Cross-validation and performance measures

How to avoid prediction blunders

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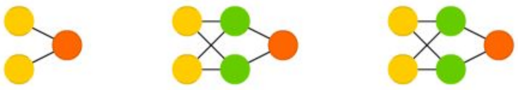
Overfitting

What is overfitting?

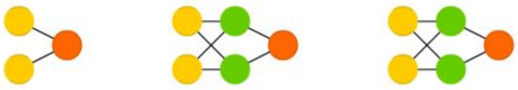
You may fit a deep learning model to your data and then measure the “accuracy”of predictions on the same data: **would this be correct?**



What is overfitting?

You may fit a deep learning model to your data and then measure the “accuracy”of predictions on the same data: **would this be correct?**

- short answer: **NO!**
- main reason: **overfitting**



What is overfitting?

Overfitting:

Fitting too well the data: R^2 too large (≃1)

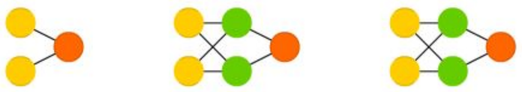
What is overfitting?

Overfitting:

Fitting too well the data: R^2 too large ($\simeq 1$)

overfitting happens with:

- using the same data to fit the model and to make predictions
- overparameterization of the model (e.g. too many effects)
- flexible methods (e.g. polynomial functions, splines, … and **deep learning!**)



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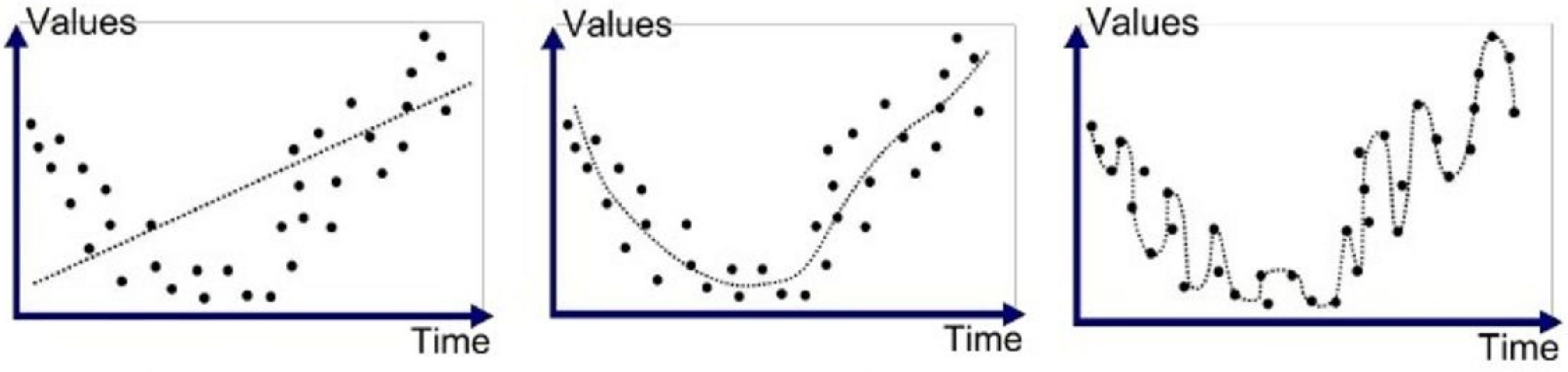


Underfitted | Good Fit/Robust | Overfitted

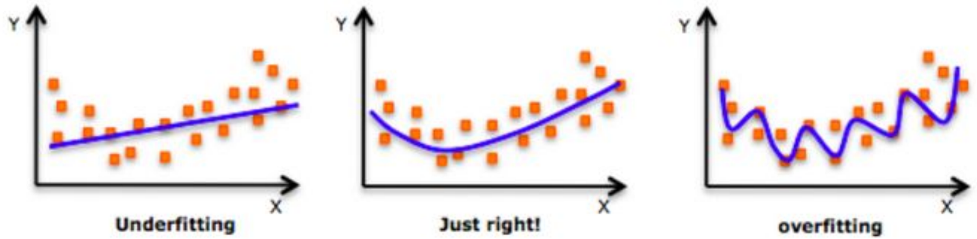
Linear regression

Polynomial (?)

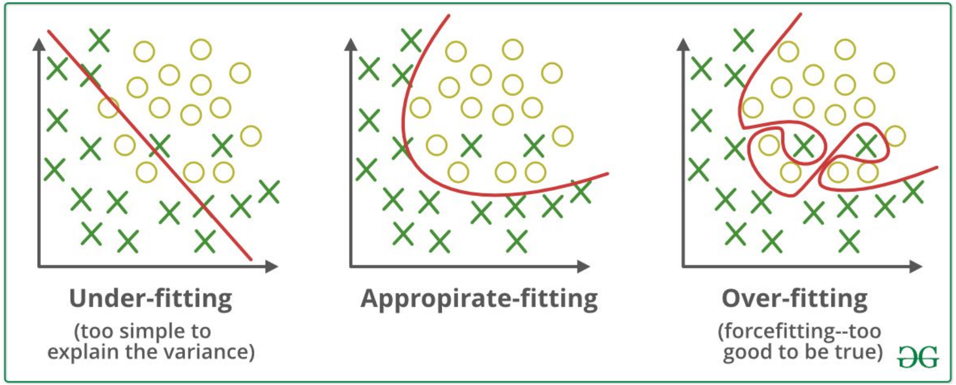
Highly non-linear model

What is overfitting?

regression



classification



Linear regression

Polynomial (?)

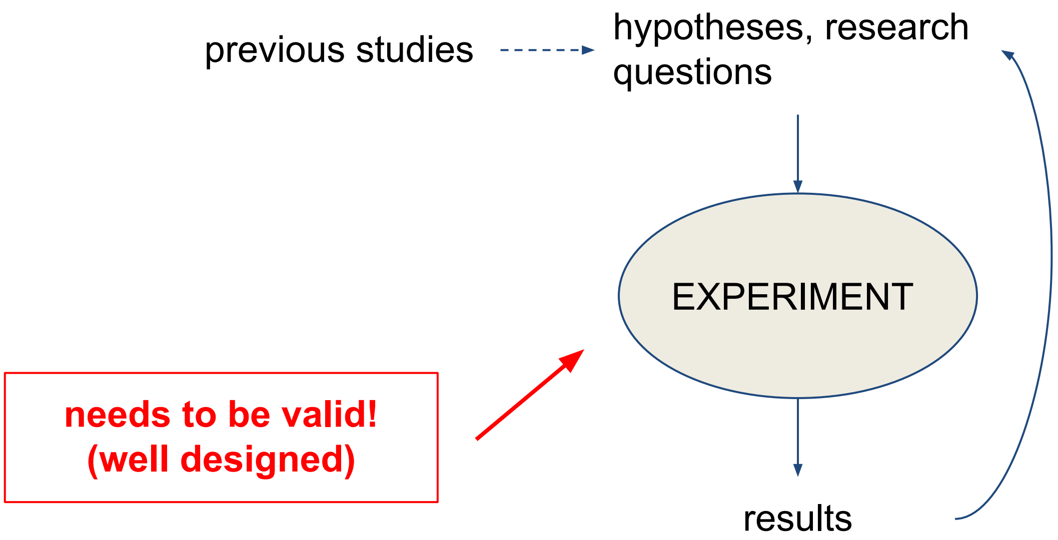
Highly non-linear model

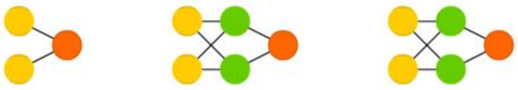
Training and validation sets

A tool to control overfitting

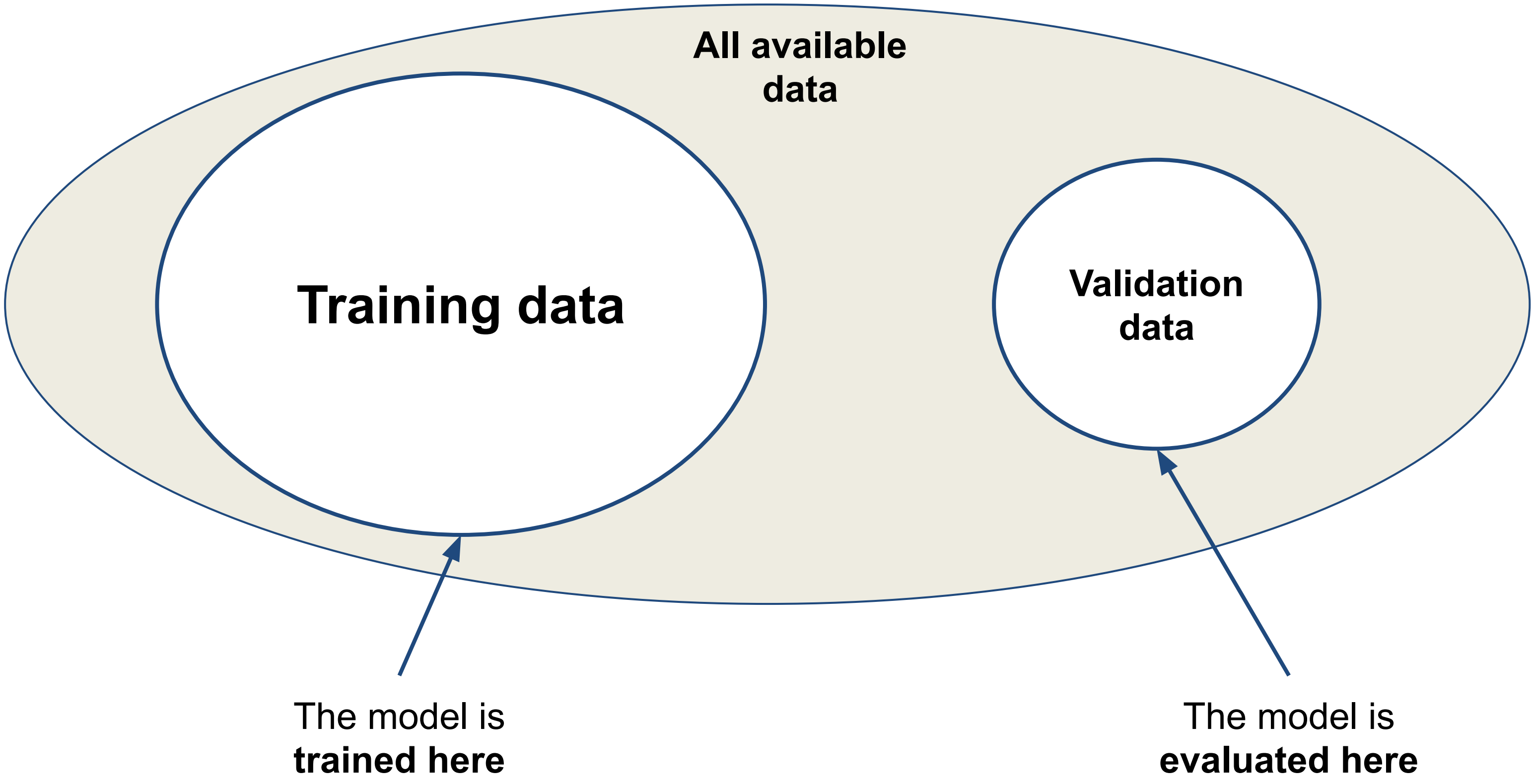
Training and validation sets

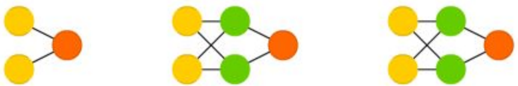
“The test of all knowledge is experiment”





Training and validation sets

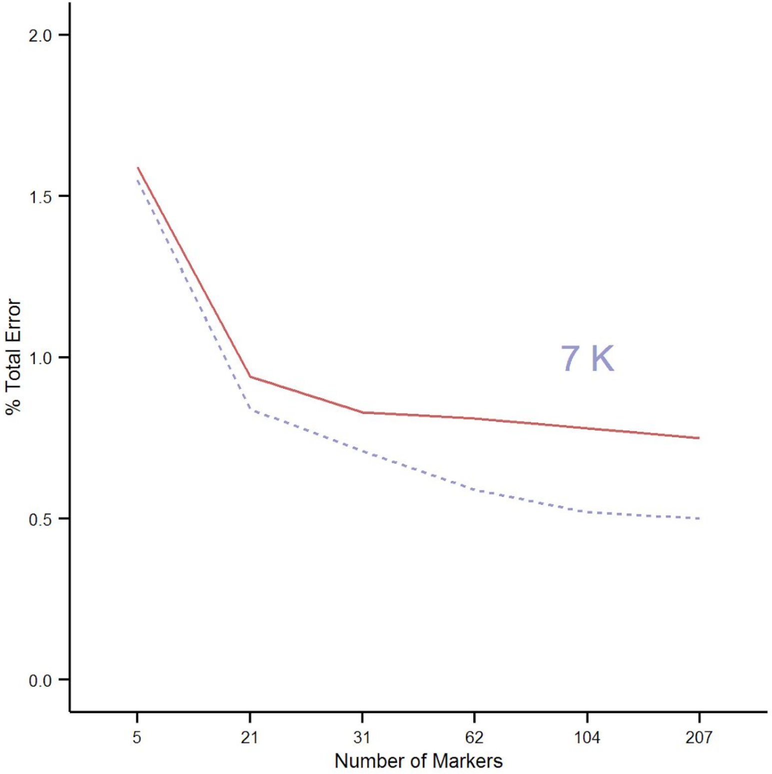


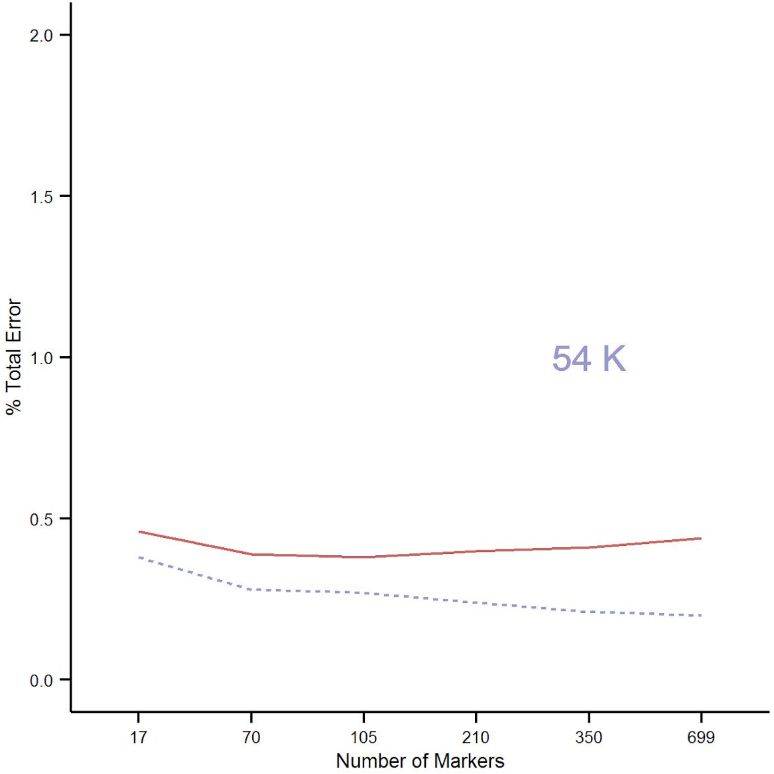


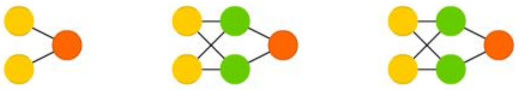
Training and validation sets

- accuracy (model performance) on the training set is “optimistic” (biased upward ← *overfitting*)
- a better estimate of model performance can be obtained from independent data
- usually we are interested in the predictive performance on new data
- accuracy in the validation set is usually lower than in the training set

An example from genomics







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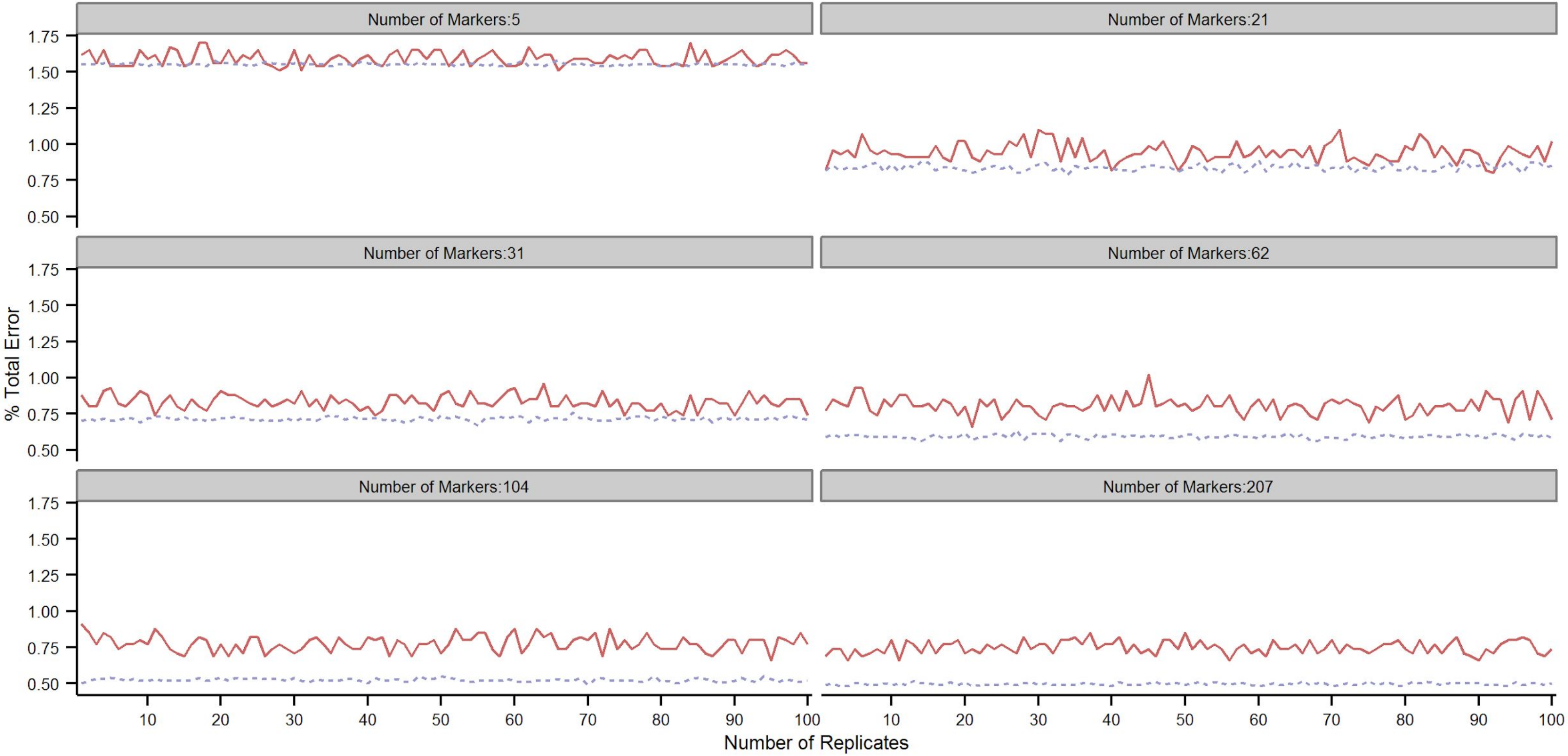


And the test set?

- “Test” and “Validation” are often considered and used as synonyms
  - But they are not! (strictly speaking)
- A test set would be a third set
  - Completely new data
  - Used only once when you finished everything else
  - An estimate of performances in real world
- We (try to) stick to Keras convention, and never talk about test sets :)

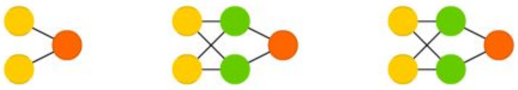
Prediction error

Prediction error

$$E\left(y-\hat{f}(x)\right) = Var\left(\hat{f}(x)\right) + \left[\mathrm{Bias}\left(\hat{f}(x)\right)\right]^2 + Var(\epsilon)$$

variance

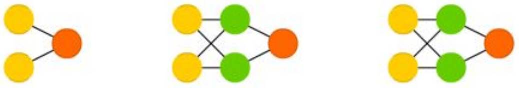
bias^2



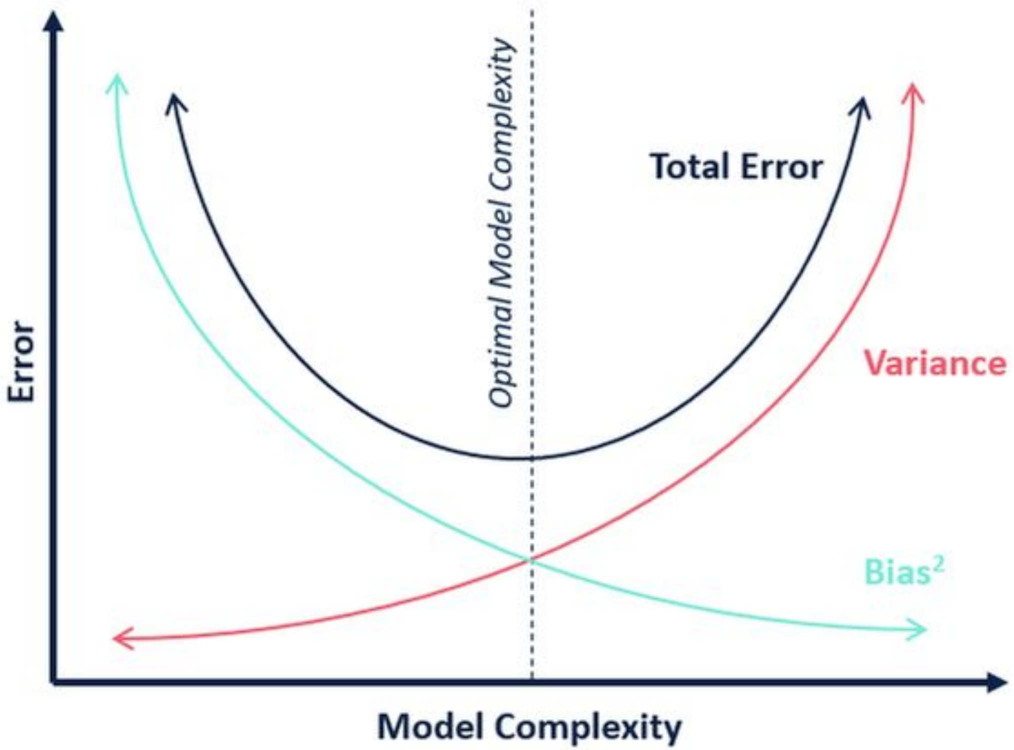
Prediction error

$$E\left(y-\hat{f}\left(x\right)\right)=Var\left(\hat{f}\left(x\right)\right)+\left[\text{Bias}\left(\hat{f}\left(x\right)\right)\right]^2+Var(\epsilon)$$

- **variance** refers to the change of the predictor if estimated using different training data
- **bias** refers to the approximation of a real problem by a simpler model

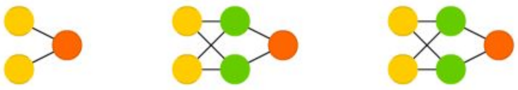


Bias-variance trade-off



- models with low bias and high variance (e.g. KNN with k=1)
- models with high bias and low variance (e.g. horizontal line crossing the data)
- → find models/methods with both low variance and low bias

Source: https://ai-pool.com/a/s/bias-variance-tradeoff-in-machine-learning



Bias-variance trade-off

Methods

low variance and high bias

- Linear regression
- Logistic regression
- Penalised regression
- SVM (linear kernel)
- Naive Bayes
- etc.

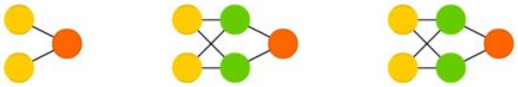
high variance and low bias

- Random Forest
- Boosting
- Polynomial regression
- Regression splines
- GAM
- **Deep learning**
- KNN
- SVM (Rbf)
- Loess/Lowess (local regression)
- etc.

Bias-variance trade-off

Related trade-offs

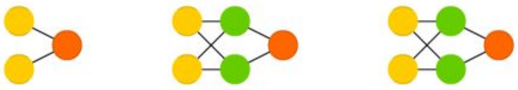
1. Prediction accuracy vs model interpretability:
   - e.g. linear regression is easy to interpret, splines are not
2. Parsimony vs "black-box":
   - e.g. variable selection, all-variables models (e.g. RF), Occam's razor



Bias-variance trade-off

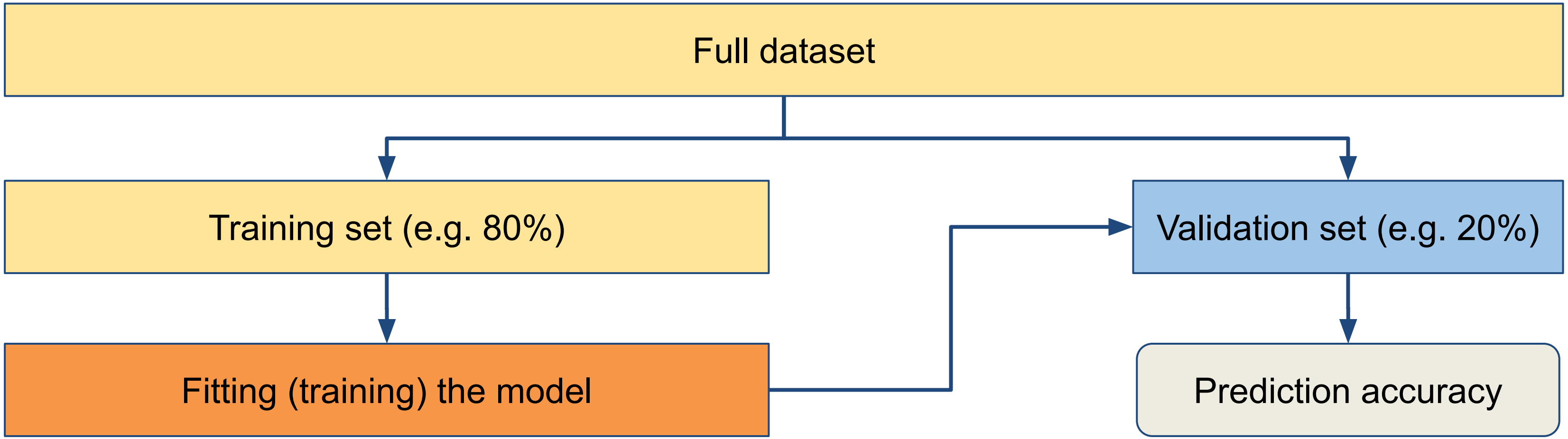
Important for:

1. **Correctly estimating the performance of a predictive machine**
2. Correctly estimating model parameters
3. Selecting between models

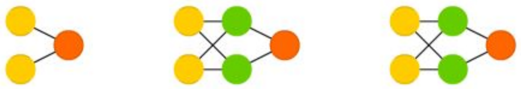


Resampling methods

Sampling the training and the validation sets

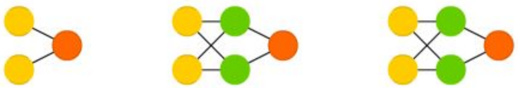


- To correctly assess the performance of a predictive model we measure it on independent data → validation data
- However we can sample many different training and test sets!



Resampling the data

- Resampling involves **repeatedly sampling** the training and validation datasets: each time, the model is **refitted** in the training set and **evaluated** in the validation 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**

The validation set approach

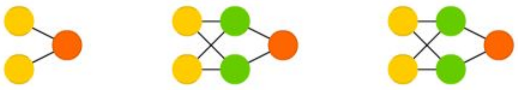
- We split the data in **two random subsets**: training and validation (test)
- 10%/90%, 20%/80%, 30%/70% etc.
- This is what we already did!
- Repeat this *n times* and you get **robust estimates** of the model performance

The validation set approach

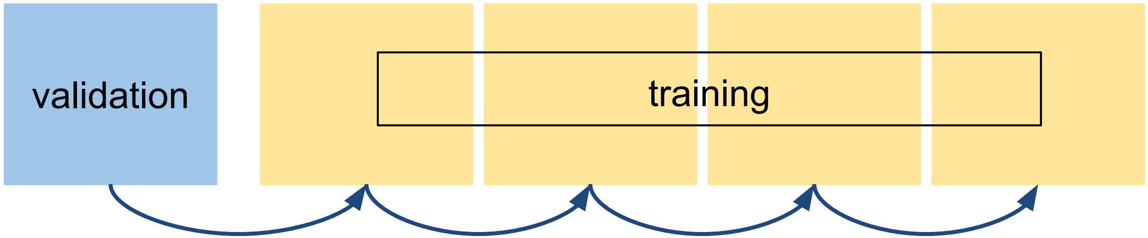
training set | **validation set**

Drawbacks:

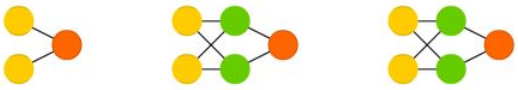
- **highly variable** (depending on the random partition of the data)
- only a subset of the data is used to train (fit) the model → **potentially underestimate model performance**



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



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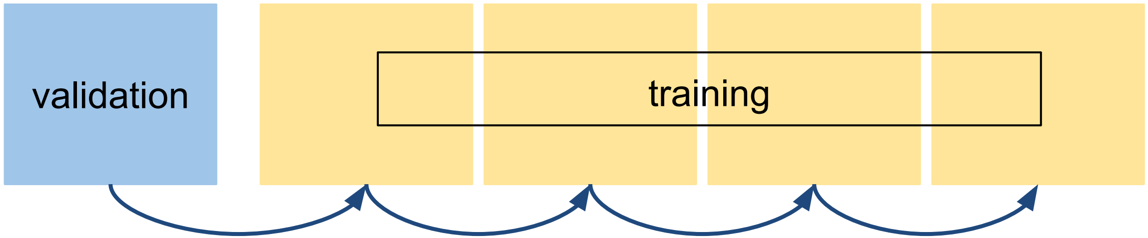

- *k* random partitions of equal size
- each partition in turn is used for validation, the rest for training
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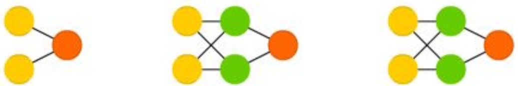
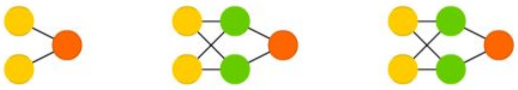
$$CV_{(k)} = \frac{1}{k}\sum_{i=1}^{k} MSE_i$$



k-fold cross-validation

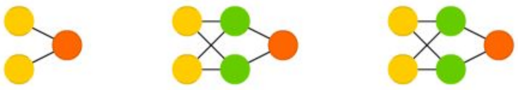
- Lower variability than the validation set approach
- cross-validation works well in **finding the minimum point** in the estimated test MSE curve → model selection
- In cross-validation each observation/record is used both to train the model and to test it → more data are used here than in the validation 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 = n → LOOCV)



Cross-validation: right and wrong

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

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



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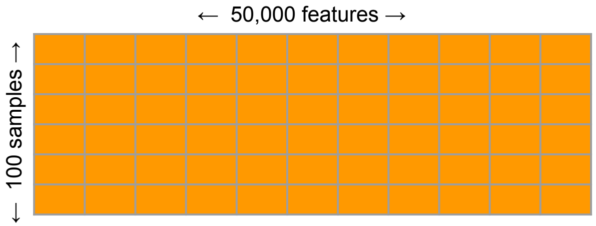
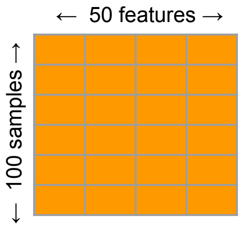
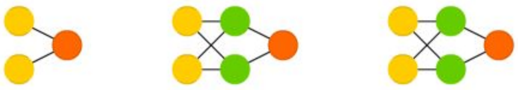


- Step 1: Find the 50 features with the **strongest correlation** with the response variable (y)



Step 2: Do the train/validation split (or k-fold CV) and build a **predictive model** (e.g. multiple linear regression) with only these 50 **selected features**

Is this the **right way to apply cross-validation** and estimate the prediction error?



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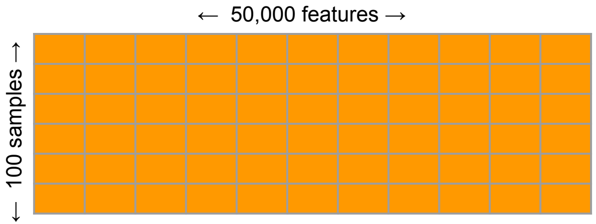

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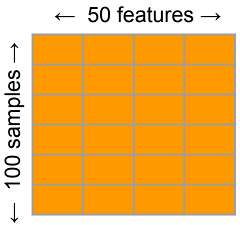


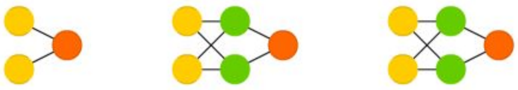
Step 2: Do the train/validation split (or k-fold CV) and build a **predictive model** (e.g. multiple linear regression) with only these 50 **selected features**

Is this the **right way to apply cross-validation** and estimate the prediction error? → NO!

Cross-validation: right and wrong

Can we apply cross-validation only in step 2? → **NO!**

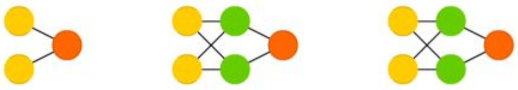
- in Step 1, the **model has already used the response** of the training data
- Features have been **"cherry picked"** based on the data: this is already **training**, and the correlation with the response may be a result of the specific configuration of this dataset (a "quirk" in the data)



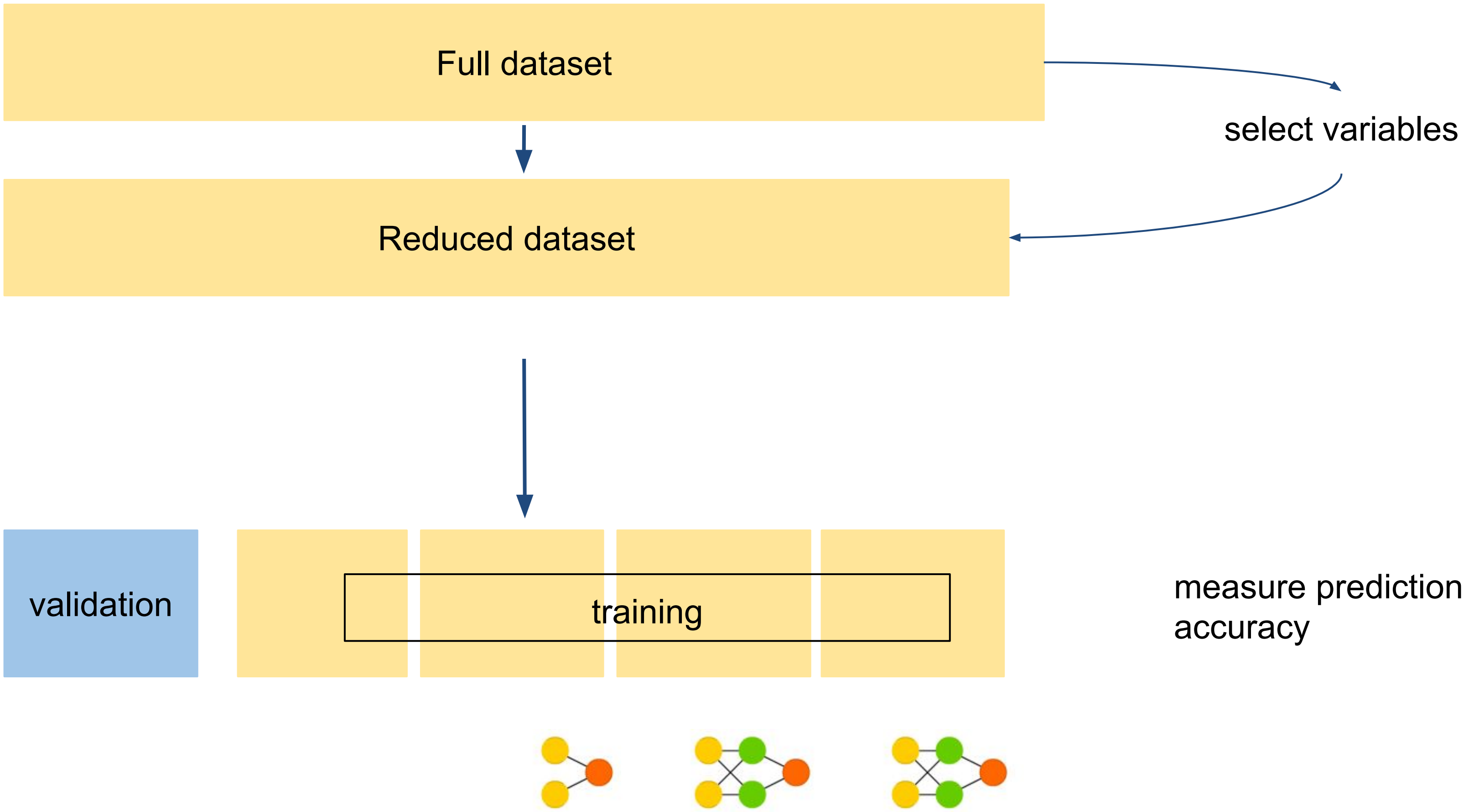
Cross-validation: right and wrong

Can we apply cross-validation only in step 2? → **NO!**

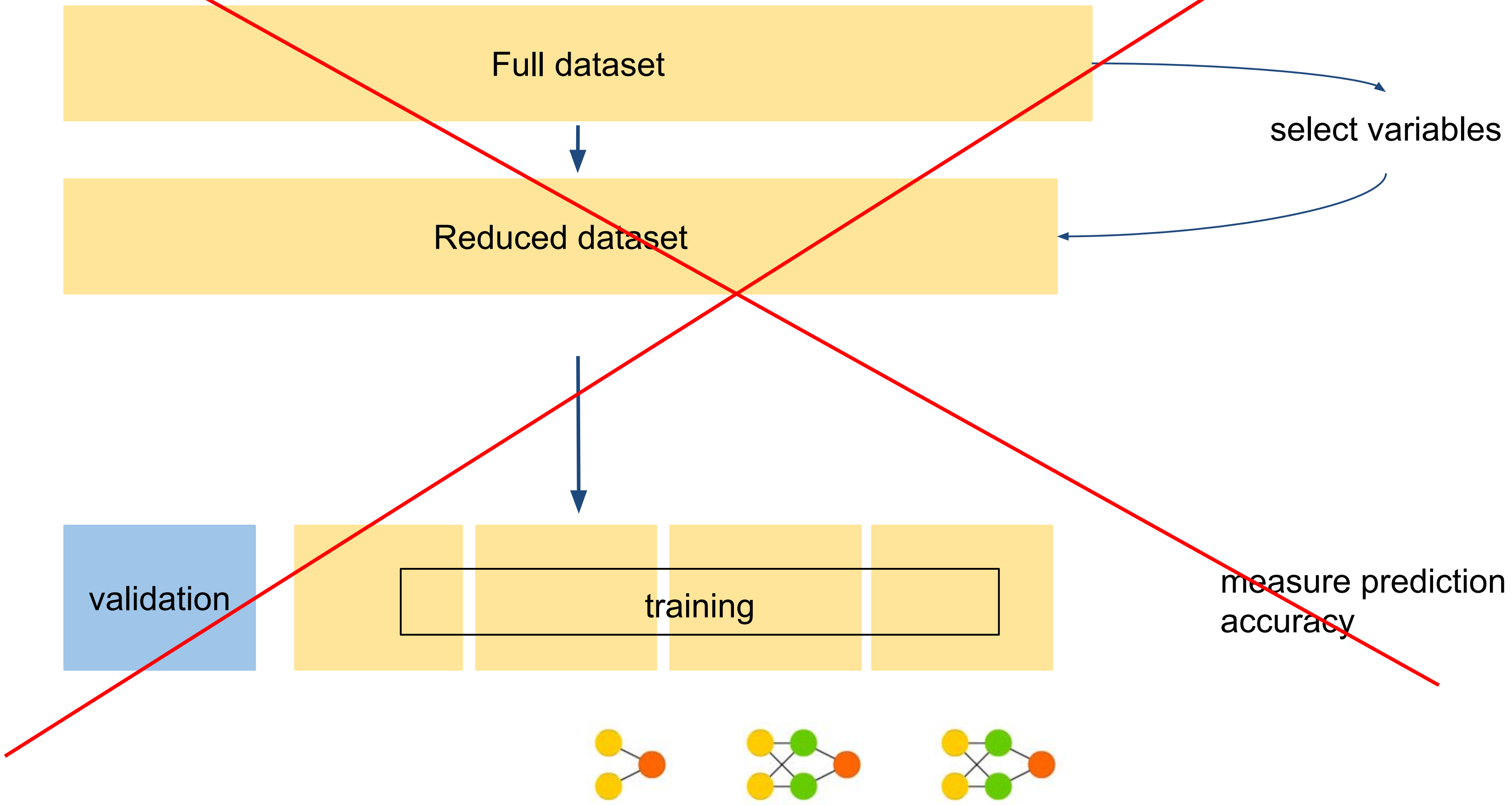
- **Wrong!** → select variables on the whole dataset, then apply cross-validation
- **Right!** → first split the data in training and test sets, then select variables (part of training)



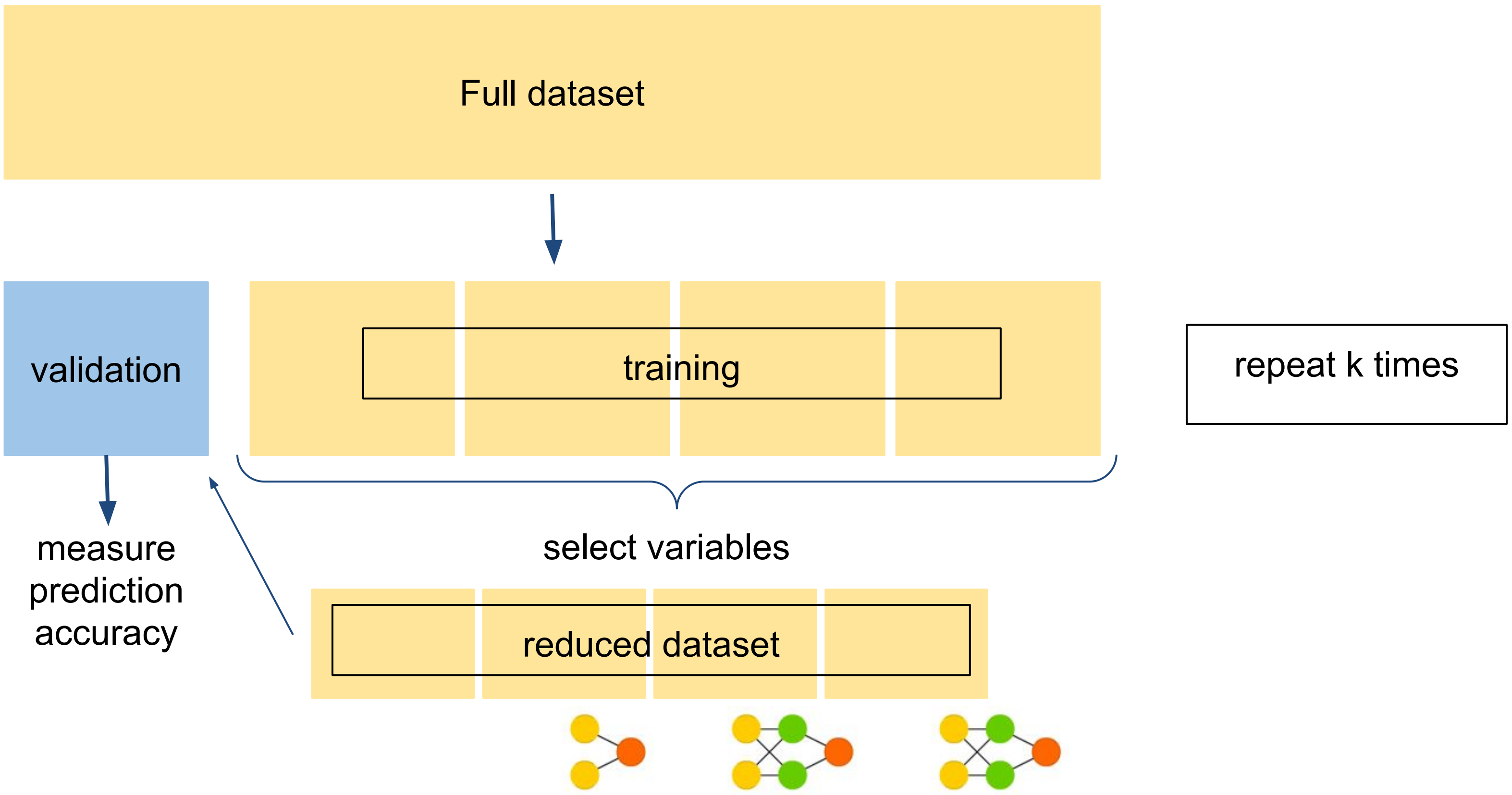
Cross-validation: wrong way



Cross-validation: **wrong way**



Cross-validation: right way



Cross-validation: right way

Full dataset

validation

training

repeat k times

measure
prediction
accuracy

select variables

You can do whatever you want in the training data, but only after you hold out the test/validation set!