Validation and Optimization of Machine Learning Models Regression

ESCAPE
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Topics

1. Introduction
2. Figures of Merit
3. Verification Schemes
4. Resampling Techniques
5. Model Stability
6. Sample Size Planning
7. Validation
8. Data-driven Model Optimization and Hyperparameter Tuning
9. Regression

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Validation and Verification

C. Beleites

Verification: Making sure/measuring/showing that the model meets the specifications.

Validation: Making sure that the model meets the application needs.

- Chemometric model validation
  ⇝ typically verification rather than validation is done.
- Characterize model by measuring its predictive performance

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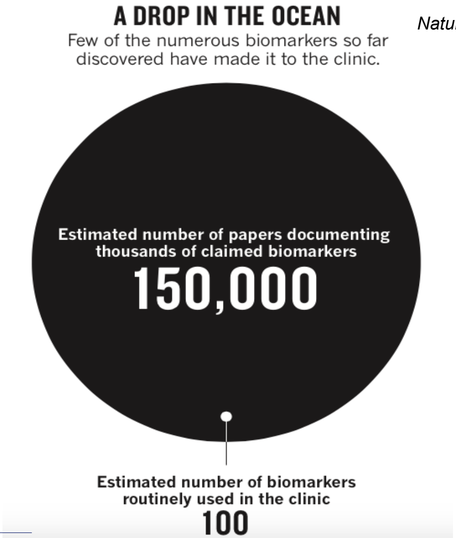
Reproducibility!?

Nature **469**, 156-157



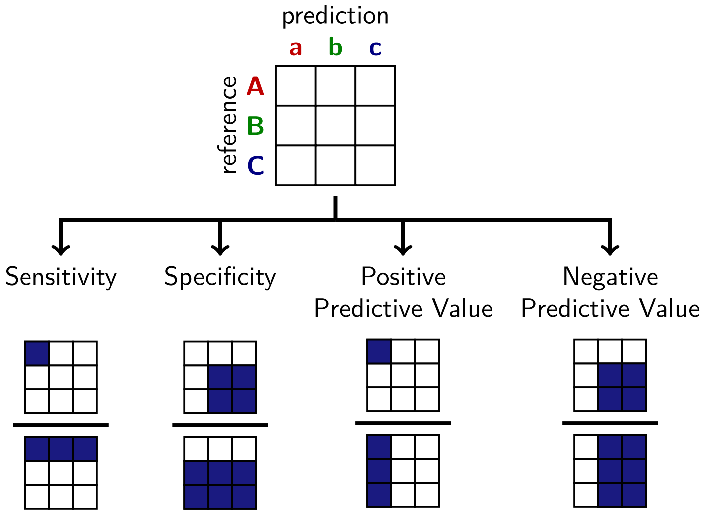
Poste: Bring on the biomarkers. Nature, 2011, 469, 156-157.

Recipe: Verification/Validation/Testing

Ingredients

- Ready-to-use model
  treated as black box: *case* $\mapsto$ *prediction*
- Figures of merit (performance measure)
  Overall Accuracy, Sensitivity, Specificity, Predictive Values, MSE, RMSE, R^2, ...
- Validation *scheme*: *How to get test cases?*
  ~~Autoprediction~~, Resampling, Test Set, Validation study

Figures of Merit: Proportions



Proportion Questions

Sensitivity = Recall: of all truly class *A* cases, which fraction is correctly recognized as class *A*?

Specificity: of all cases truly not belonging to class *A*, which fraction is correctly recognized as not belonging to class *A*?

Positive Predictive Value = Precision: of all cases predicted to belong to class *A*, which fraction does truly belong to class *A*?

Negative Predictive Value: of all cases predicted not to belong to class *A*, which fraction does truly not belong to class *A*?

accuracy: correct proportion among all predicted cases

error rate: misclassified proportion among all predicted cases

κ: chance-corrected accuracy, inter-observer agreement

Proportions: Characteristics

✔ well-known, widely used

✘ often misunderstood:

- sensitivity & specificity
  - ✔ easy to measure: test *n* cases of each class, record results
  - ✘ low relevance for application
- predictive values (positive/negative)
  - ✔ high relevance for application
  - ✘ difficult to measure: need to know relative class fequencies under application conditions
    weight rows of confusion matrix accordingly
- figures of merit spanning rows of confusion matrix
  - ✘ correct for relative class fequencies under application conditions

More figures of merit

- chance-corrected: κ
  - ✔ rescaling possible for other figures of merit
  - ✔ alternative: report chance agreement (or naive model performance) together with figure of merit

- Information gain
  - **positive likelihood ratio:** $LR_A^+ = \frac{Sens_A}{1 - Spez_A}$
    How much do the odds to belong to class A increase when a case is predicted to belong to class A?
  - **negative likelihood ratio:** $LR_A^- = \frac{Spez_A}{1 - Sens_A}$
    How much do the odds to belong to class A decrease when a case is predicted not to belong to class A?
  - ✔ independent of relative class fequencies under application conditions

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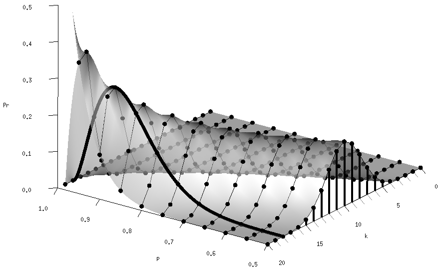
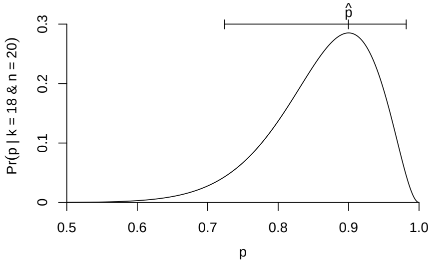
Confidence Intervals for Sensitivity





- Statistical description: Bernoulli trial

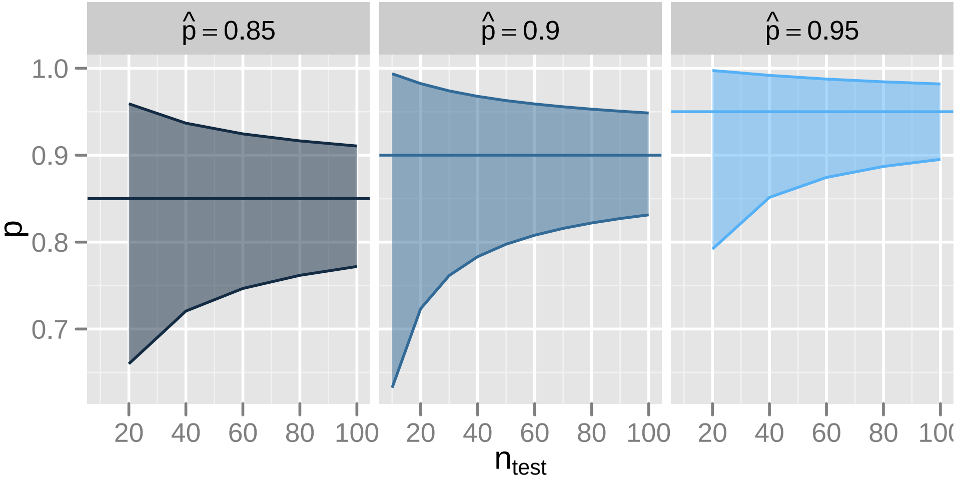
✔ ⇝ use binomial distribution

- Uncertainty on proportion: $var(\hat{p}) = \frac{p(1-p)}{n_{test}}$

✘ normal approximation appropriate only with $np \geq 5$ and $n(1-p) \geq 5$

⇝ Estimate necessary n_{test}

Sample size from Confidence Interval



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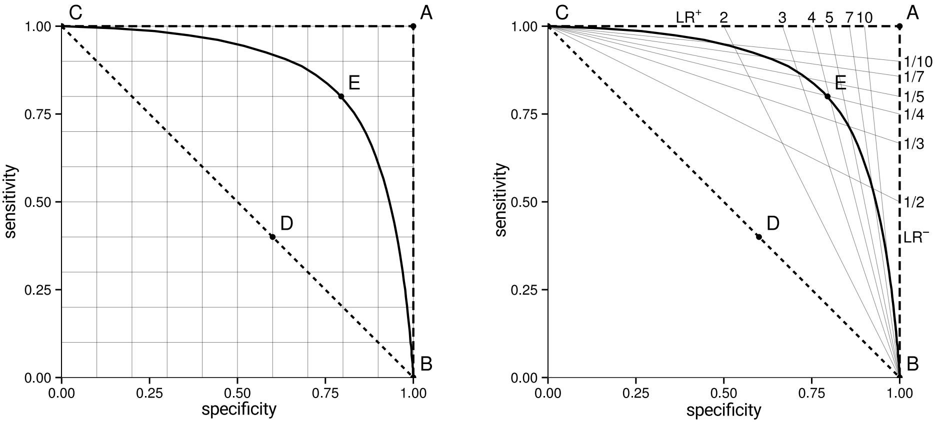
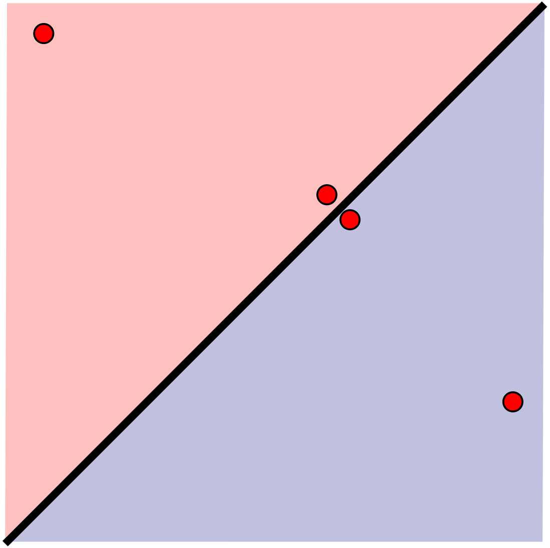
Beleites, C. *et al.*:Sample size planning for classification models. Anal Chim Acta, 2013, 760, 25-33

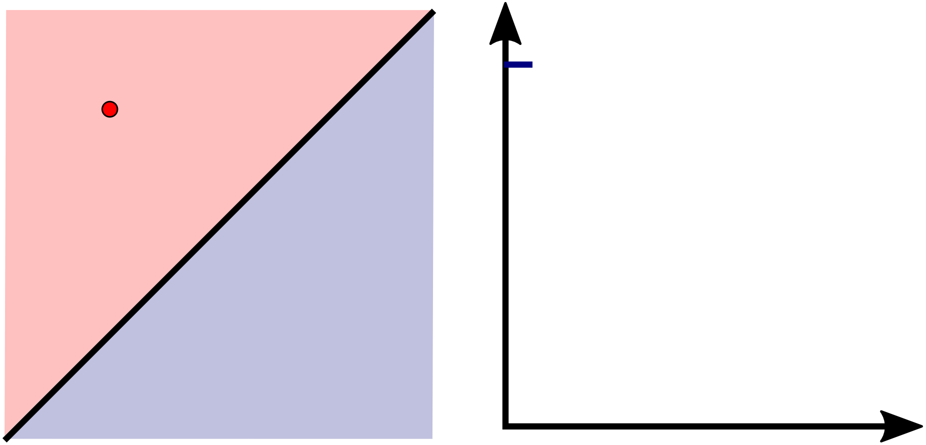
Receiver Operating Charcteristic/Specificity-Sensitivity-Diagram



Proportions: Behaviour in Hyperparameter Optimization



Proportions: Behaviour



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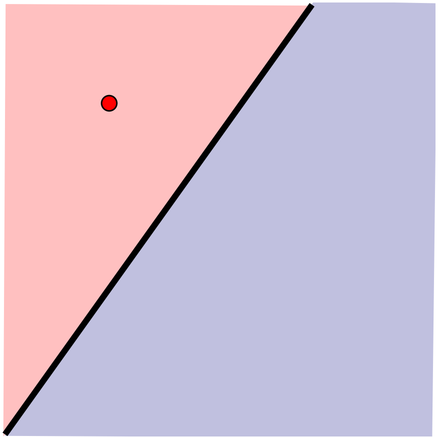

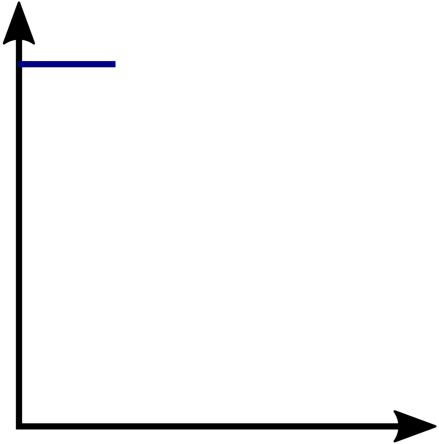

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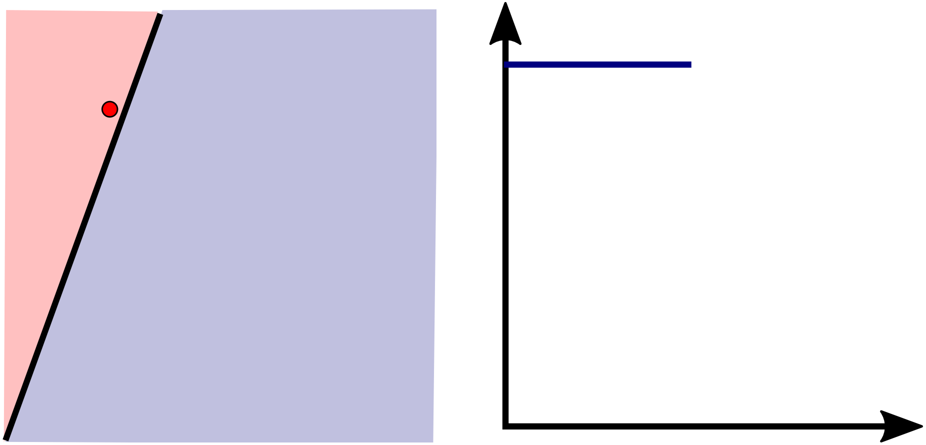

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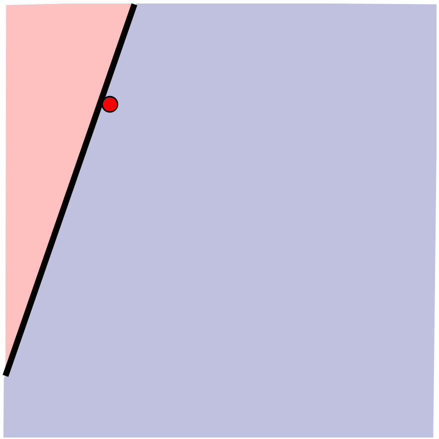

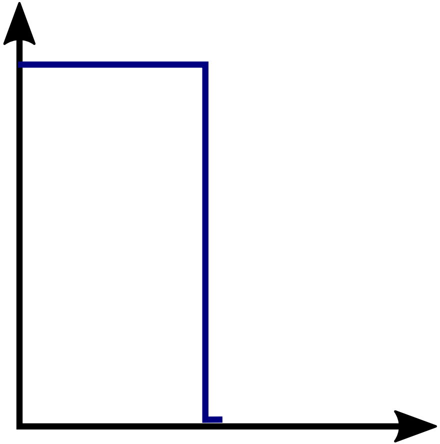

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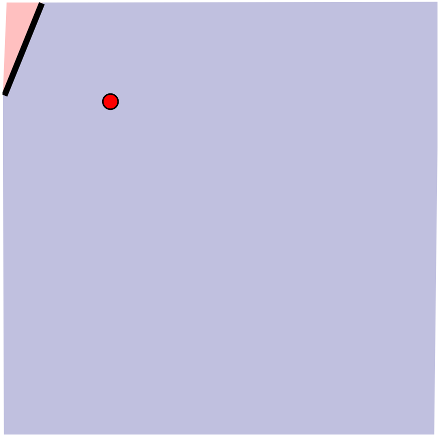
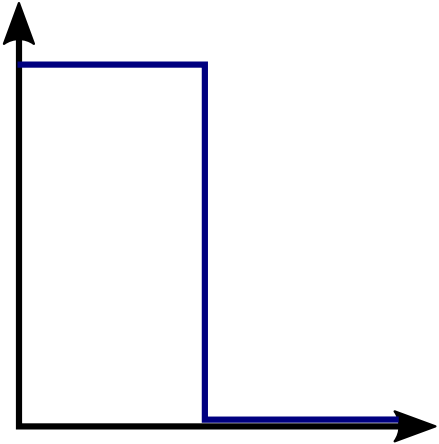
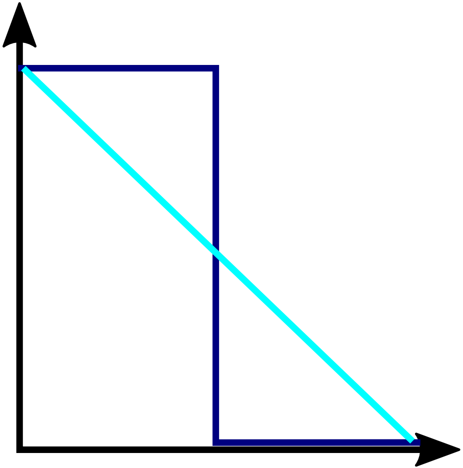




(Strictly) Proper Scoring Rules



Wanted: Figure of merit that . . .

- . . . continuously penalizes closeness to class boundary
- . . . continuously reacts to changes in the model
- . . . slight deterioration ⇝ slight drop in measured performance
- . . . has exactly one optimum
- at the best classifier.

Regression: (Root) Mean Squared Error

- Loss behind e.g. Gaussian Least Squares
- penalizes large deviations
- $MSE = \frac{1}{N} \sum_{i=1}^{N} (\hat{y}_i - y_i)^2$
  $N \ldots$ number of cases
  $i \ldots$ case in question
- $MSE = bias^2 + variance$
- $RMSE = \sqrt{\frac{1}{N} \sum_{i=1}^{N} (\hat{y}_i - y_i)^2}$
  same scale as y

Brier's Score: Mean Squared Error for Classification

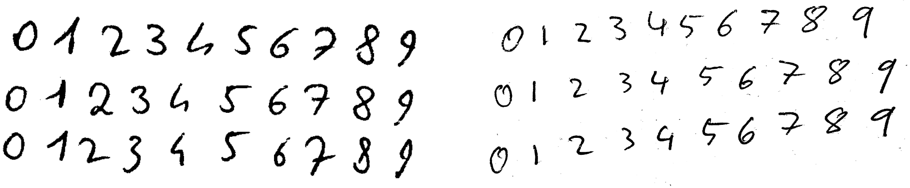
- Classifier that predicts class membership probability rather than labels
- Idea: of all cases where classifier predicts x % class membership, x % should belong to class in question
  a.k.a. *well calibrated prediction*
- Brier's score: $BS = \frac{1}{N} \sum_{i=1}^{N} (\hat{p}_i - p_i)^2$ or
  $BS = \frac{1}{N} \sum_{j=1}^{R} \sum_{i=1}^{N} (\hat{p}_i j - p_i j)^2$ (multiclass version) with
  N ... number of cases
  i ... case in question
  R ... number of classes
  j ... class in question
  p ... class membership, usually $\in \{0, 1\}$
  $\hat{p}$ ... predicted class membership $\in [0, 1]$

Summary Figures of Merit

- Many exist ⇝ choose relevant ones
- Usually, several figures of merit are needed for characterization
- Figures of merit are *measured* ⇝ subject to bias and variance like any other measurement
- Regression: figures of merit “well-behaved”,
  but no back-of-the-envelope variance guesstimates
- Classification: proportions easy to understand & widespread
  but have bad variance properties & discontinuous behaviour

⇝ use (strictly) proper scoring rules for optimization

Cases and Statistical Independence



- structure in data: clusters, spatial and/or temporal
- e.g. repeated measurements: repetitions are more similar to each other
- special case: time series

✔ Think hard about factors affecting independence

Model Testing: Measure the Model's Performance

Different kinds of test samples
⇝ different performance measures

Goodness of fit: *training samples*
⇝ residuals

Generalization error: statistically independent samples
resampling,
test set measured at same time as training set

Future performance: samples measured *after* training samples
dedicated test set for detection of drift

Resampling for Model Validation

✘ We don't have enough samples

- Training:
  - Model quality depends on ratio $n_{train} : d.f.$
  - Linear model: $5\,\text{samples}/(\text{variate} \cdot \text{class})$
  - ✔ We want to use all samples for training

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✘ We don't have enough samples

- Training:
  - Model quality depends on ratio $n_{train} : d.f.$
  - Linear model: 5 samples/(variate · class)
  - ✔ We want to use all samples for training

- Testing:
  - ✔ We want to know whether the model is stable
  - Quality of the performance measure depends on n_{test}
  - Width of 95 % confidence interval $\overset{!}{\leq}$ 10 % for $p = 90\,\%$: $n_{test} \geq 140$
  - ✔ We want to use all samples for testing

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Validation Schemes: Overview

autoprediction
reclassification
resubstitution

Resampling Validation

set validation

leave one out

cross validation

iterated *k*-fold
repeated *k*-fold

out-of-bootstrap

.632+ bootstrap

.632 bootstrap

hold-out
independent
test set

validation study

R Kohavi: A Study of Cross-Validation and Bootstrap for Accuracy Estimation and Model Selection. In: Proc. 14th International Joint Conference on Artificial Intelligence, 1995, Morgan Kaufmann, USA, 1995, 1137–1145.

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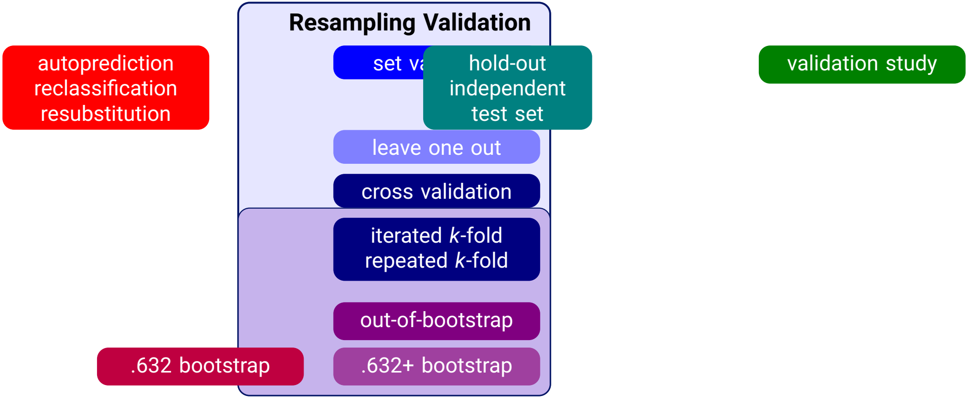

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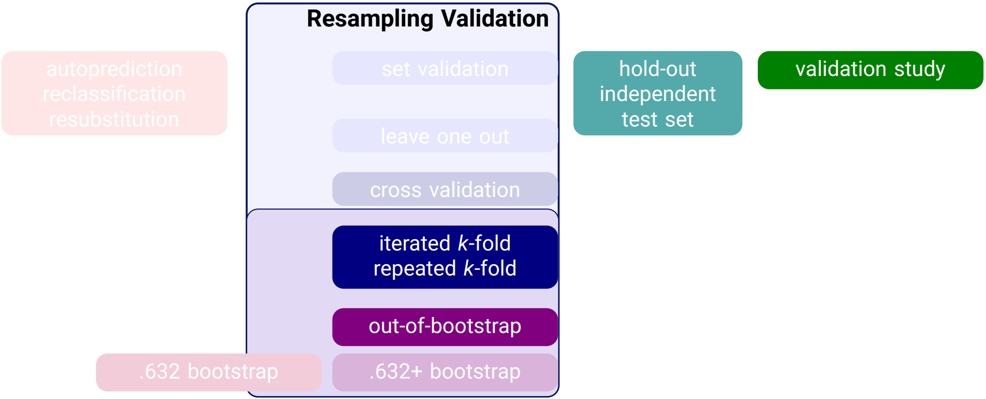
Validation Schemes: Recommendations



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Resampling vs. Validation Study

	Resampling	Validation Study
statistical properties		
bias	✔ pessimistic (low)	✔ unbiased
variance	$f(n)$	$f(n_{test})$
efficient use of cases	✔	✔
measure model stability	✔ iterated	✔/✘
measure drift	✘	✔ DoE
future case performance	✘	✔ DoE
out-of-spec cases	✘	✔ DoE
practical properties		
independence	⚠ splitting error prone	✔
effort	✔ computational	✘ experimental

Beleites, C. & Salzer, R.: Assessing and improving the stability of chemometric models in small sample size situations Anal Bioanal Chem, 2008, 390, 1261-1271
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Resampling vs. Hold Out

	Resampling	Split off Hold Out Set
statistical properties		
bias	✔ pessimistic (low)	✔ unbiased
variance	✔ $f(n)$ lower	✘ $f(n_{test})$ large
efficient use of cases	✔	✘
measure model stability	✔ iterated	✘
measure drift	✘	✘
future case performance	✘	✘
out-of-spec cases	✘	✘(✔)
practical properties		
independence	⚠ splitting error prone	⚠ same as resampling
effort	✔ computational	✔ low

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Validation Check List

- Randomize order of measurements
- Split at highest level in sample hierarchy/data structure
- Split before 1st step that involves multiple cases
- Additional independent validation for data-driven optimization/tuning/model selection
- Test cases: reference labels must be independent of cases (measurements, spectra, . . .)
- Make sure labelling procedure does not distort difficulty for test cases
- Ensure correctness of code

Validation Check List

- Randomize order of measurements
- Split at highest level in sample hierarchy/data structure
  patients, strains, cell lines,
- Split before 1st step that involves multiple cases
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Validation Check List

- Randomize order of measurements
- Split at highest level in sample hierarchy/data structure
  patients, strains, cell lines,
  day of measurement, before/after new calibration, . . .
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  patients, strains, cell lines,
  day of measurement, before/after new calibration, . . .
- Split before 1st step that involves multiple cases
  centering, PCA preprocessing, . . .
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- Additional independent validation for data-driven optimization/tuning/model selection
  nested/double cross validation or train-validate-test ⇝ necessary case numbers HUGE
- Test cases: reference labels must be independent of cases (measurements, spectra, . . .)
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  cluster analysis to assign labels → OK for training cases
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  cluster analysis to assign labels → OK for training cases semi-supervised learning → OK for training cases
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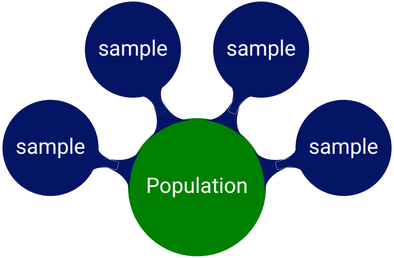
The Concept behind Resampling



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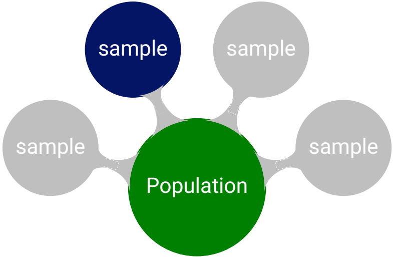

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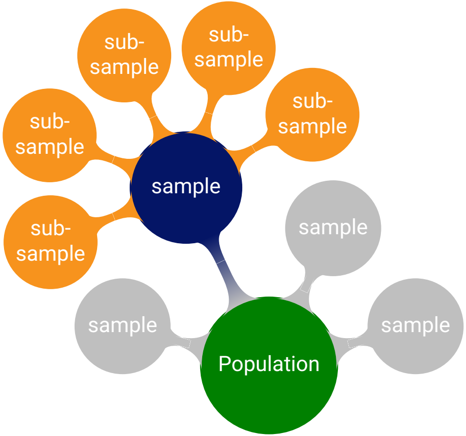


- Subsamples are approximations of (more) real samples
- Subsample is perturbed version of the real sample

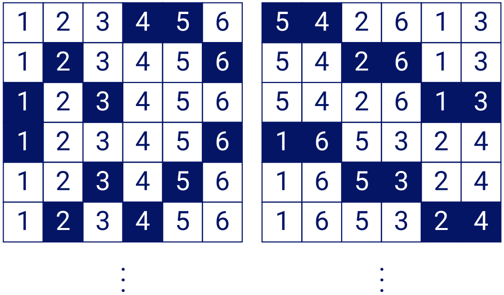
Cross Validation: Drawing without Replacement

1	2	3	**4**	**5**	6
1	**2**	3	4	5	**6**
1	2	**3**	4	5	6

5	**4**	2	6	1	3
5	4	**2**	**6**	1	3
5	4	2	6	**1**	**3**

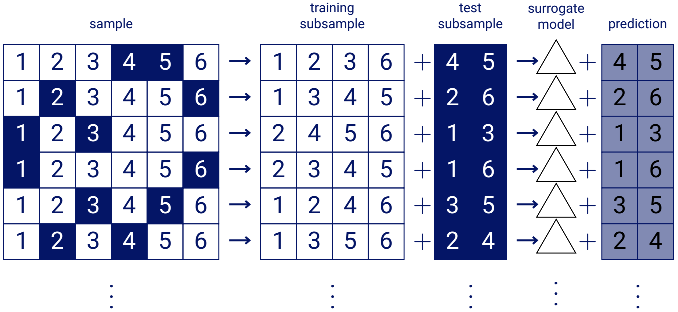
✔ Each case is left out exactly once

Cross Validation: Drawing without Replacement



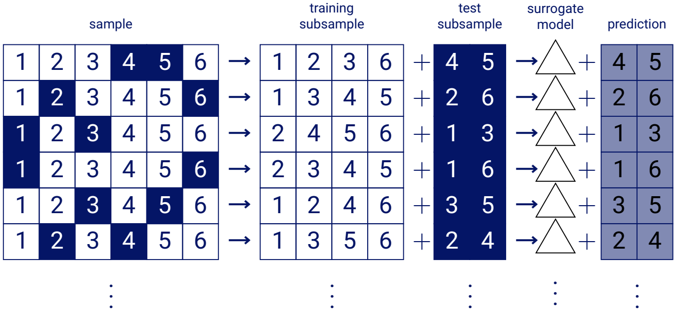
- ✔ Each case is left out exactly once per iteration
- Repetitions aka iterations possible with *k*-fold or leave-*n*-out cross validation
- ✘ Leave-one-out cannot be iterated

Resampling for Model Validation: Assumptions



- Surrogate model equals model of whole sample
- Surrogate models equal to each other
- All cases come from the same distribution

Resampling for Model Validation: Assumptions



- Surrogate model equals model of whole sample

✘ Violation ⇝ pessimistic bias

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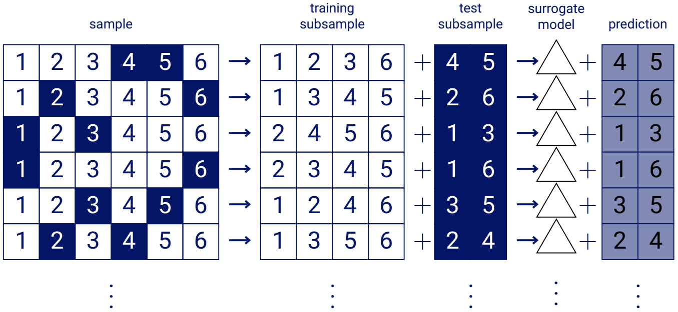
Resampling for Model Validation: Assumptions



- Surrogate model equals model of whole sample
- ✘ Violation ⇝ pessimistic bias

- Surrogate models equal to each other
- ✘ Violation (instability) ⇝ higher variance

- All cases come from the same distribution

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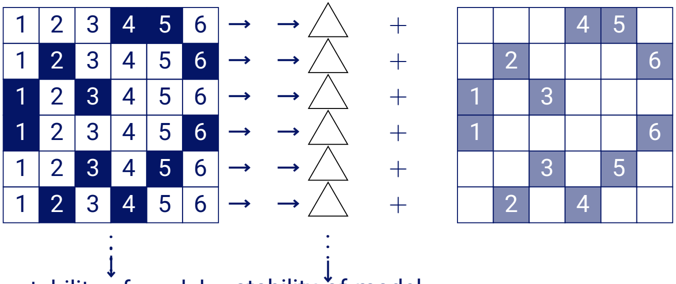
Model Stability



stability of model predictions

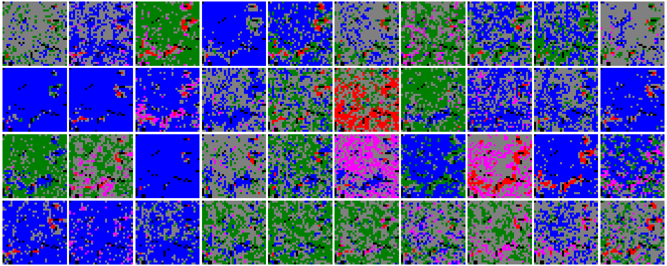
stability of model parameters

- Subsamples are perturbed versions of real sample

✔ Measure stability of model
  - Stability of model parameters
  - Stability of predictions

- Repetitions reduce variance due to instability of surrogate models.

Model Stability: 40× 8-fold cross validation



- FTIR images of tumour sections (normal, °II, °III, °IV)
- total: 150 images of 58 patients: 133 000 spectra
  smallest class: °II, 4 800 spectra (3 patients, 5 images)
- LDA after automatic selection of 8 spectral regions
- reject spectra with posterior probability <0.85

How many cases do we need?

. . . **to train a good classifier?**

– rules of thumb
linear model: $\frac{n}{p} \geq 3 - 5$ in each class

⇒ learning curve

. . . **to measure the model's performance?**

⇝ confidence intervals for test results

– Rules of thumb
100 test cases to estimate a proportion

– Regression ⇝ needs preliminary experiment

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Validation: Questions

- Did you ask the right question?
- Or did you use a surrogate?
  - Is that surrogate appropriate?
  - What are the limits?
- Is your model set up correctly?
  - Is it really a classification problem?
  - one-class vs. discriminative?
  - open-world vs. closed-world?
  - correct scale of *y*? Other transformation better?
- Do you use the correct controls/base class or correct 0-point (center, origin) of regression?
- What happens with out-of-spec cases (unknown class? bad measurements?)

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Validation: Questions

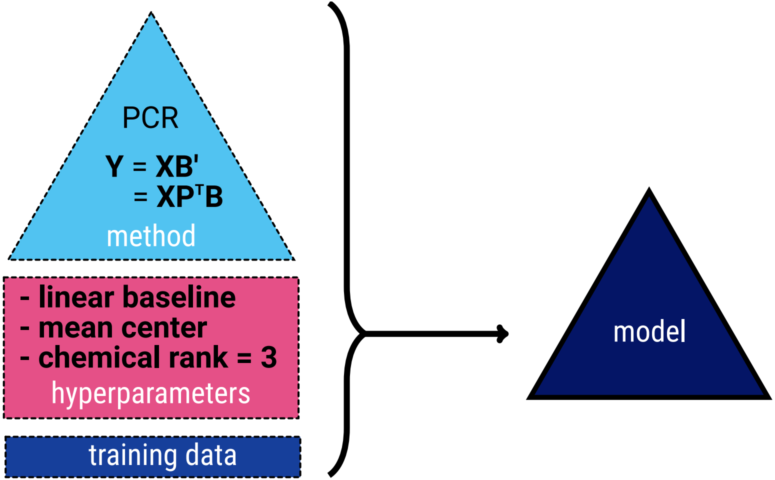
- Bias introduced by data acquisition procedure?
  - Labeling procedure with self-fulfilling prophecies (e.g. cluster analysis as basis for labeling, semi-supervised label generation)?
- What about borderline cases?
  - Do your *labeled* cases correctly represent them?
  - No exclusion of “difficult” cases in the reference labeling step?
- What other confounders could exist?
- What are the limits of your method?
- reading suggestions on reproducibility issues in medical research:
  - Buchen, L.: Cancer: Missing the mark. Nature, 2011, 471, 428 – 432
  - Begley, C. G. & Ellis, L. M.: Drug development: Raise standards for preclinical cancer research. Nature, 2012, 483, 531 – 533
  - Ioannidis, J. P. A.: Why Most Published Research Findings Are False, PLoS Med 2(8): e124
  - . . .

Ruggedness: Perturb Data

- How robust are the predictions?
- Which factors (confounders) have most influence?
- Perturb Data
  - Repeated cross validation:
    How do predictions vary if *a few* training cases are exchanged?
    ⇝ stability of predictions
  - Simulate instrument related distortions:
    Measure respective drop in performance

Beleites, C. & Salzer, R.: Assessing and improving the stability of chemometric models in small sample size situations Anal Bioanal Chem, 2008, 390, 1261-1271
Sattlecker, M. et al.: Assessment of robustness and transferability of classification models built for cancer diagnostics using Raman spectroscopy J Raman Spectrosc, 2010, 897-903

Hyperparameters



- available: PCR ($\mathbf{X}_{train}$, no_PCs, center)
- wanted: PCR_tuned ($\mathbf{X}_{train}$)

Data-driven Model Optimization

training data

Idea:

1. sensible range of hyperparameters
2. build covering this search space
3. measure performance
4. take the best

⇒ **Optimize predictive performance**

✔ Large variety of numerical optimizers available

exhaustive grid search, genetic optimizers, simulated annealing, . . .

Data-driven Model Optimization

training data | validation data

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⇒ need another independent set to validate the *final* model

Data-driven Model Optimization

training data | validation data | test data

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- fit normal parameters (coefficients) with *training* set
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✔ resampling version: nested/double cross validation

✔ `train (X, hyperparameters)` vs. `tuned_train (X)`
  - tuned training function: additional internal split for tuning

Data-driven Model Optimization

training data

test data

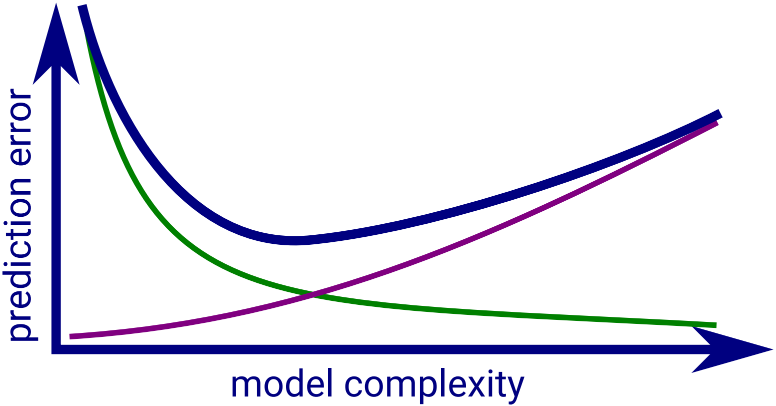
- fit normal parameters (coefficients) with *training* set
- fit hyperparameters with ~~validation set~~ optimization aka development set
- validate chosen model with ~~test set~~ final verification set

✔ resampling version: nested/double cross validation

✔ `train (X, hyperparameters)` vs. `tuned_train (X)`
  - tuned training function: additional internal split for tuning
  - ✔ treat `tuned_train (X)` like any other training function

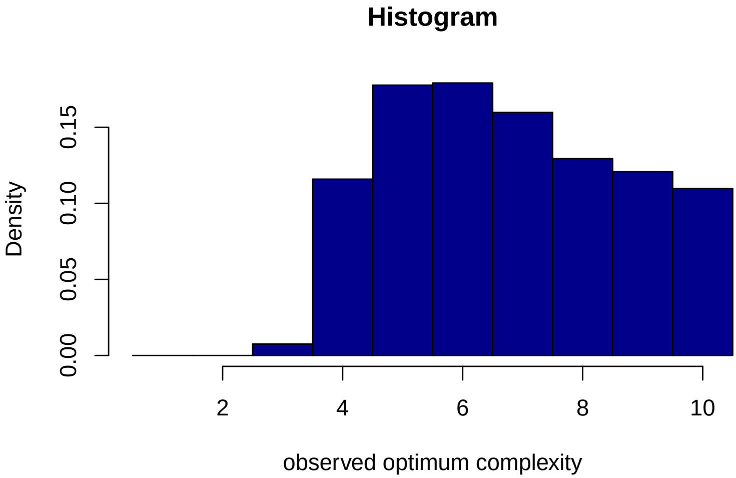
CHEMO METRIX

Grid search: Stability of Solution



Hastie, Tibshirani, Friedman: The Elements of Statistical Learning, Springer

Grid search: Stability of Solution



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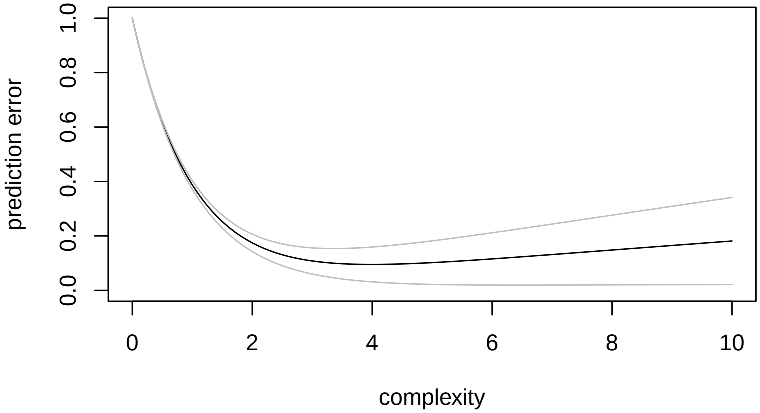

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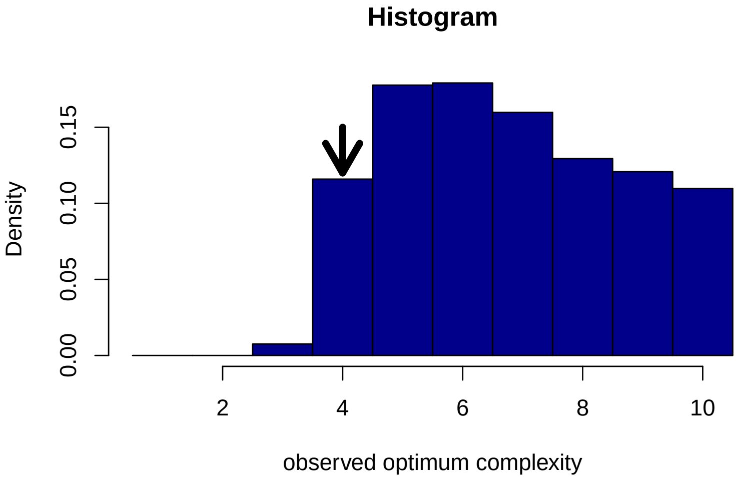

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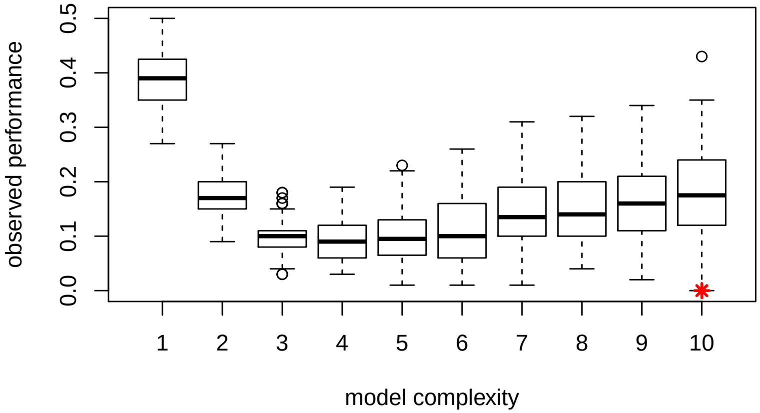

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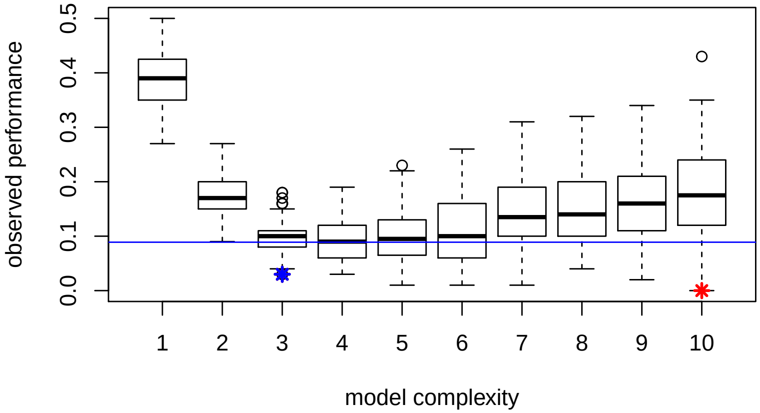

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Summary: Validation

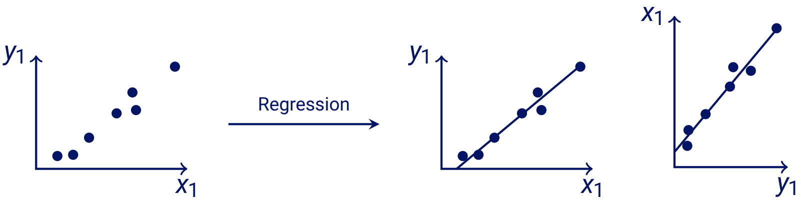
- ✔ Think hard about your data, model, and application!
- ✔ Sample size planning: calculate from required precision of validation results possibly from preliminary experiment
- At some point, validation studies are needed.
  Before that, use repeated cross validation or out-of-bootstrap.
- ✔ Determine independent splitting
- ✔ Check stability of predictions and – if possible – model parameters
- ✘ Resampling cannot detect drift
- ✘ Hold-out is inefficient and prone to the same errors as resampling!

Summary: Data-driven model Optimization

- ✔ Needs internal performance estimate plus outer independent validation
- ✘ ⇝ large sample size required
- ✔ wrap optimization in `tuned_model` function
- ✔ validate output of `tuned_model` like any other model training function
- ✔ Check stability of optimization
- ✔ Use 1-sd-rule to guard against overfitting
- ✔ Class membership probability predicted: MSE (Brier's Score) has low variance and is proper scoring rule
  ⇝ suitable for optimization

CHEMO METRIX

Regression



Ordinary Regression

$\mathbf{Y}^{(n \times m)} = \mathbf{X}^{(n \times p)} \mathbf{B}^{(p \times m)}$

- assume error on y (I)
- ✔ causality: $I = f(c)$
- ✔ efficient estimation of calibration line parameters

Inverse Regression

- assume error on x (c)
- ✔ prediction: $c = f(I)$
- ✔ efficient estimation of y
- ✘ needs $p \leq m$

Univariate Linear Regression

$$\mathbf{Y}^{(n \times m)} = \mathbf{X}^{(n \times p)} \mathbf{B}^{(p \times m)}$$

y	**x**
1	2
2	3
3	4
4	5
5	6

Multivariate Linear Regression

$$\mathbf{Y}^{(n \times m)} = \mathbf{X}^{(n \times p)} \mathbf{B}^{(p \times m)}$$

$\mathbf{y}$	$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$
1	2	7	3
2	3	5	5
3	4	3	-2
4	5	1	7
5	6	-1	0

Linear Models: Polynomial Features

$$\mathbf{Y}^{(n \times m)} = \mathbf{X}^{(n \times p)} \mathbf{B}^{(p \times m)}$$

y	x
1	2
2	3
3	4
4	5
5	6

Linear Models: Polynomial Features

$$\mathbf{Y}^{(n \times m)} = \mathbf{X}^{(n \times p)} \mathbf{B}^{(p \times m)}$$

y	x^0	x^1	x^2
1	1	2	4
2	1	3	9
3	1	4	16
4	1	5	25
5	1	6	36

Questions?

Please contact me (**Claudia.Beleites@chemometrix.gmbh**) if you

- have questions, or
- want to reuse these slides.