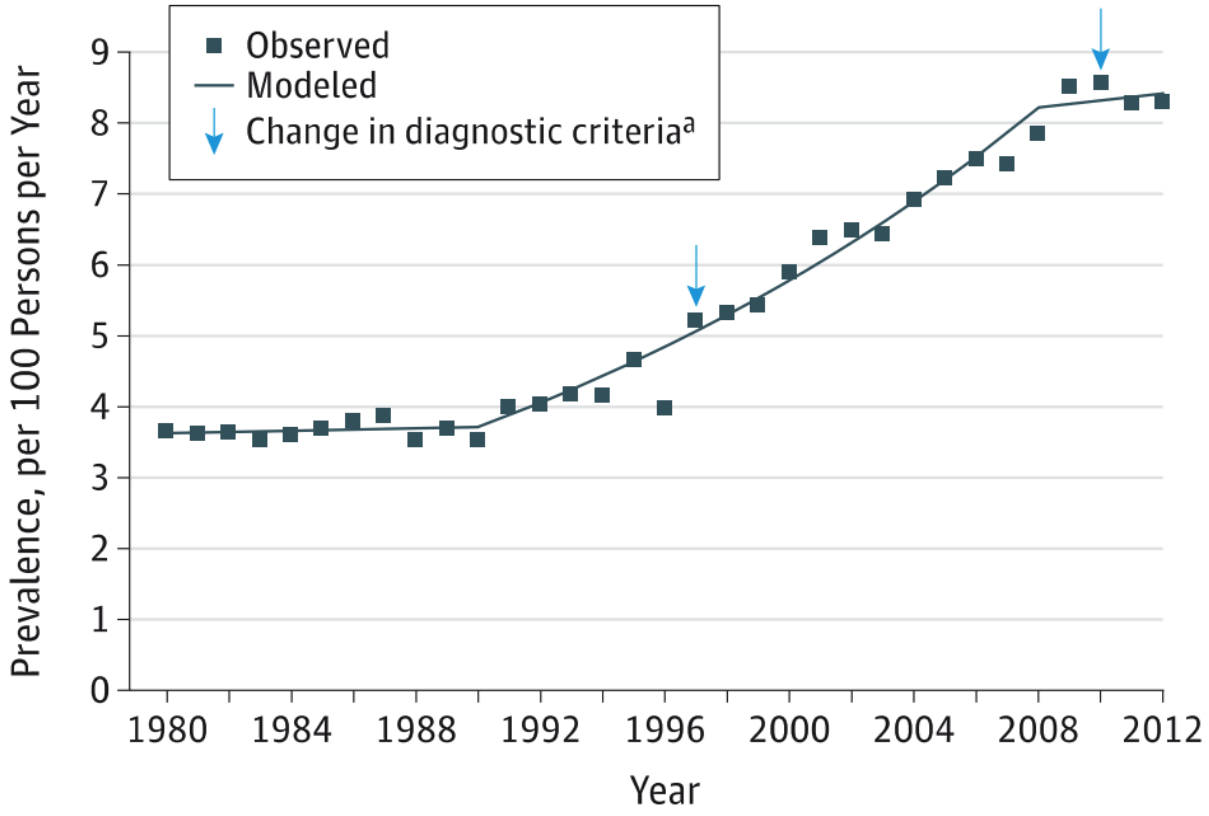


Data 146: Foundations for CPH

Distribution Shift

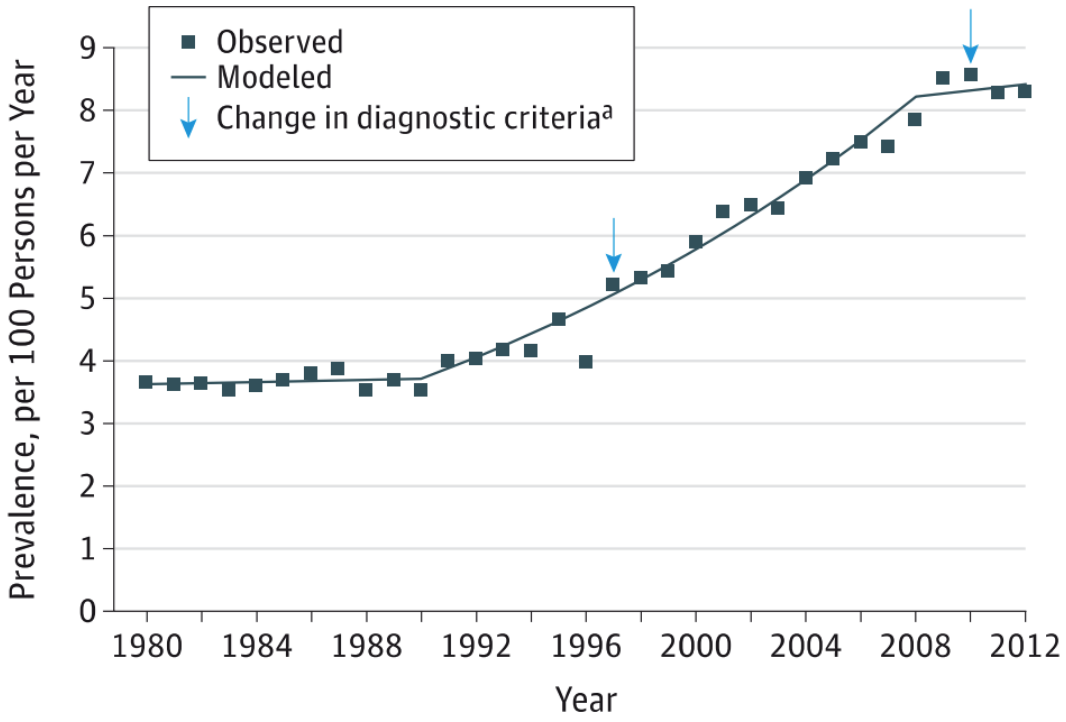
Irene Y. Chen

Dataset shift / non-stationarity: *Diabetes Onset After 2009*



Why might diabetes go up over time?

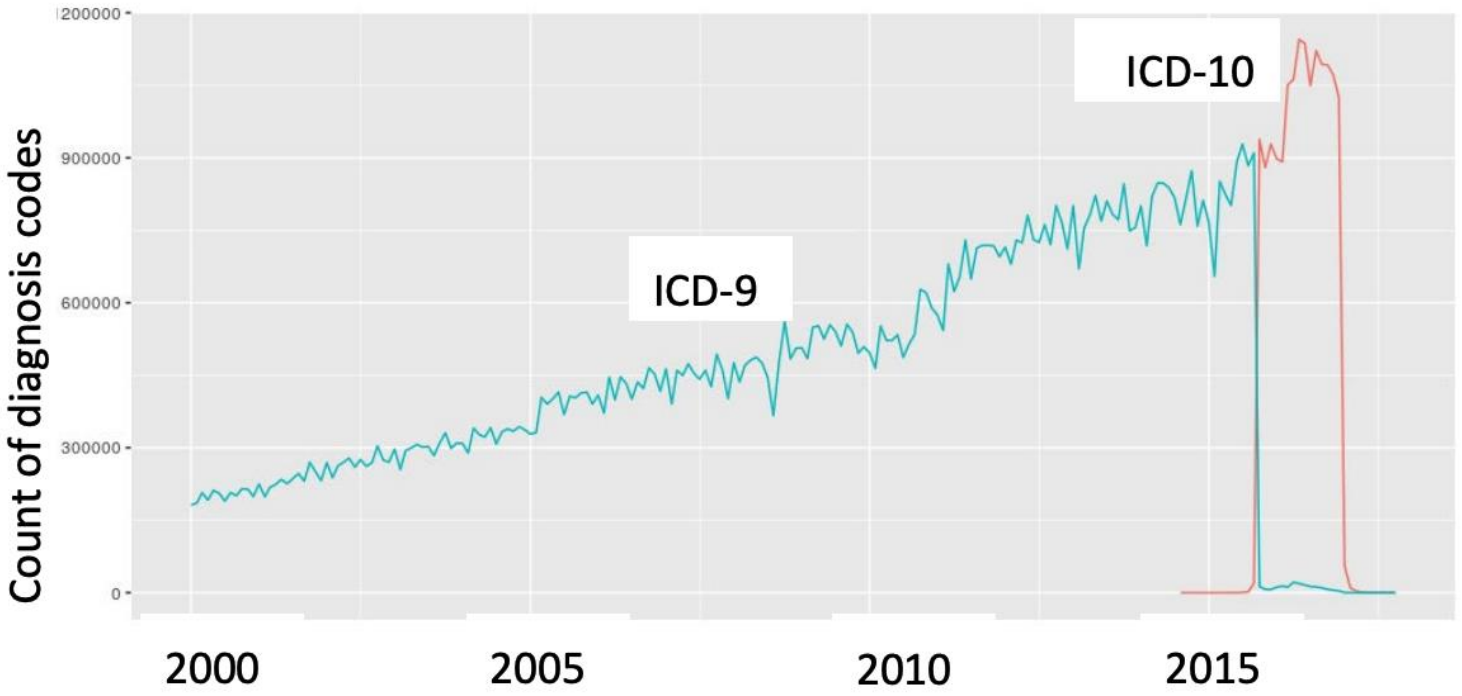
Dataset shift / non-stationarity: *Diabetes Onset After 2009*



- Better diagnosis criteria
- Insulin / glucose biomarkers
- Obesity rates
- Definition of disease
- Meaning of label
- T1D vs T2D

[Geiss LS, Wang J, Cheng YJ, et al. Prevalence and Incidence Trends for Diagnosed Diabetes Among Adults Aged 20 to 79 Years, United States, 1980-2012. JAMA, 2014.]

Dataset shift / non-stationarity: *Diabetes Onset After 2009*



ICD-9 to ICD-10 | ICD-10 to ICD-9

2501 | Display ICD long descriptions

ICD-9	Description		ICD-10	Description
25010	DIABETES MELLITUS WITH KETOACIDOSIS TYPE II OR UNSPECIFIED TYPE NOT STATED AS UNCONTROLLED	→	E1169	TYPE 2 DIABETES MELLITUS WITH OTHER SPECIFIED COMPLICATION
25011	DIABETES MELLITUS WITH KETOACIDOSIS TYPE I NOT STATED AS UNCONTROLLED	→	E1010	TYPE 1 DIABETES MELLITUS WITH KETOACIDOSIS WITHOUT COMA
25012	DIABETES MELLITUS WITH KETOACIDOSIS TYPE II OR UNSPECIFIED TYPE UNCONTROLLED	→	E1165	TYPE 2 DIABETES MELLITUS WITH HYPERGLYCEMIA
		→	E1169	TYPE 2 DIABETES MELLITUS WITH OTHER SPECIFIED COMPLICATION
	1-to-2 mapping			
25013	DIABETES MELLITUS WITH KETOACIDOSIS TYPE I UNCONTROLLED	→	E1010	TYPE 1 DIABETES MELLITUS WITH KETOACIDOSIS WITHOUT COMA
		→	E1065	TYPE 1 DIABETES MELLITUS WITH HYPERGLYCEMIA
	1-to-2 mapping			

Significance of features may change over time. Note ICD10 to ICD9 isn't 1-1

[Figure credits: (Left) Mike Oberst, (Right) http://www.icd10codesearch.com/]

Outline

- **Examples and formulation of dataset shift** (20 mins)
- **Testing for dataset shift** (10 mins)
- **Mitigating dataset shift** (15 mins)
- **Discussion** (5 mins)



How can we make Data 146 better for you?

Learning Objective: Understand criteria and formalization of dataset shift

Formalizing Dataset Shift

- General Task: Perform well on a “target domain” Q
  - Train: Population **P** (e.g., MGH)
  - Apply: Population **Q** (e.g., UCSF)
- Assumptions: What is changing vs. what is stable?
  - Covariate Shift
  - Label Shift
  - More General Shift

Formalizing Dataset Shift

- General Task: Perform well on a “target domain” Q
- Assumptions: What is changing vs. what is stable?

An Impossible Problem

Given $\{X_i, Y_i\}_{i=1}^n$ from a *source domain* $\boldsymbol{P}(X, Y)$, find a model that performs well on some *target domain* $\boldsymbol{Q}(X, Y)$

$$\min_{f \in \mathcal{F}} \mathbb{E}_{\boldsymbol{Q}}[\ell(Y, f(X)]$$

Minimize the expected loss between truth Y and prediction *f*(X) in domain Q
Find the function *f* that minimizes this

Examples:
- P and Q are two different hospital systems
- P is the past, Q is the future
- …

Not well-posed without further assumptions or information about Q!

Formalizing Dataset Shift

- General Task: Perform well on a “target domain” Q
- Assumptions: What is changing vs. what is stable?

Example: Covariate Shift Assumption

$$P(X) \neq Q(X)$$

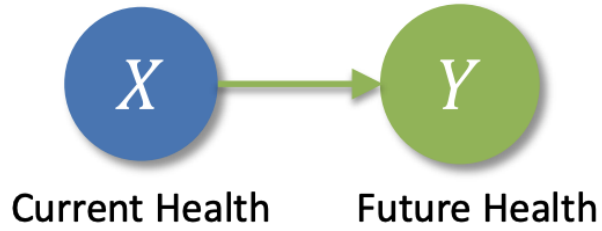
$$P(Y \mid X) = Q(Y \mid X)$$

Why might this be true? One rationale: $P(Y \mid X)$ encodes some "causal" mechanism

Example: Covariate Shift Assumption

$$P(X) \neq Q(X)$$
$$P(Y \mid X) = Q(Y \mid X)$$

Why might this be true? One rationale: $P(Y \mid X)$ encodes some "causal" mechanism



Example: Risk stratification for different patient populations

Common assumption: distribution of future health will be the same. But doesn't usually hold

Example: Label Shift Assumption

$$P(Y) \neq Q(Y)$$

$$P(X \mid Y) = Q(X \mid Y)$$

(flip directionality from previous slide)

Why might this be true? One rationale: $P(X \mid Y)$ encodes some "causal" mechanism

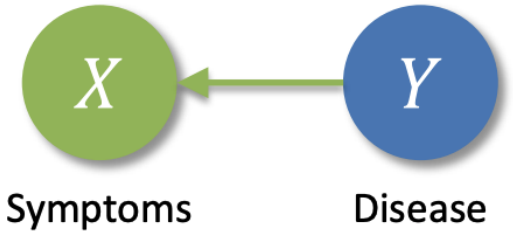
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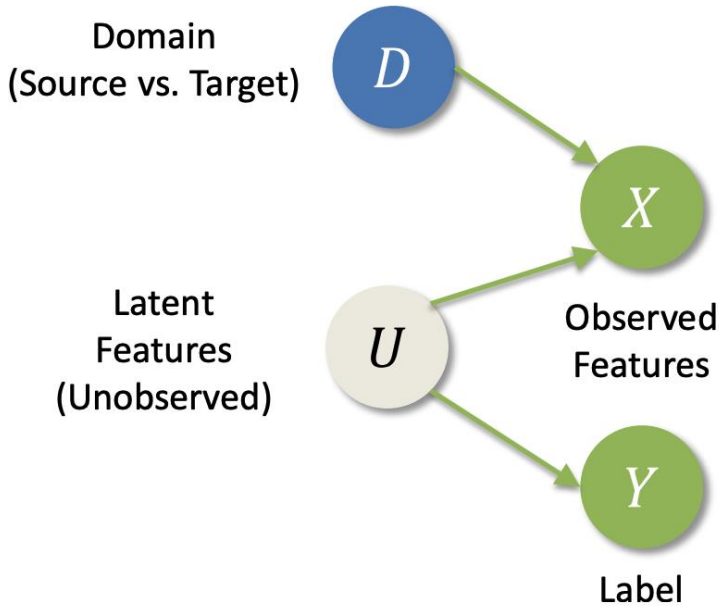
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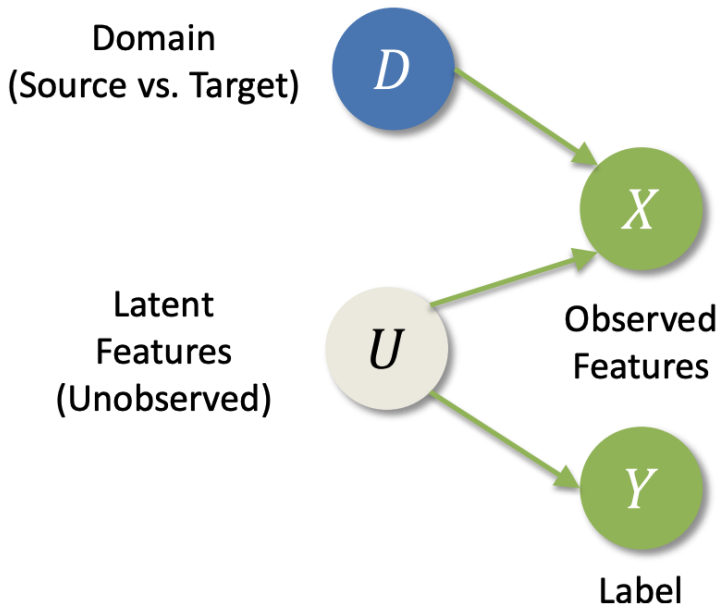
Example: Diagnostic testing under changes in disease prevalence.

Disease informative of symptoms. Prior vs. posterior probability.
Generative model vs. data-conditional posterior-probability inference

Example: “Domain Shift”



Example: “Domain Shift”



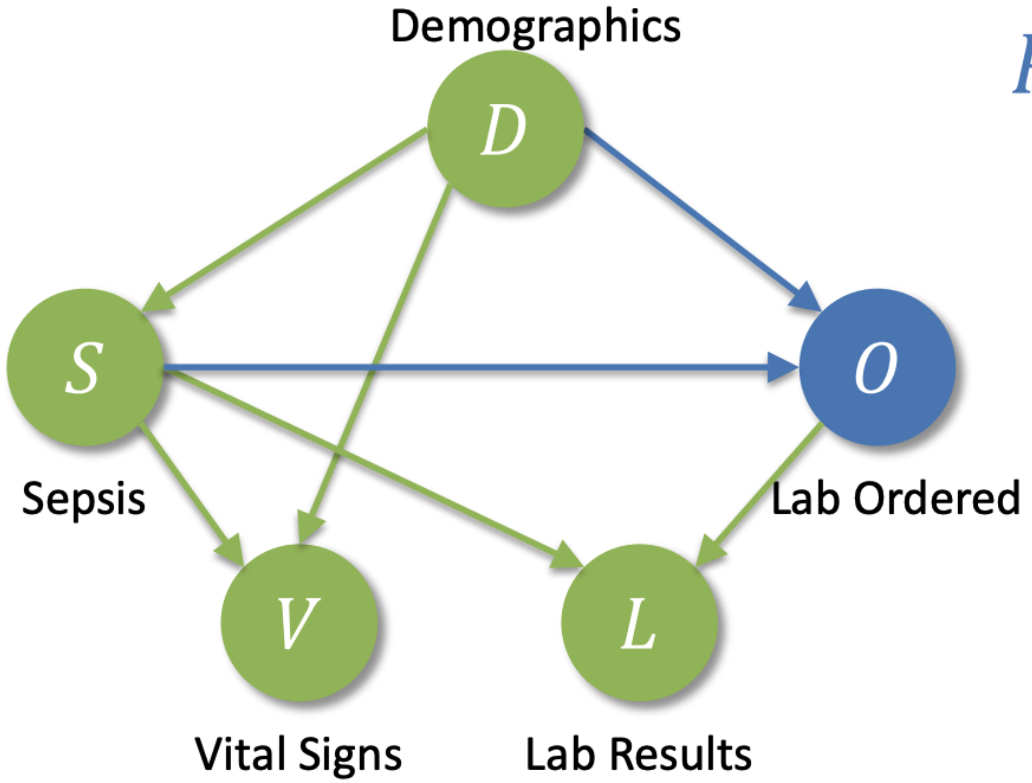
Example: Changes in how features are derived (e.g., ICD-9 versus ICD-10)

We can also view the domain itself as a variable that influences others

Note: So far, we have not discussed how to mitigate these shifts. In this example, more information is required!

Quinonero-Candela et al., (2008). *Dataset Shift in Machine Learning*, MIT Press.

Example: Using causal graphs to reason about shifts



$$P(O \mid D, S) \neq Q(\mathrm{O} \mid \mathrm{D}, \mathrm{S})$$

More fine-grained shifts can be reasoned about as changes in marginal/conditional distributions

Example: Changes in lab ordering patterns across hospitals

$$P(D, S, O, V, L) = P(D)P(S|D)P(V \mid D, S)P(O|D, S)P(L|O, S)$$

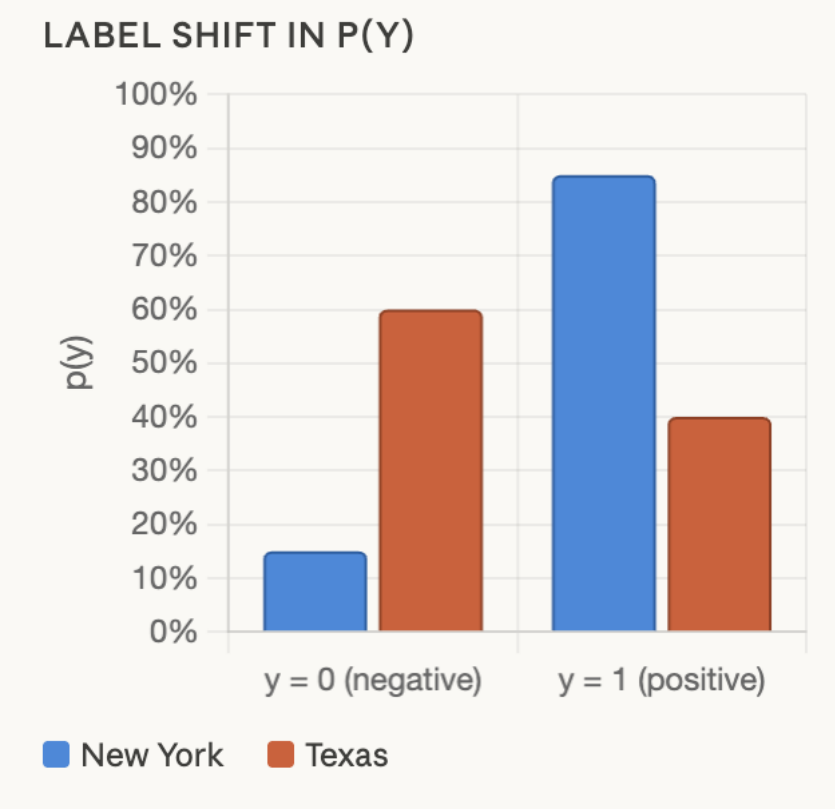
Example from Subbaswany et al. (2021). Evaluating Model Robustness and Stability to Dataset Shift. AISTATS

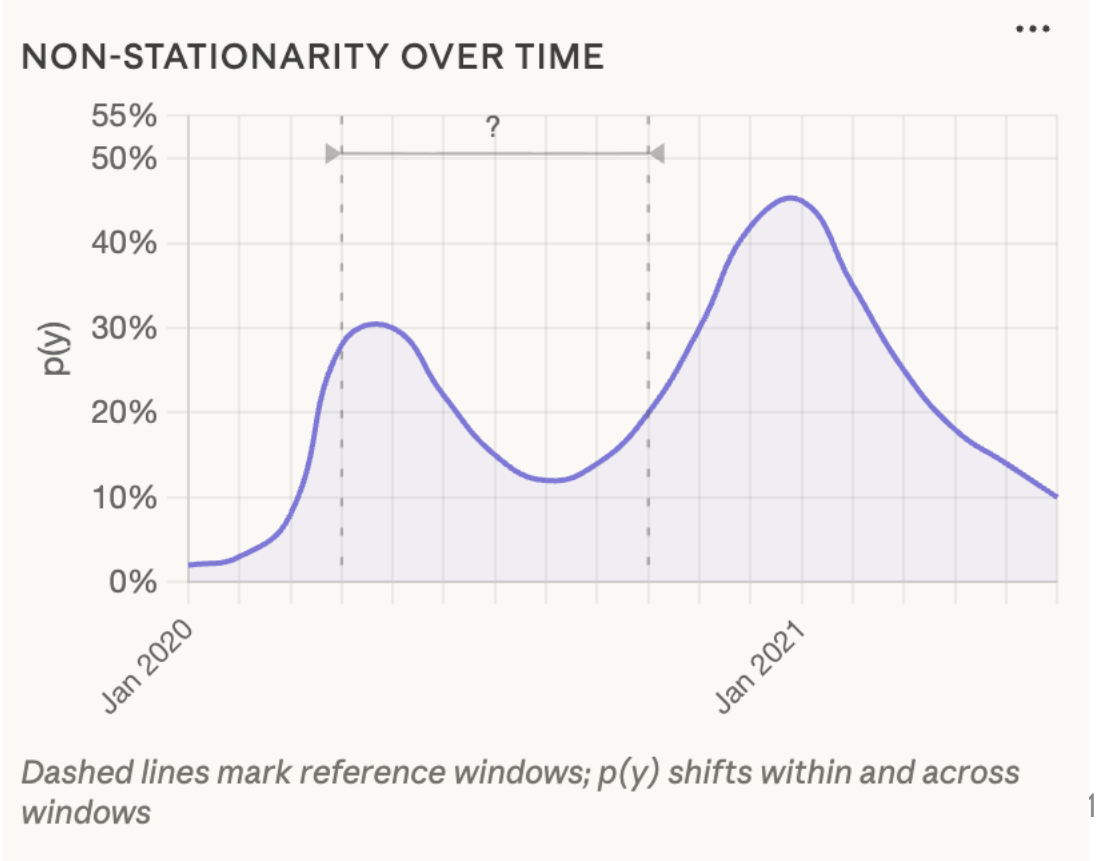
Distribution Shift Topics

- Examples & formalization of dataset shift
- **Testing for dataset shift**
- Mitigating dataset shift

Testing for dataset shift

- Shift in p(y)
- Plot distributions (across populations, across time)





Testing for dataset shift

- Shift in p(x) or p(x|y):
  - Different: x is multidimensional

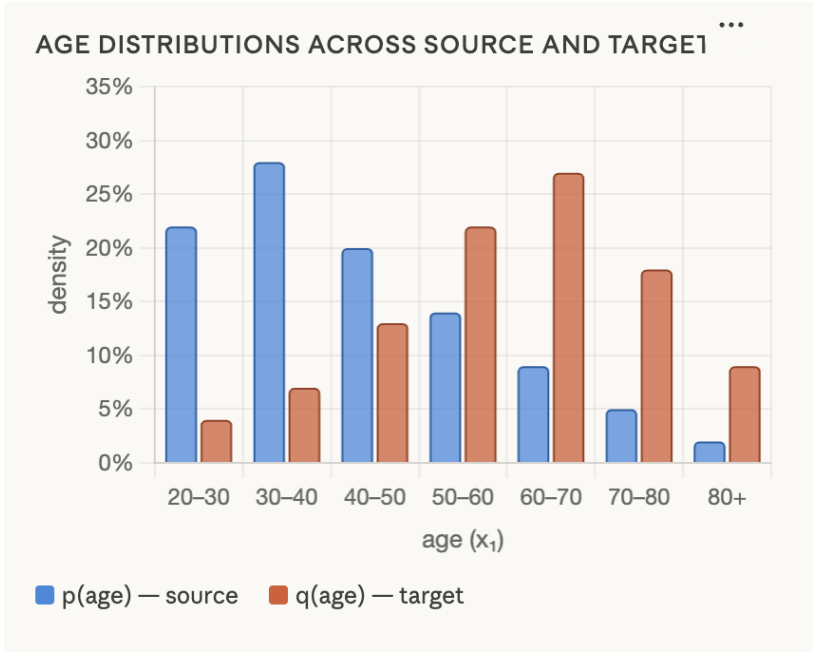
Testing for dataset shift

- Shift in p(x) or p(x|y):
  - Different: x is multidimensional
  - Compare feature means -> could miss bimodal or unimodal differences
  - Could look for additional moments

feature x_1 = age

source p		target q
$\hat{E}_p[x_1]$	vs.	$\hat{E}_q[x_1]$
$\hat{E}_p[x_2]$	vs.	$\hat{E}_q[x_2]$
⋮		⋮

significant differences → $p(x) \neq q(x)$



Testing for dataset shift

- Shift in p(x) or p(x|y):
  - Compare feature means (repeat of Y, assuming discrete)
  - However, means can be identical even if two distributions are different!
  - E.g., variance, co-variance

- Thus, we must check the higher-order moments
  - $\mathbb{E}_p[x_1^2]$ vs $\mathbb{E}_q[x_1^2]$
  - $\mathbb{E}_p[x_1\ x_2]$ vs $\mathbb{E}_q[x_1\ x_2]$

Testing for dataset shift

- Shift in p(x) or p(x|y):
  - Compare feature means
  - Use kernel two-sample test (Gretton et al, JMLR 2012)
  - Integral probability metric (Muller 197)
    - $\mathcal{L} = \{\ell\colon \mathbb{R}^d \to \mathbb{R}\}$ for vector $\vec{x}$
    - E.g., $\mathcal{L} = \{x_1, x_2, \ldots, x_d, x_1^2, x_1 x_2\}$

$$\mathrm{IPM}_{\mathcal{L}}(p, q) := \sup_{\ell \in \mathcal{L}} |\mathbb{E}_p[\ell(x)] - \mathbb{E}_q[\ell(x)]|$$

Testing for dataset shift

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  - Maximum mean discrepancy (MMD): L are functions with norm 1 in a RKHS: (Gretton et al., 2012)

$$\text{samples } x_1, ..., x_m \sim p,\ x'_1, ..., x'_n \sim q$$

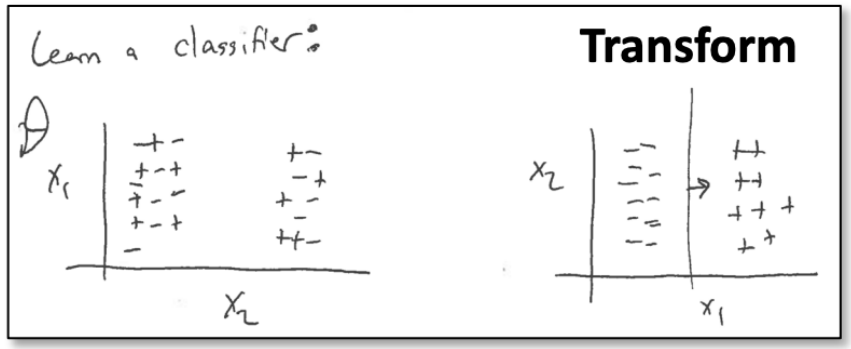
$$\mathrm{M\hat{M}D}_k^2(p,q) := \frac{1}{m(m-1)} \sum_{i=1}^{m} \sum_{j=1}^{m} k(x_i, x_j) - \frac{2}{mn} \sum_{i=1}^{m} \sum_{j=1}^{n} k(x_i, x'_j) + \frac{1}{n(n-1)} \sum_{i=1}^{n} \sum_{j=1}^{n} k(x'_i, x'_j)$$

Testing for dataset shift

- Shift in p(x) or p(x|y):
  - Compare feature means
  - Use kernel two-sample test such as maximum mean discrepancy/MMD (Gretton et al., JMLR '12)
  - (Attempt to) learn a classifier to distinguish one dataset from the other

Draw samples from p and q $\quad \text{samples } x_1, ..., x_m \sim p,\ x'_1, ..., x'_n \sim q$

Binary classification $\quad \mathcal{D} = \{(x_1, 1), \ldots, (x_m, 1), (x'_1, 0), \ldots, (x'_n, 0)\}$

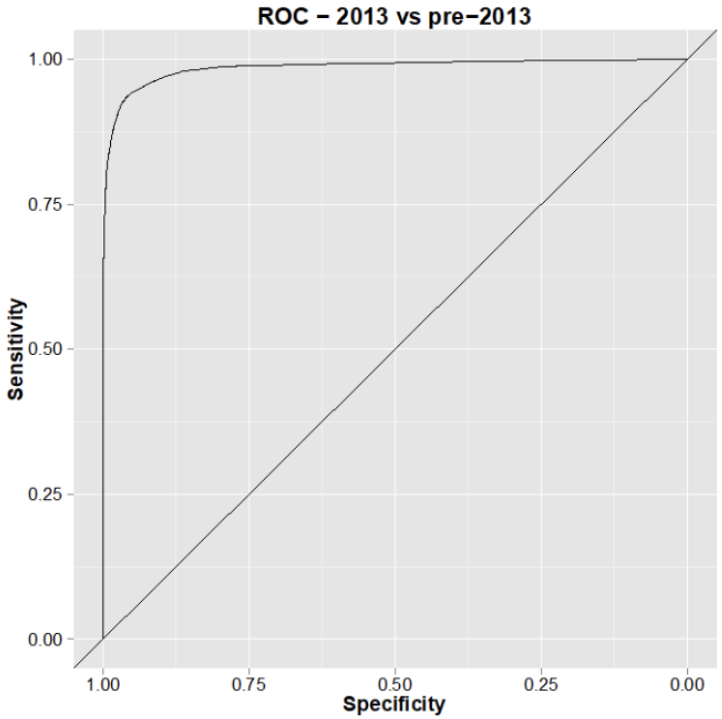


Can we find any non-linear transformation (kernel) that makes the data separable?

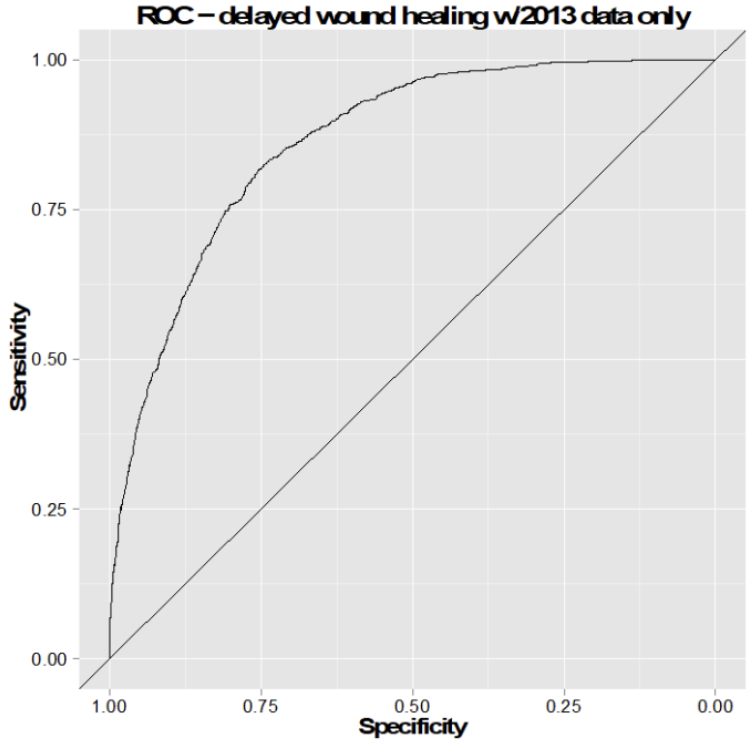
Testing for dataset shift

(Figures from Ken Jung. See also Jung & Shah, Implications of non-stationarity on predictive modeling using EHRs, Journal of Biomedical Informatics, 2015)

- Testing for covariate shift (wound healing):



2013 vs pre-2013



First 2/3 of 2013 vs last 1/3 of 2013

Distribution Shift Topics

- Examples & formalization of dataset shift
- Testing for dataset shift
- **Mitigating dataset shift**

Some practical answers

- **Domain shift** – can we transform the features?

Some practical answers

- **Domain shift** – transform features
  - imputation of missing values
  - artificially introduce noise/missingness during training
  - reprocess images
  - map to a common space
  - drop features that do not transfer

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  - Retrain the model with most recent data
  - Research question: how to automate the above?

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  - Application to different population: younger, healthier, etc

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Covariate shift: nonparametric regression just “works”

- When can we expect training on p(x,y) and testing on q(x,y) to give good results, for p ≠ q?

Covariate shift: nonparametric regression just “works”

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- **Theorem**: If p(x) > 0 whenever q(x) > 0 and p(y|x) = q(y|x), then in the limit of infinite data from p, can achieve Bayes’ error on q

Covariate shift: nonparametric regression just "works"

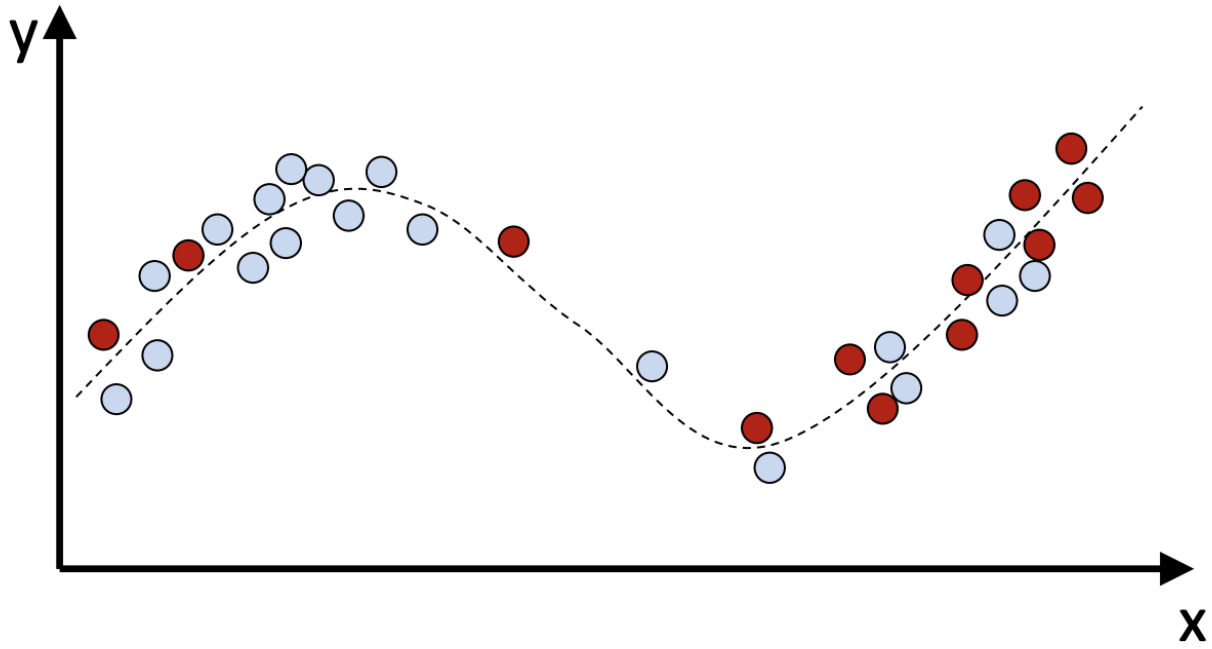
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- **Theorem**: If p(x) > 0 whenever q(x) > 0 and p(y|x) = q(y|x), then in the limit of infinite data from p, can achieve Bayes' error on q

- We never have infinite data! May have to use a more restricted model to prevent overfitting (e.g. a linear model despite true one being non-linear)

Effect of covariate shift when (naively) learning with misspecified models

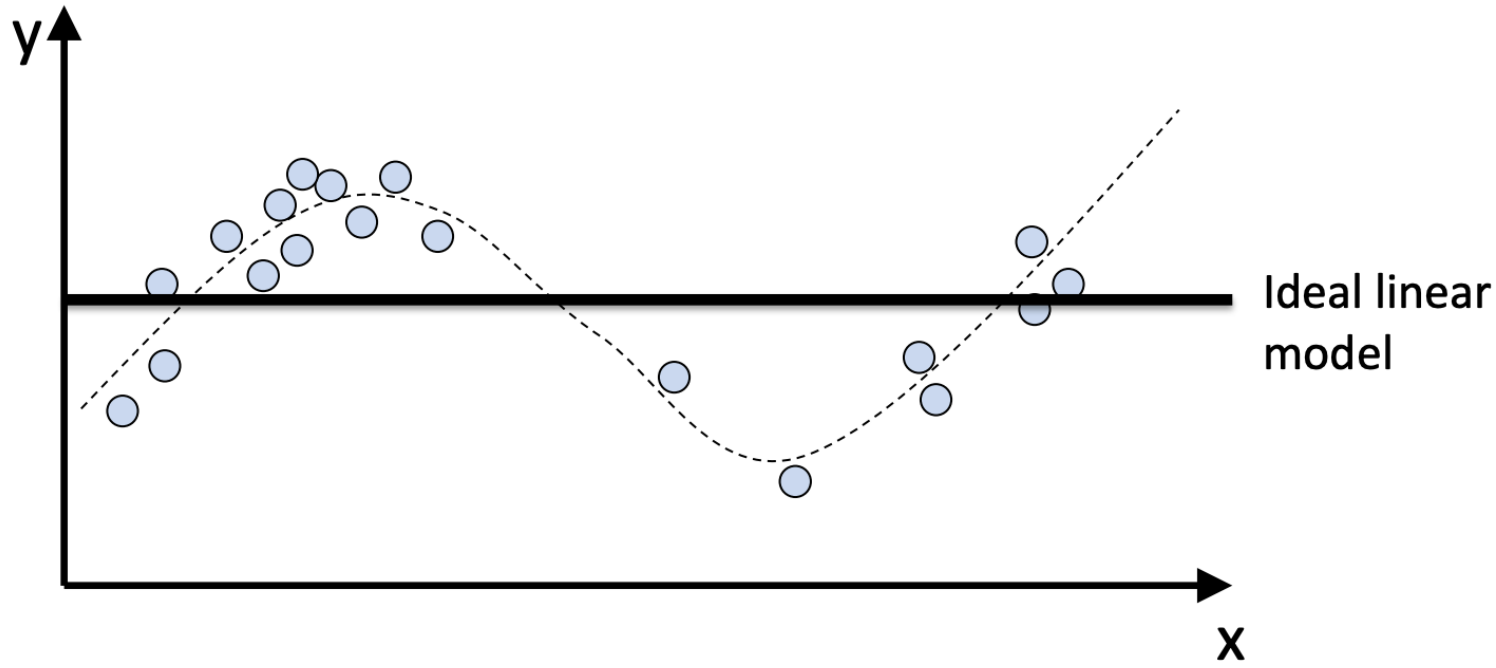
- Training data p(x,y)= red and test data q(x,y)= blue



[Storkey, “When Training and Test Sets are Different”, Dataset in Machine Learning, MIT Press 2009]

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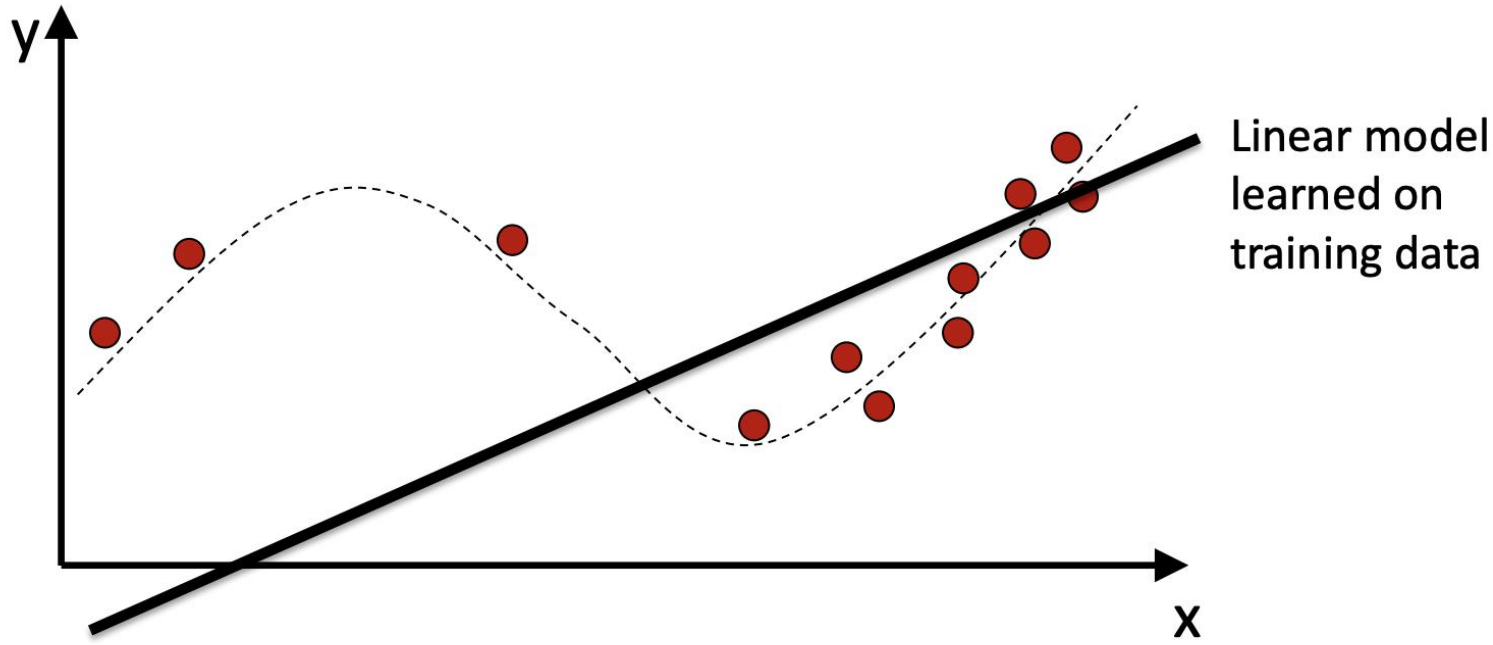
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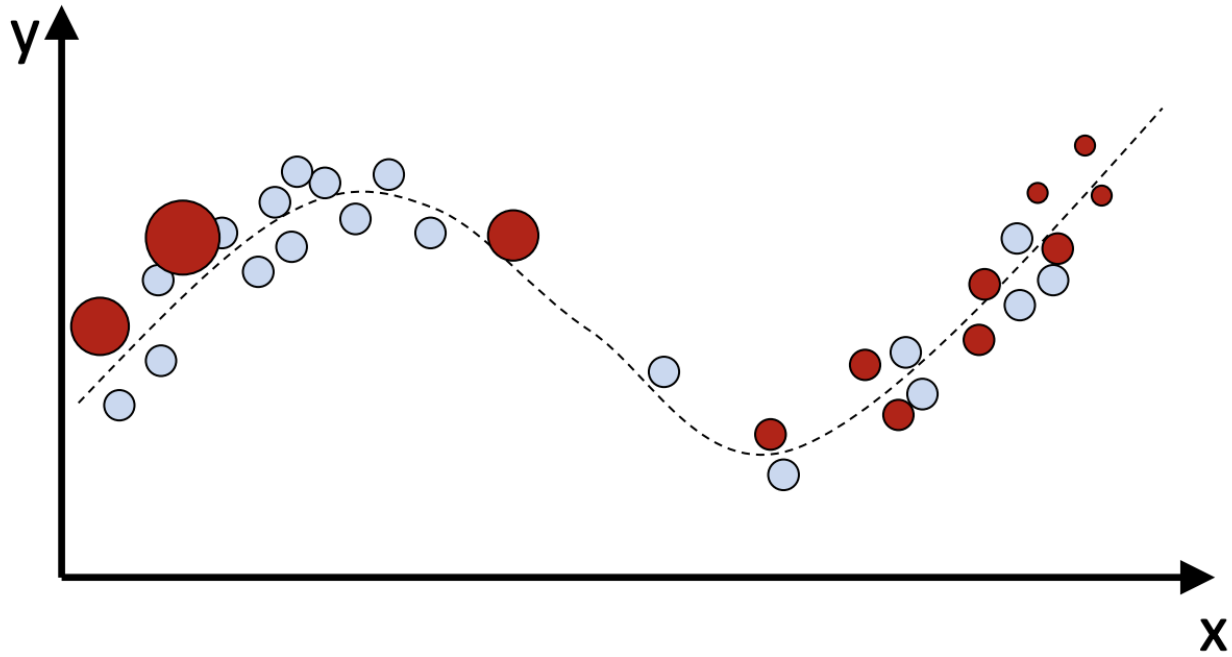
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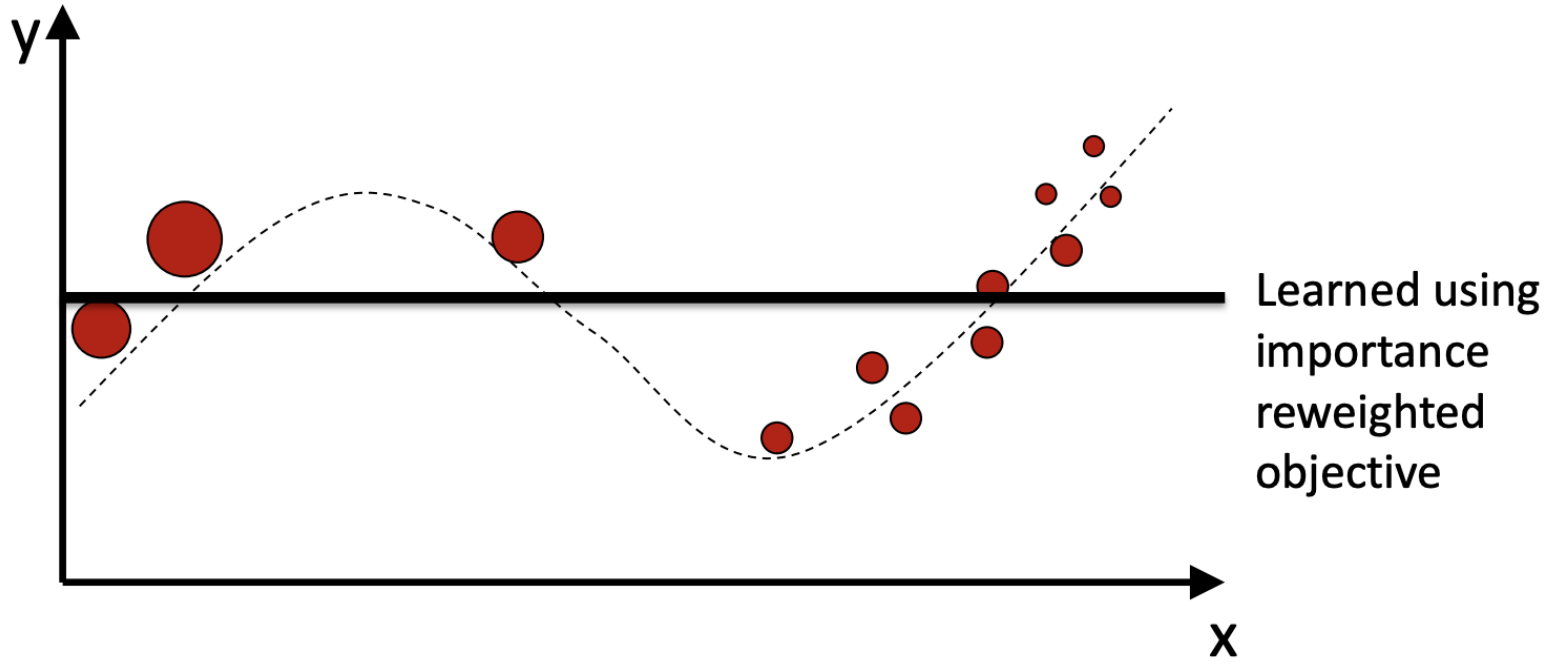
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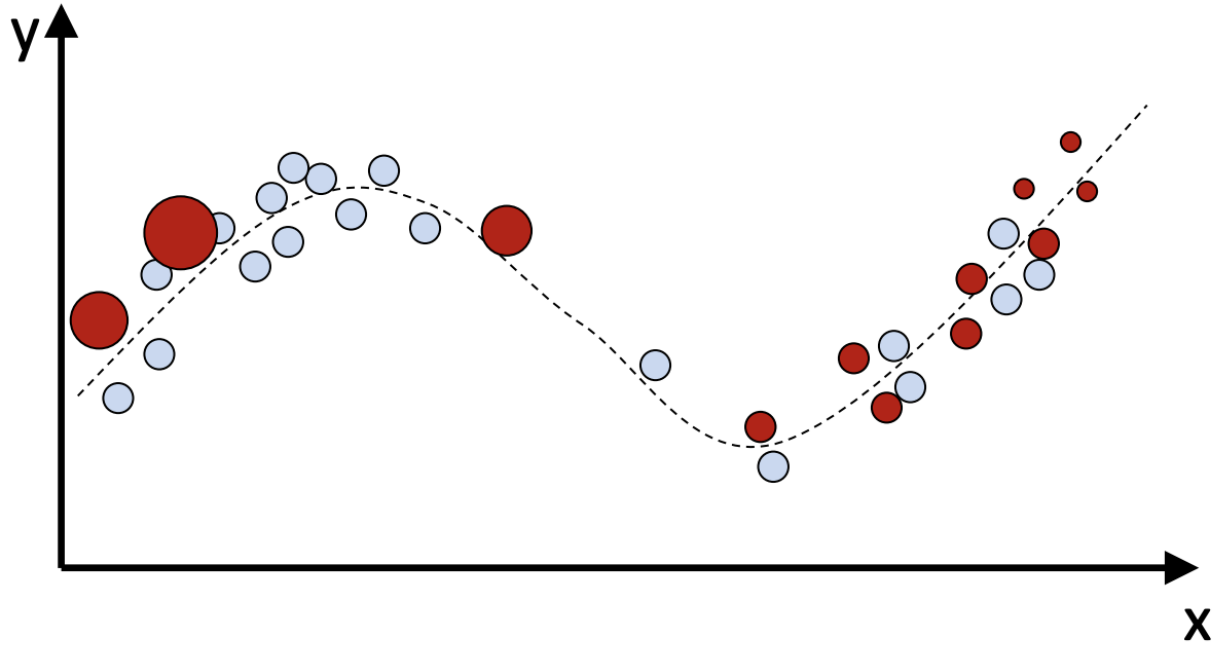
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Effect of covariate shift when (naively) learning with misspecified models

- Training data p(x,y)= red and test data q(x,y)= blue



Key insight: We only need to know q(x) to reweight the training data!

Example of unsupervised domain adaptation. No need for y values!

Learning using importance reweighting under covariate shift

- Goal of learning: $\min_\theta \mathbb{E}_{(x,y)\sim q} L(x, y; \theta)$

Example – squared loss, linear model

$$L(x, y; \theta) = (y - \theta \cdot x)^2$$

- But, suppose we only have samples $(x_1, y_1), \ldots, (x_m, y_m) \sim p(x, y)$
- Learn using: $\frac{1}{m} \sum_{i=1}^{m} \frac{q(x_i)}{p(x_i)} L(x_i, y_i; \theta)$

Importance reweighting

Recall $p(y|x) = q(y|x)$

$$\mathbb{E}_p\left[\frac{q(x)}{p(x)} L(x, y; \theta)\right] = \int_{x,y} p(x) p(y|x) \frac{q(x)}{p(x)} L(x, y; \theta)\, dx\, dy$$

$$= \int_{x,y} q(x, y) L(x, y; \theta)\, dx\, dy = \mathbb{E}_q[L(x, y; \theta)].$$

Learning using importance reweighting under covariate shift

- How do we obtain q(x) / p(x)?
- Approach 1: Empirically estimate the probabilities

$$\text{samples } x_1, ..., x_m \sim p,\ x'_1, ..., x'_n \sim q \longrightarrow \mathcal{D} = \{(x_1, 1), \ldots, (x_m, 1), (x'_1, 0), \ldots, (x'_n, 0)\}$$

$$\frac{q(x)}{p(x)} \leftarrow \frac{\Pr(d = 1 \mid x)}{1 - \Pr(d = 1 \mid x)} \frac{n}{m}$$

- Approach 2: Density estimation of p and q

When importance reweighting is not enough

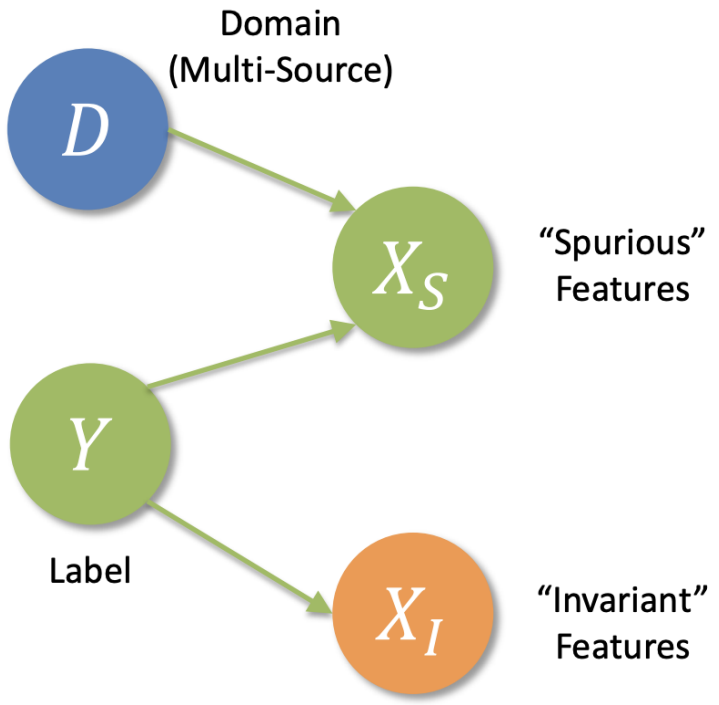
- Importance reweighted estimator can be high variance

- If there is *no overlap*, then in general impossible – even with infinite data

Current state of research on dataset shift

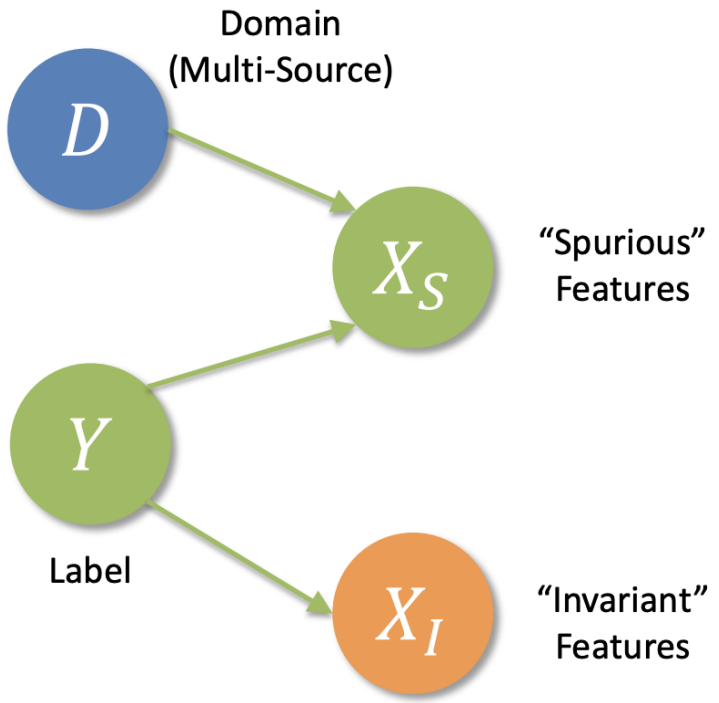
- Seek “invariant” representations that will work well even after dataset shift

- What properties should a representation have?
  - Here, the domain only influences (some) features. Learn only on those features.
  - Lower performance, but better translation between domains
  - But, how do we know which ones?
  - We just saw several methods to do so



Current state of research on dataset shift

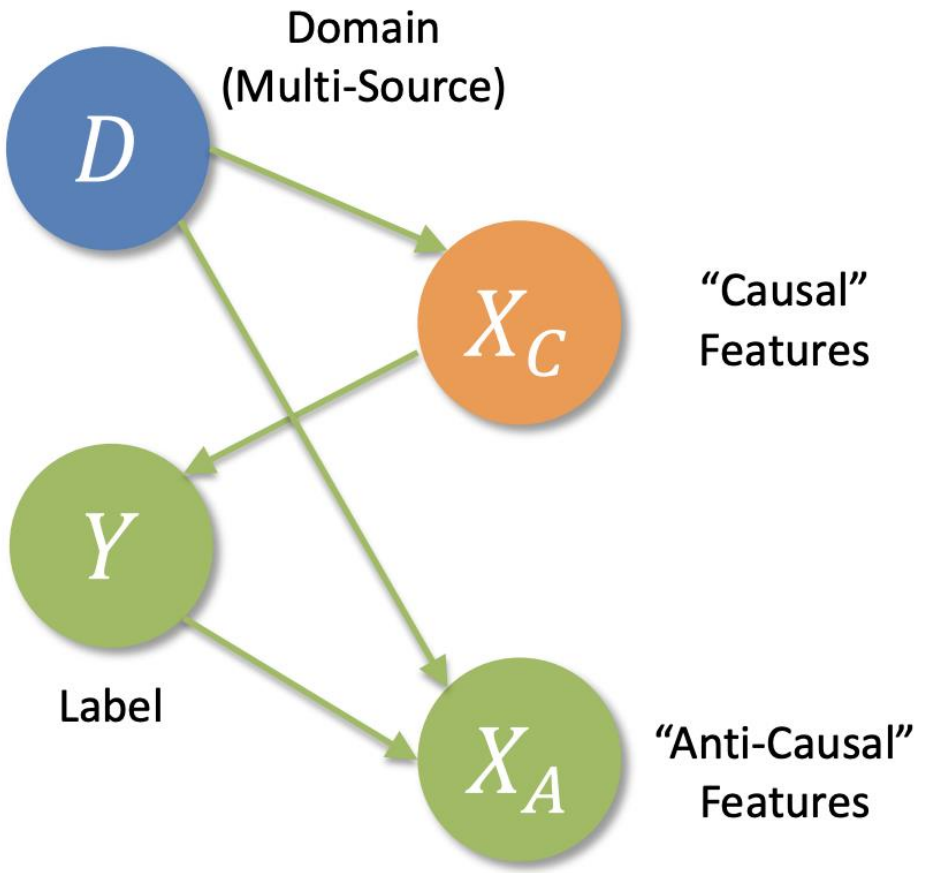
- **Observe**: The distribution P(X,Y) does not depend on D. Can we encourage our representation to recover X_I?
- **Potential approach**: Given multiple source environments, learn a representation such that $\phi(X) \perp D$
- ***Caveat***: The right "invariance" depends on the generative structure, and how D impacts X, Y



Current state of research on dataset shift

- Here, the domain influences all features.
- **Observe**: The distribution $P(Y|X_C)$ does not depend on D. Can we encourage our representation to recover X_C?
- **Potential approach**: Given multiple source environments, learn a representation such that

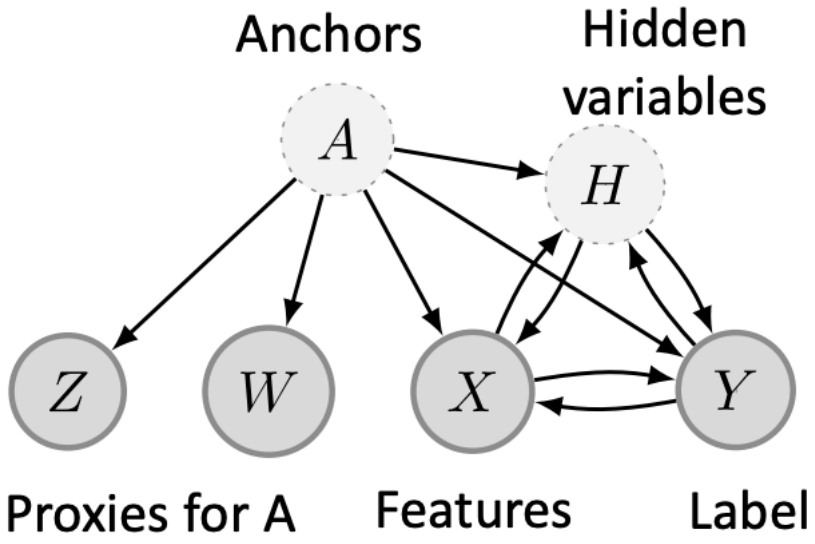
$$Y \perp D \mid \phi(X)$$



Note: Under this generative structure, it no longer makes sense to seek $\phi(X) \perp D$

Current state of research on dataset shift

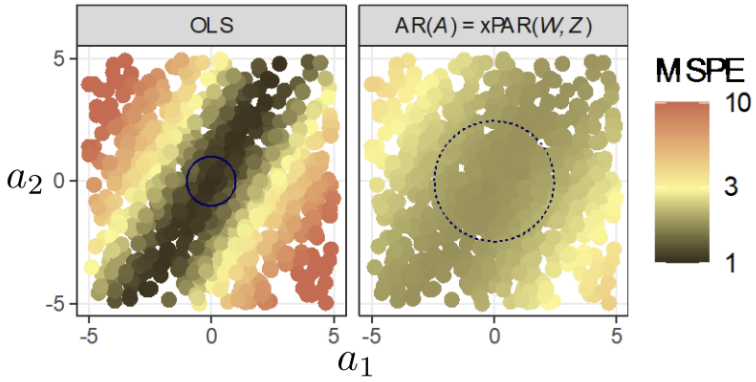
- Assume knowledge of ‘anchors’ that tell you what can change; learn to extrapolate



Assume p(*A*) will change in test distribution, and use distributionally robust training

$$f^* = \arg\min_{f \in \mathcal{F}} \sup_{\mathbb{P} \in \mathcal{P}} \mathbb{E}_{\mathbb{P}}[\ell(Y, f(X))]$$

Change in A is assumed to be *bounded*.



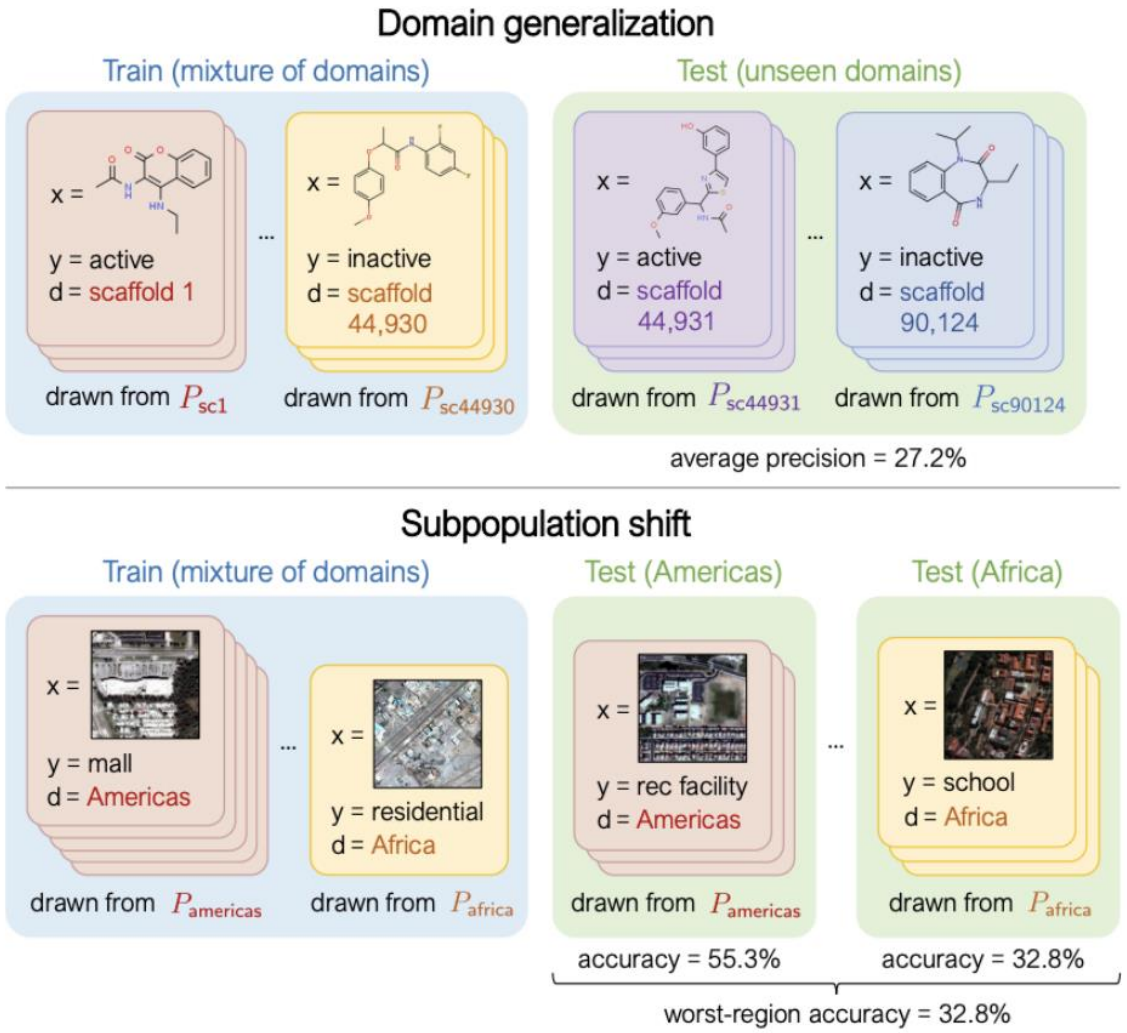
[Rothenhausler et al., Anchor regression: heterogeneous data meets causality. J. of the Royal Statistical Society: Series B, ’18; Oberst, Thams, Peters, Sontag. Regularizing towards Causal Invariance: Linear Models with Proxies, ICML, ‘21]

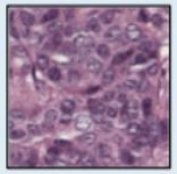
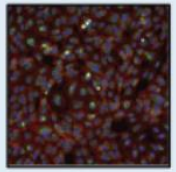
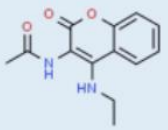
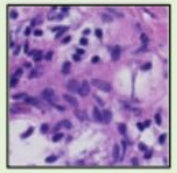
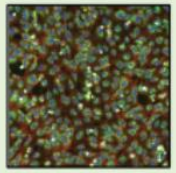
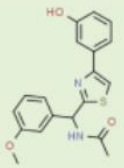
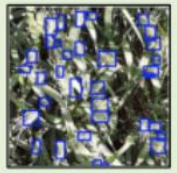
Distribution Shift Benchmarking

WILDS: A Benchmark of in-the-Wild Distribution Shifts

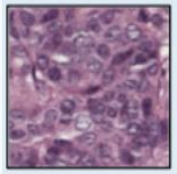
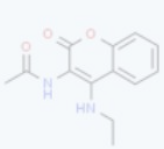
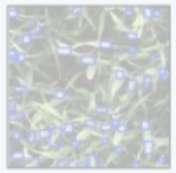
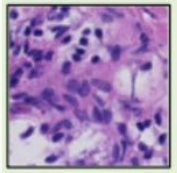
Pang Wei Koh* and **Shiori Sagawa***	{pangwei, ssagawa}@cs.stanford.edu
Henrik Marklund	marklund@stanford.edu
Sang Michael Xie	xie@cs.stanford.edu
Marvin Zhang	marvin@eecs.berkeley.edu
Akshay Balsubramani	abalsubr@stanford.edu
Weihua Hu	weihuahu@stanford.edu
Michihiro Yasunaga	myasu@stanford.edu
Richard Lanas Phillips	richard@cs.cornell.edu
Irena Gao	igao@stanford.edu
Tony Lee	tonyhlee@stanford.edu
Etienne David	etienne.david@inrae.fr
Ian Stavness	stavness@usask.ca
Wei Guo	guowei@g.ecc.u-tokyo.ac.jp
Berton A. Earnshaw	berton.earnshaw@recursionpharma.com
Imran S. Haque	imran.haque@recursionpharma.com
Sara Beery	sbeery@caltech.edu
Jure Leskovec	jure@cs.stanford.edu
Anshul Kundaje	akundaje@stanford.edu
Emma Pierson	epierson@microsoft.com
Sergey Levine	svlevine@eecs.berkeley.edu
Chelsea Finn	cbfinn@cs.stanford.edu
Percy Liang	pliang@cs.stanford.edu

Correspondence to: wilds@cs.stanford.edu



	Domain generalization					Subpopulation shift	Domain generalization + subpopulation shift			
Dataset	**iWildCam**	**Camelyon17**	**RxRx1**	**OGB-MolPCBA**	**GlobalWheat**	**CivilComments**	**FMoW**	**PovertyMap**	**Amazon**	**Py150**
Input (x)	camera trap photo	tissue slide	cell image	molecular graph	wheat image	online comment	satellite image	satellite image	product review	code
Prediction (y)	animal species	tumor	perturbed gene	bioassays	wheat head bbox	toxicity	land use	asset wealth	sentiment	autocomplete
Domain (d)	camera	hospital	batch	scaffold	location, time	demographic	time, region	country, rural-urban	user	git repository
# domains	323	5	51	120,084	47	16	16 x 5	23 x 2	2,586	8,421
# examples	203,029	455,954	125,510	437,929	6,515	448,000	523,846	19,669	539,502	150,000
Train example						What do Black and LGBT people have to do with bicycle licensing?			Overall a solid package that has a good quality of construction for the price.	`import numpy as np … norm=np.___`
Test example						As a Christian, I will not be patronizing any of those businesses.			I *loved* my French press, it's so perfect and came with all this fun stuff!	`import subprocess as sp p=sp.Popen() stdout=p.___`
Adapted from	Beery et al. 2020	Bandi et al. 2018	Taylor et al. 2019	Hu et al. 2020	David et al. 2021	Borkan et al. 2019	Christie et al. 2018	Yeh et al. 2020	Ni et al. 2019	Raychev et al. 2016

[Koh et al., WILDS: A Benchmark of in-the-Wild Distribution Shifts. arXiv:2012.07421, 2021.]

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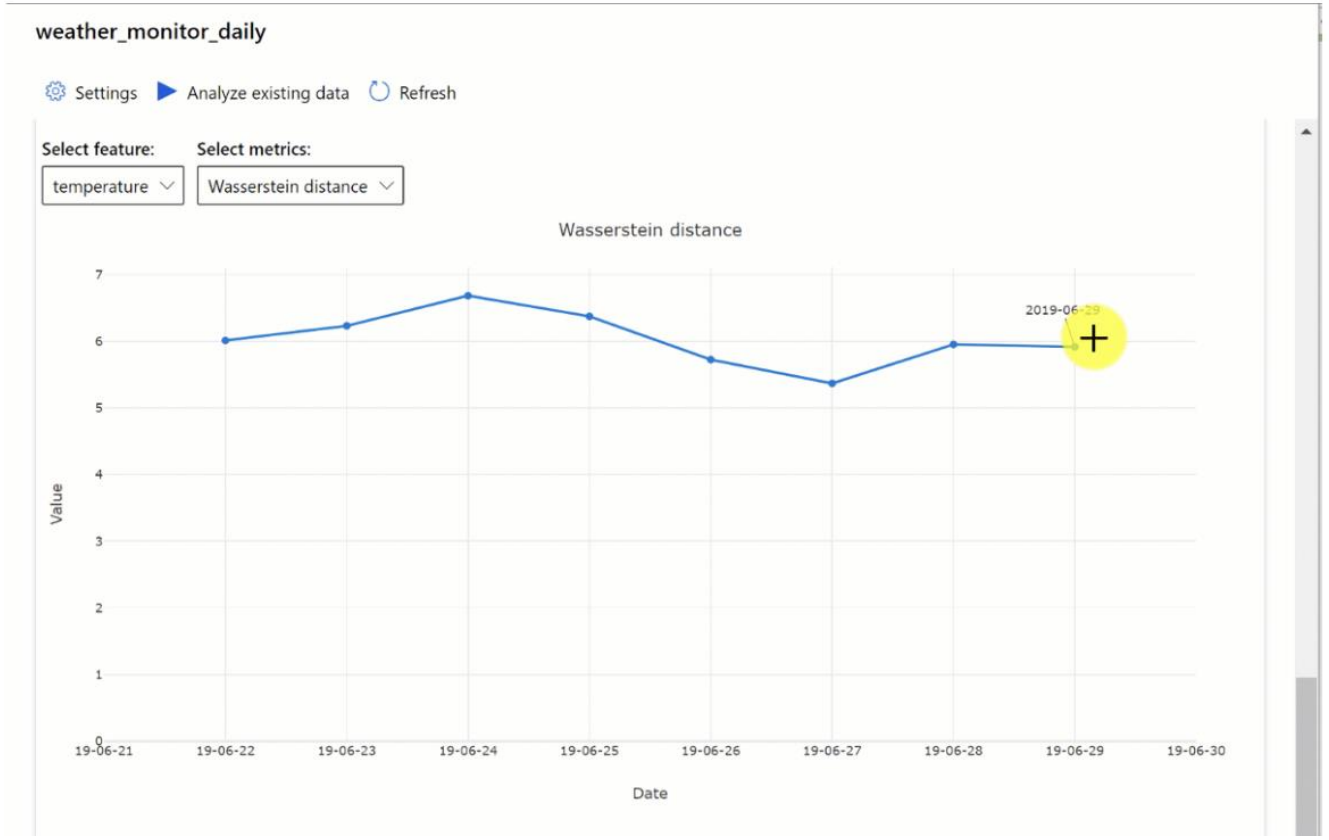
TL;DR: Existing algorithms don't substantially improve over Empirical Risk Minimization (ERM)

where ERM = estimate risk empirically on training data, bc we don't know all possible distributions of datasets

Table 2: The out-of-distribution test performance of models trained with different baseline algorithms: CORAL, originally designed for unsupervised domain adaptation; IRM, for domain generalization; and Group DRO, for subpopulation shifts. Evaluation metrics for each dataset are the same as in Table 1; higher is better. Overall, these algorithms did not improve over empirical risk minimization (ERM), and sometimes made performance significantly worse, except on CivilComments-WILDS where they perform better but still do not close the in-distribution gap in Table 1. For GlobalWheat-WILDS, we omit CORAL and IRM as those methods do not port straightforwardly to detection settings; its ERM number also differs from Table 1 as its ID comparison required a slight change to the OOD test set. Parentheses show standard deviation across 3+ replicates.

Dataset	Setting	ERM	CORAL	IRM	Group DRO
iWildCam2020-WILDS	Domain gen.	31.0 (1.3)	**32.8 (0.1)**	15.1 (4.9)	23.9 (2.1)
Camelyon17-WILDS	Domain gen.	**70.3 (6.4)**	59.5 (7.7)	64.2 (8.1)	68.4 (7.3)
RxRx1-WILDS	Domain gen.	**29.9 (0.4)**	28.4 (0.3)	8.2 (1.1)	23.0 (0.3)
OGB-MolPCBA	Domain gen.	**27.2 (0.3)**	17.9 (0.5)	15.6 (0.3)	22.4 (0.6)
GlobalWheat-WILDS	Domain gen.	**51.2 (1.8)**	—	—	47.9 (2.0)
CivilComments-WILDS	Subpop. shift	56.0 (3.6)	65.6 (1.3)	66.3 (2.1)	**70.0 (2.0)**
FMoW-WILDS	Hybrid	**32.3 (1.3)**	31.7 (1.2)	30.0 (1.4)	30.8 (0.8)
PovertyMap-WILDS	Hybrid	**0.45 (0.06)**	0.44 (0.06)	0.43 (0.07)	0.39 (0.06)
Amazon-WILDS	Hybrid	**53.8 (0.8)**	52.9 (0.8)	52.4 (0.8)	53.3 (0.0)
Py150-WILDS	Hybrid	**67.9 (0.1)**	65.9 (0.1)	64.3 (0.2)	65.9 (0.1)

Current state of industry on dataset shift



Source: https://docs.microsoft.com/en-us/azure/machine-learning/how-to-monitor-datasets
See also: https://cloud.google.com/solutions/machine-learning/ml-modeling-monitoring-identifyingtraining-server-skew-with-novelty-detection & https://docs.seldon.io/projects/alibi-detect/en/latest/

Conclusion

- Dataset shift happens all the time with healthcare data
- It doesn’t always hurt performance
- Interpretability methods can help with detecting and mitigating dataset shift
- Safe deployments should include automated checks for dataset shift
- Active area of research in ML

Summary

- Examples and formulation of dataset shift
- Testing for dataset shift
- Mitigating dataset shift
- Discussion



How can we make Data 146 better for you?

Next class: Pediatric datasets