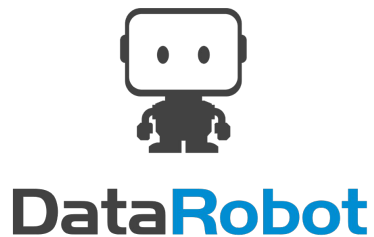


Target Leakage in ML

Yuriy Guts





Machine Learning Engineer

Automated ML, time series forecasting, NLP

Lecturer

AI, Machine Learning, Summer/Winter ML Schools

Compete sometimes

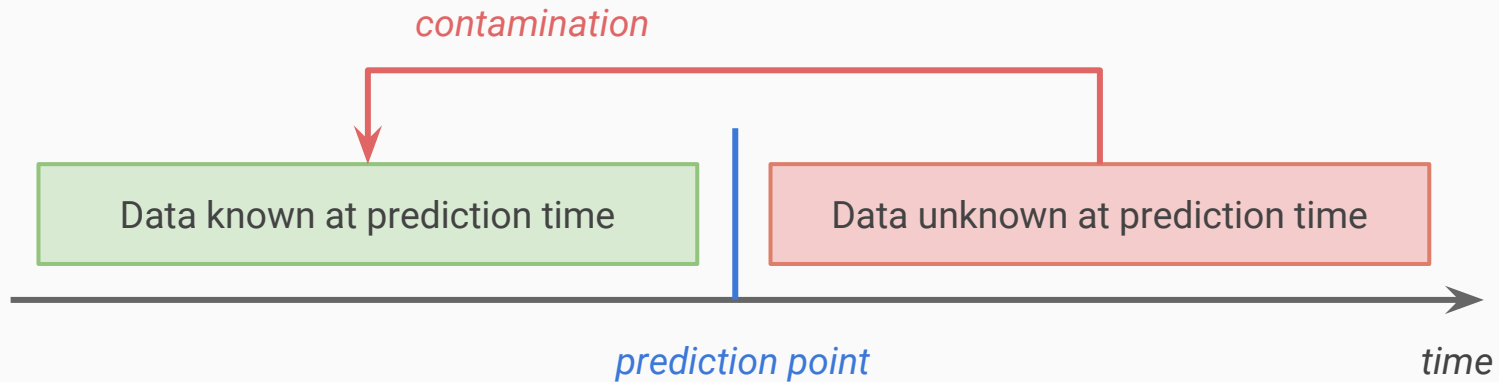
Currently hold an Expert rank, top 2% worldwide



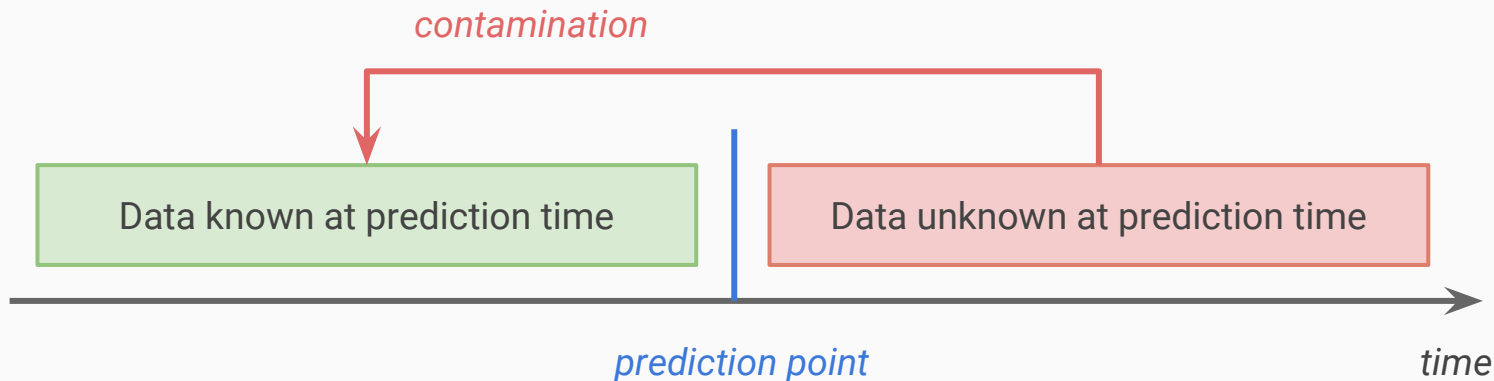
Follow my presentation and code at:

<https://github.com/YuriyGuts/odsc-target-leakage-workshop>

Leakage in a Nutshell



Leakage in a Nutshell



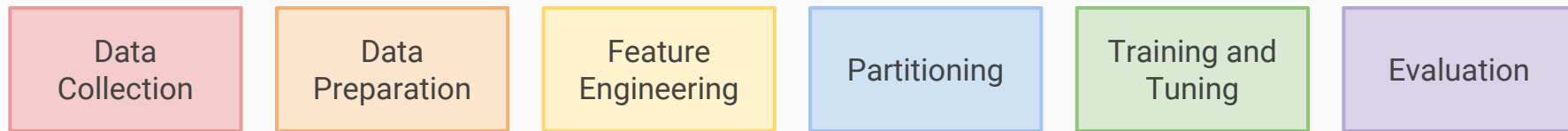
Training on **contaminated data** leads to overly optimistic expectations about model performance in production

"But I always validate on random K-fold CV. I should be fine, right?"



They suspect nothing





Leakage can happen anywhere during the project lifecycle



Leakage in Data Collection

Where is the leakage?

EmployeeID	Title	ExperienceYears	MonthlySalaryGBP	AnnualIncomeUSD
315981	Data Scientist	3	5,000.00	78,895.44
4691	Data Scientist	4	5,500.00	86,784.98
23598	Data Scientist	5	6,200.00	97,830.35

Target is a function of another column

EmployeeID	Title	ExperienceYears	MonthlySalaryGBP	AnnualIncomeUSD
315981	Data Scientist	3	5,000.00	78,895.44
4691	Data Scientist	4	5,500.00	86,784.98
23598	Data Scientist	5	6,200.00	97,830.35

The target can have different formatting or measurement units in different columns.

Forgetting to remove the copies will introduce target leakage.

Check out the example: **example-01-data-collection.ipynb**

Where is the leakage?

SubscriberID	Group	DailyVoiceUsage	DailySMSUsage	DailyDataUsage	Gender
24092091	M18-25	15.31	25	135.10	0
4092034091	F40-60	35.81	3	5.01	1
329815	F25-40	13.09	32	128.52	1
94721835	M25-40	18.52	21	259.34	0

Feature is an aggregate of the target

SubscriberID	Group	DailyVoiceUsage	DailySMSUsage	DailyDataUsage	Gender
24092091	M18-25	15.31	25	135.10	0
4092034091	F40-60	35.81	3	5.01	1
329815	F25-40	13.09	32	128.52	1
94721835	M25-40	18.52	21	259.34	0

E.g., the data can have derived columns created after the fact for reporting purposes

Where is the leakage?

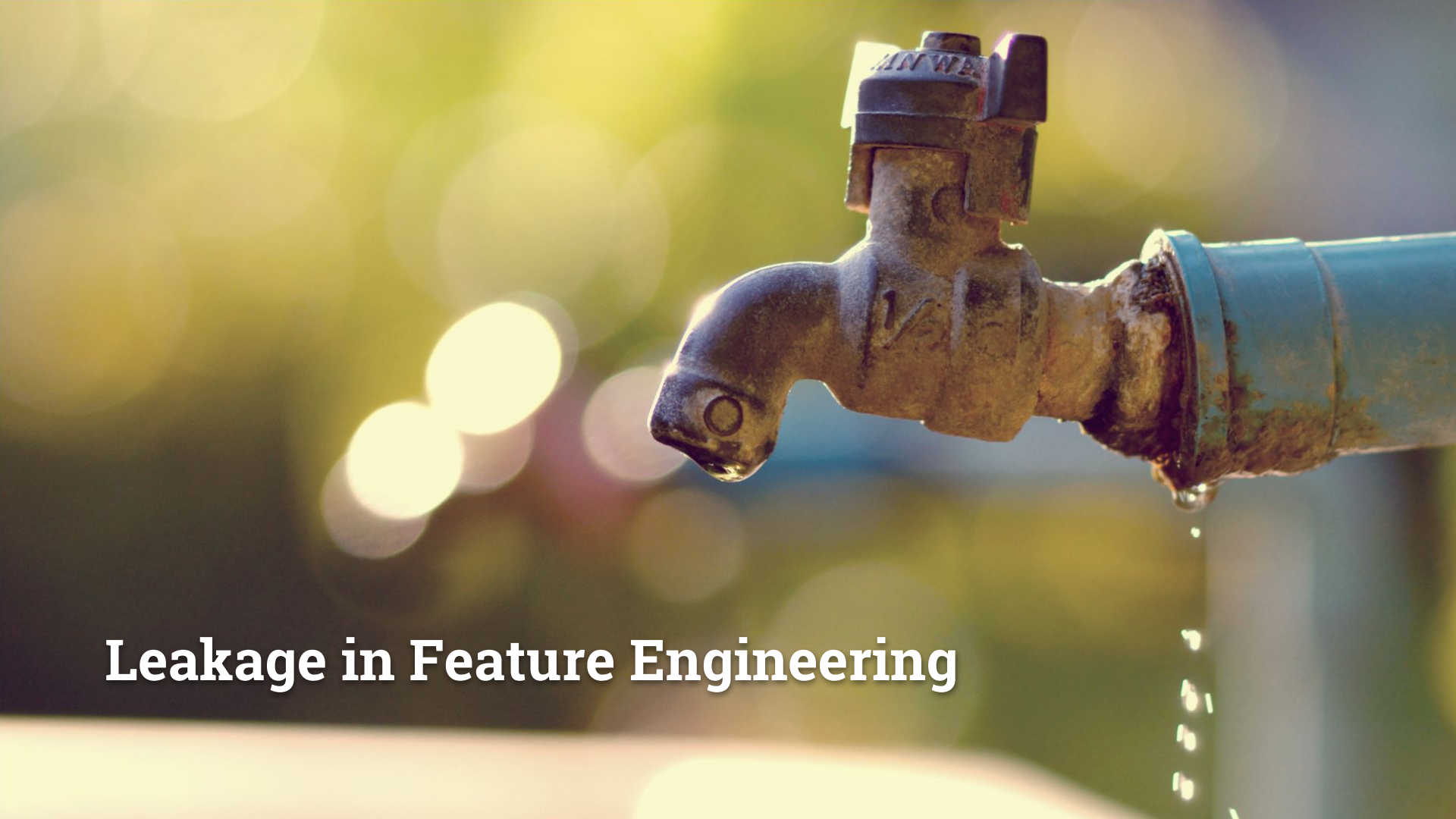
Education	Married	AnnualIncome	Purpose	LatePaymentReminders	IsBadLoan
1	Y	80k	Car Purchase	0	0
3	N	120k	Small Business	3	1
1	Y	85k	House Purchase	5	1
2	N	72k	Marriage	1	0

Mutable data due to lack of snapshot-ability

Education	Married	AnnualIncome	Purpose	LatePaymentReminders	IsBadLoan
1	Y	80k	Car Purchase	0	0
3	N	120k	Small Business	3	1
1	Y	85k	House Purchase	5	1
2	N	72k	Marriage	1	0

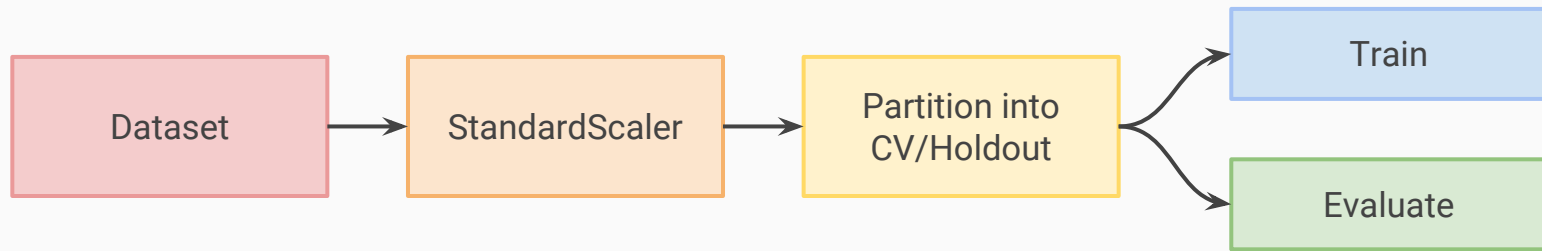
Database records get overwritten as more facts become available.

But these later facts won't be available at prediction time.

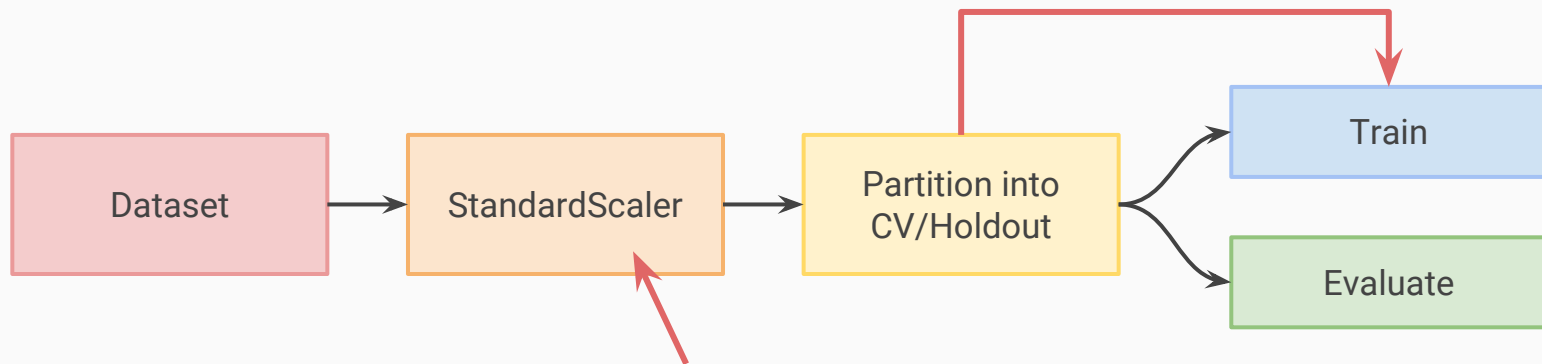


Leakage in Feature Engineering

My model is sensitive to feature scaling...



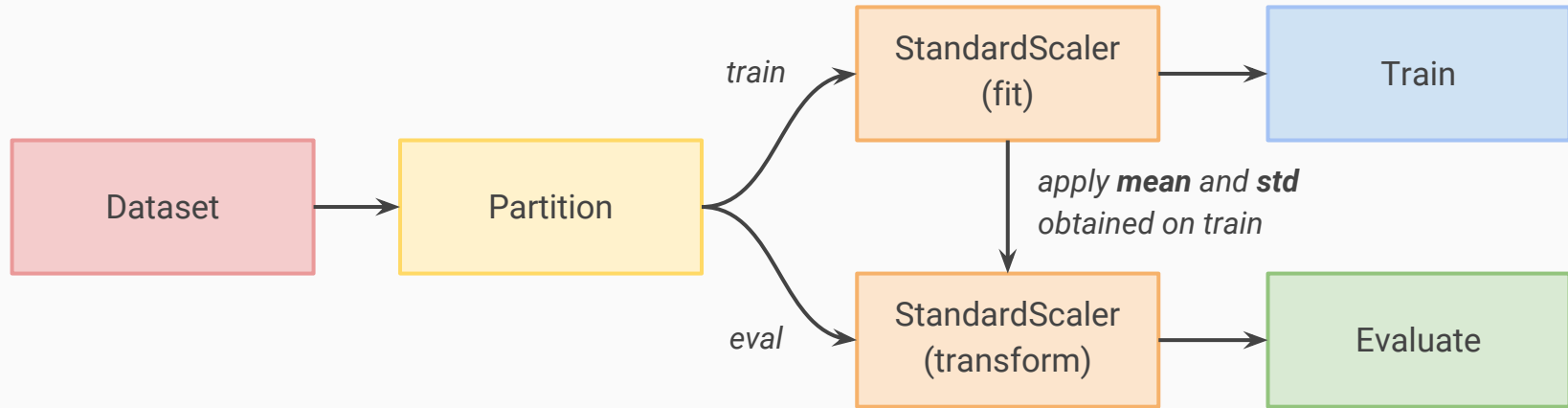
My model is sensitive to feature scaling...



OOPS. WE'RE LEAKING THE TEST FEATURE DISTRIBUTION INFO INTO THE TRAINING SET

Check out the example: **example-02-data-prep.ipynb**

Removing leakage in feature engineering



Obtain feature engineering/transformation parameters only on the training set

Apply them to transform the evaluation sets (CV, holdout, backtests, ...)

Encoding of different variable types

Text:

Learn DTM columns from the **training set only**, then transform the evaluation sets
(avoid leaking possible out-of-vocabulary words into the training pipeline)

Categoricals:

Create mappings on the **training set only**, then transform the evaluation sets
(avoid leaking cardinality/frequency info into the training pipeline)

Leakage in Partitioning





Andrew Ng ✓

@AndrewYNg

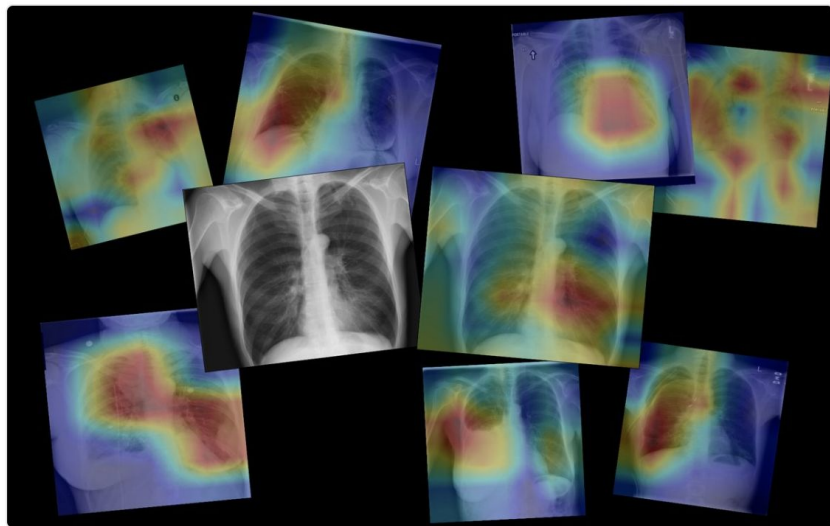
Follow



Our full paper on Deep Learning for pneumonia detection on Chest X-Rays.

@pranavrajpurkar @jeremy_irvin16

@matlungrenMD arxiv.org/abs/1711.05225



9:09 PM - 15 Nov 2017 from [Mountain View, CA](#)

665 Retweets 1,352 Likes





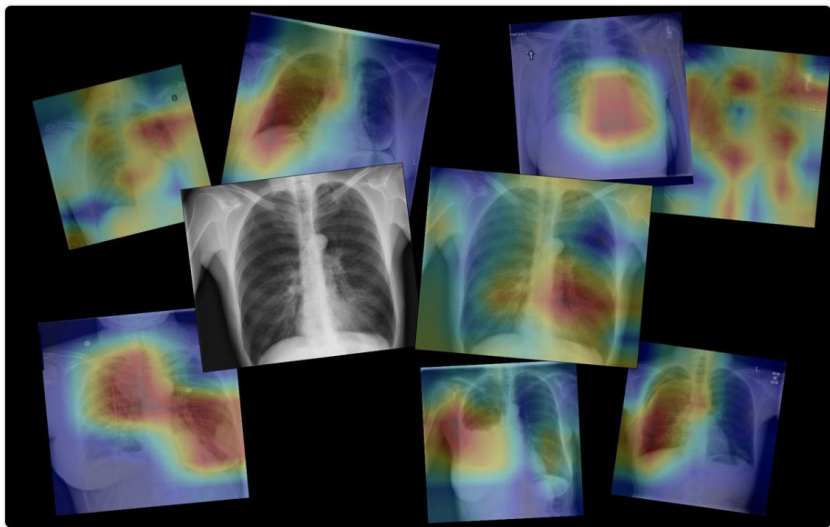
Andrew Ng ✓

@AndrewYNg

Follow



Our full paper on Deep Learning for pneumonia detection on Chest X-Rays.
[@pranavrajpurkar](#) [@jeremy_irvin16](#)
[@mattlungrenMD](#) arxiv.org/abs/1711.05225



9:09 PM - 15 Nov 2017 from Mountain View, CA

665 Retweets 1,352 Likes



3. Data

3.1. Training

We use the ChestX-ray14 dataset released by Wang et al. (2017) which contains 112,120 frontal-view X-ray images of 30,805 unique patients. Wang et al. (2017) annotate each image with up to 14 different thoracic pathology labels using automatic extraction methods on radiology reports. We label images that have pneumonia as one of the annotated pathologies as positive examples and label all other images as negative examples for the pneumonia detection task. We randomly split the entire dataset into 80% training, and 20% validation.

Before inputting the images into the network, we downscale the images to 224×224 and normalize based on the mean and standard deviation of images in the ImageNet training set. We also augment the training data with random horizontal flipping.

<https://twitter.com/AndrewYNg/status/931026446717296640>

Group Leakage



Nick Roberts

@nizkroberts

Follow



Replying to @AndrewYNg @pranavrajpurkar and 2 others

Were you concerned that the network could memorize patient anatomy since patients cross train and validation?

“ChestX-ray14 dataset contains 112,120 frontal-view X-ray images of 30,805 unique patients. We randomly split the entire dataset into 80% training, and 20% validation.”

OOPS. THERE ARE FOUR TIMES MORE UNIQUE IMAGES THAN PATIENTS

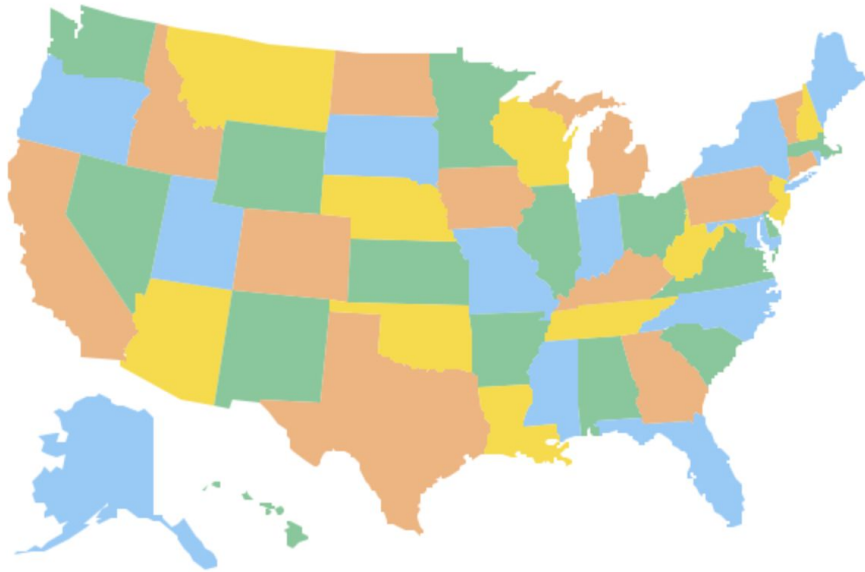
ples. For the pneumonia detection task, we randomly split the dataset into training (28744 patients, 98637 images), validation (1672 patients, 6351 images), and test (389 patients, 420 images). There is no patient overlap between the sets.

Pathology	Wang et al. (2017)	Yao et al. (2017)	CheXNet (ours)
Atelectasis	0.716	0.772	0.8209
Cardiomegaly	0.807	0.904	0.9048
Effusion	0.784	0.859	0.8831
Infiltration	0.609	0.695	0.7204
Mass	0.706	0.792	0.8618
Nodule	0.671	0.717	0.7766
Pneumonia	0.633	0.713	0.7632
Pneumothorax	0.806	0.841	0.8932
Consolidation	0.708	0.788	0.7939
Edema	0.835	0.882	0.8932
Emphysema	0.815	0.829	0.9260
Fibrosis	0.769	0.767	0.8044
Pleural Thickening	0.708	0.765	0.8138
Hernia	0.767	0.914	0.9387

Paper v1 (AUC)

CheXNet (ours)
0.8094
0.9248
0.8638
0.7345
0.8676
0.7802
0.7680
0.8887
0.7901
0.8878
0.9371
0.8047
0.8062
0.9164

Paper v3 (AUC)



Observe:



Illinois

Oklahoma



Texas

Predict:



North Carolina

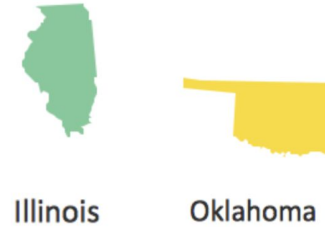
Group Partitioning, Out-of-Group Validation



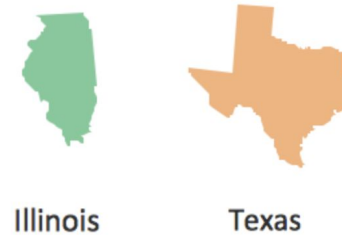
Fold 1

Training:

Validation:



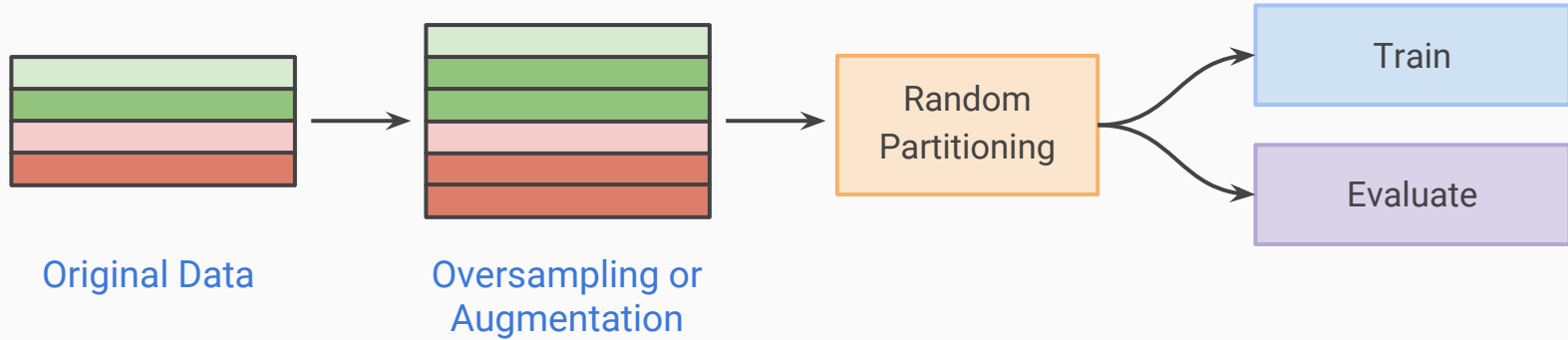
Fold 2



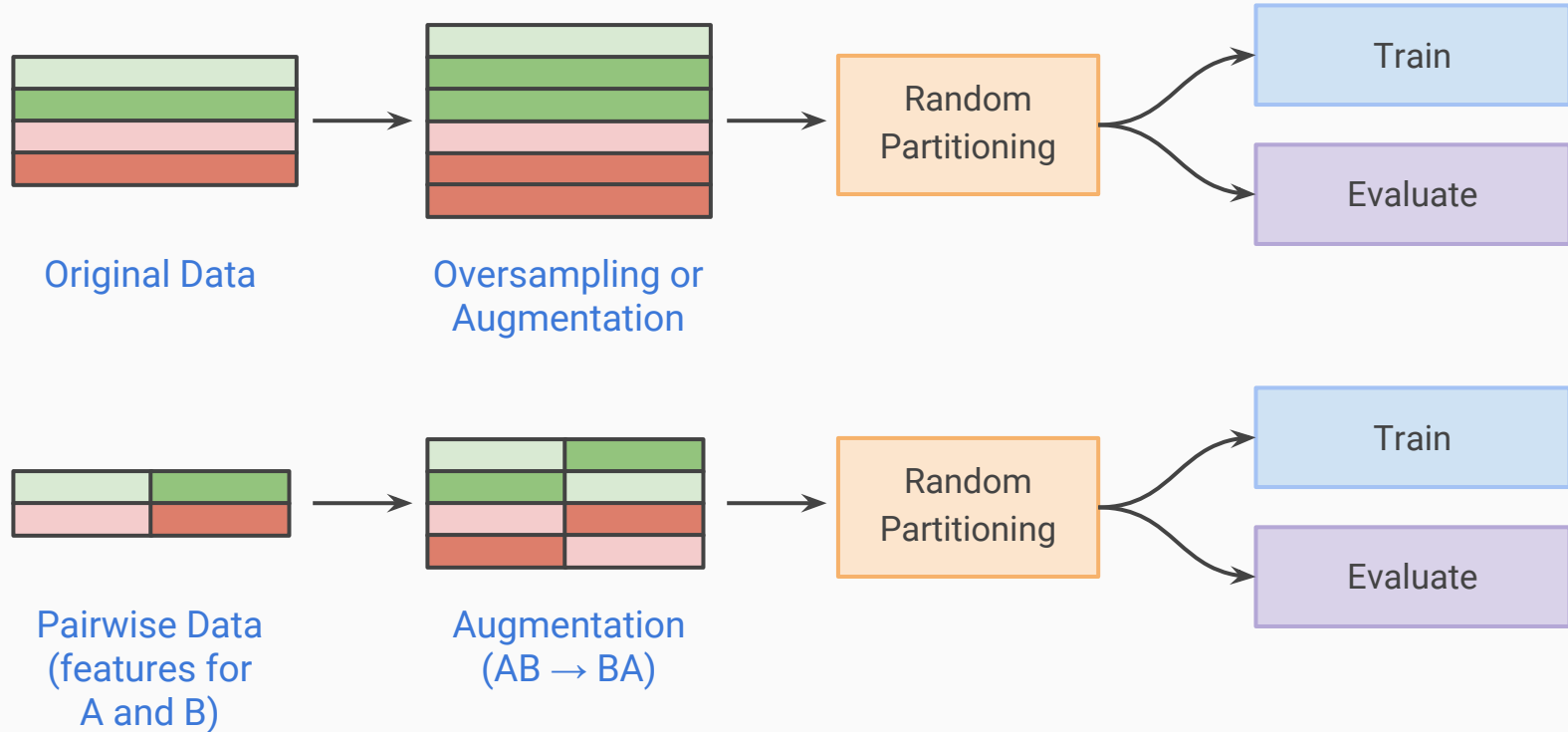
Fold 3



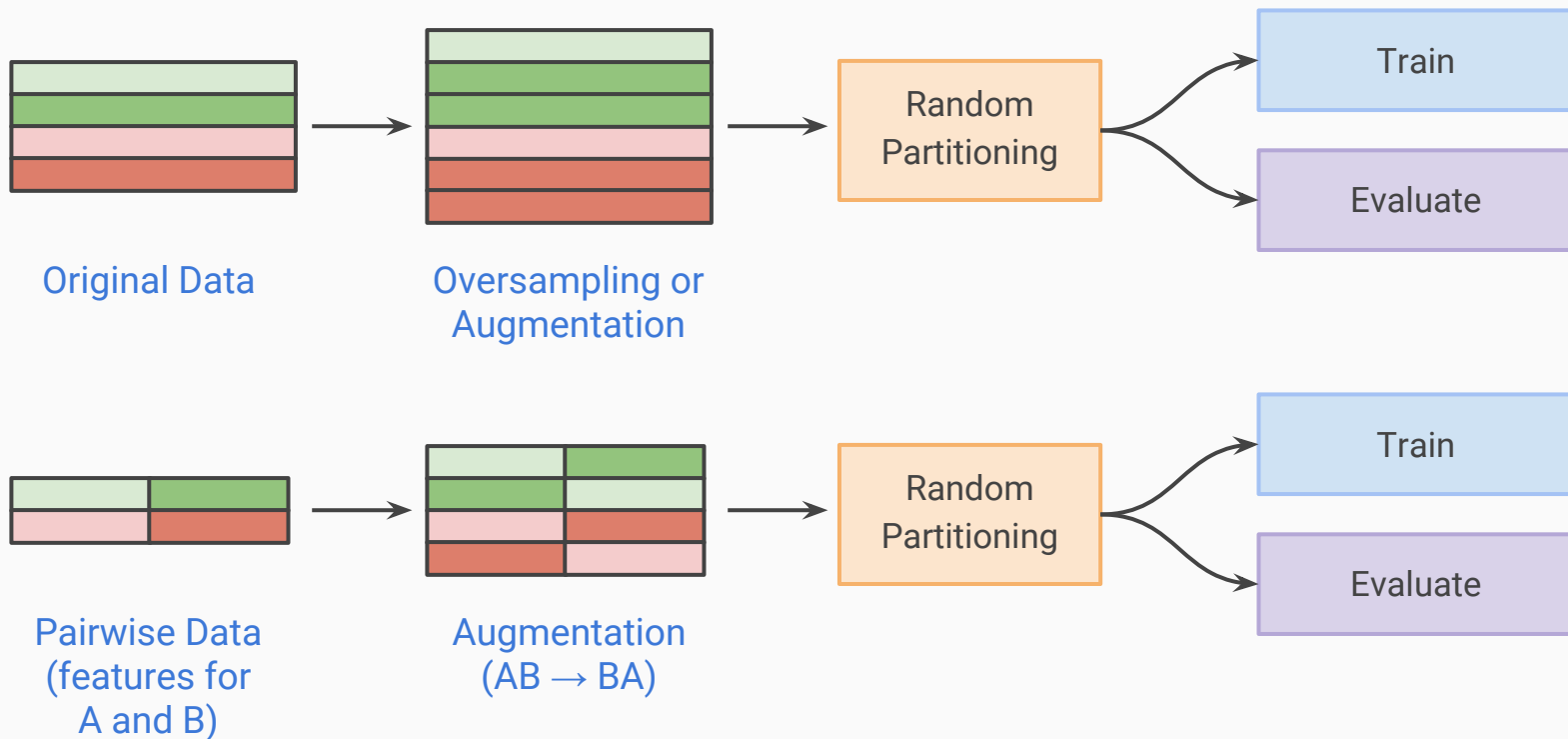
Leakage in oversampling / augmentation



Leakage in oversampling / augmentation

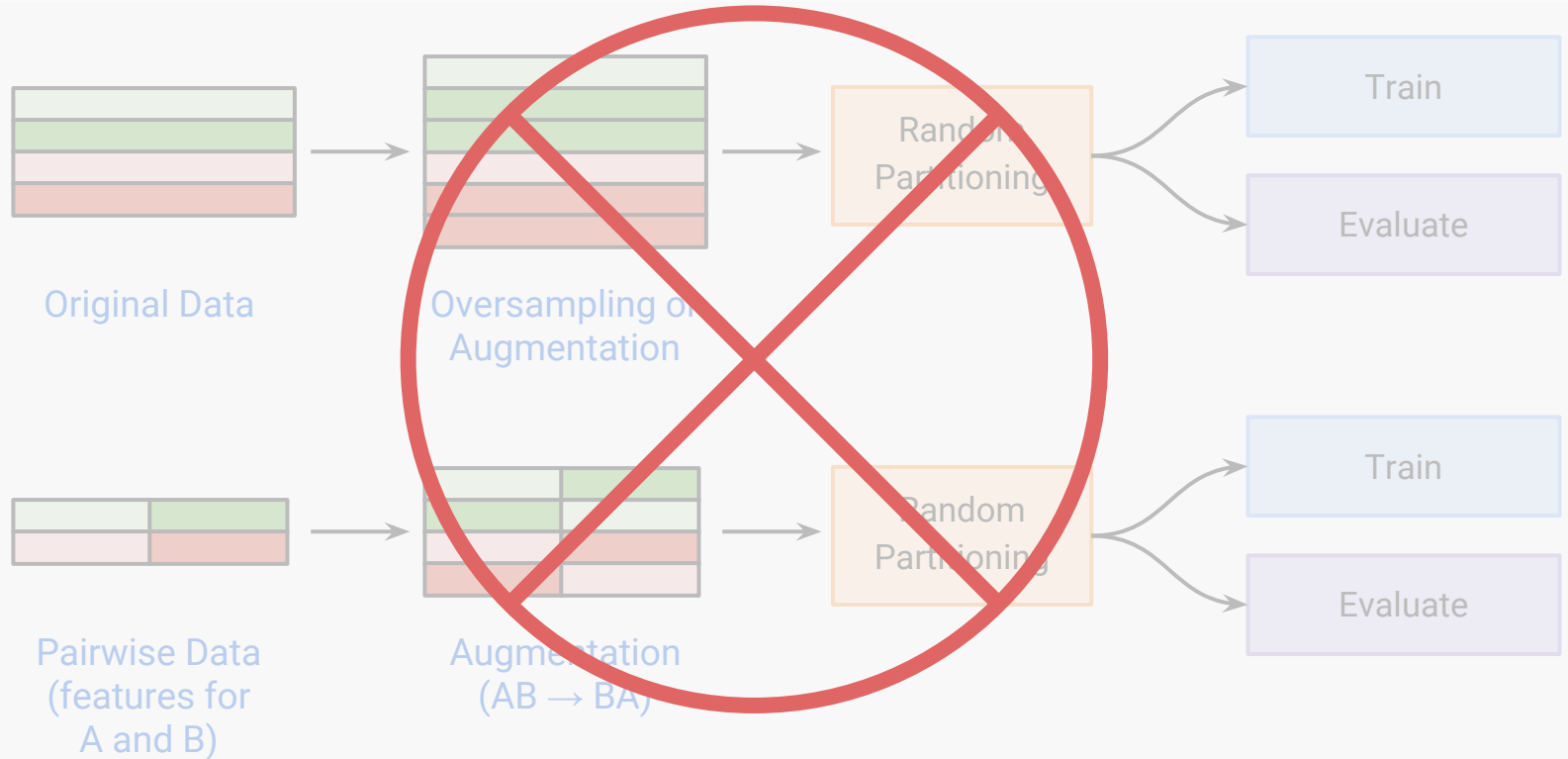


Leakage in oversampling / augmentation



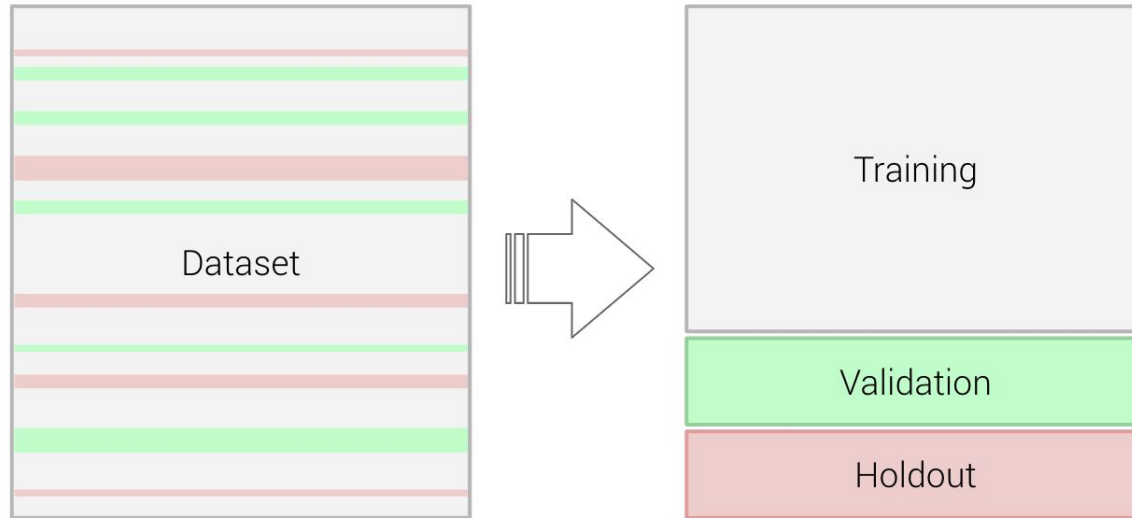
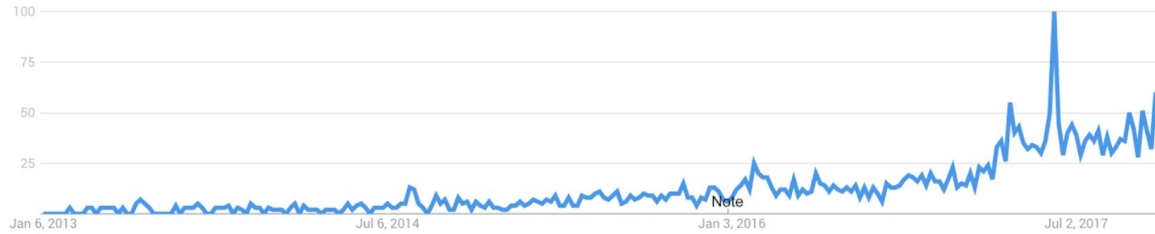
OOPS. WE MAY GET COPIES SPLIT BETWEEN TRAINING AND EVALUATION

Leakage in oversampling / augmentation



First partition, then augment the training data.

Random Partitioning for Time-Aware Models

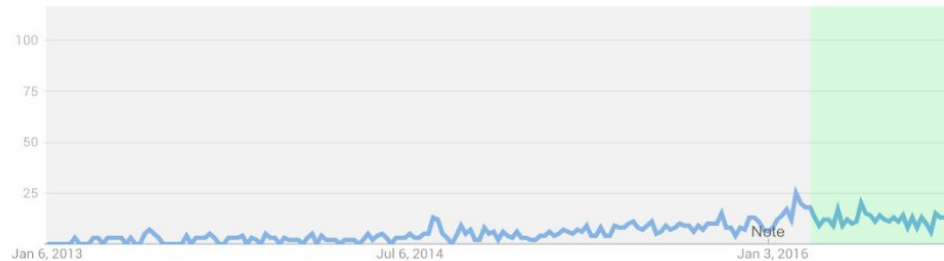


Random Partitioning for Time-Aware Models



Out-of-Time Validation (OTV)

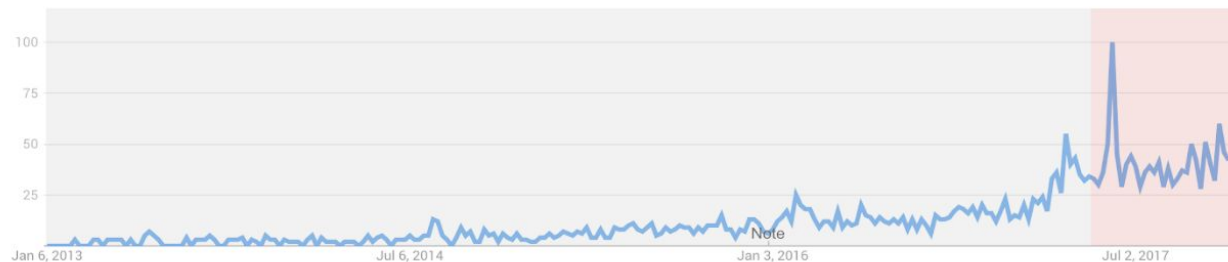
Backtest 2



Backtest 1



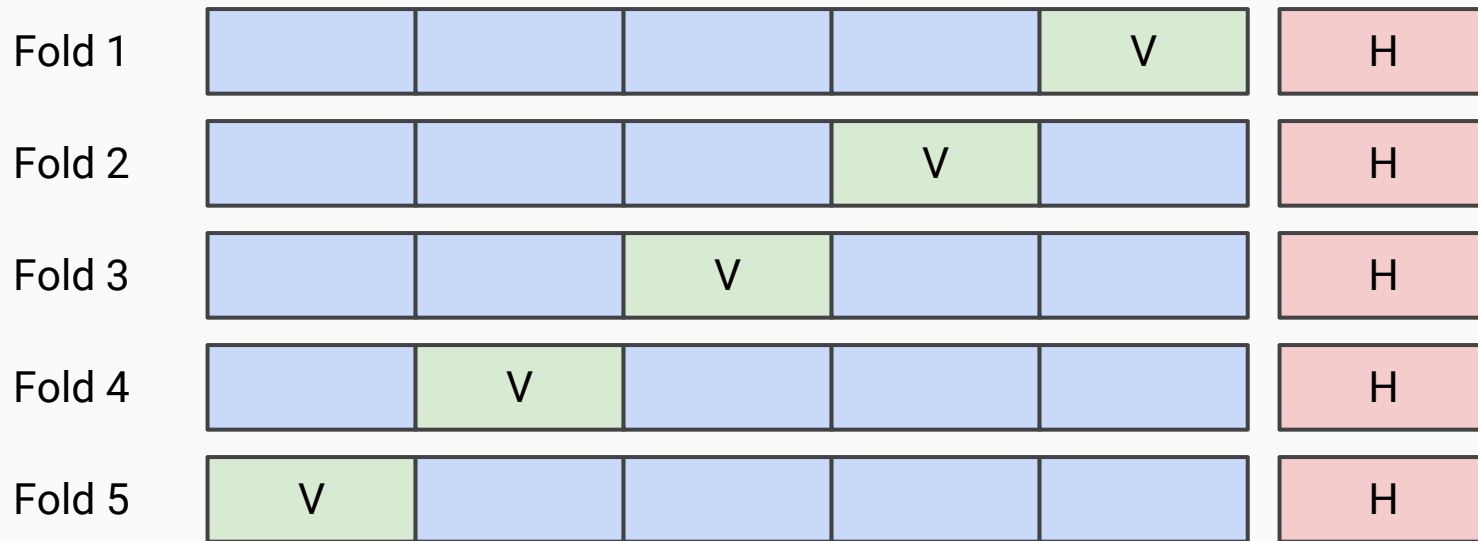
Holdout





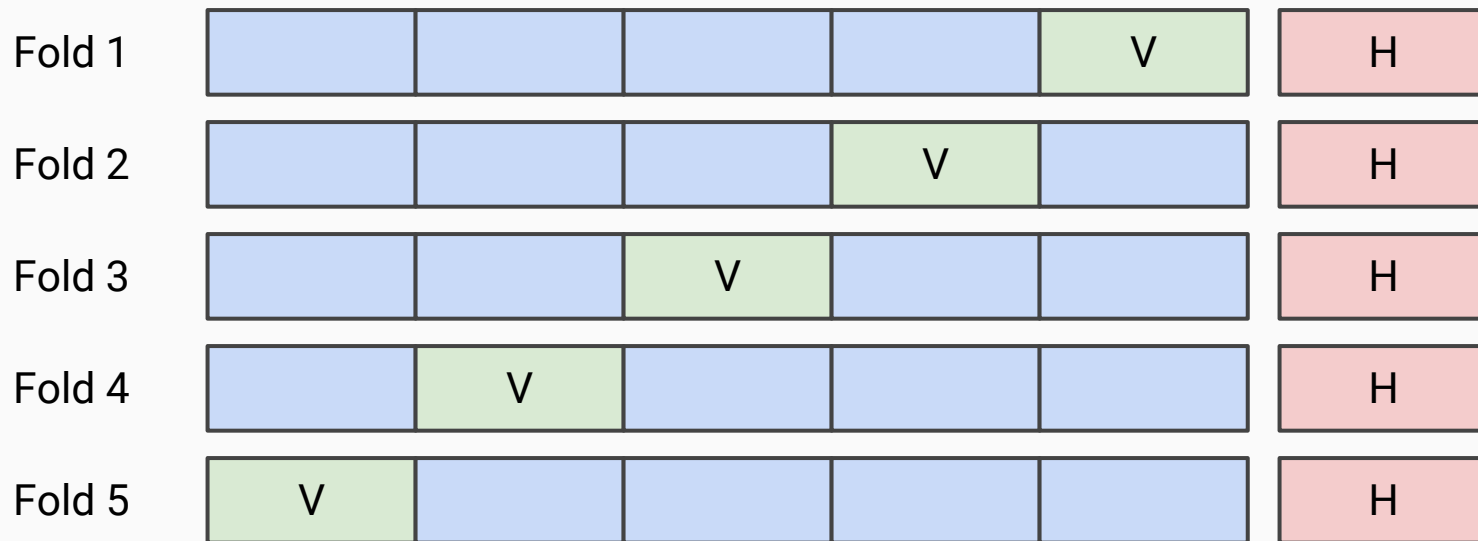
Leakage in Training & Tuning

Reusing a CV split for multiple tasks



Feature selection, hyperparameter tuning, model selection...

Reusing a CV split for multiple tasks



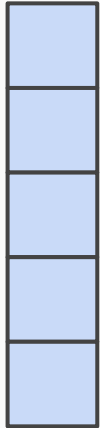
Feature selection, hyperparameter tuning, model selection...

***OOPS. CAN OVERTUNE TO THE VALIDATION SET
BETTER USE DIFFERENT SPLITS FOR DIFFERENT TASKS***

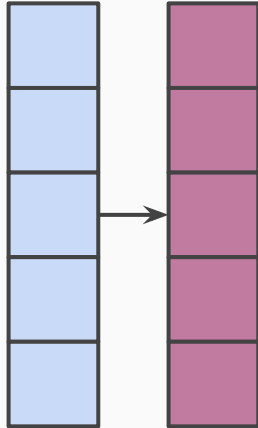
Model stacking on in-sample predictions

Model 1

Train



Predict

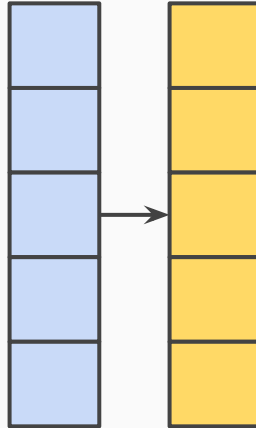


Model 2

Train

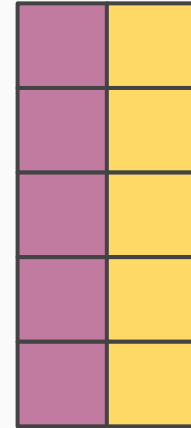


Predict



2nd Level Model

Train



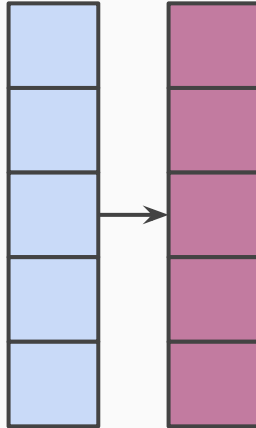
Model stacking on in-sample predictions

Model 1

Train



Predict

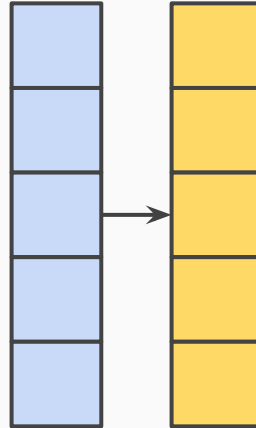


Model 2

Train

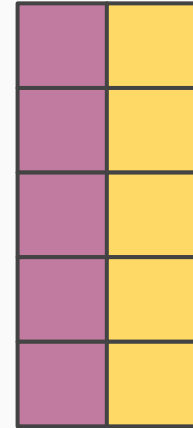


Predict



2nd Level Model

Train

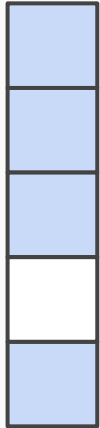


OOPS. WILL LEAK THE TARGET IN THE META-FEATURES

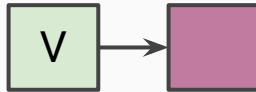
Better way to stack

Model 1

Train



Predict

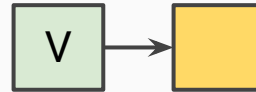


Model 2

Train

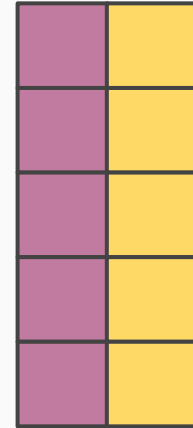


Predict



2nd Level Model

Train



Compute all meta-features only out-of-fold



Leakage in Competitive ML

Case Studies

- Removing user IDs does not necessarily mean data anonymization
(Kaggle: Expedia Hotel Recommendations, 2016)
- Anonymizing feature names does not mean anonymization either
(Kaggle: Santander Value Prediction competition, 2018)
- Target can sometimes be recovered from the metadata or external datasets
(Kaggle: Dato “Truly Native?” competition, 2015)
- Overrepresented minority class in pairwise data enables reverse engineering
(Kaggle: Quora Question Pairs competition, 2017)

Prevention Measures



Leakage prevention checklist (not exhaustive!)

- Split the holdout away immediately and do not preprocess it in any way before final model evaluation.
- Make sure you have a data dictionary and understand the meaning of every column, as well as unusual values (e.g. negative sales) or outliers.
- For every column in the final feature set, try answering the question: “Will I have this feature at prediction time in my workflow? What values can it have?”
- Figure out preprocessing parameters on the training subset, freeze them elsewhere.
- Treat feature selection, model tuning, model selection as separate “machine learning models” that need to be validated separately.
- Make sure your validation setup represents the problem you need to solve with the model.
- Check feature importance and prediction explanations: do top features make sense?

Thank you!

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[linkedin.com/in/yuriyguts](https://www.linkedin.com/in/yuriyguts)