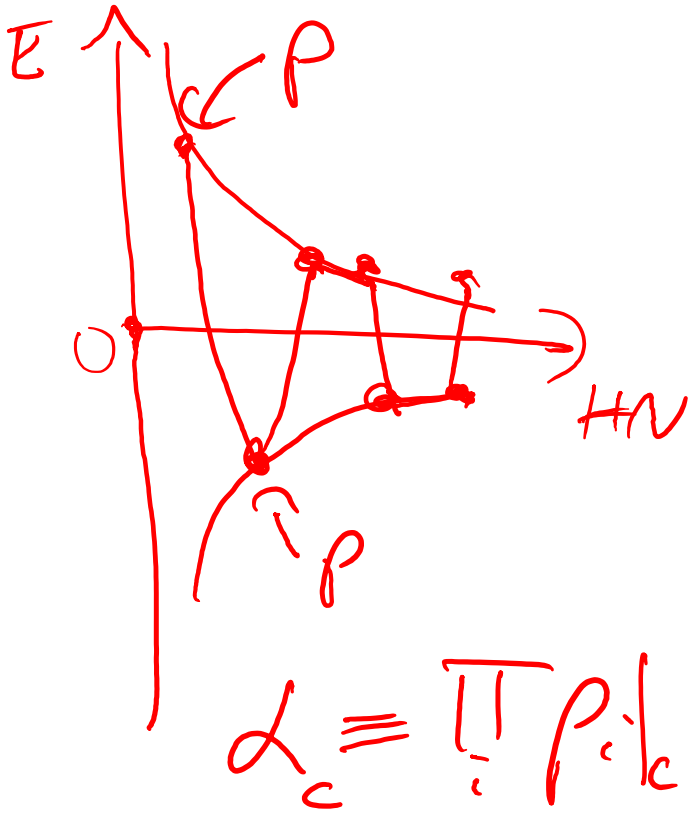
- Use all but p entries for training, rest validation
- Do **some** combinations (choose p entries randomly)

Advantages

- Converges to leave-p-out
- Chooses all data points equally

Disadvantages

- Needs quite few random selections to converge



$$\alpha_c \equiv \prod_i p_{i|c}$$

$$\operatorname{argmax}_c \alpha_c$$

Stratification

- Training data could be imbalanced: Detecting vans in the city
- Subsets become imbalanced despite random selection: Sock drawer problem

Solution: Stratification

- Choose any subset / split s.t. it is closely representative of the full data set
  - Mean label / distribution of labels
  - Prevalence of groups
  - Prevalence of features
- Independent of method of cross-validation / actual model

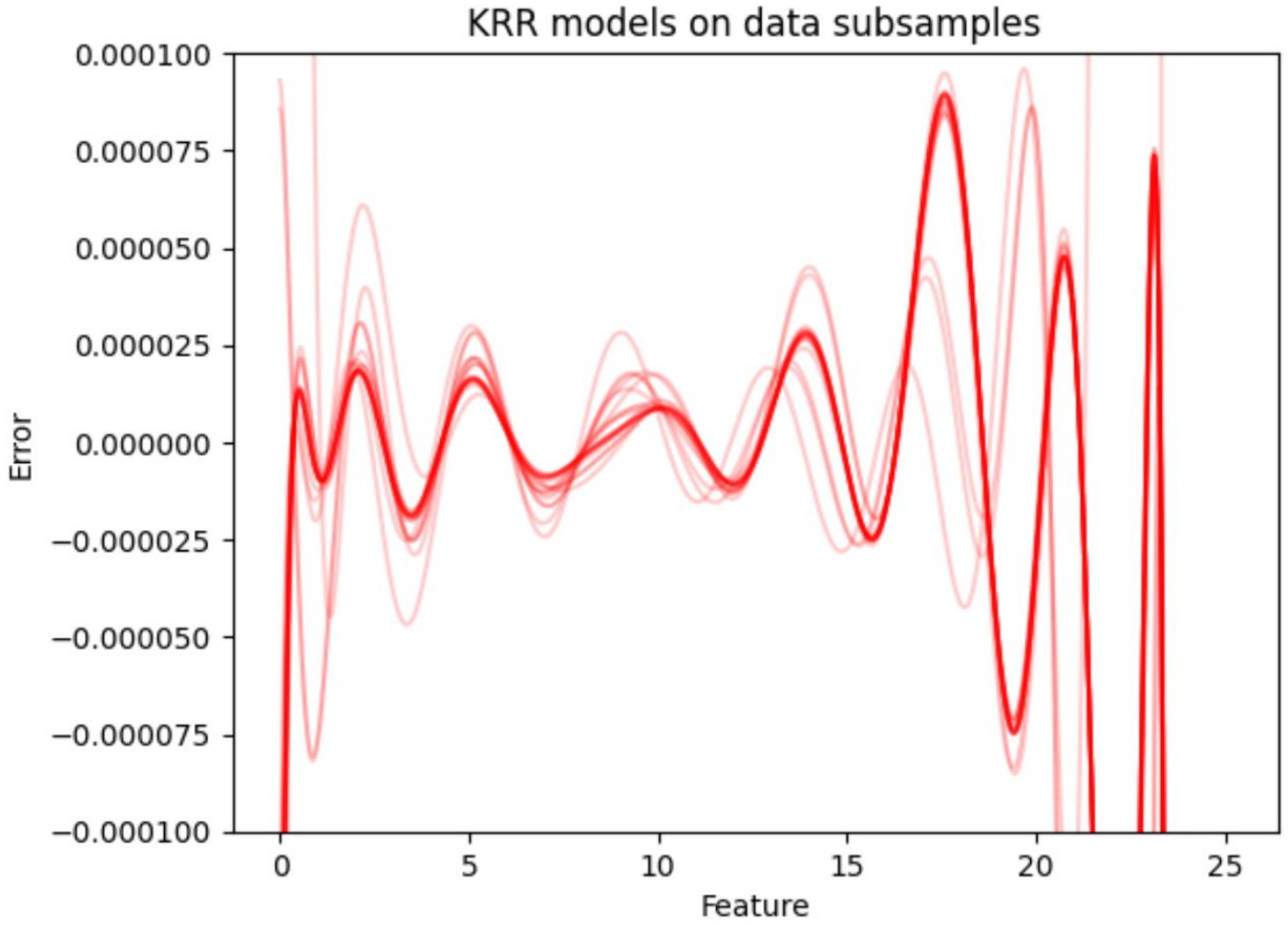
Note on split ratios

Too small:
Bad estimate of generalisation error

Too large:
Loosing training data

Solution: fully nesting k-fold
- Average k-fold over all choices for test data

Note on subsampling



Best practices

- Shuffle all data — Removes bias of ordering
- Stratify into 5 groups — Prevents overfitting; Helps if test set is small
- Repeat until converged:
  - For each of these groups:
    - One group as test set, rest as training — Test on all data points
    - Split train into stratified random sets — Estimate hyperparameters
  - Check whether hyperparameters and performance is converged

Summary Cross-validation

- Key target is reliable estimation of generalization error
- May require stratification to avoid bias
- Different methods differ in cost, simplicity, and convergence
- Relevant representatives: Leave-p-out, k-fold, shuffle split
- Common split ratio 80%/20% (no hard justification except experience)