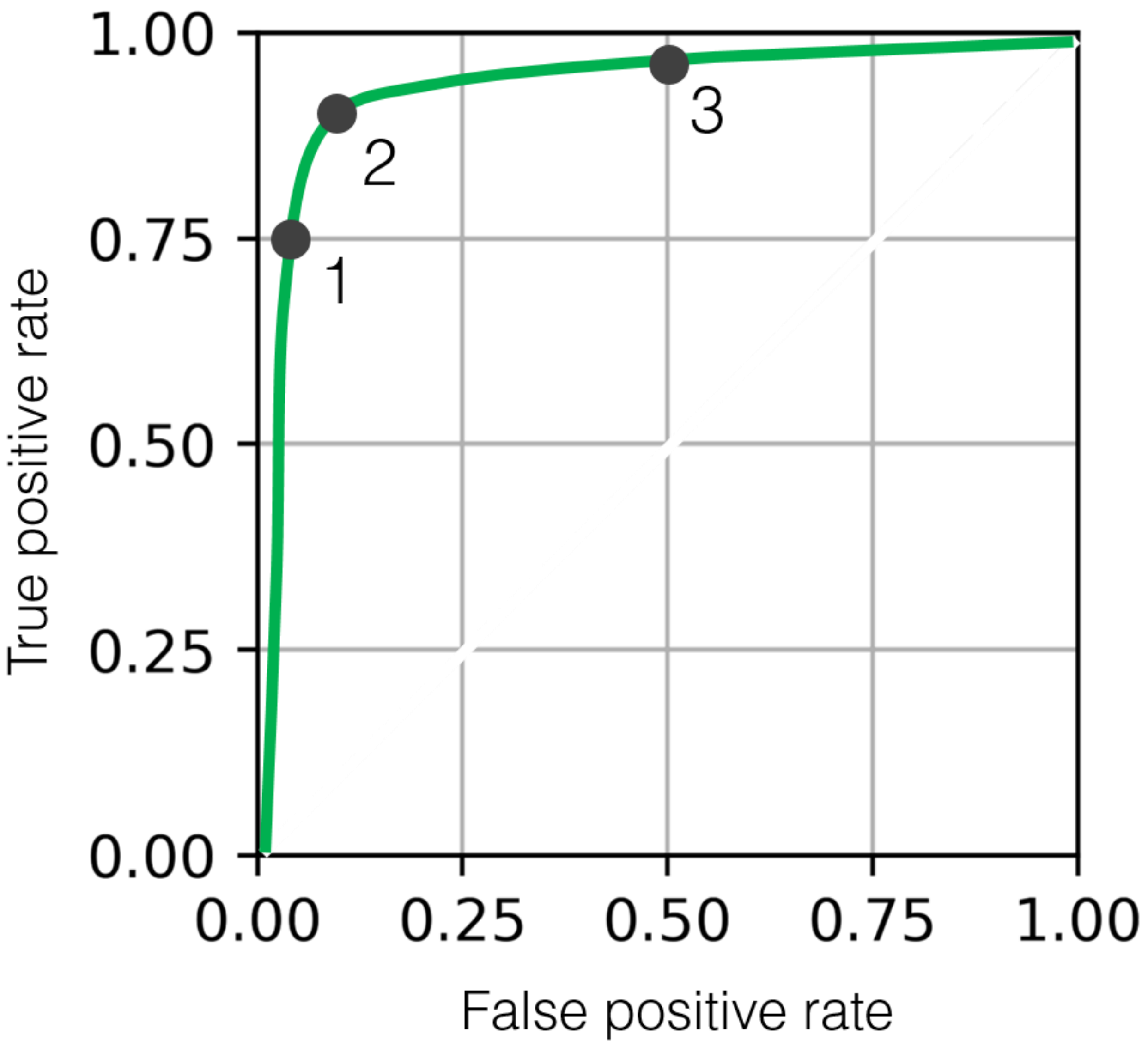
Evaluating Performance II

You are in charge of a landmine clearing operation. If you predict there is a mine in a given plot of land, it costs $500 to check (and twice that to remove it). If you miss the mine, the expected damage would be $10,000,000. If you can pick any of the three points below, where on the ROC curve do you operate to minimize potential costs?



Modeling Considerations

Accuracy

Computational Efficiency

Interpretability

Accuracy
Supervised Learning Performance Evaluation

Regression

Classification

Binary

Multiclass

Cost / Loss Functions

Regression:

- Mean squared error (MSE)
- Mean absolute error (MAE)
- Huber loss

Classification:

- Cross entropy / log loss

Performance Evaluation Metrics and Tools

Regression:

- Root mean squared error (RMSE)
- R^2, coefficient of determination

Binary:

- Classification accuracy
- True positive rate (Recall)
- False positive rate
- Precision
- F_1 Score
- Area under the ROC curve (AUC)
- Receiver Operating Characteristic (ROC) curves

Multiclass:

- Classification accuracy
- Micro-averaged F_1 Score
- Macro-averaged F_1 Score
- Confusion matrices
- Per class metrics (recall, precision, etc.)

We can always compute our accuracy metrics of a trained model on our test set…

…BUT, they may not be valid (i.e. may not reflect generalization performance) if:

1. The underlying data are NOT representative of what we will encounter in practice

2. The test data set DOES NOT remain separate from our model training process

Goal: estimate generalization performance

Spot the misstep

1

1. Your train a logistic regression algorithm on training data
2. You evaluate the generalization performance of your trained algorithm on the training data
3. Your estimated performance is exceptional!

NEVER USE THE SAME DATA USED FOR TRAINING FOR ESTIMATING GENERALIZATION PERFORMANCE

2

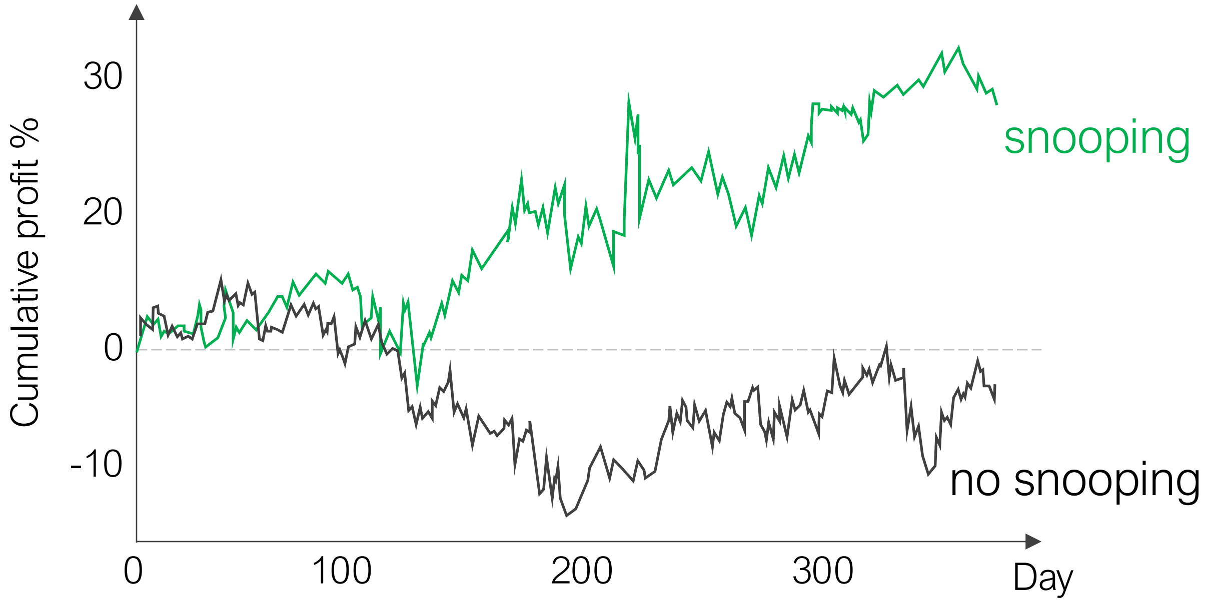
1. Goal: predict the exchange rate for the U.S. Dollar vs British Pound (using 20 past observations)

2. You take your historical data, normalize it, then split it randomly into a training and test set
   DATA SNOOPING!

3. You train on the training data, test on the test data

Results:
Your predictions are correct 56% of the time

Estimate your profits…



All preprocessing should be based on the training data alone

Abu-Mostafa, Learning From Data

3

1. Goal: predict the Dow Jones Industrial average

2. You randomly split your data into a training and test dataset

3. Choose a model with lots of flexibility

4. You iterate on the following process hundreds of times:
    1. Train your model on the training data
    2. Test your model on the test data
    3. Evaluate performance on the test data

DATA SNOOPING!

5. Report that you were able to achieve 75% accuracy on your test set!

4

1. Goal: predict long-term performance of a “buy and hold” strategy in stocks

2. You collect 50 years of historical data and include all companies that are currently traded in the S&P500

   SAMPLING BIAS!

3. You randomly split your data into a training and test dataset.

4. You assume you will strictly follow the “buy and hold” strategy

5. You then use apply your model on the current portfolio and predict that you will be rich in retirement!

Abu-Mostafa, Learning From Data

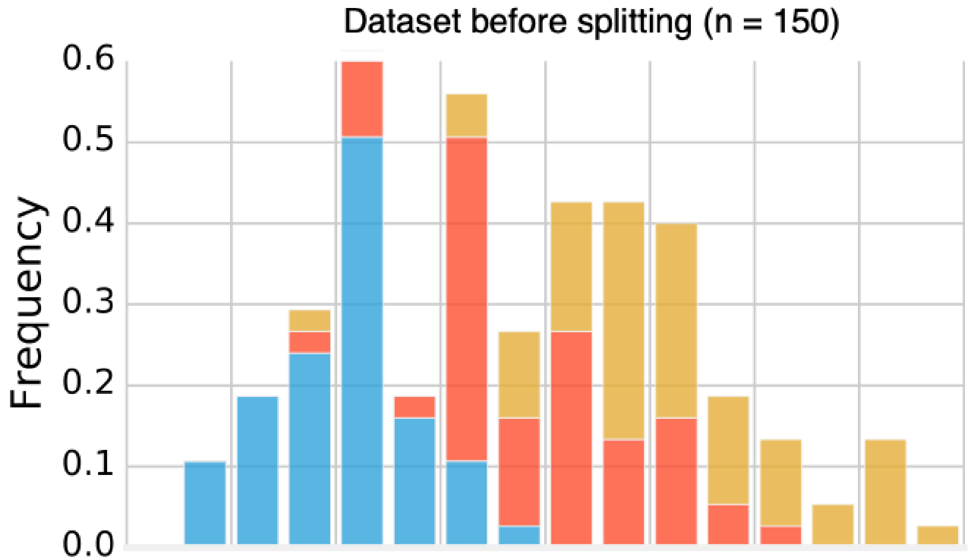
Data snooping / leakage

If a test data set has affected **any step** in the learning process, its ability to assess the generalization performance has been **compromised**.

Abu-Mostafa, Learning From Data

Sampling bias

Are the data we're using for machine learning **representative of the population you will apply on in practice**?



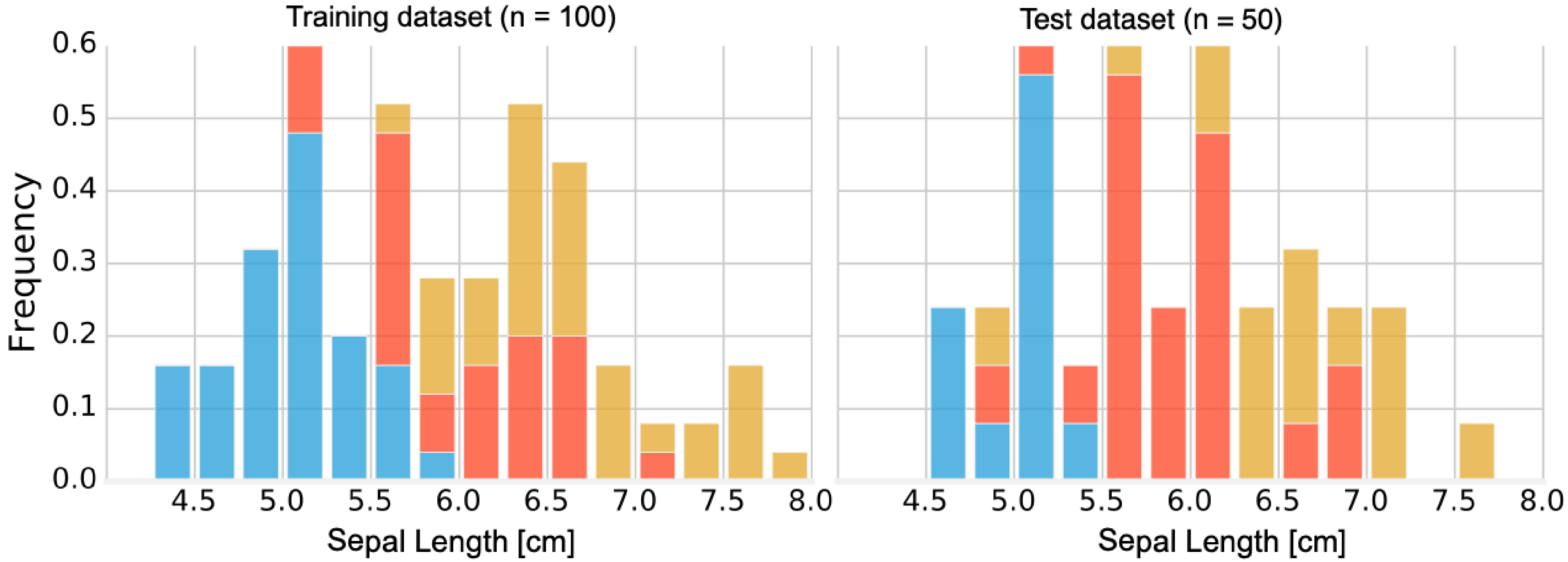
Setosa
Versicolor
Virginica

All: 50 Setosa, 50 Versicolor, 50 Virginica

Train: 38 Setosa, 28 Versicolor, 34 Virginica

Test: 12 Setosa, 22 Versicolor, 16 Virginica

One form of sampling bias



Ideally training and test sets are independent and statistically representative of the population

Dividing up your dataset we violate independence assumptions

Reduce this bias with **stratified sampling**

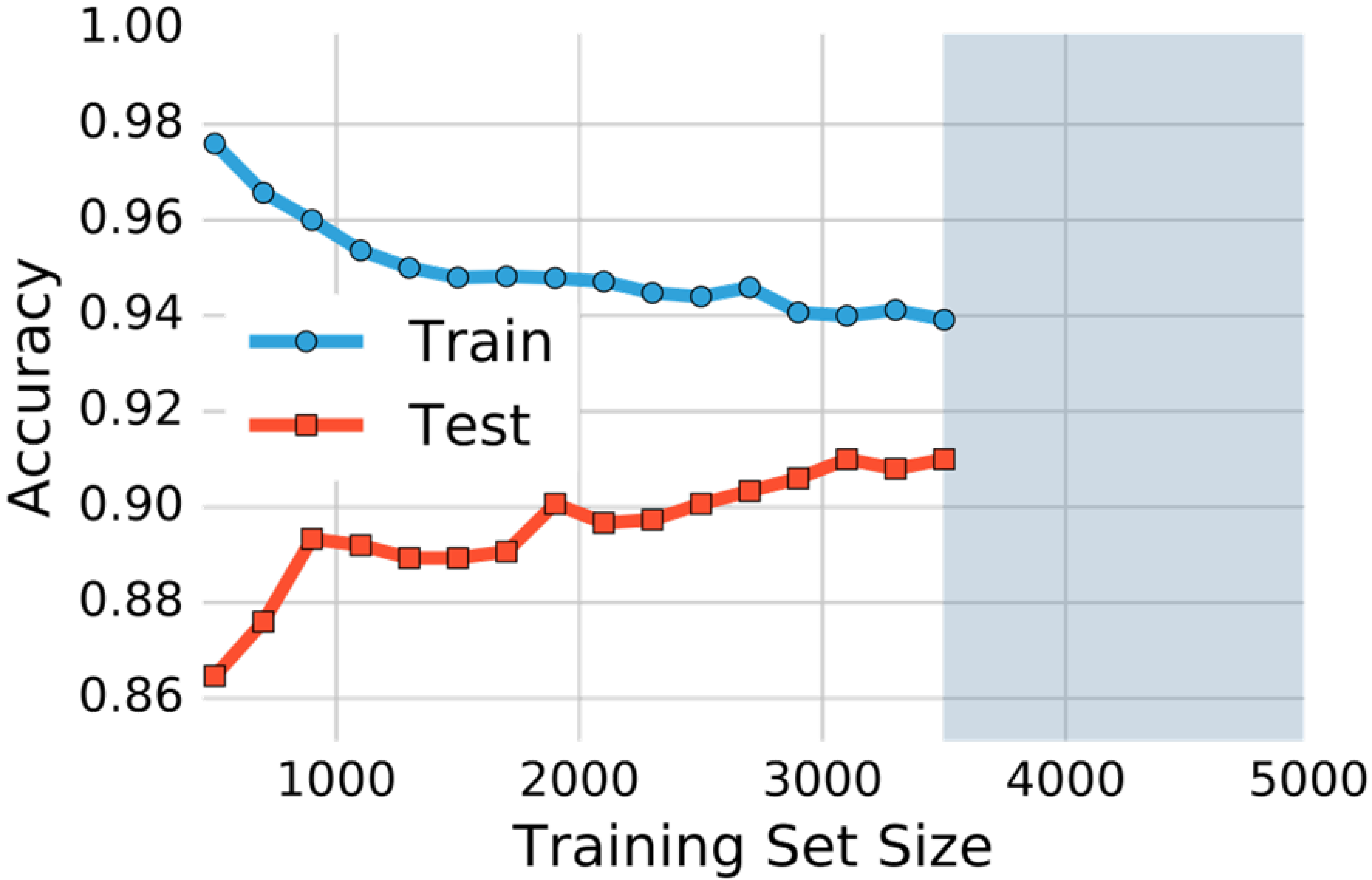
Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part1.html)

Sample Size

Ideally, we would use infinite samples in our training set representing the population

In practice, we try to use as much data as possible

Larger datasets may also reduce overfit



Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part2.html)

1 How do we use the metrics to **evaluate performance**?

Basic ML Experimental Design

1 Generalization Performance Evaluation

Model → Evaluation Framework → Performance metrics

	no hyperparameter optimization	hyperparameter optimization
Large Dataset	**Train-test split**	**Train-validation-test split**
Small Dataset	**Cross-validation**	**Nested Cross-validation**

2 Model Comparison

(experiment to determine the best-performing algorithm)

Model A → Evaluation Framework → Performance metrics

Model B → Evaluation Framework → Performance metrics

Model C → Evaluation Framework → Performance metrics

Compare models according to metrics

Only vary the model!

(don't vary the data, evaluation framework, etc. for a fair comparison)

Train-Test Split

Learning model parameters and evaluating performance

Commonly ~80/20

Used for model training: select model parameters

Evaluate generalization performance

1. If our test split is too small, our estimate of generalization performance will have high variance
2. Not using all data for training produces an algorithm that is pessimistically biased
3. For small datasets, this reduction in dataset size may be detrimental

What are Hyperparameters?

Parameters: Configuration variable that control model predictions that are adjusted during the training process based on data

Hyperparameters: parameters set prior to model training; they are not modified during the training procedure, but often impact the training procedure.

Hyperparameter Examples

- k in KNN
- Learning rates for gradient descent of your model fitting procedure
- Model architectures (e.g. number and types of layers in neural networks)

What happens if we re-evaluate the model with different hyperparameters?

We may overfit to our held-out test data!

Model w/ hyperparameter set A	Train	Test
Model w/ hyperparameter set B	Train	Test
Model w/ hyperparameter set C	Train	Test
Model w/ hyperparameter set D	Train	Test
Model w/ hyperparameter set E	Train	Test
Model w/ hyperparameter set F	Train	Test

Training, Validation, Test Split

Learning model parameters AND **hyperparameters** and evaluating performance

Train	Validation	Test
Used for model training / fitting	Used to optimize hyperparameters and/or compare models	Used to evaluate generalization performance of the final model(s)

→ Performance metrics

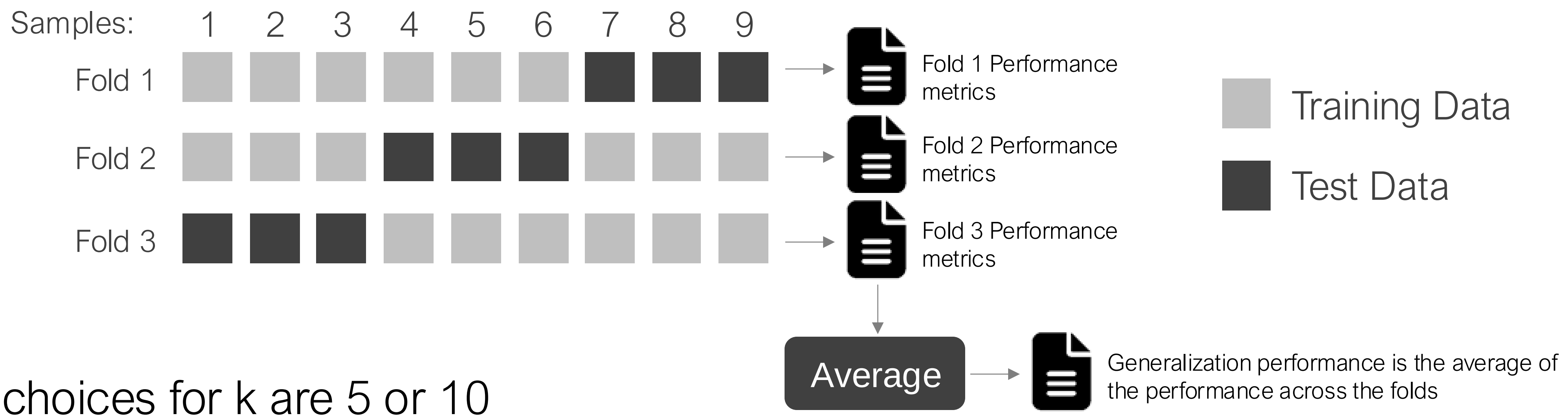
Hyperparameters: parameters that control how your algorithm learns; typically set before training begins (e.g. k in KNN, learning rate, etc.)

What if you have a small dataset?

K-folds cross-validation

K-fold cross validation K = 3

❶ **Performance evaluation**: Train your model K times, once for each fold



Typical choices for k are 5 or 10

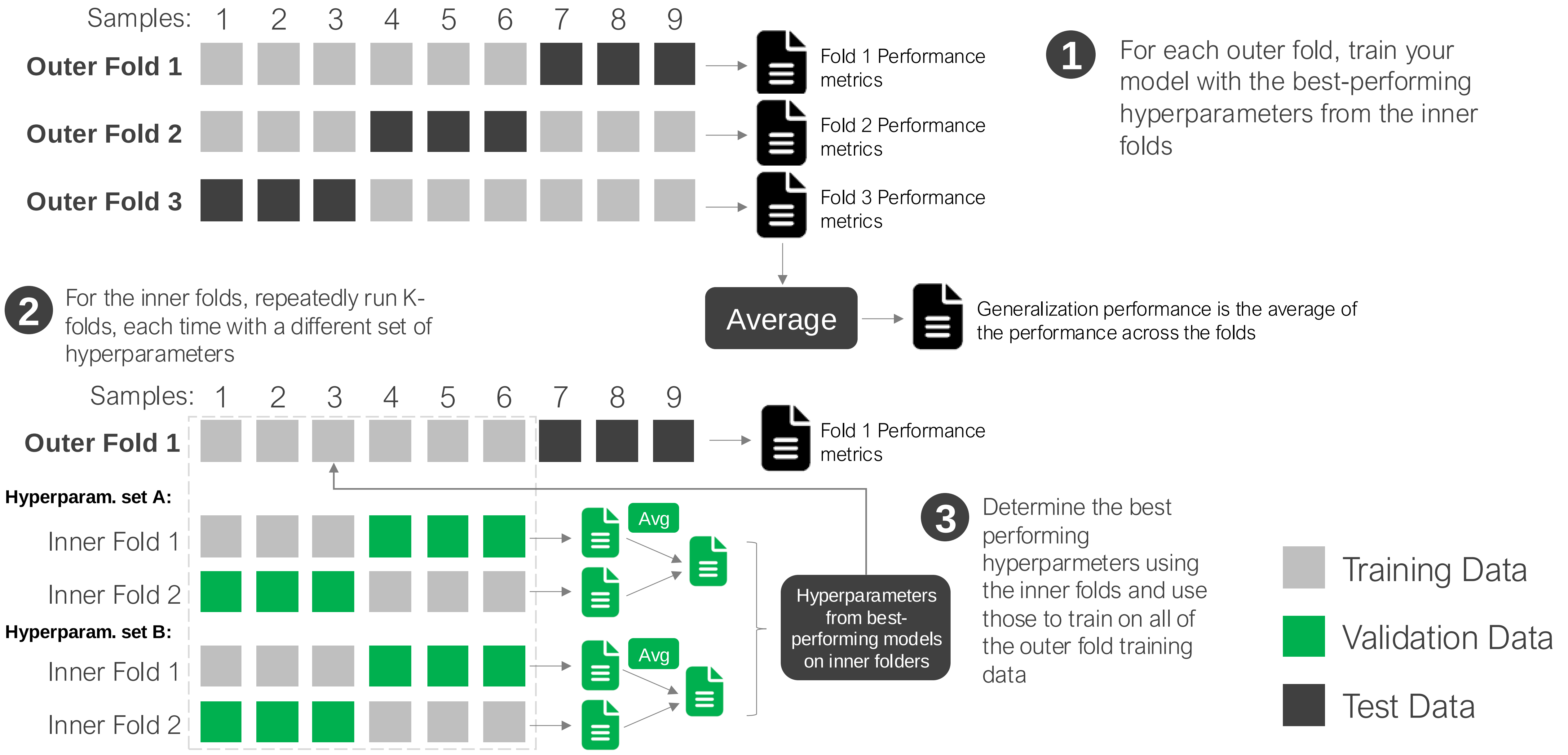
Average performance metrics across the splits

If k = N (number of samples): Leave-one-out cross validation

The number of splits impacts the bias-variance tradeoff of your performance estimates
(larger k means lower bias on the performance estimate, but with higher variance)

What if you need to select hyperparameters for a small dataset?

Nested cross-validation with hyperparameters



When to use each technique for **performance evaluation**?

	no hyperparameter optimization	hyperparameter optimization
Large Dataset	**Train-test split**	**Train-validation-test split**
Small Dataset	**Cross-validation**	**Nested Cross-validation**

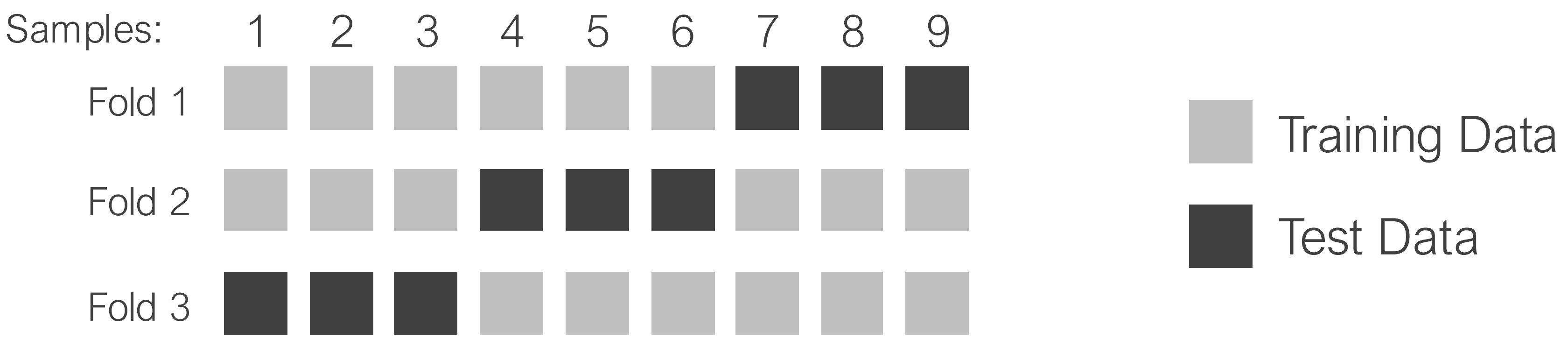
Note: hyperparameter optimization can be considered a form of model comparison

K-folds cross validation results in **k models**

How do we pick which to use?

After performance has been validated, **train on all the data you have** before you apply the model in practice

1 **Performance evaluation**: Train your model K times, once for each fold



2 **Model application**: Once you've evaluated model performance and are ready apply the model then retrain the model on ALL of your data to prepare it for unseen data

(this is not a model evaluation step, but only when you're ready to apply in practice)

Basic ML Experimental Design

1 Generalization Performance Evaluation

Model → **Evaluation Framework** → Performance metrics

	no hyperparameter optimization	hyperparameter optimization
Large Dataset	**Train-test split**	**Train-validation-test split**
Small Dataset	**Cross-validation**	**Nested Cross-validation**

2 Model Comparison

Model A → **Evaluation Framework** → Performance metrics

Model B → **Evaluation Framework** → Performance metrics

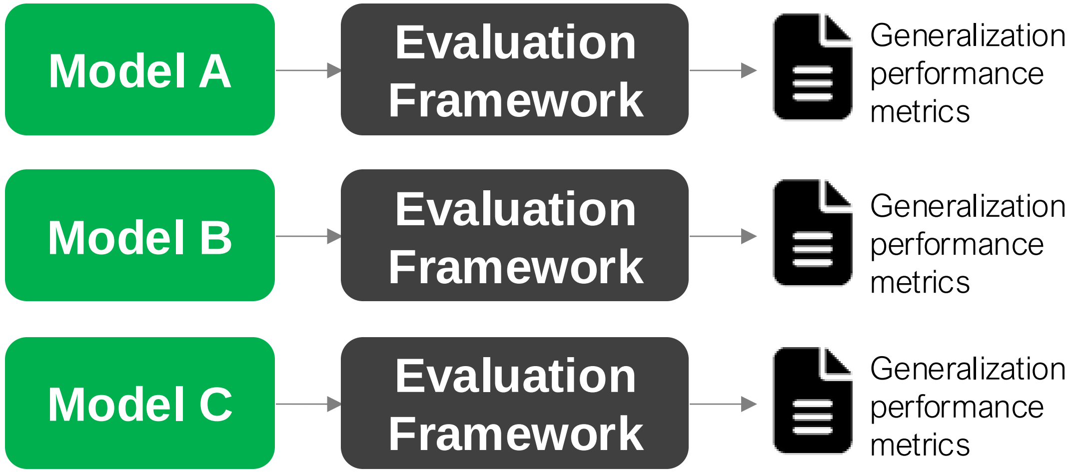
Model C → **Evaluation Framework** → Performance metrics

Compare models according to metrics

2 How do we use the metrics to **compare models**?

We can compare models and hyperparameters using the evaluation frameworks

2 Model Comparison



Select the model with the best performance metric

Note: once we use generalization performance metrics to select a model (or hyperparameter), they are **no longer unbiased metrics**

We can always use a further held-out dataset to estimate unbiased generalization performance

But is the performance "better"?

2 Model Comparison

Model A → **Evaluation Framework** → Accuracy = 0.89

Model B → **Evaluation Framework** → Accuracy = 0.88

Model C → **Evaluation Framework** → Accuracy = 0.90

Is Model C actually better than A and B?

Is the comparison fair?

Model	Learning Rate	Batch Size	Training data size	Test data size
A (ResNet)	0.001	16	500	100
B (Inception v3)	0.001	32	500	100
C (VGG16)	0.010	32	505	100

What other questions do I need to ask here?

Are my metrics uncertain?

Model-based uncertainty
(Inherent stochasticity in the model training process)

- Order of training data
- Random initializations of model weights

Data-based uncertainty

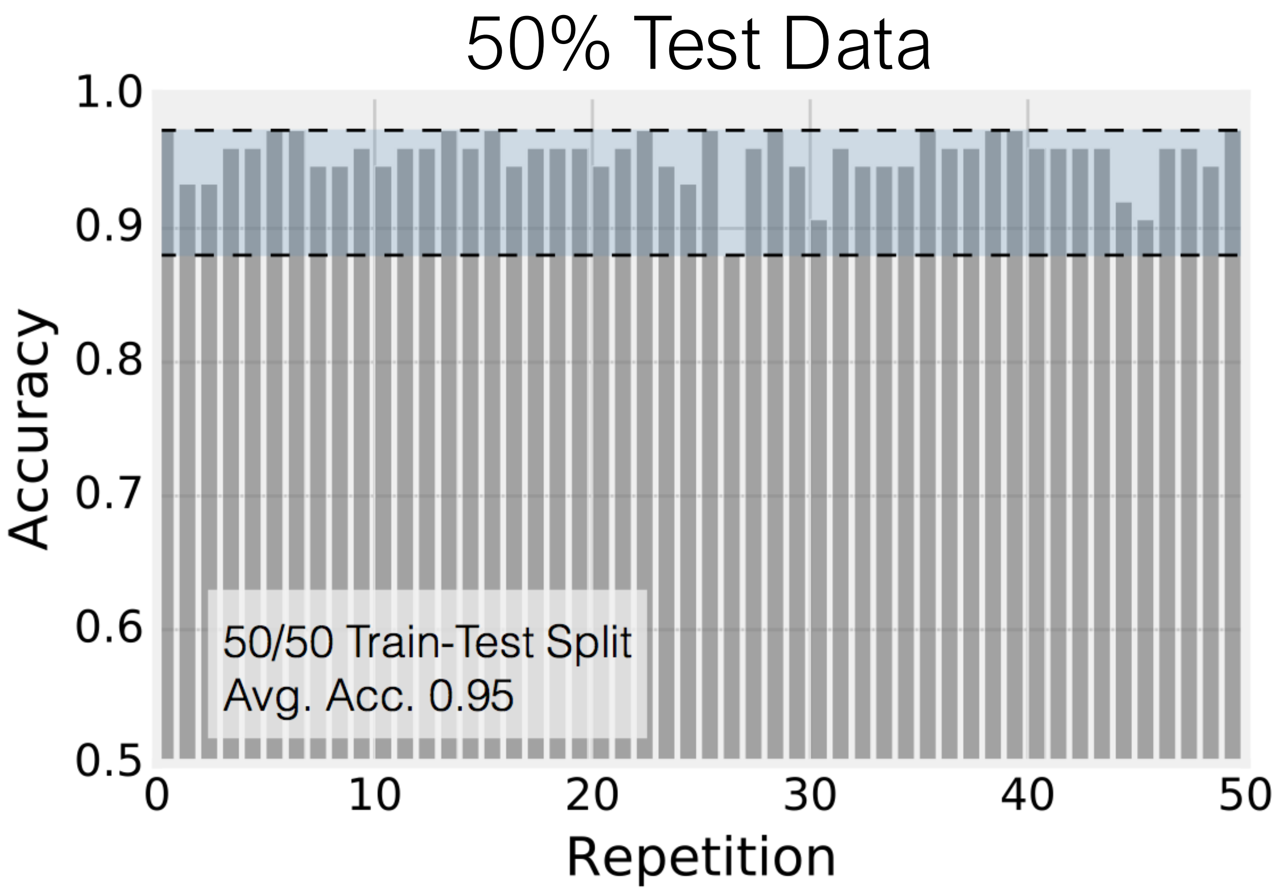
- Train/test split sampling
- Noise in the data
- Errors in the target variable

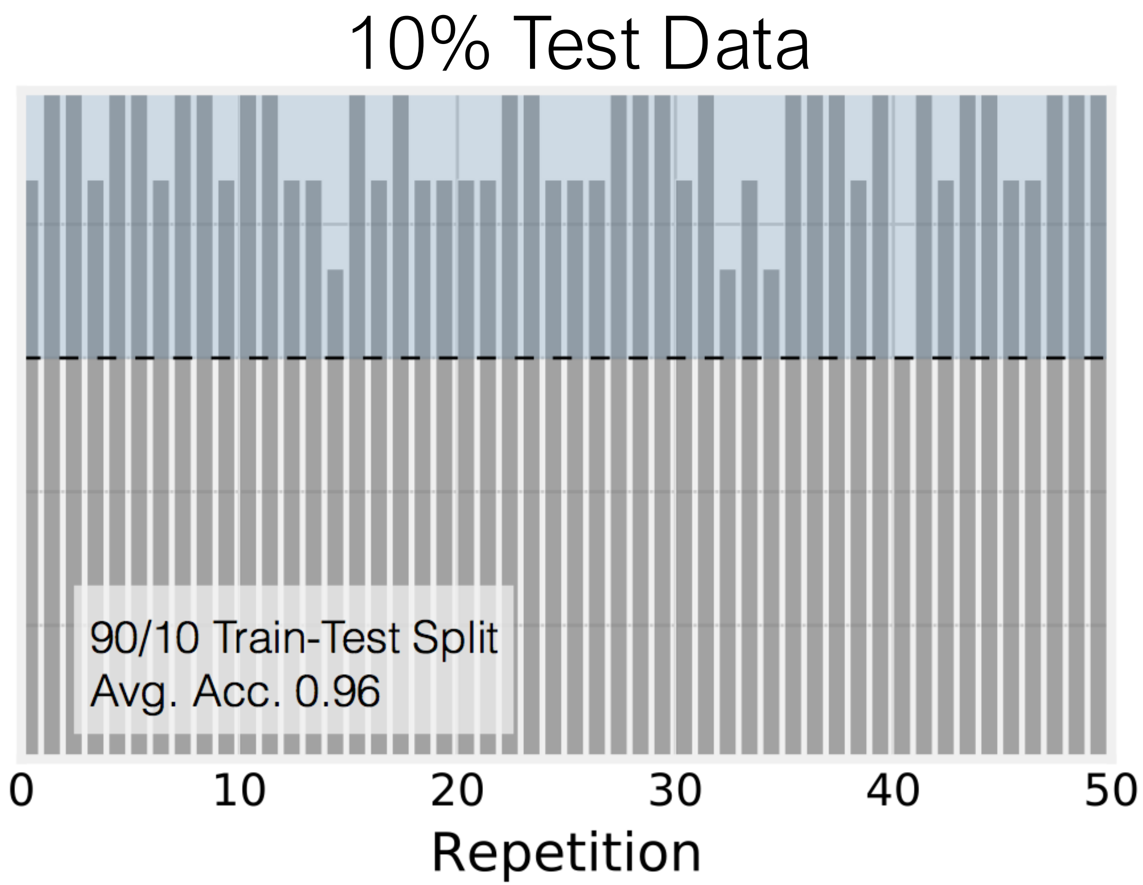
Solution: retrain the model multiple times, varying the variable components; evaluate the variation of the estimates

Different data splits produce different results

Each bar represents test performance for model trained on different random splits of data

Smaller test datasets lead to greater variance in the estimate of generalization performance

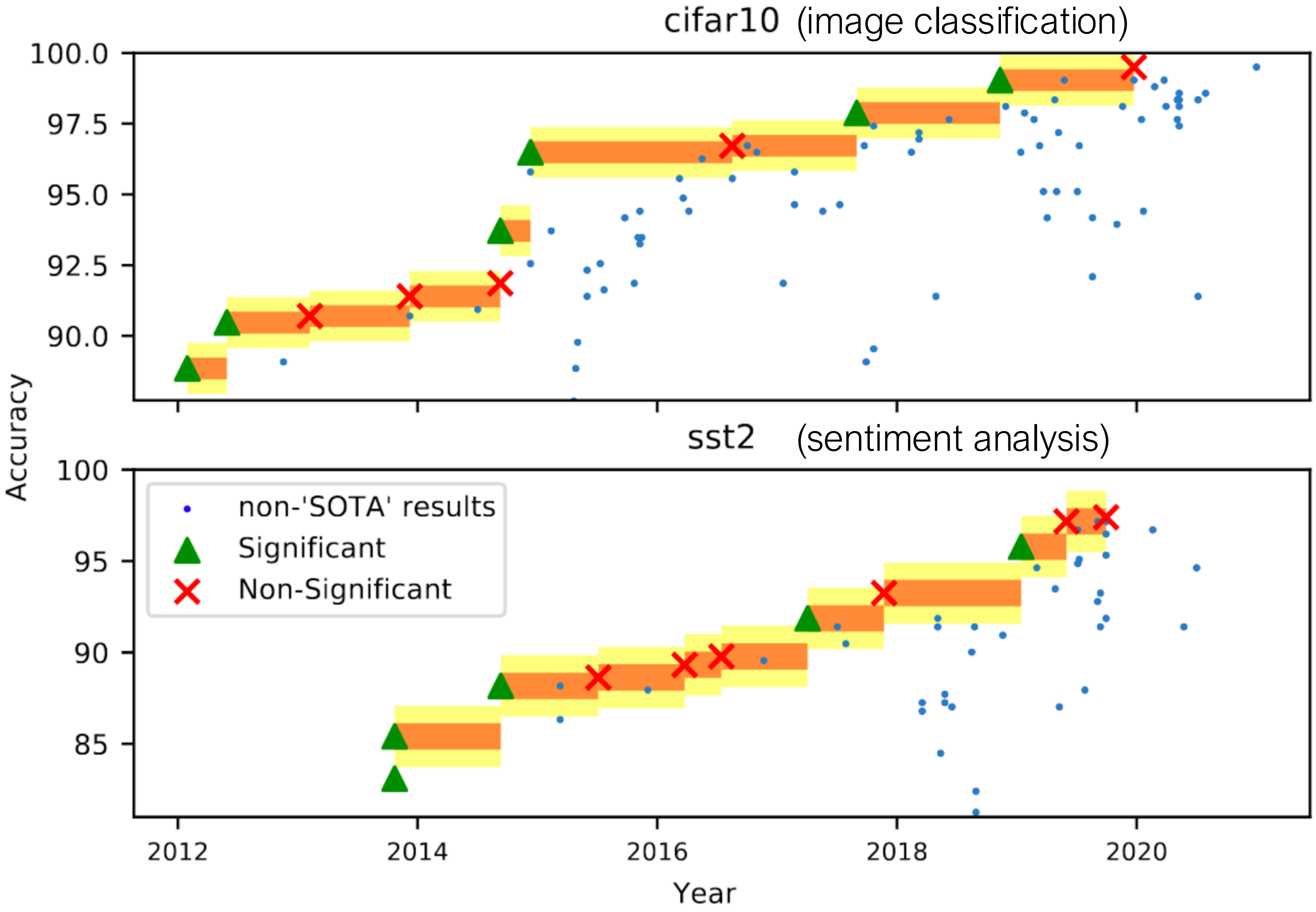




Images from Sebastian Raschka (https://sebastianraschka.com/blog/2016/model-evaluation-selection-part2.html)

Iris dataset, KNN, k=3

Performance metrics have uncertainty



Bouthillier, X., Delaunay, P., Bronzi, M., Trofimov, A., Nichyporuk, B., Szeto, J., Sepah, N., Raff, E., Madan, K., Voleti, V., Kahou, S.E., Michalski, V., Serdyuk, D., Arbel, T., Pal, C., Varoquaux, G., Vincent, P., 2021. Accounting for Variance in Machine Learning Benchmarks. https://doi.org/10.48550/arXiv.2103.03098

Performance metric distributions

Model → **Evaluation Framework** →

Performance metrics

Performance metrics

Performance metrics

Performance metrics

Performance metrics

Performance metrics

Repeat the performance evaluation process allowing stochastic components to vary
(e.g. model initialization, cross validation folds)

The model and evaluation framework are unchanged

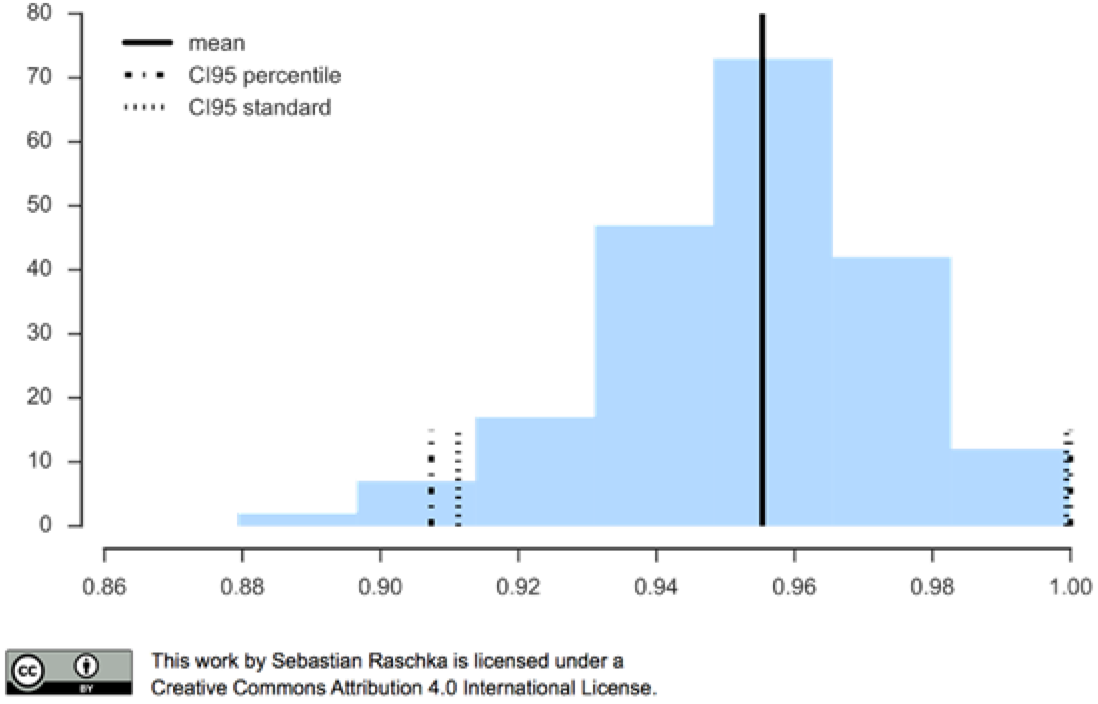


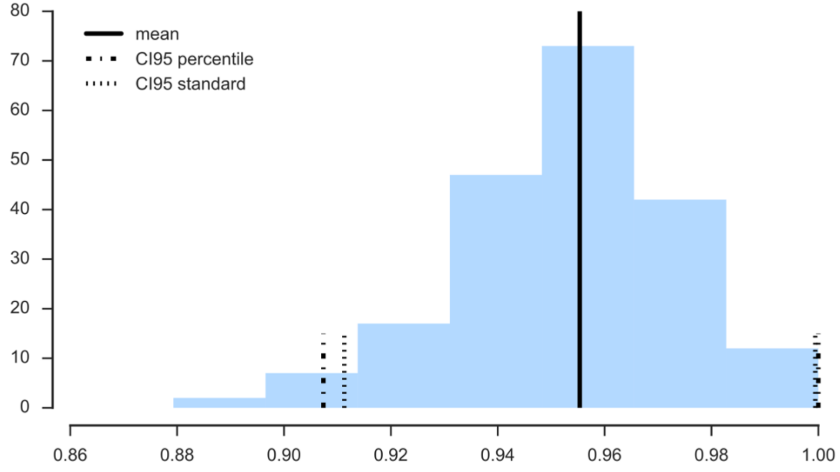
Image from Sebastian Raschka

Confidence intervals via bootstrap sampling

Sampling **with replacement**

Often used to **estimate standard errors and confidence intervals**

Integral part of model ensembles (i.e. bagging in random forests)



Images from Sebastian Raschka

3 Other performance analyses?

Sensitivity / robustness analysis - vary one model hyperparameter and evaluate its effect on performance

Ablation study – remove one or more aspect of a model and compare performance before and after

Example Experimental Design

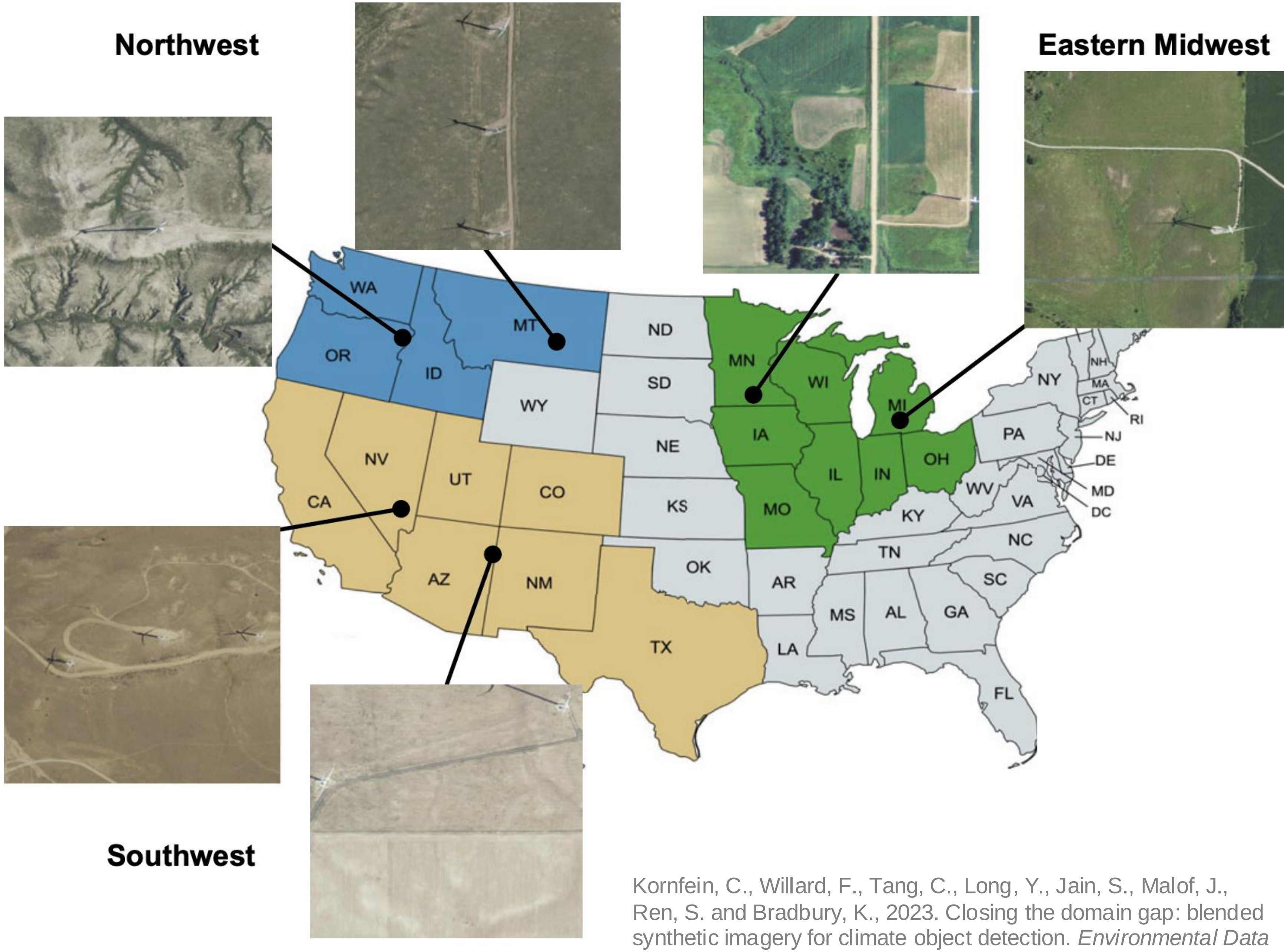
- Enables us to answer questions, typically related to comparing models (e.g. does Model A or Model B perform better)

- Requires that you ONLY vary one characteristic at a time (e.g. model architecture, hyperparameters, training data)
  (unless you are actively looking to estimate the variation induced by that characteristic)

- Requires that you control for uncertainty (in the model AND in the data)

Experimental Design Example

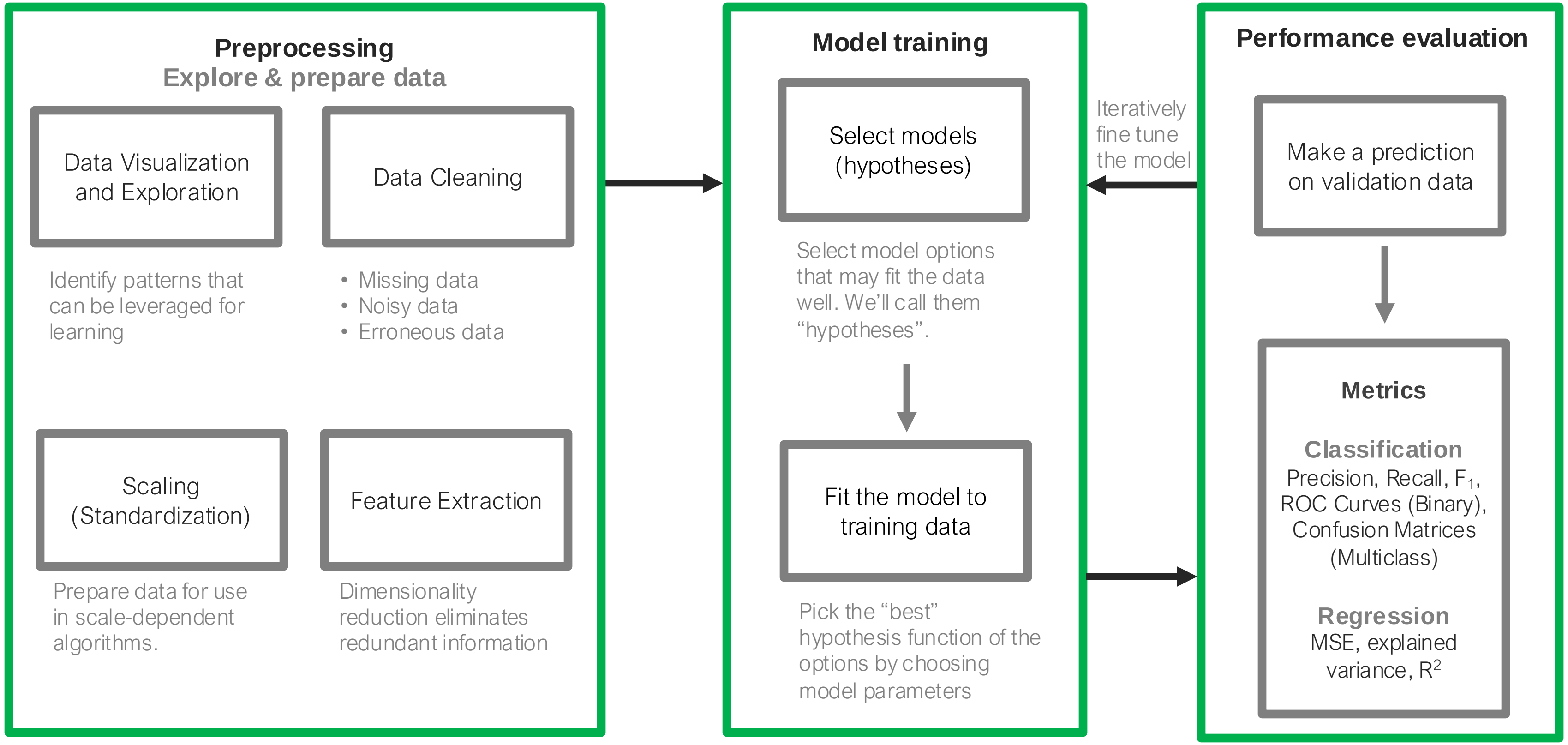
How well do models transfer to new domains?



Kornfein, C., Willard, F., Tang, C., Long, Y., Jain, S., Malof, J., Ren, S. and Bradbury, K., 2023. Closing the domain gap: blended synthetic imagery for climate object detection. *Environmental Data Science*, *2*, p.e39.

Experimental Design

What do we need to check to make sure that there is only one change between experimental conditions?

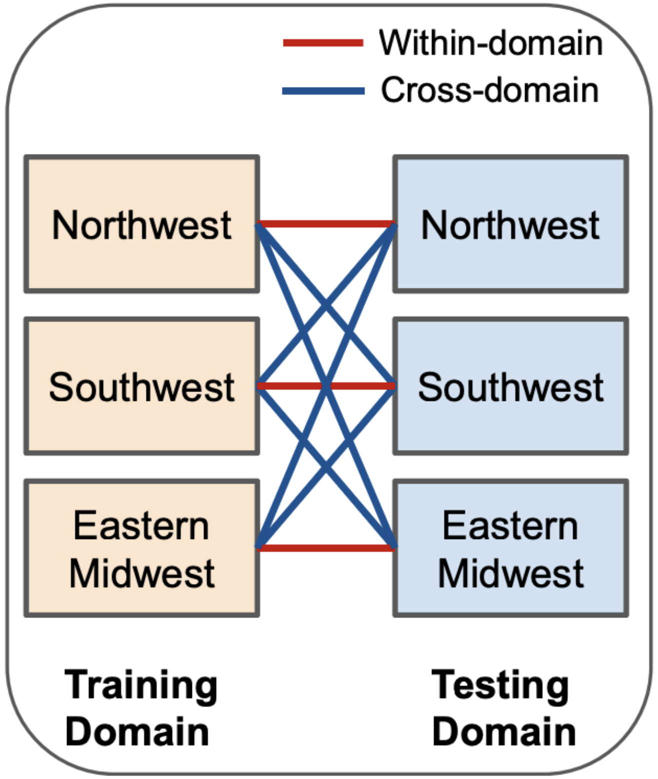


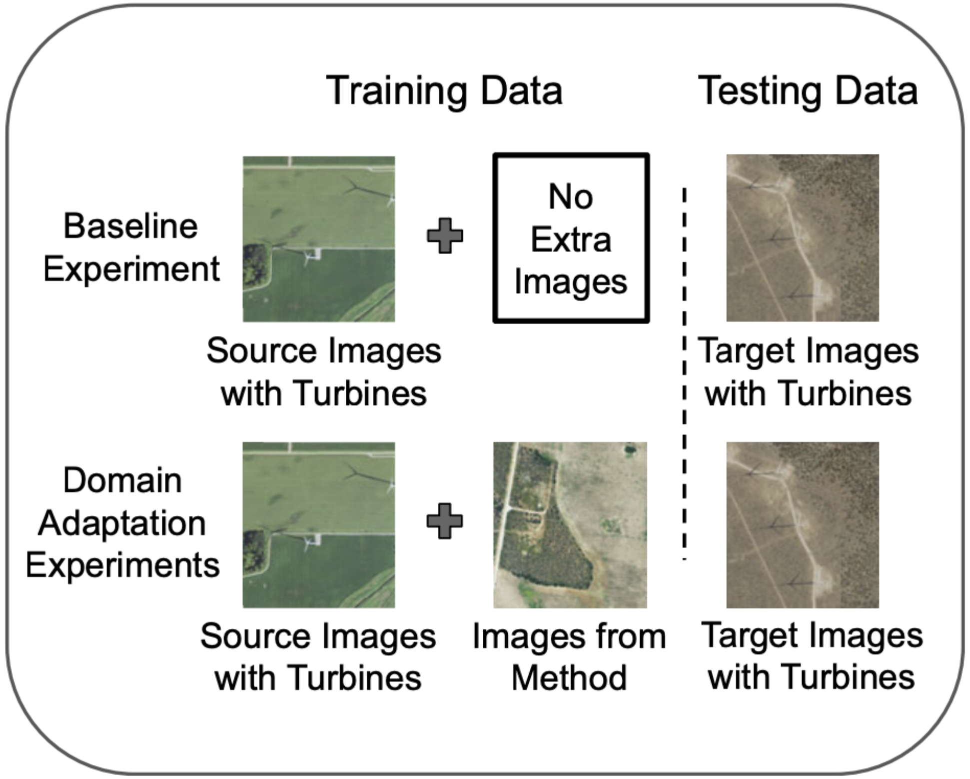
- Train/validation/test split
  - How it was split
  - The split itself
- Data imputation
- Feature selection
- Scaling
- Dimensionality reduction
- Feature transformations

- Model architecture
- Hyperparameters (e.g. learning rate, batch size, stopping criterion, choice of regularization)

Validation / test data should be the same for each model evaluation instance

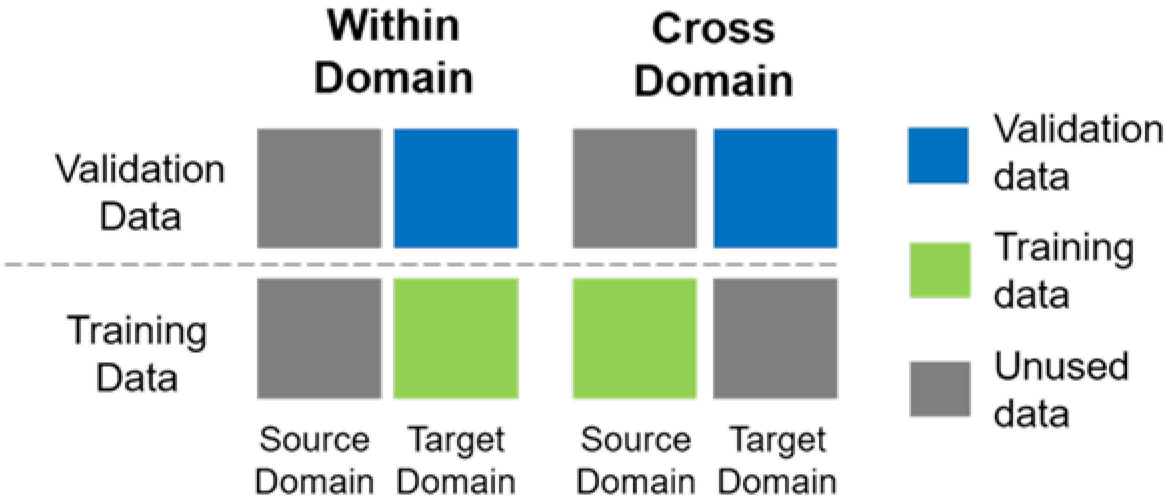
Experimental Design Example





Experimental Design
The only change between experimental conditions was the content of the training data

Training Procedure



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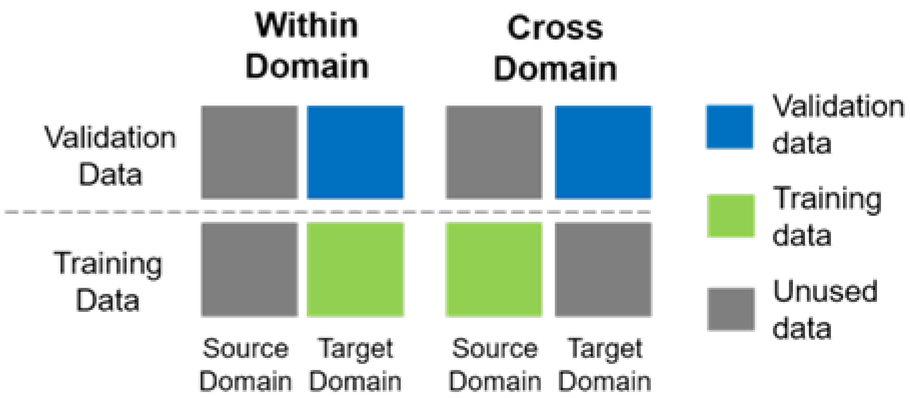
Experimental Design Example

How well do models transfer to new domains?



Results shown in units of mean average precision (mAP)

Source domain	Target domain	Baseline $\pm 2\sigma$	Adding synthetic $\pm 2\sigma$	Average improvement%
EM	EM	0.822 ± 0.067	$\mathbf{0.919} \pm 0.016$	11.8%
NE		0.567 ± 0.019	$\mathbf{0.698} \pm 0.038$	23.1%
NW		0.358 ± 0.061	$\mathbf{0.424} \pm 0.114$	18.4%
SW		0.449 ± 0.160	$\mathbf{0.626} \pm 0.180$	39.4%
EM	NE	0.387 ± 0.031	$\mathbf{0.487} \pm 0.114$	25.8%
NE		0.812 ± 0.028	$\mathbf{0.842} \pm 0.013$	3.7%
NW		0.666 ± 0.061	$\mathbf{0.709} \pm 0.049$	6.5%
SW		0.412 ± 0.045	$\mathbf{0.521} \pm 0.089$	26.5%
EM	NW	0.485 ± 0.064	$\mathbf{0.521} \pm 0.054$	7.4%
NE		0.746 ± 0.018	$\mathbf{0.770} \pm 0.032$	3.2%
NW		0.895 ± 0.071	$\mathbf{0.915} \pm 0.023$	2.2%
SW		0.659 ± 0.111	$\mathbf{0.693} \pm 0.066$	5.2%
EM	SW	0.093 ± 0.016	$\mathbf{0.113} \pm 0.008$	20.9%
NE		0.121 ± 0.029	$\mathbf{0.134} \pm 0.030$	10.7%
NW		0.149 ± 0.029	$\mathbf{0.197} \pm 0.024$	32.2%
SW		0.566 ± 0.035	$\mathbf{0.568} \pm 0.104$	0.4%
Within-domain average		0.774 ± 0.050	$\mathbf{0.811} \pm 0.039$	4.8%
Cross-domain average		0.425 ± 0.054	$\mathbf{0.491} \pm 0.067$	15.7%

Bolded items represent best model (comparing a baseline model and experimental condition model)

Standard deviations contextualize model uncertainty
- This represents retraining the model multiple times to measure performance variability
- For a result to be significant, the performance change needs to be large enough to be unlikely to be due to model variability

Kornfein, C., Willard, F., Tang, C., Long, Y., Jain, S., Malof, J., Ren, S. and Bradbury, K., 2023. Closing the domain gap: blended synthetic imagery for climate object detection. *Environmental Data Science*, *2*, p.e39.

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Modeling Considerations

Accuracy (and techniques to measure it)

Computational Efficiency

Interpretability

Computational Efficiency

Measure of how an algorithm's run time (or space requirements) grows as the input size grows

Complexity of making predictions with kNN
(compare an unseen sample to the training samples)

Assume we have n = 10,000, p = 2

The Euclidean distance between $\begin{bmatrix} x_{1,1} \\ x_{1,2} \end{bmatrix}$ and $\begin{bmatrix} x_{2,1} \\ x_{2,2} \end{bmatrix}$ can be measured as:

$$\sqrt{(x_{2,1} - x_{1,1})^2 + (x_{2,2} - x_{1,2})^2}$$

That's two (p) distinct sets of operations dependent on the data
We repeat that n times – once for each sample in the training dataset

$$O(np)$$

Computational Efficiency

Training time efficiency?

Test time efficiency?

How do each change with the size of our data?

Interpretability

Transparency (can I tell how the model works)

- **Simulatability**: can I contemplate the whole model at once?
- **Decomposability**: is there an intuitive explanation for each part of the model?
  (e.g. all patients with diastolic blood pressure over 150)

Explainability (post-hoc explanations)

Visualization, local explanations, explanations by example

(e.g. this tumor is classified as malignant because to the model it looks a lot like these other tumors)

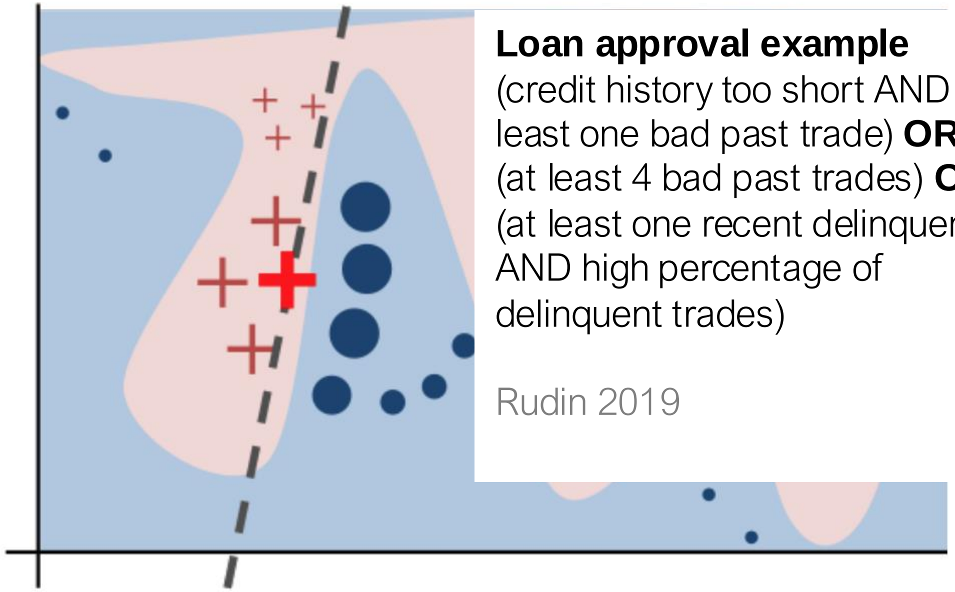
Lipton, Zachary C. "The Mythos of Model Interpretability: In Machine Learning, the Concept of Interpretability Is Both Important and Slippery." Queue 16, no. 3 (2018): 31–57.

Recidivism prediction algorithm

Performance as good as a black box model with 130+ factors; might include socio-economic info; expensive (software license); within software used in US justice system

IF	age between 18-20 and sex is male	THEN predict arrest (within 2 years)
ELSE IF	age between 21-23 and 2-3 prior offences	THEN predict arrest
ELSE IF	more than three priors	THEN predict arrest
ELSE	predict no arrest	

Rudin, Cynthia. "Stop Explaining Black Box Machine Learning Models for High Stakes Decisions and Use Interpretable Models Instead." Nature Machine Intelligence 1, no. 5 (2019): 206–15.



Loan approval example
(credit history too short AND at least one bad past trade) **OR** (at least 4 bad past trades) **OR** (at least one recent delinquency AND high percentage of delinquent trades)

Rudin 2019

Ribeiro, Marco Tulio, Sameer Singh, and Carlos Guestrin. "Model-Agnostic Interpretability of Machine Learning." ArXiv Preprint ArXiv:1606.05386, 2016.

For further reading…

Raschka, Sebastian. “Model Evaluation, Model Selection, and Algorithm Selection in Machine Learning.” *ArXiv:1811.12808 [Cs, Stat]*, November 10, 2020. http://arxiv.org/abs/1811.12808.

Kohavi, Ron. “A Study of Cross-Validation and Bootstrap for Accuracy Estimation and Model Selection.” In *IJCAI*, 14:1137–45. Montreal, Canada, 1995. (link)