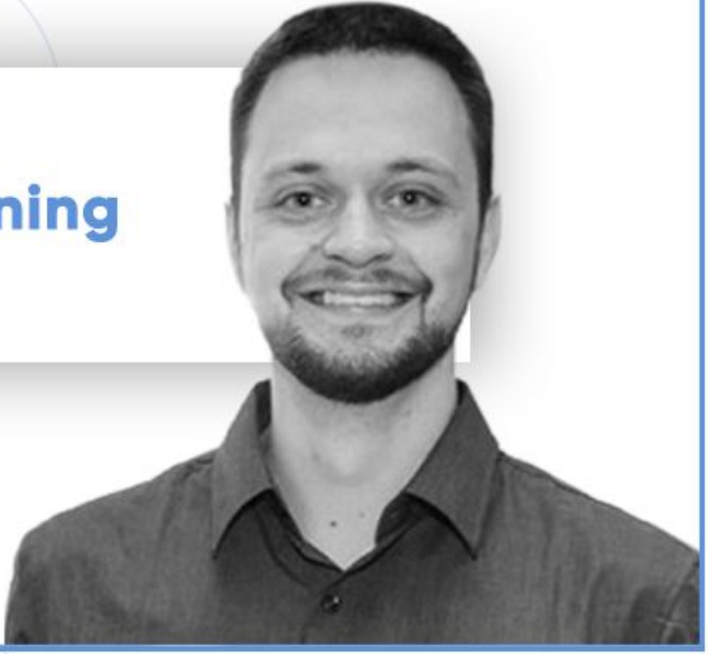
#ODSC

BOSTON

APR 30 - MAY 3

Target Leakage in Machine Learning



Yuriy Guts

Machine Learning Engineer,
DataRobot

DataRobot

Machine Learning Engineer

Automated ML, time series forecasting, NLP

Ukrainian Catholic University
APPLIED SCIENCES FACULTY

Lecturer

AI, Machine Learning, Summer/Winter ML Schools

kaggle™

Compete sometimes

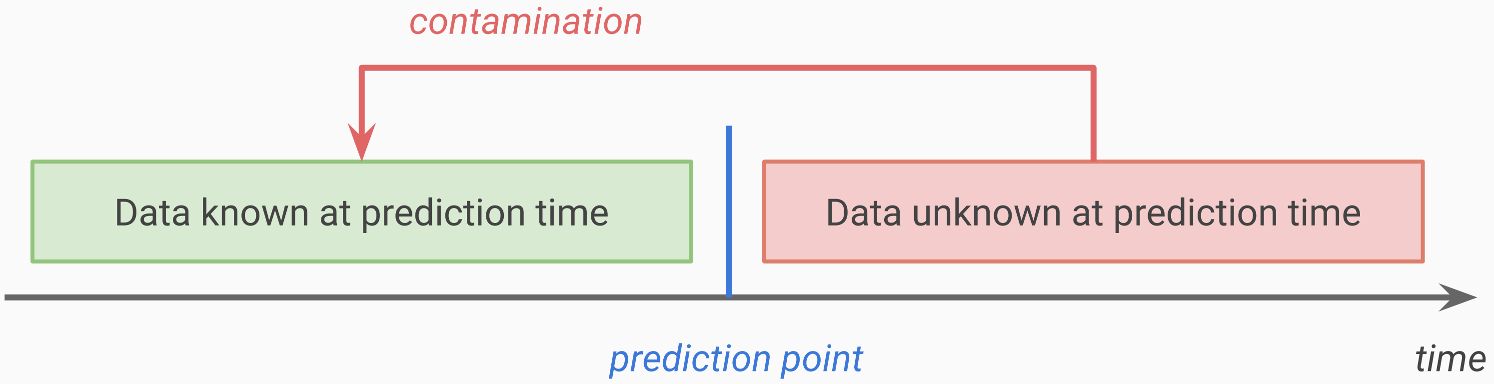
Currently hold an Expert rank, top 2% worldwide

Follow my presentation and code at:

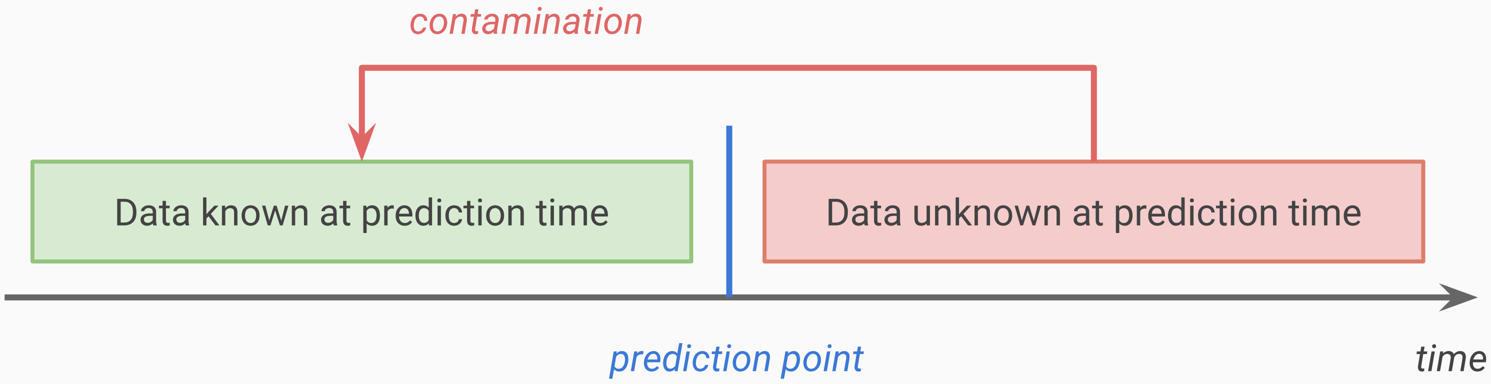
https://github.com/YuriyGuts/odsc-target-leakage-workshop

Target Leakage in ML

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

Data Collection | Data Preparation | Feature Engineering | Partitioning | Training and Tuning | Evaluation

Leakage can happen anywhere during the project lifecycle

Leakage in Data Collection

Where is the leakage?

INSTNM	CITY	STABBR	(500 Cols Skipped)	MD_EARN_WNE_P10
Empire Beauty School-Jackson	Jackson	TN	...	17,100
Geneva College	Beaver Falls	PA	...	38,700
The Art Institute of Austin	Austin	TX	...	34,100
College of Business and Technology-Cutler Bay	Cutler Bay	FL	...	23,800
University of Hartford	West Hartford	CT	...	47,800

Median earnings of students 10 years after entry

Source: **https://collegescorecard.ed.gov/**

Where is the leakage?

INSTNM	CITY	STABBR	MD_EARN_WNE_P6	MD_EARN_WNE_P10
Empire Beauty School-Jackson	Jackson	TN	15,900	17,100
Geneva College	Beaver Falls	PA	33,000	38,700
The Art Institute of Austin	Austin	TX	27,300	34,100
College of Business and Technology-Cutler Bay	Cutler Bay	FL	21,600	23,800
University of Hartford	West Hartford	CT	38,400	47,800

6-year median earnings are highly predictive of 10-year median earnings.
But they are unavailable at prediction (admission) time

Target is a function of another column

MEDIAN_EARNINGS_MONTHLY	MEDIAN_EARNINGS_GROUP	MD_EARN_WNE_P10
1425	LOW	17,100
1985	MED	23,800
3985	HIGH	47,800

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

It can also have derived columns created after the fact for reporting purposes.

Forgetting to remove the copies will introduce target leakage.

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

Where is the leakage?

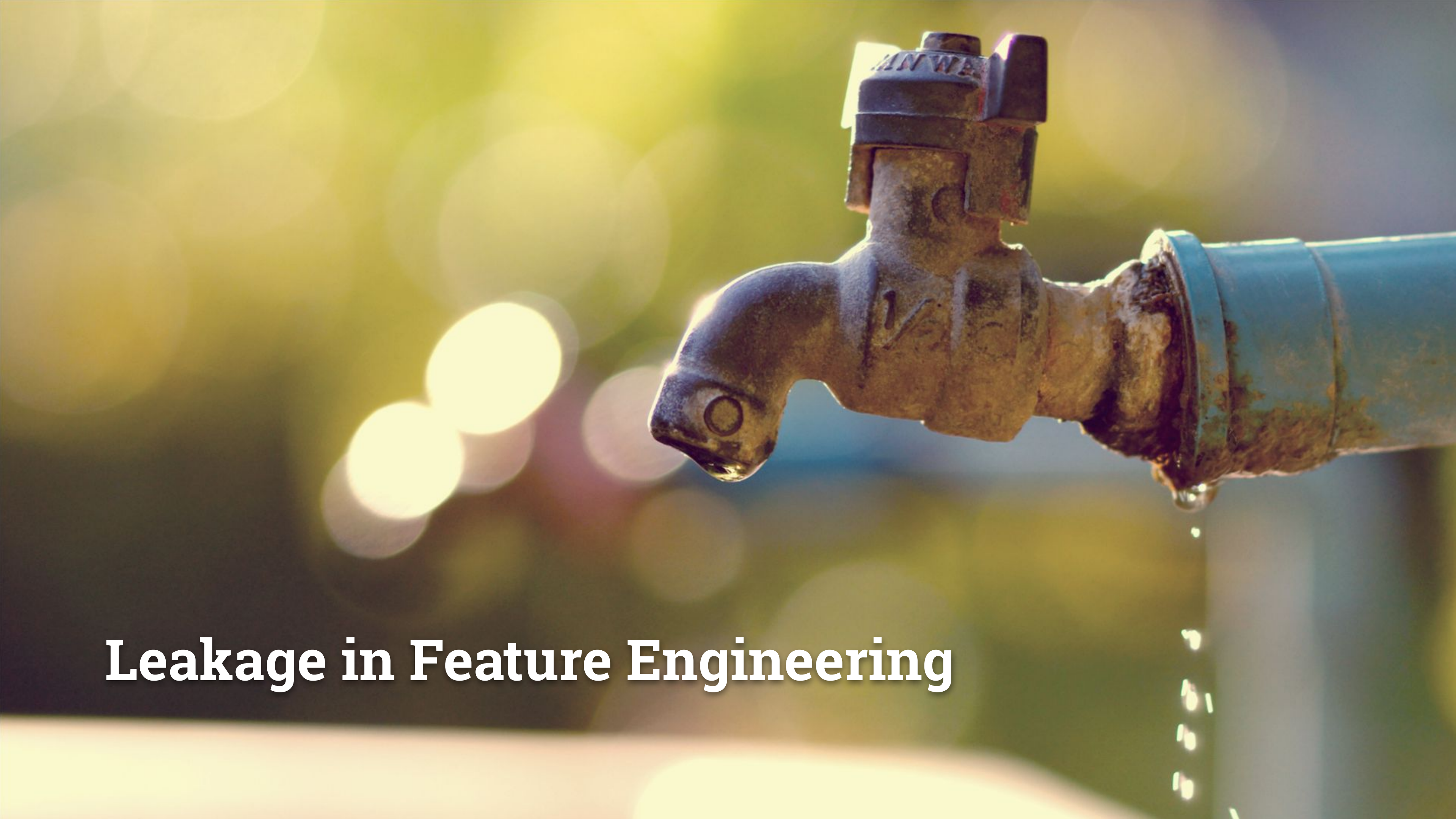
Education	Married	AnnualIncome	Purpose	LatePaymentReminders	IsBadLoan
1	Y	80k	Car Purchase	0	0
3	N	120k	Small Business	3	1
1	Y	85k	House Purchase	5	1
2	N	72k	Marriage	1	0

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

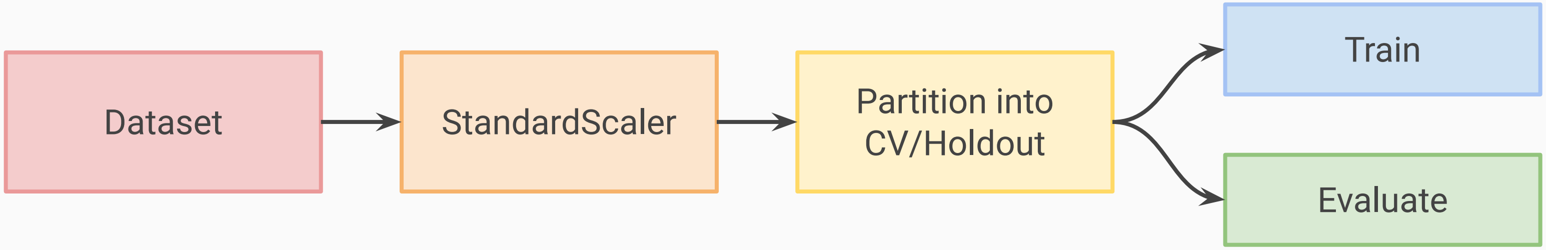
Database records get overwritten as more facts become available.

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

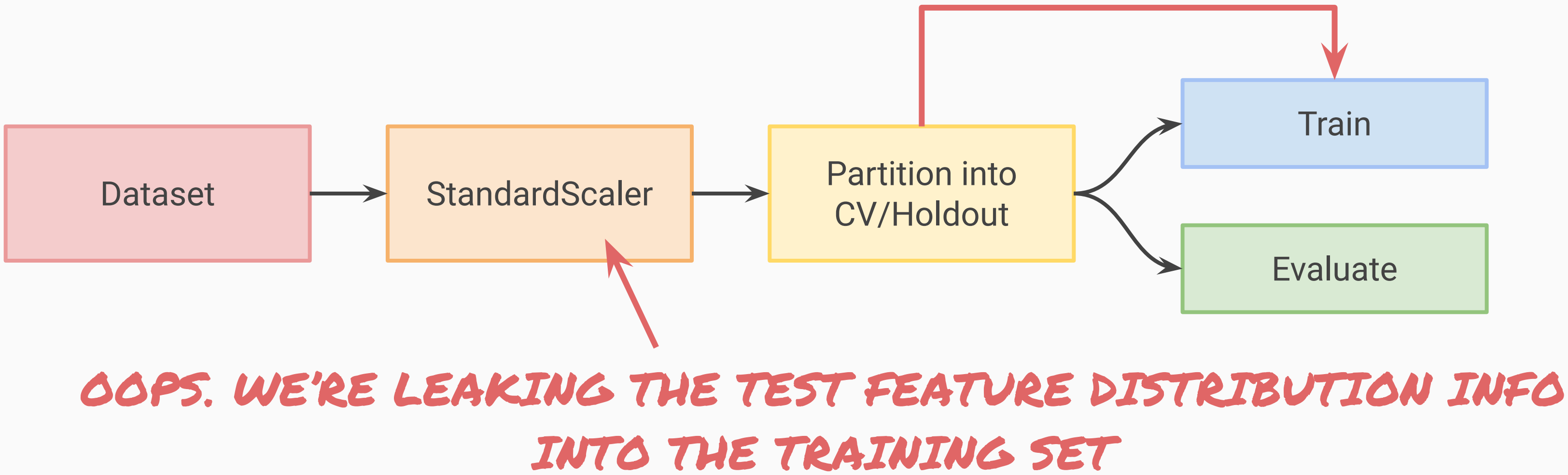


Leakage in Feature Engineering

My model is sensitive to feature scaling...

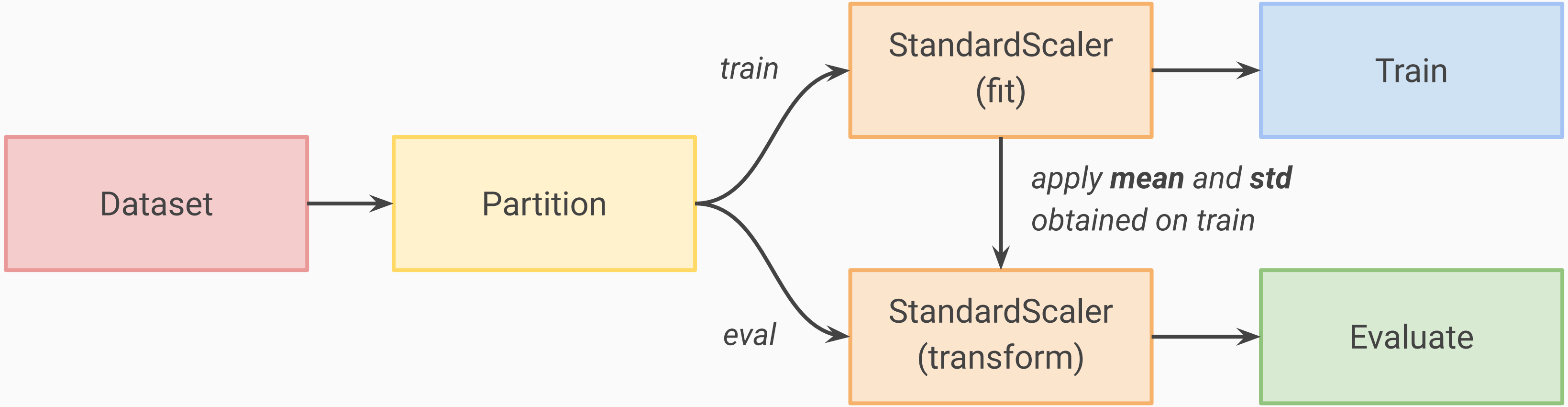


My model is sensitive to feature scaling...



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)


left_overs
655 rows

no_food
519 rows

closed_lids
277 rows

new_food
275 rows

What about deep learning?

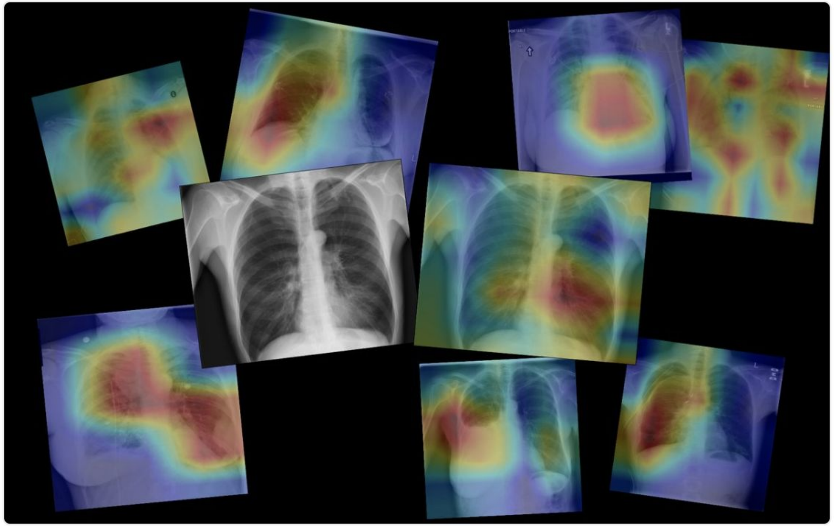
What about deep learning?

Leakage in Partitioning

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



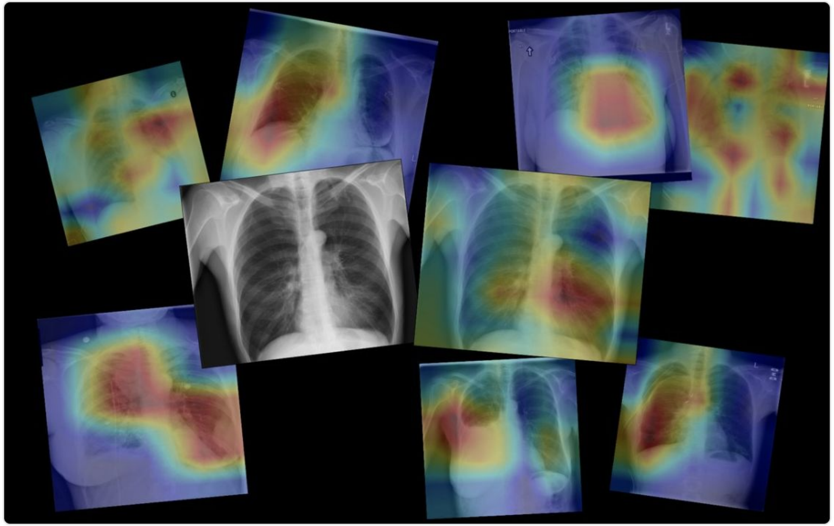
9:09 PM - 15 Nov 2017 from Mountain View, CA

665 Retweets **1,352** Likes

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



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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.

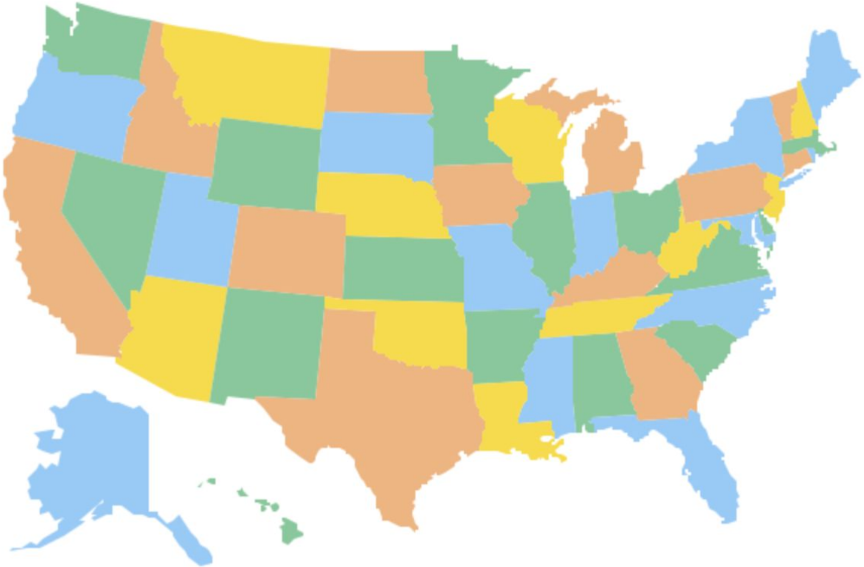
Pathology	Wang et al. (2017)	Yao et al. (2017)	CheXNet (ours)
Atelectasis	0.716	0.772	**0.8209**
Cardiomegaly	0.807	0.904	**0.9048**
Effusion	0.784	0.859	**0.8831**
Infiltration	0.609	0.695	**0.7204**
Mass	0.706	0.792	**0.8618**
Nodule	0.671	0.717	**0.7766**
Pneumonia	0.633	0.713	**0.7632**
Pneumothorax	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)

The Cold Start Problem



Observe:

Illinois

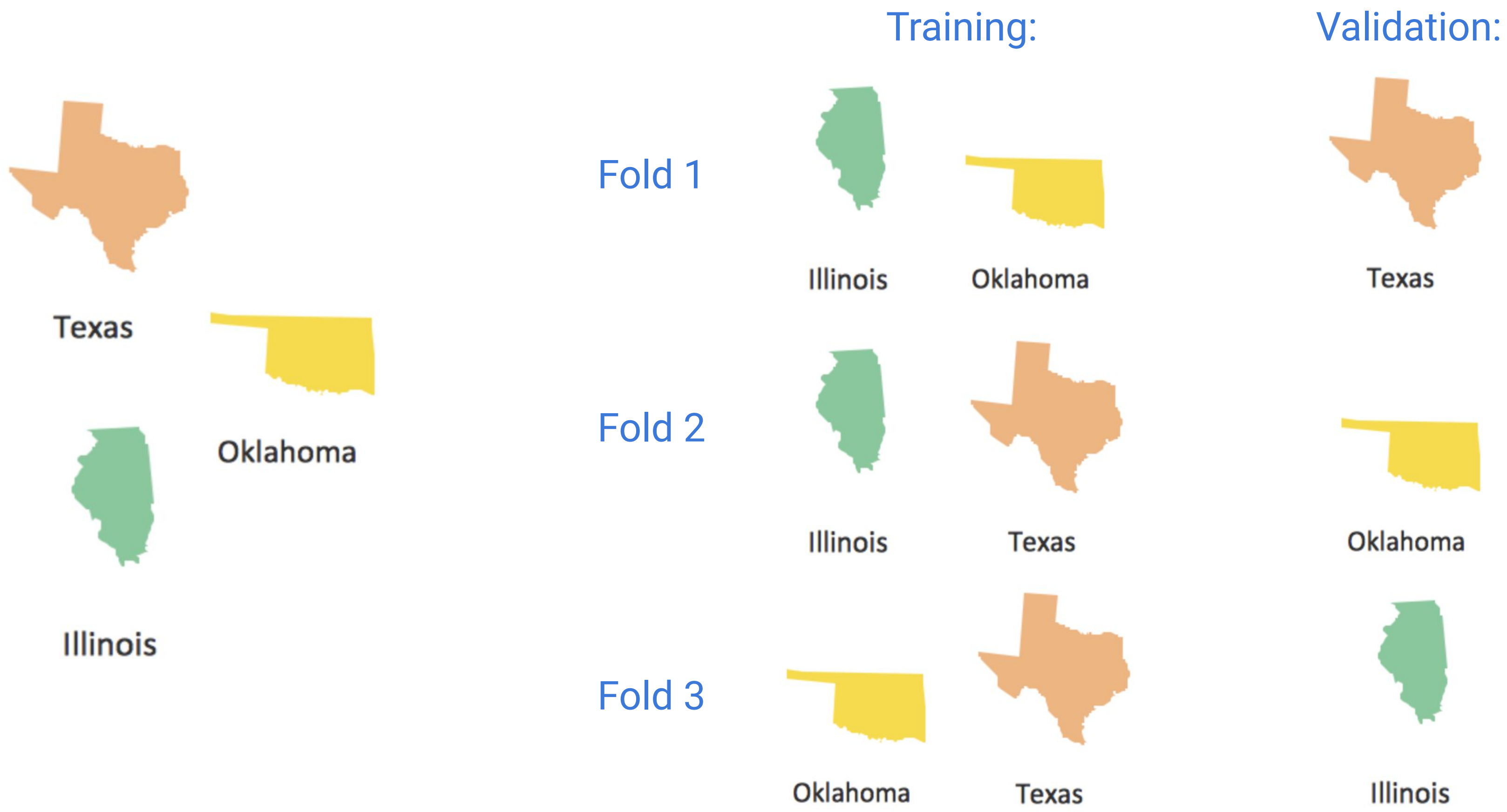
Oklahoma

Texas

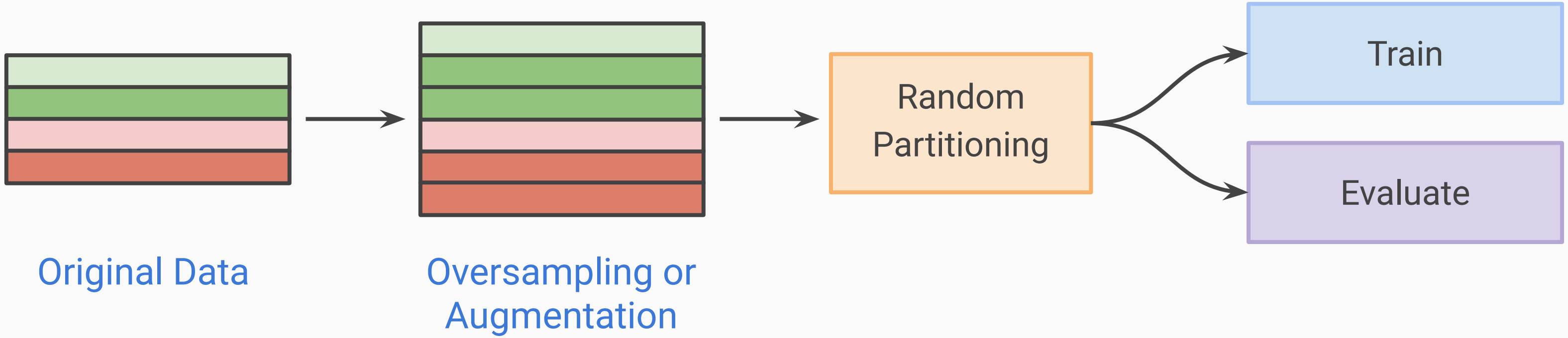
Predict:

North Carolina

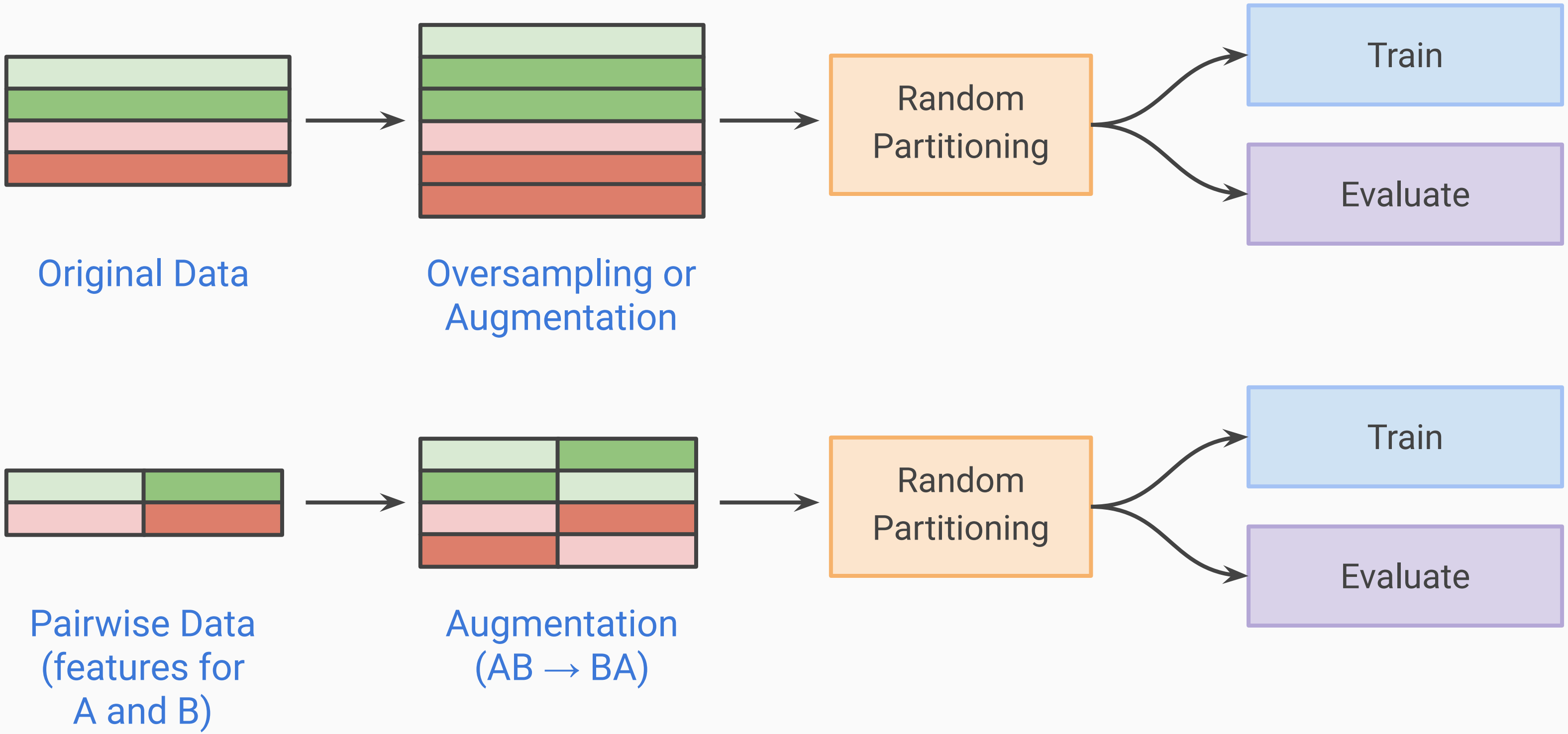
Group Partitioning, Out-of-Group Validation



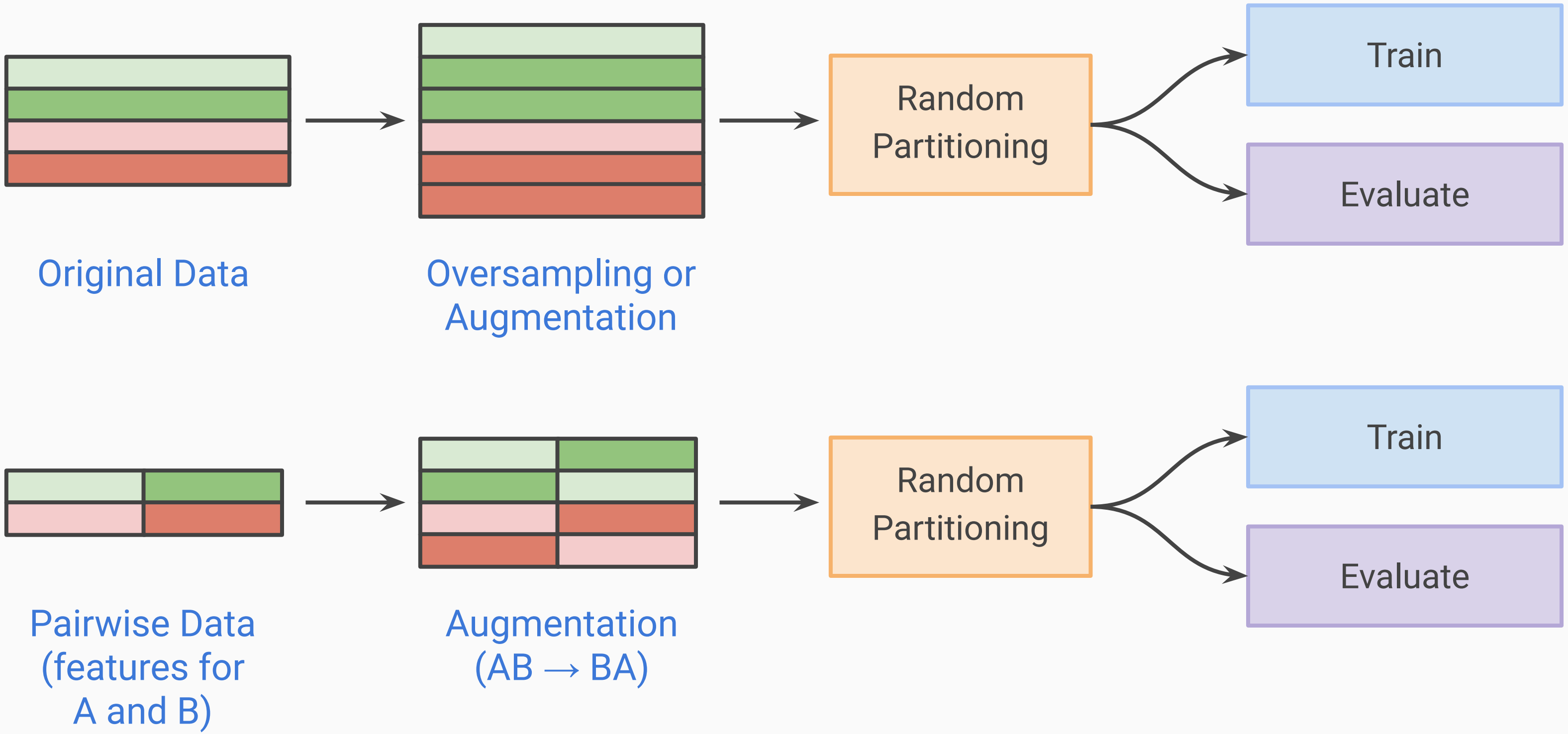
Leakage in oversampling / augmentation



Leakage in oversampling / augmentation

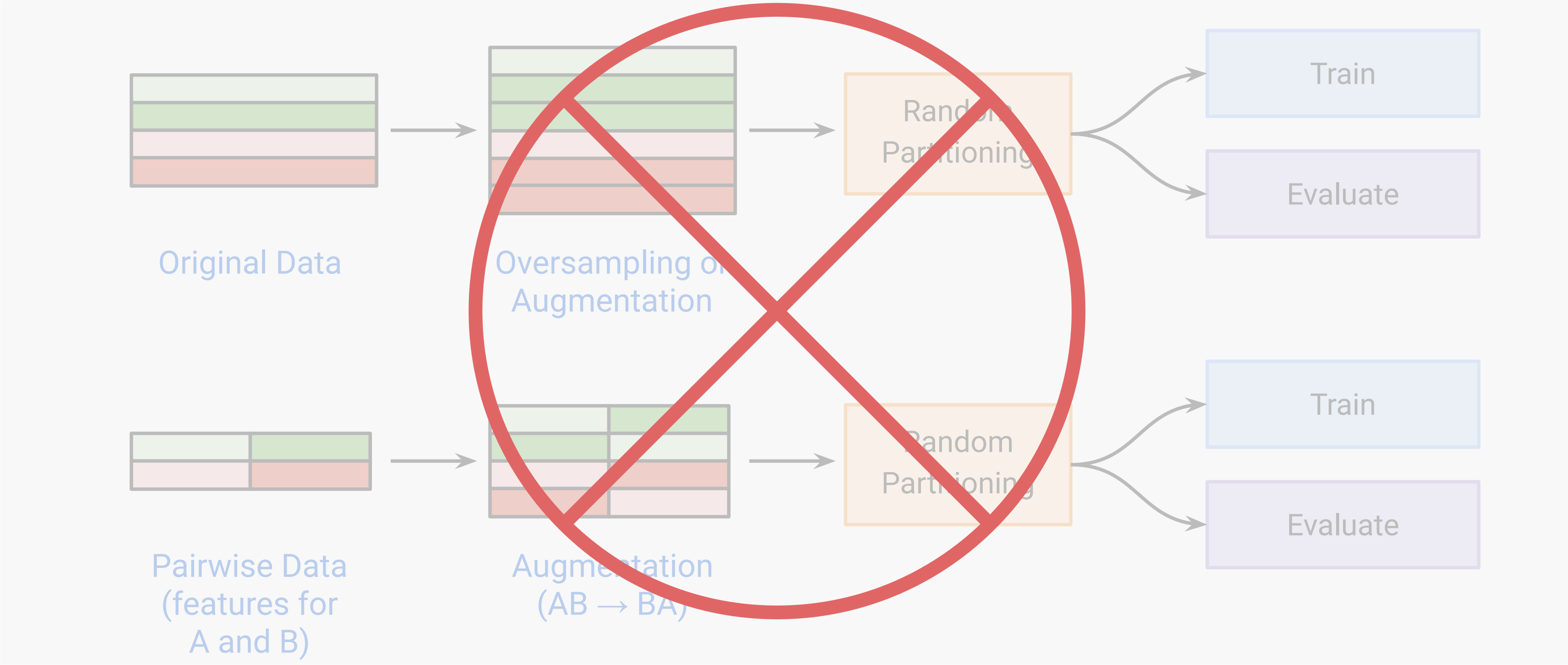


Leakage in oversampling / augmentation



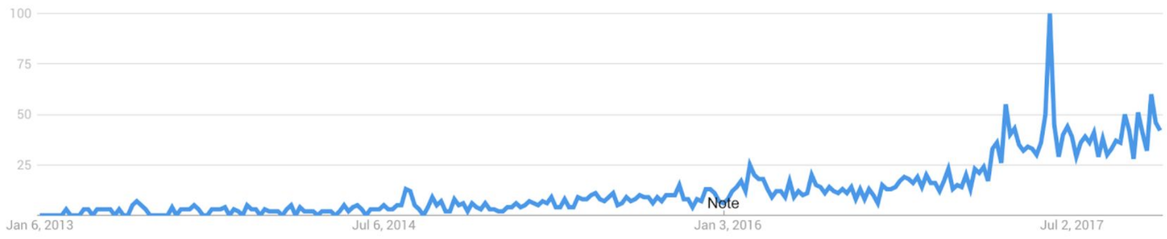
OOPS. WE MAY GET COPIES SPLIT BETWEEN TRAINING AND EVALUATION

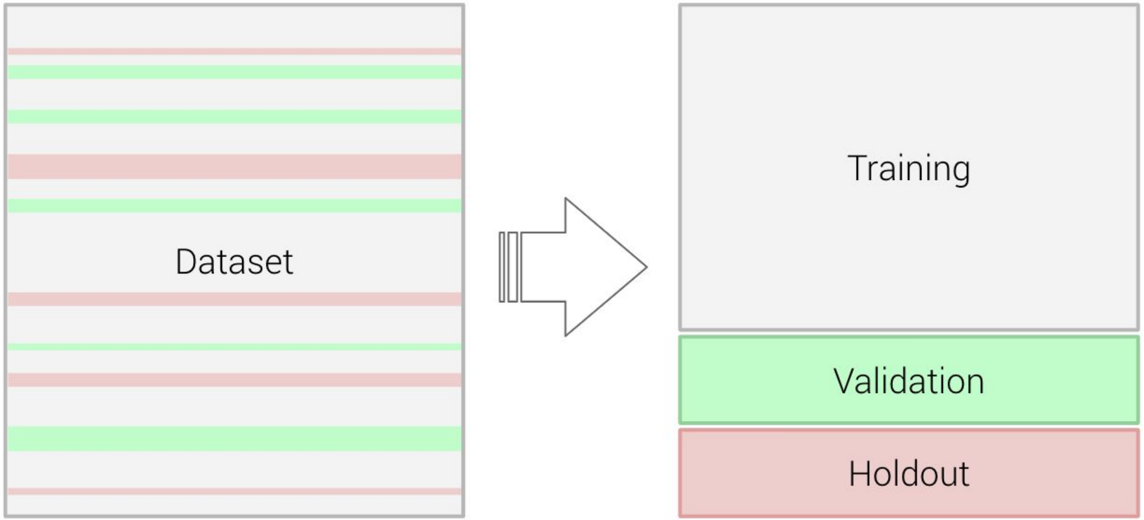
Leakage in oversampling / augmentation



First partition, then augment the training data.

Random Partitioning for Time-Aware Models

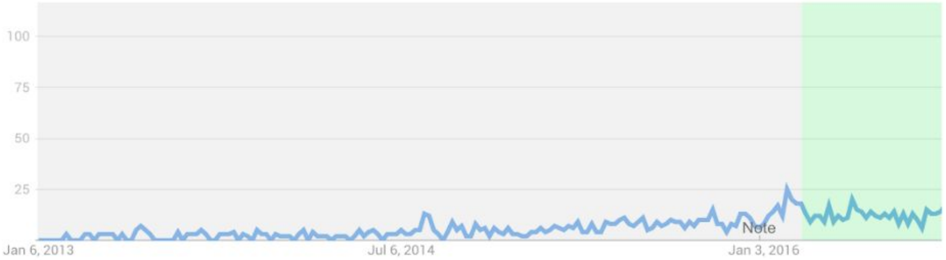




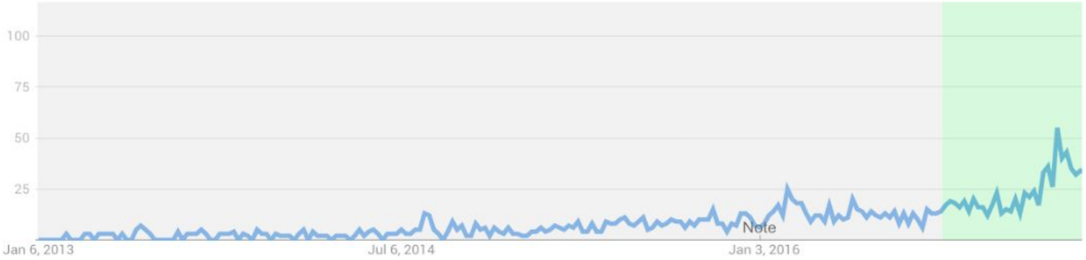
Random Partitioning for Time-Aware Models

Out-of-Time Validation (OTV)

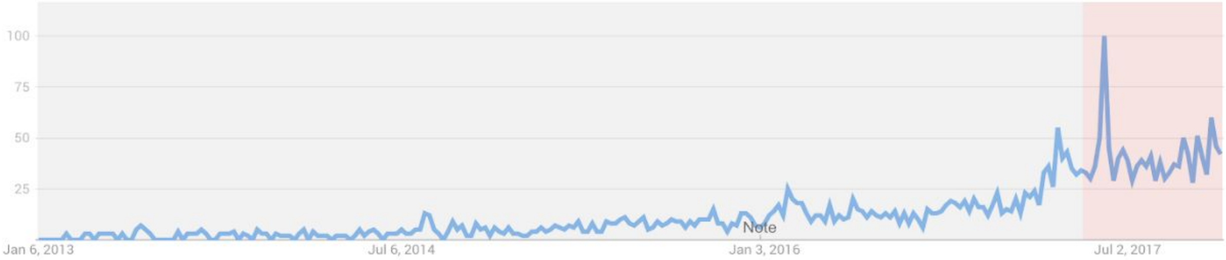
Backtest 2



Backtest 1

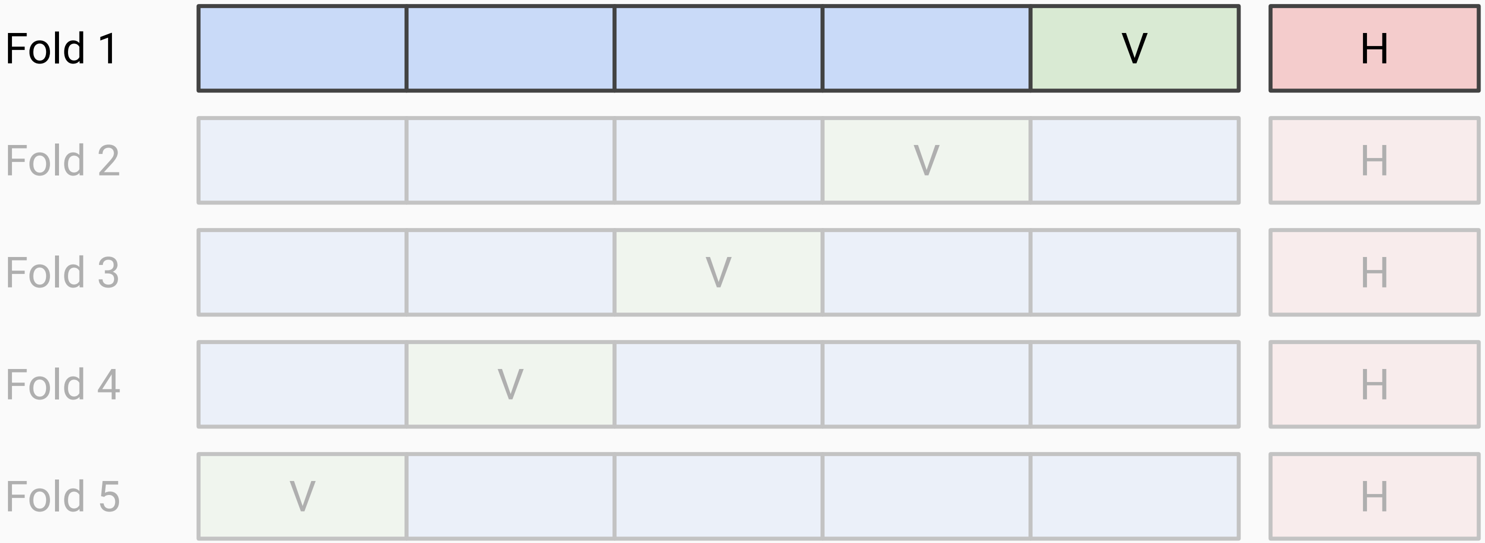


Holdout



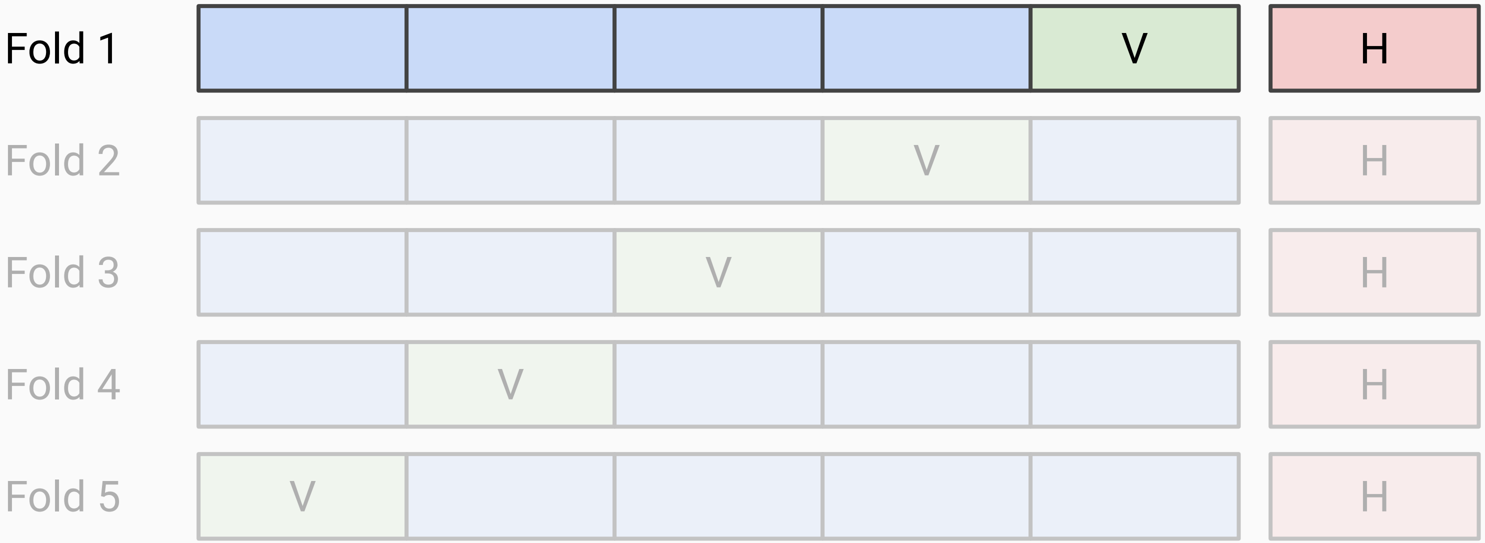
Leakage in Training & Tuning

Reusing a CV split for multiple tasks



Feature selection, hyperparameter tuning, model selection...

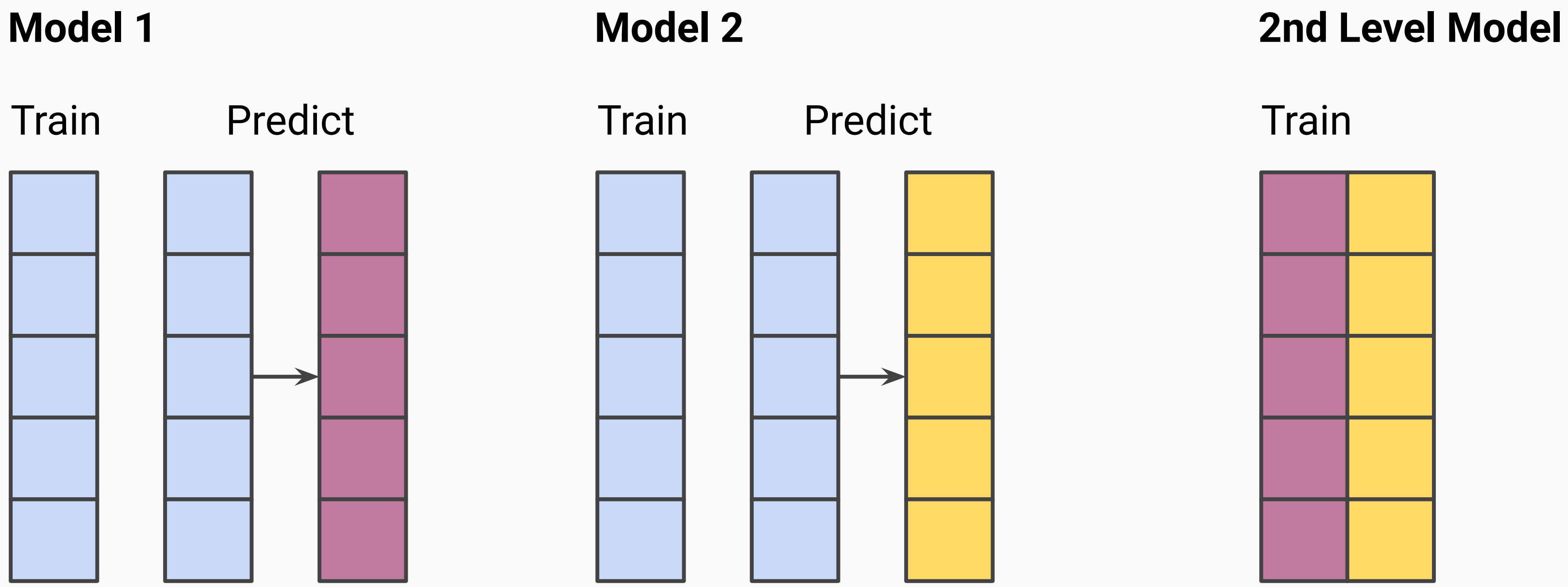
Reusing a CV split for multiple tasks



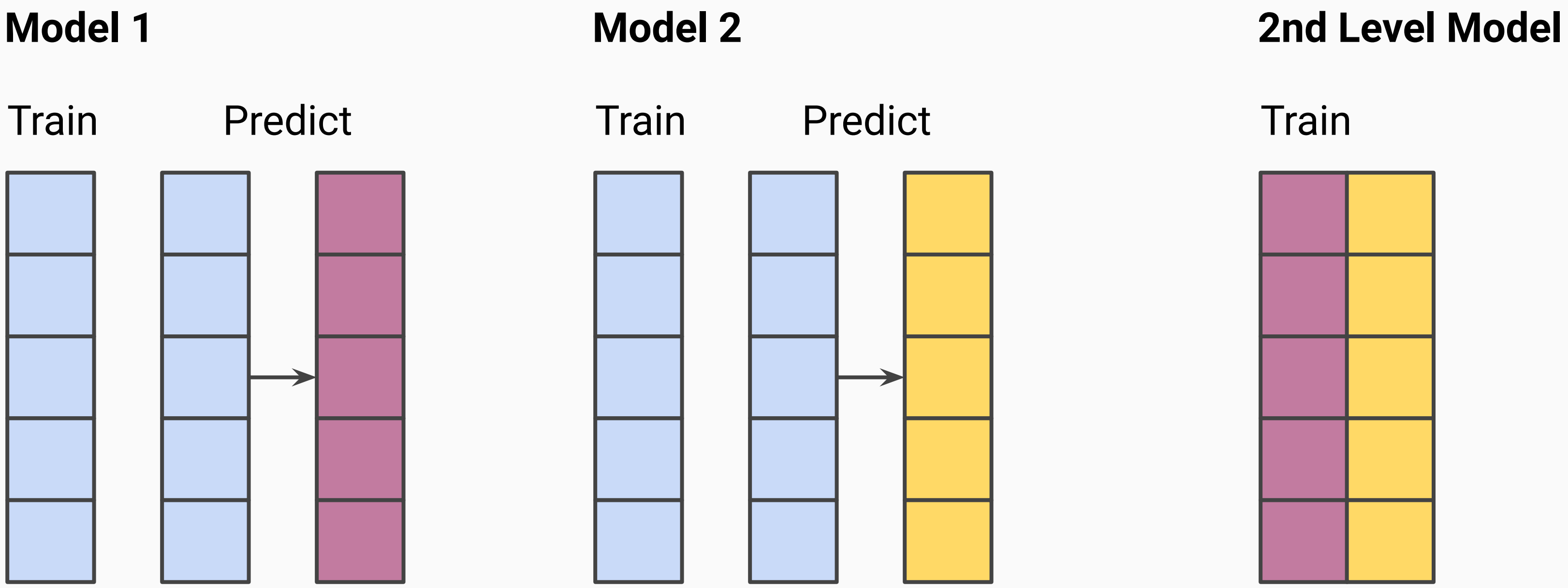
Feature selection, hyperparameter tuning, model selection...

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

Model stacking on in-sample predictions

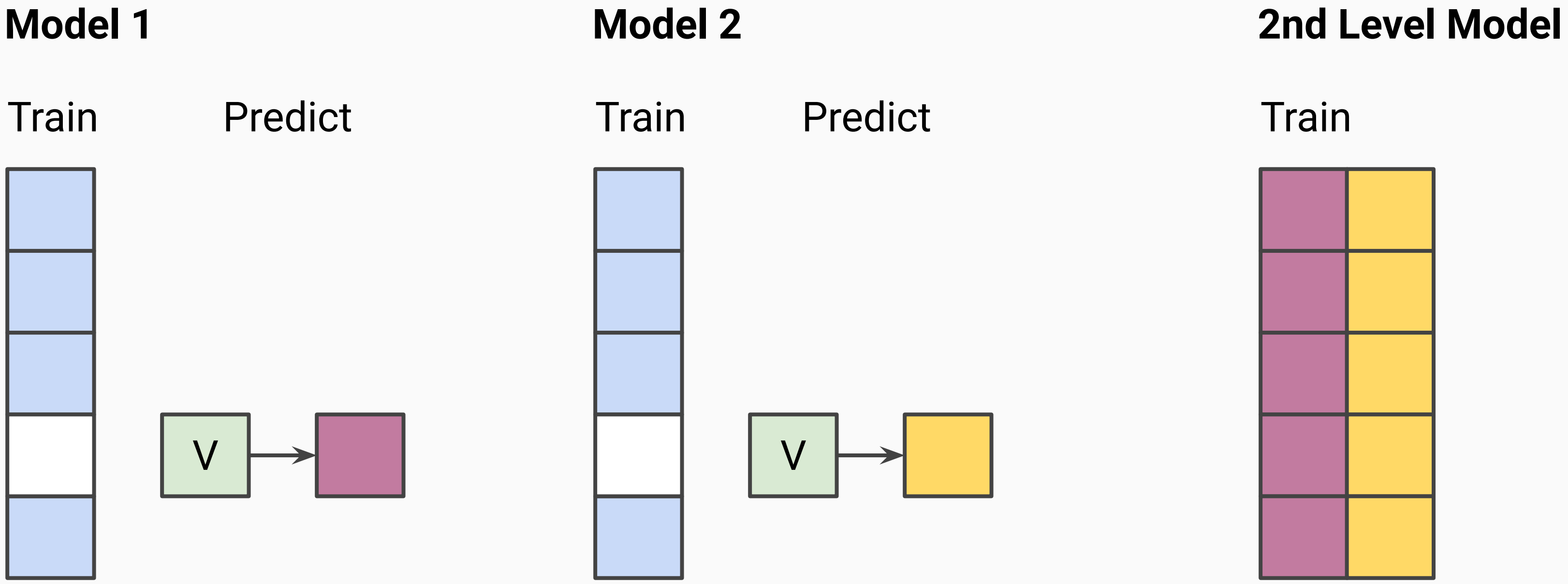


Model stacking on in-sample predictions



OOPS. WILL LEAK THE TARGET IN THE META-FEATURES

Better way to stack



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 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.
  For scikit-learn, use Pipelines.
- 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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