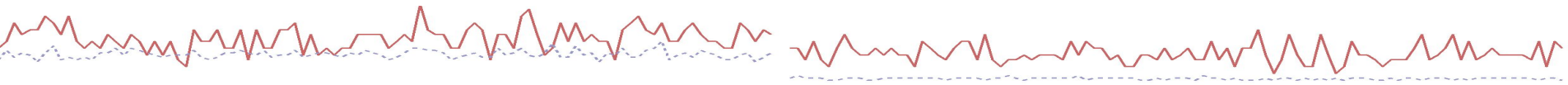


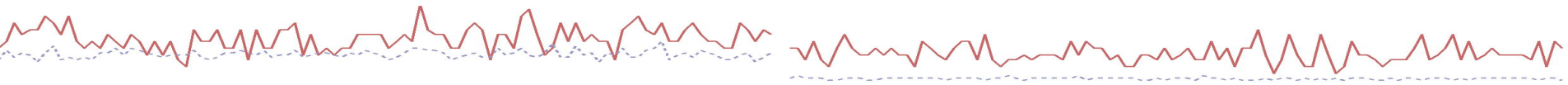
Resampling methods

Filippo Biscarini (CNR, Milan, Italy)

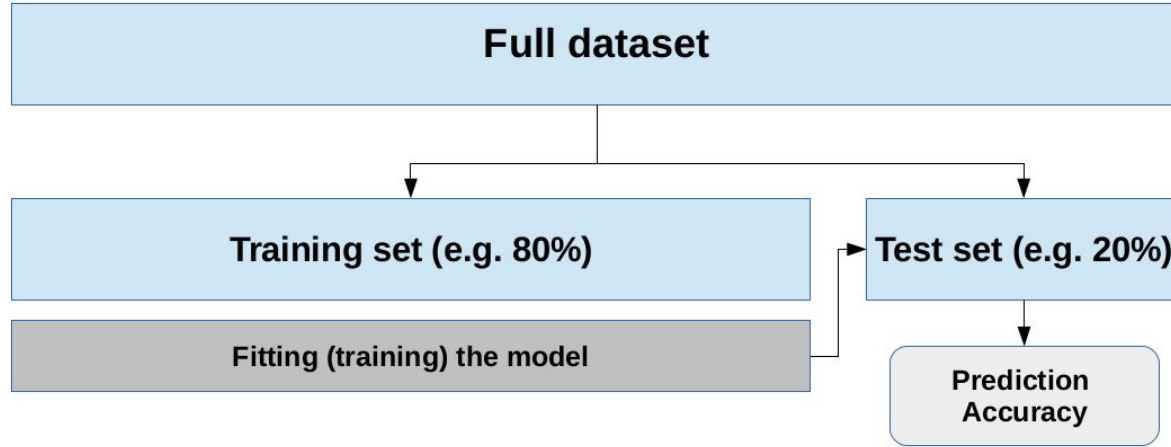
filippo.biscarini@cnr.it



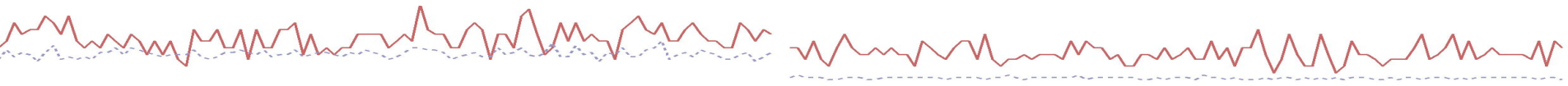
Training and test sets



Sampling the training and the test sets



- To correctly assess the performance of a predictive model we measure it on independent data → test data
- However we can sample many different training and test sets!



Resampling the data

- Resampling involves **repeatedly sampling** the training and test datasets: each time, the model is **refitted** in the training set and **evaluated** in the test set
- You can e.g. estimate the **variability** of a predictive model or the effect of modifying the model or method:
 - **Model assessment**
 - **Model selection**



Resampling the data

- Several resampling methods exist
- We will examine two such methods:
 1. **validation set approach**
 2. **cross-validation**

[validation set ~ test set]



The validation set approach

training set

validation set

- We split the data in **two random subsets**: training and validation (test)
- 10%/90%, 20%/80%, 30%/70% etc.
- This is what we already did!
- Repeat this n times and you get **robust estimates** of the model performance



The validation set approach

training set

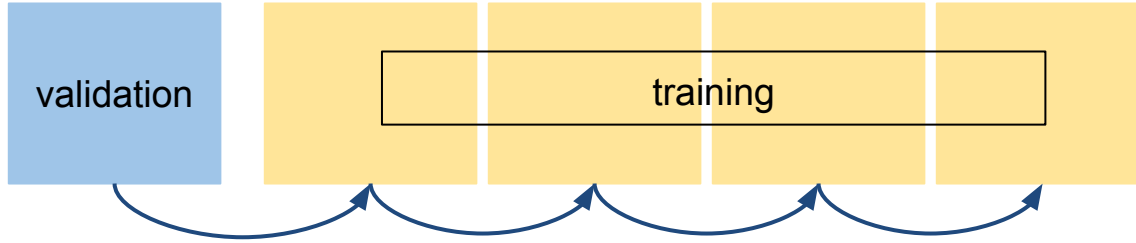
validation set

Drawbacks:

- **highly variable** (depending on the random partition of the data)
- only a subset of the data is used to train (fit) the model → **potentially underestimate model performance**



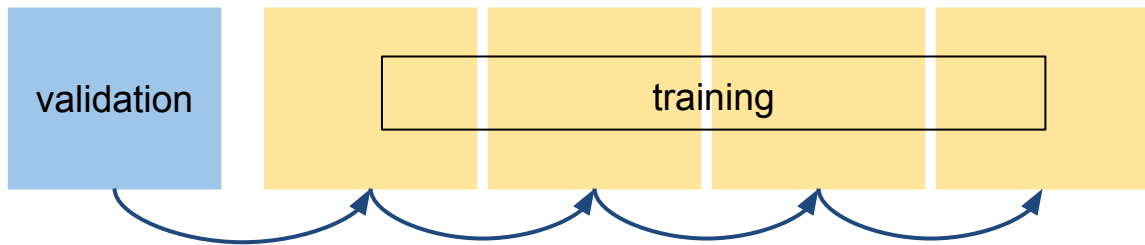
k-fold cross-validation



- k random partitions of equal size
- each partition in turn is used for validation, the rest for training
- k estimates of model performance



k-fold cross-validation



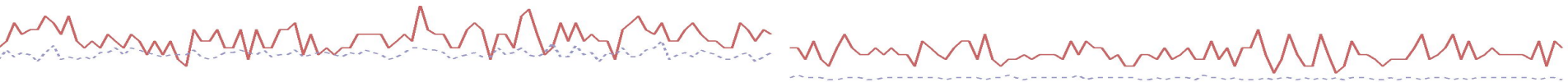
- k random partitions of equal size
- each partition in turn is used for validation, the rest for training

- **k estimates** of model performance $\longrightarrow CV_{(k)} = \frac{1}{k} \sum_{i=1}^k MSE_i$



k-fold cross-validation

- Lower variability than the validation set approach
- cross-validation works well in **finding the minimum point** in the estimated test MSE curve → model selection
- In cross-validation each observation/record is used both to train the model and to test it → more data are used here than in the validation set approach → lower bias
- cross-validation is therefore expected to have **both lower variance** and **lower bias** than the validation set approach → more accurate estimate of model performance
- typical values for k are **$k=5$** and **$k=10$**



k-fold cross-validation

validation-set approach

k-fold cross-validation

Exercise 3.2

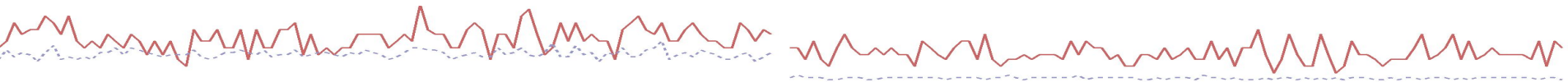
→ 3.training_testing.ipynb



Cross-validation: right and wrong

- Consider a **regression problem**: 100 samples, 50,000 features (variables, e.g. 'omics data):
 1. Find the 50 features with the **strongest correlation** with the response variable
 2. Apply a **predictor** (e.g. multiple linear regression) with only these 50 **selected features**

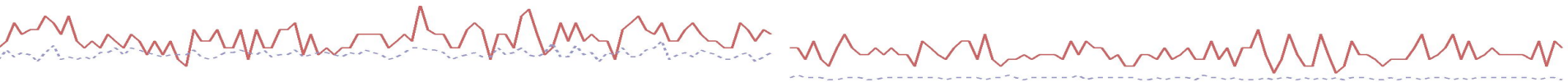
Estimate the **prediction error**: can we apply cross-validation in step 2?



Cross-validation: right and wrong

- Consider a **regression problem**: 100 samples, 50,000 features (variables, e.g. 'omics data):
 1. Find the 50 features with the **strongest correlation** with the **response variable**
 2. Apply a **predictor** (e.g. multiple linear regression) with only these 50 **selected features**

Estimate the **prediction error**: can we apply cross-validation in step 2? → **NO!**



Cross-validation: right and wrong

Estimate the **prediction error**: can we apply cross-validation in step 2? → **NO!**

- in Step 1, the **model has already used the response** of the training data
- Features have been “**cherry picked**” based on the data: this is already **training**, and the correlation with the response may be a result of the specific configuration of this dataset (a “quirk” in the data)



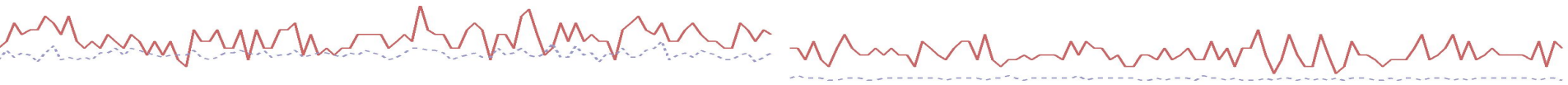
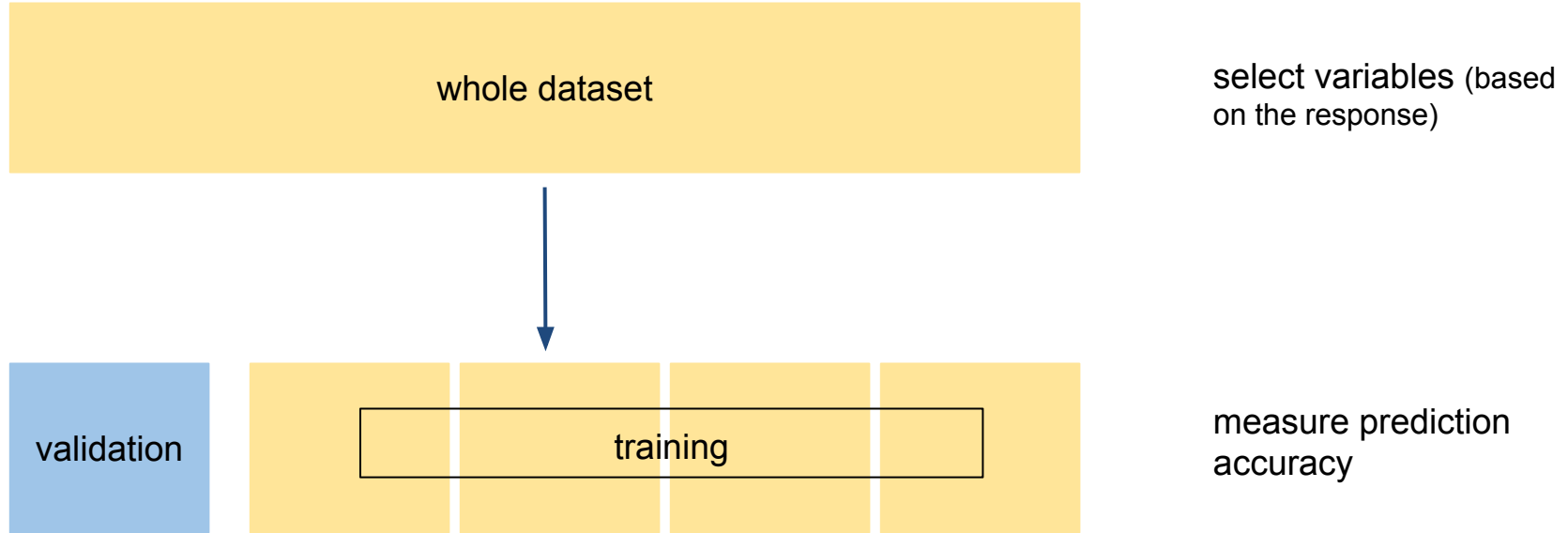
Cross-validation: right and wrong

Estimate the **prediction error**: can we apply cross-validation in step 2? → **NO!**

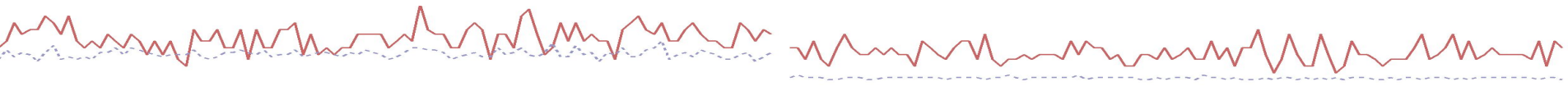
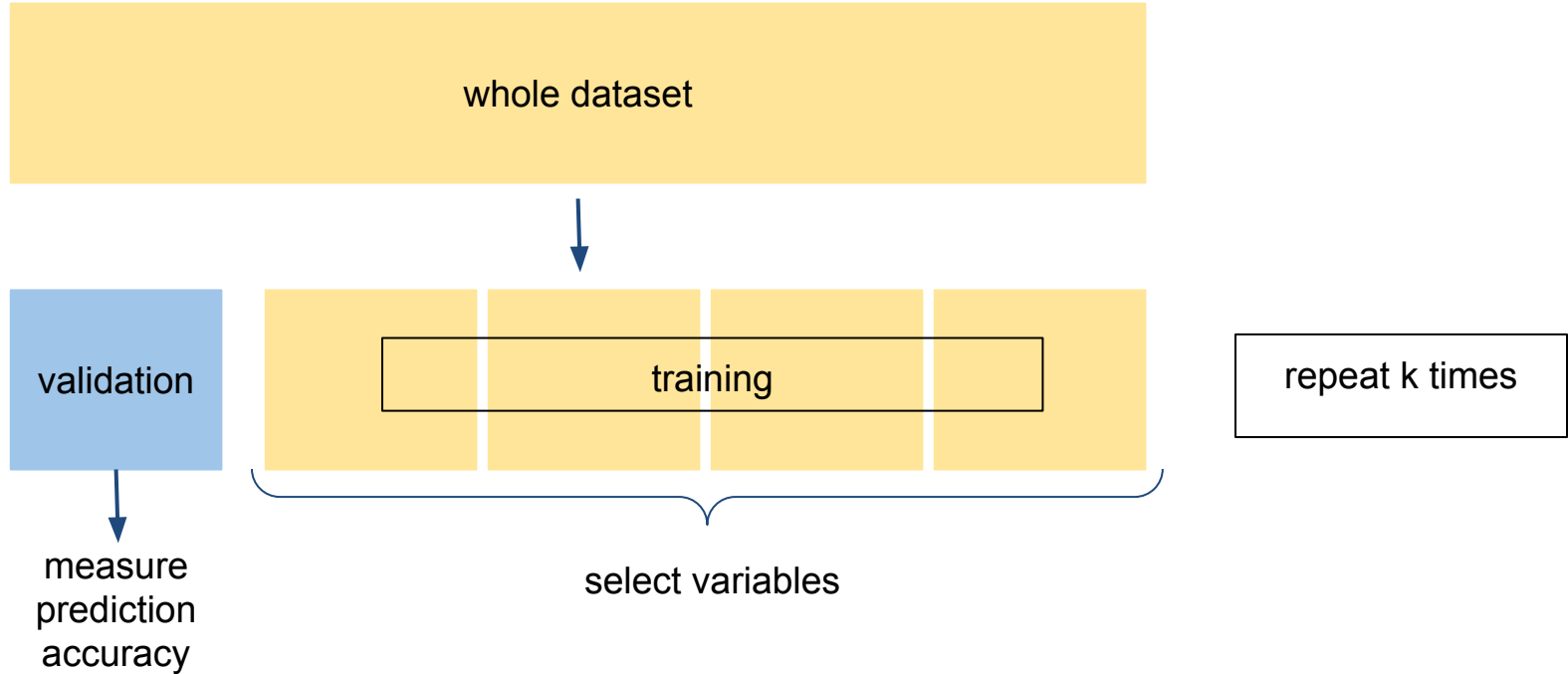
- **Wrong!** → select variables on the whole dataset, then apply cross-validation
- **Right!** → first split the data in training and test sets, then select variables (part of training)



Cross-validation: **wrong way**



Cross-validation: **right way**



Cross-validation: right way

