TRAIL Brownbag
Covariate Shift Tutorial

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COLUMBIA | MAILMAN SCHOOL OF PUBLIC HEALTH

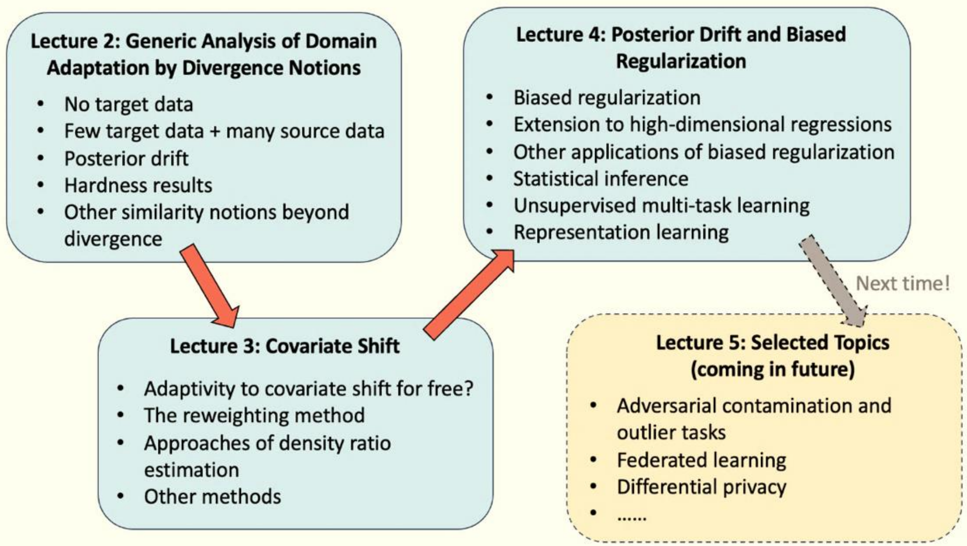
Acknowledgement

This tutorial is modified based on the Theoretical Covariate Shift Lecture from Ye Tian

A (Selective) Introduction to the Statistics Foundations of Transfer Learning

Time: 9AM-5PM, May 20, 2024

Schedule

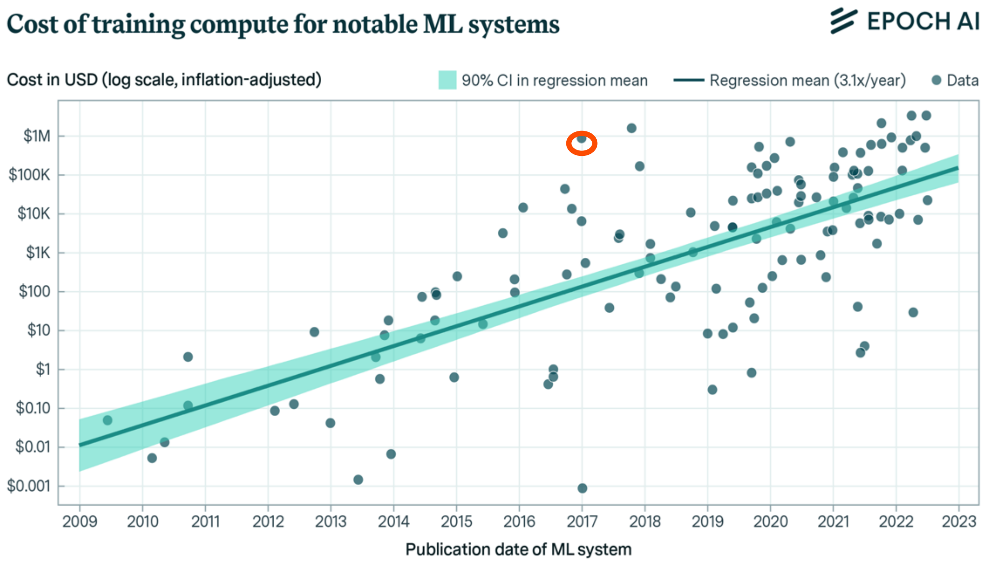


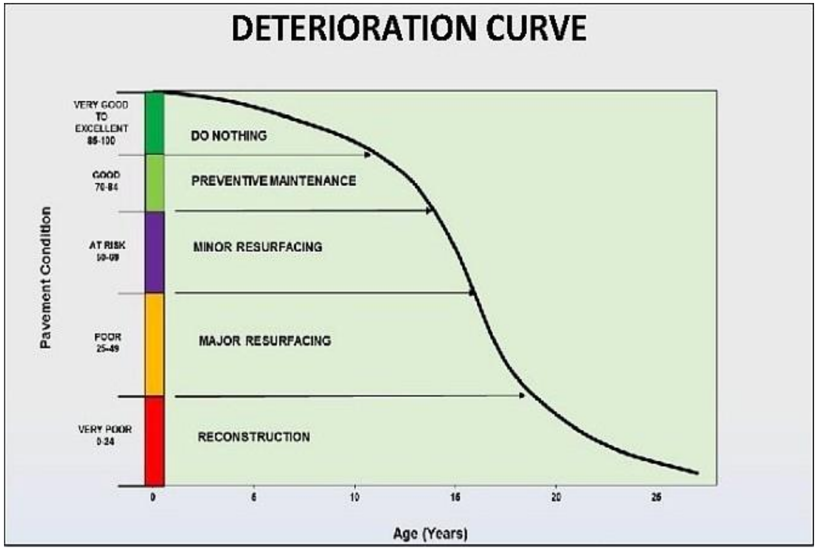
https://www.columbia.edu/~yt2661/STL.html

Machine Learning Dilemma

Machine learning is powerful but **expensive**, because it requires:

- large labeled datasets
- significant computing power and training time





Ruiz, Victor M. et al.
The Journal of Thoracic and Cardiovascular Surgery, Volume 164, Issue 1, 211 - 222.e3

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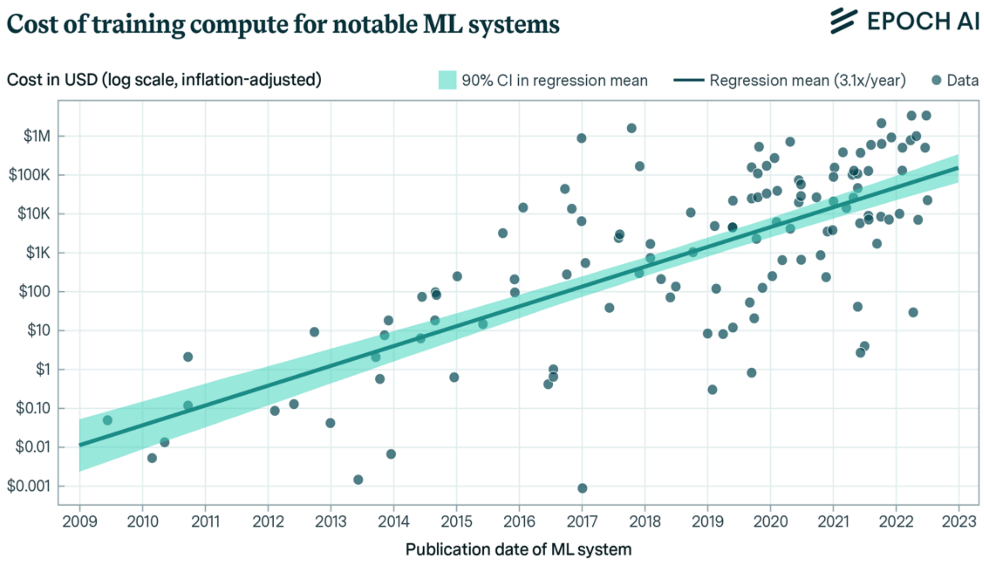
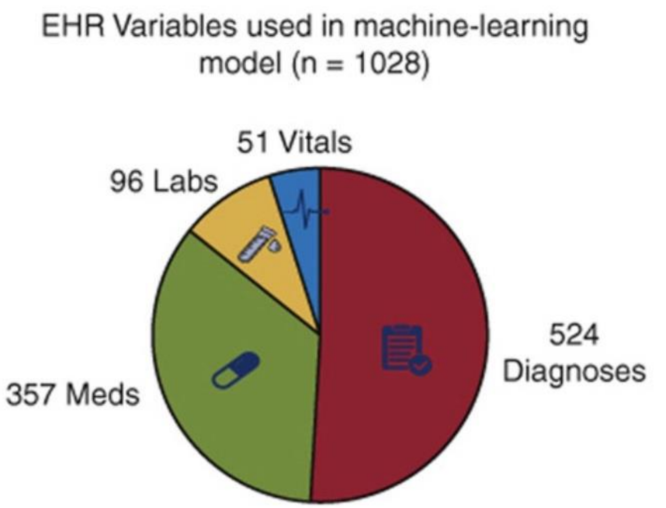
Annotation (eg. chart review) by doctors is costly





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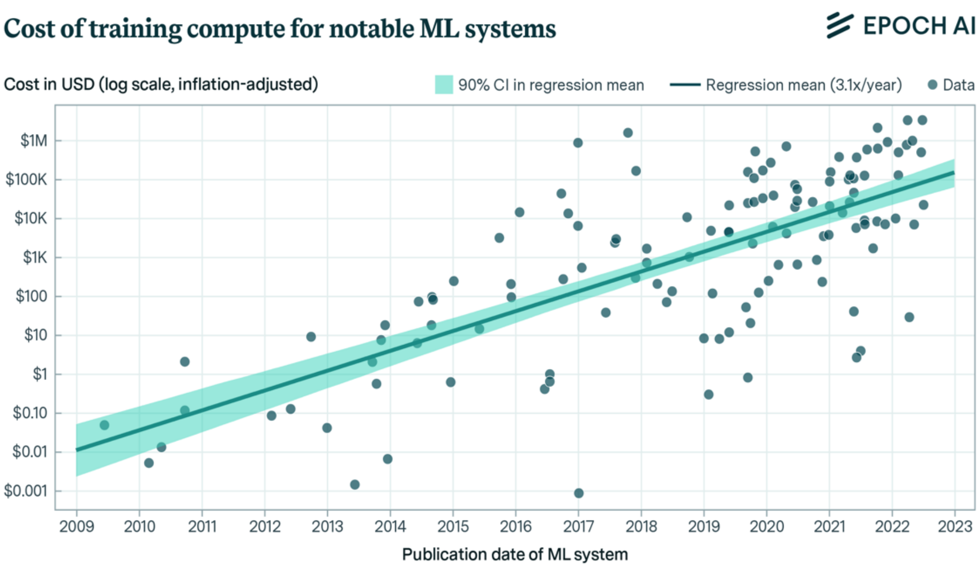

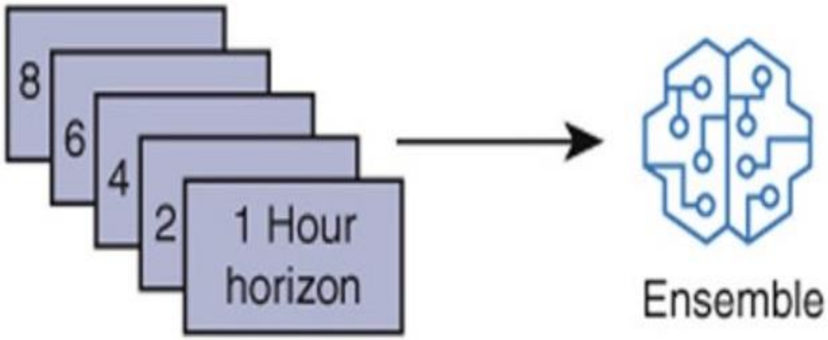

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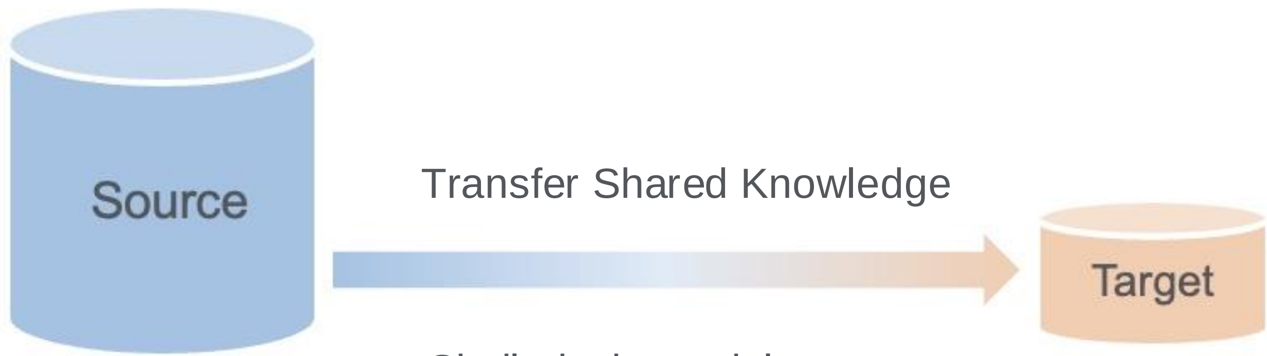
Transfer Learning

Leverage knowledge from a model trained for one task and reused to help with a similar, related task



- Similarity in model parameters
- Shared model structure
- Shared embedding structure
- …

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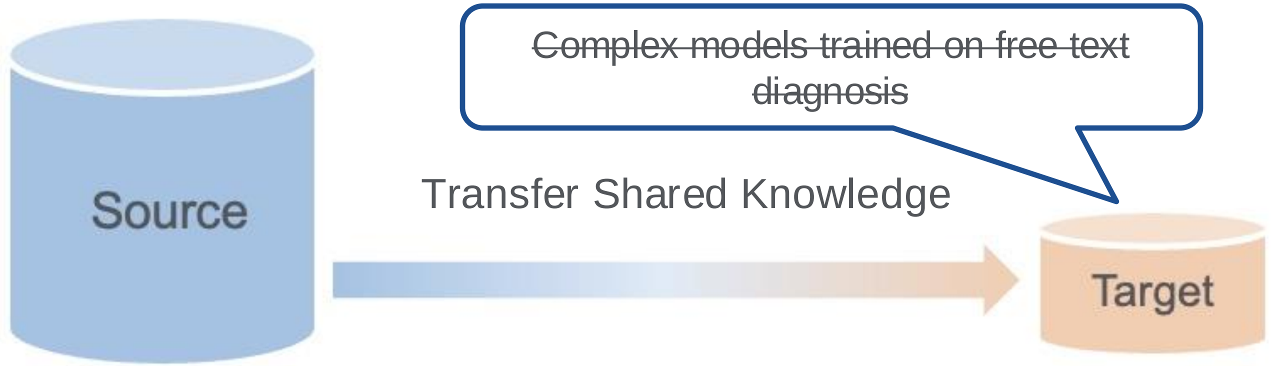
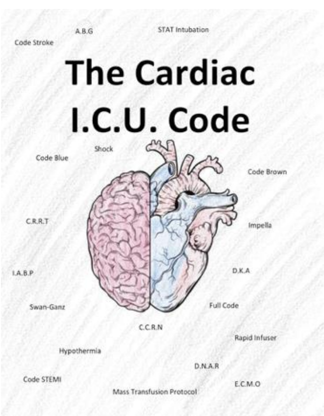
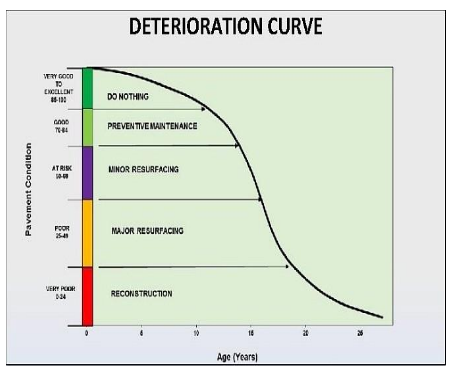
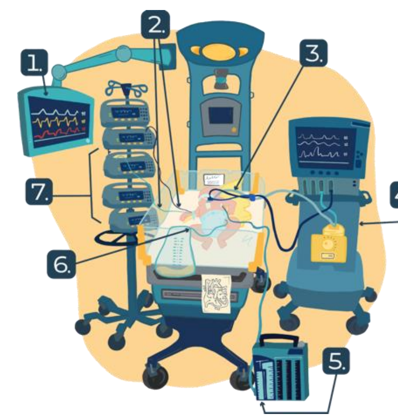




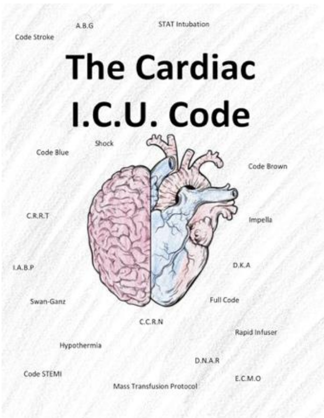


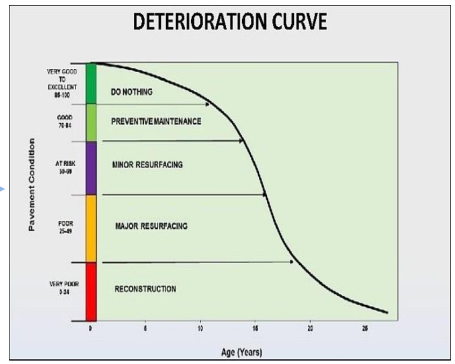


Target Deterioration Curve

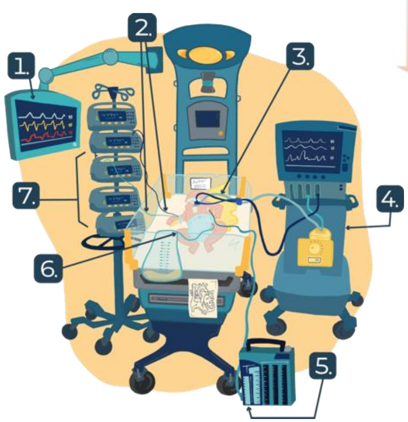
Transfer Learning

Difference between source and target dataset:





- Sample size
  Rich vs Scarce
- Variables/Features
  Young vs Old



Target
Deterioration
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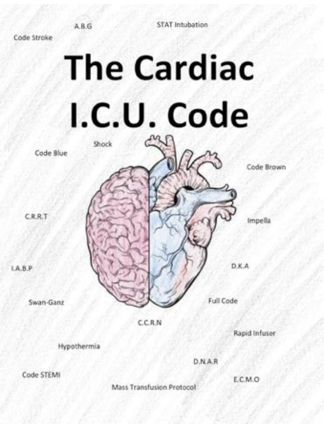

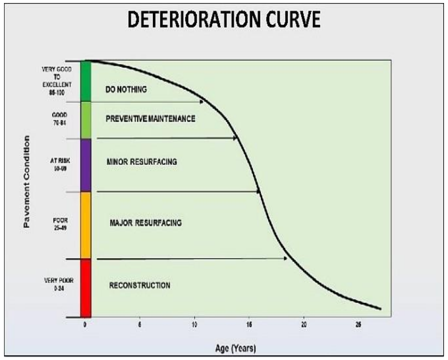

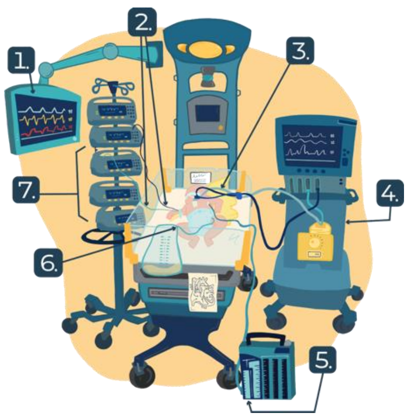

Target Deterioration Curve

Domain Adaptation: address the challenge of training a model on one data distribution and applying it to a related but different data distribution

Domain Adaptation (a solution)

- Model finetuning
- Covariate shift adjustment
- Learning invariant representations
- …

Distributional Shift

- Target T, $(X,Y)_T$
  Source S, $(X,Y)_S$
- Probability Chain Rule: $\boxed{P(X,Y)} = P(Y|X)\ P(X)$
- Distribution Shift types:
  - Joint Shift: $P_S(X,Y) \neq P_T(X,Y)$

Distributional Shift

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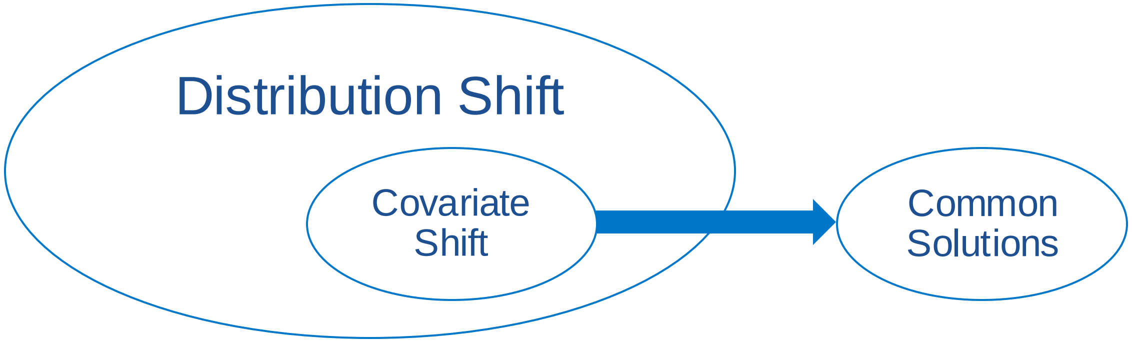
  - Joint Shift: $P_S(X, Y) \neq P_T(X, Y)$
  - Model Shift: $P_S(Y|X) \neq P_T(Y|X)$
  - **Covariate Shift:** $P_S(X) \neq P_T(X)$



Tutorial Plan

- Separate Density Estimation
    - Kernel Density Estimation
    - Histogram-based Method

April 18th

- Estimating Weight as a whole
    - Kernel Mean Matching
    - Least Square Method
    - Kullback-Leibler Method
    - Discriminative Learning
    - Profile Likelihood Method
- Beyond Reweighting Technique and Covariate Shift
    - Marginal Transfer Learning
    - Domain Invariant Method
    - Optimal Transformation

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April 25th

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Fall 2025

  - Profile Likelihood Method
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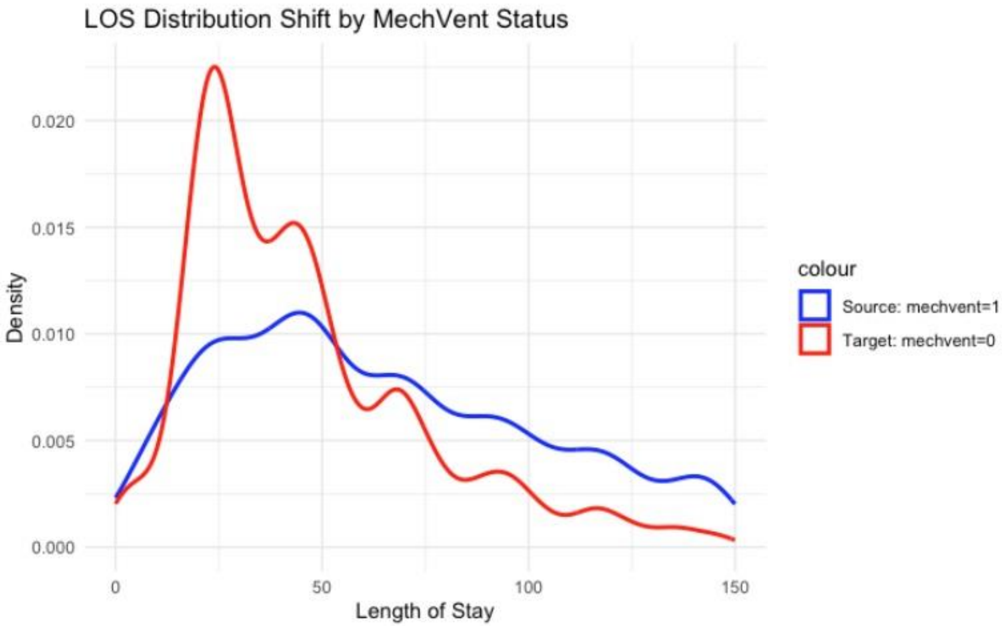
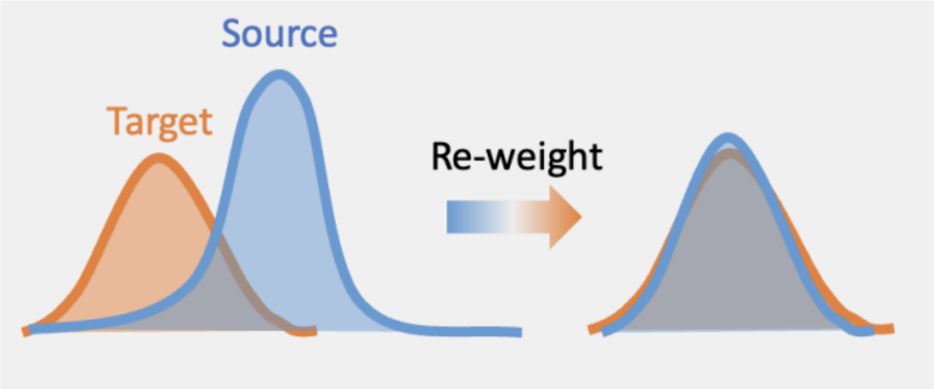
Covariate Shift



Importance Weighting Framework



Density ratio model: $\omega(\boldsymbol{X}) = \frac{P^{\mathcal{T}}(\boldsymbol{X})}{P^{\mathcal{S}}(\boldsymbol{X})}$

$$\mathrm{E}^{\mathcal{T}}[f(\boldsymbol{X})] = \mathrm{E}^{\mathcal{S}}[\omega(\boldsymbol{X})f(\boldsymbol{X})]$$

holds for any $f(\boldsymbol{X})$

$$\int f(\boldsymbol{X})\, P^{\mathcal{T}}(\boldsymbol{X})\, dX = \int \frac{P^{\mathcal{T}}(\boldsymbol{X})}{\cancel{P^{\mathcal{S}}(\boldsymbol{X})}} f(\boldsymbol{X})\, \cancel{P^{\mathcal{S}}(\boldsymbol{X})}\, dX$$

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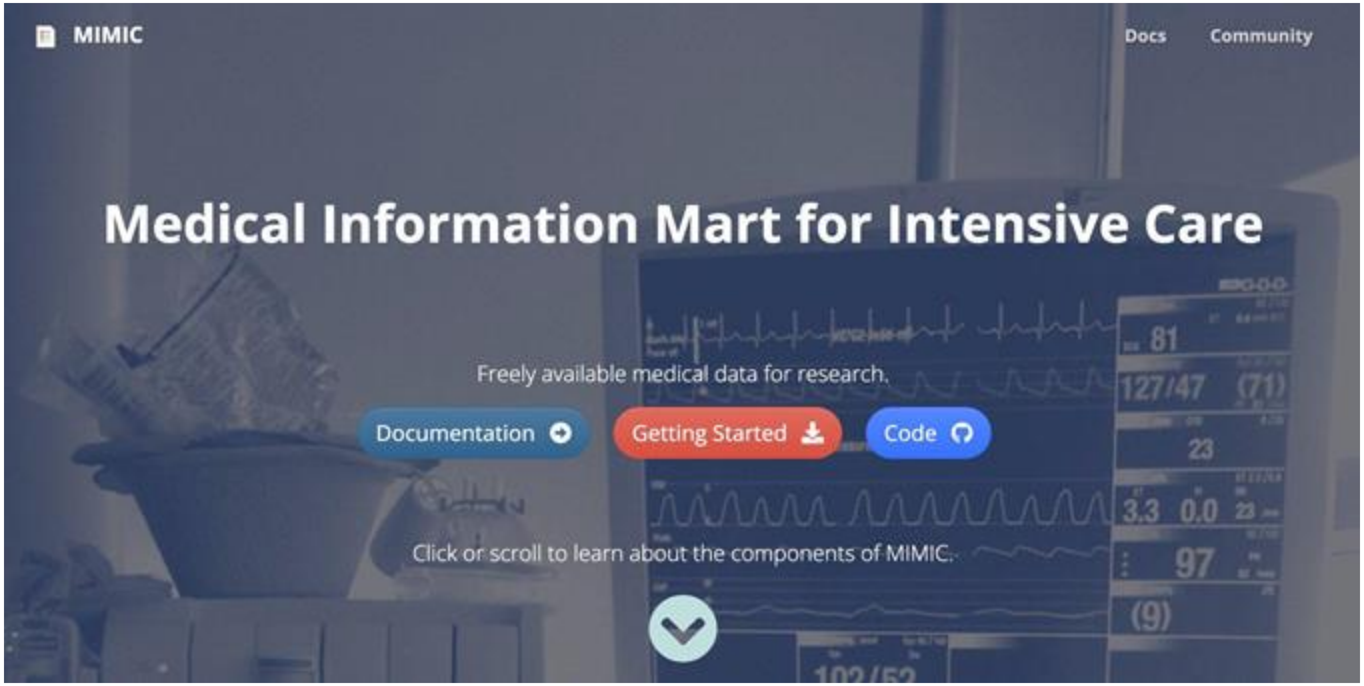
MIMIC-III Dataset

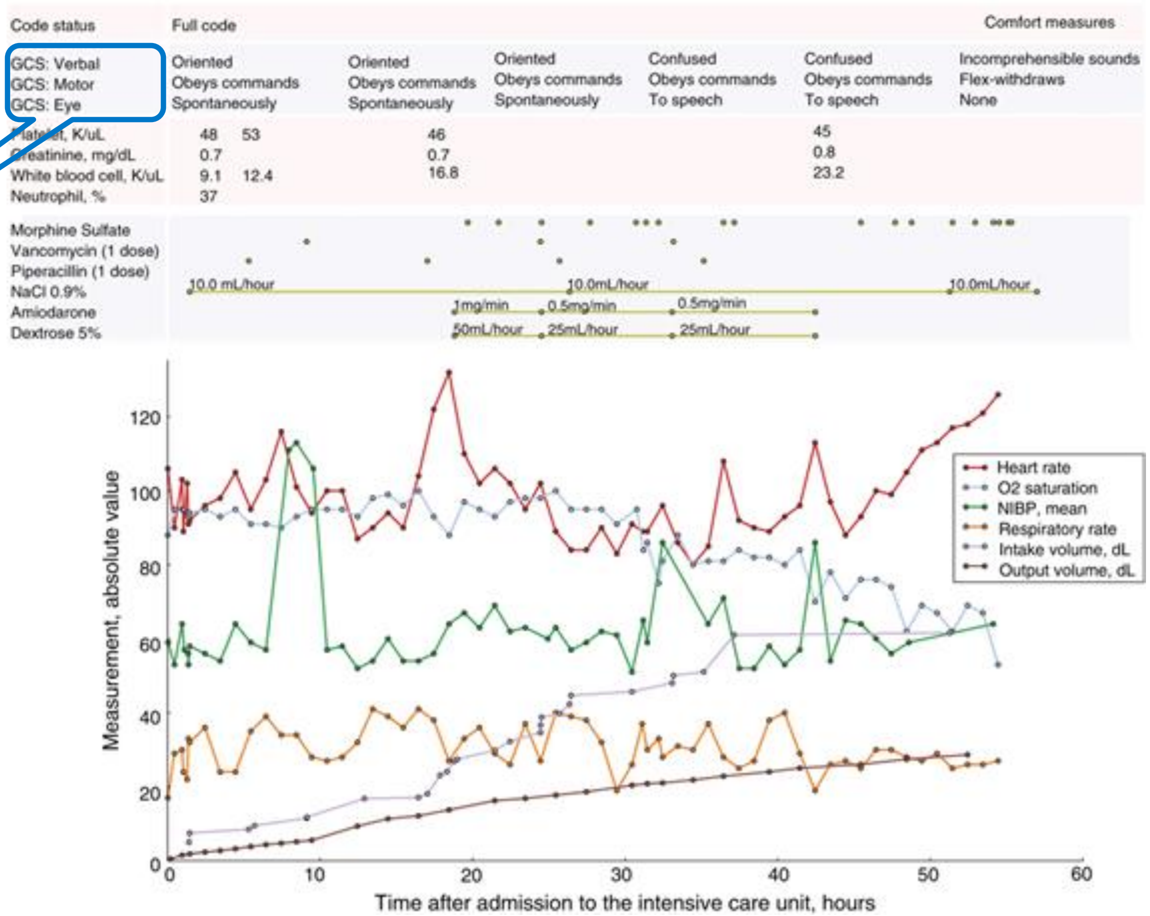


- PhysioNet: https://physionet.org/
  - The Research Resource for Complex Physiologic Signals
  - Need to get credentialed and trained

MIMIC-III Dataset

Sample data for a single patient stay in a medical intensive care Unit including:

- Consciousness
- Blood test result
- Drug
- Vital sign measurement



https://www.nature.com/articles/sdata201635#Fig2

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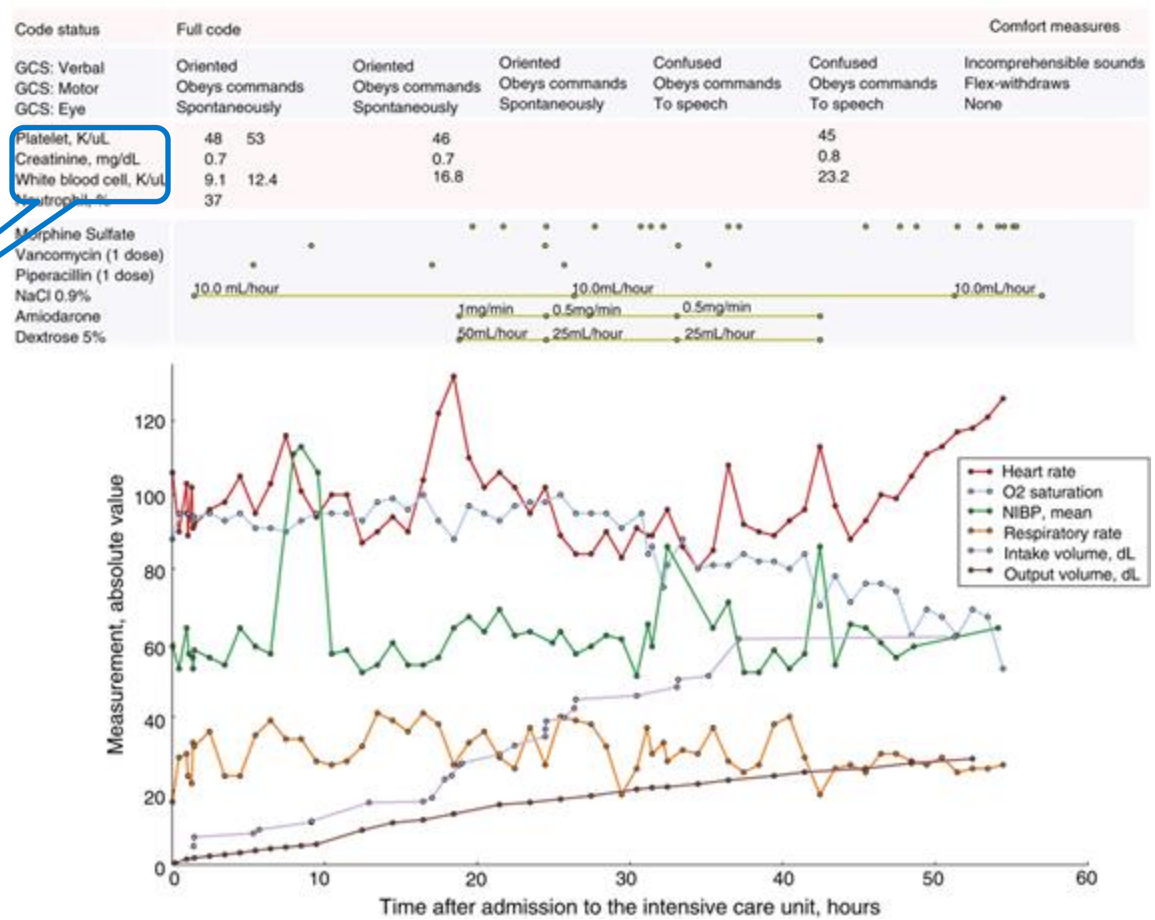

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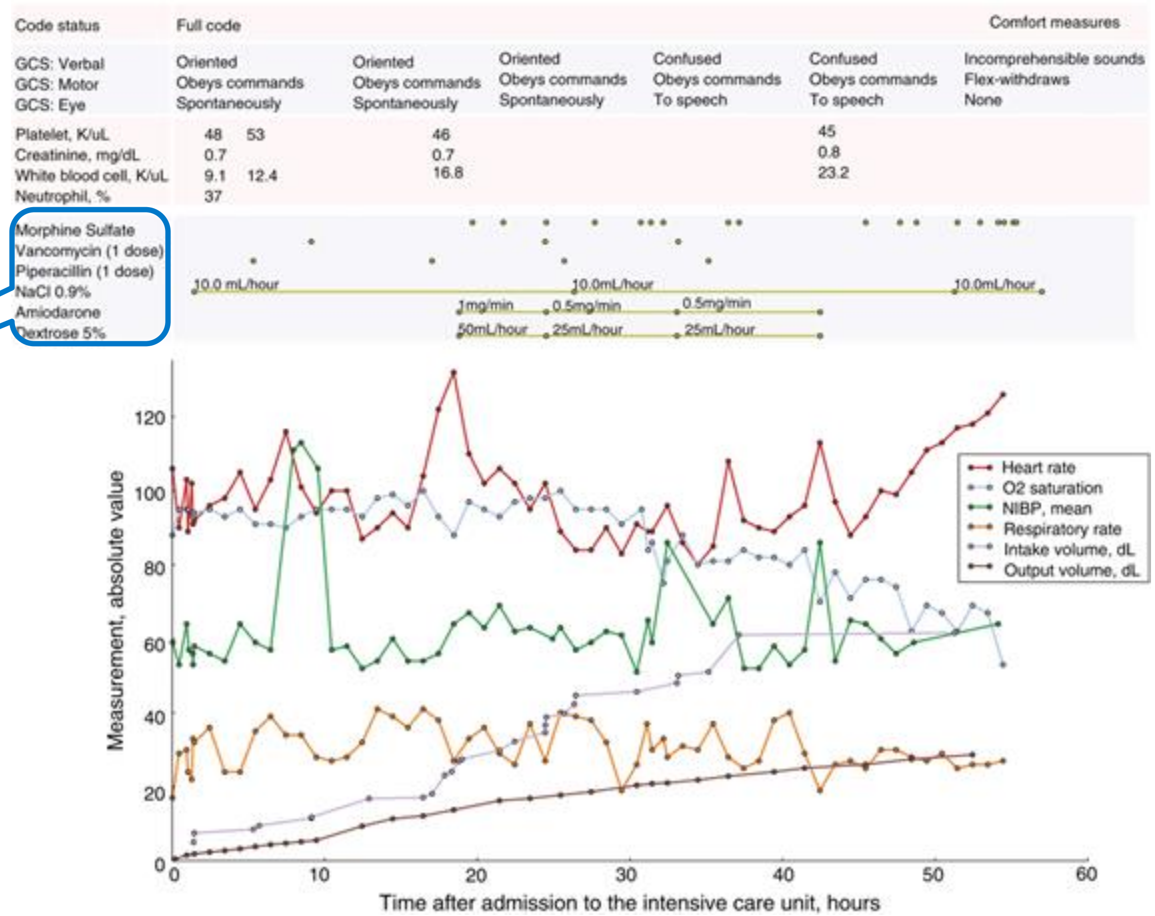

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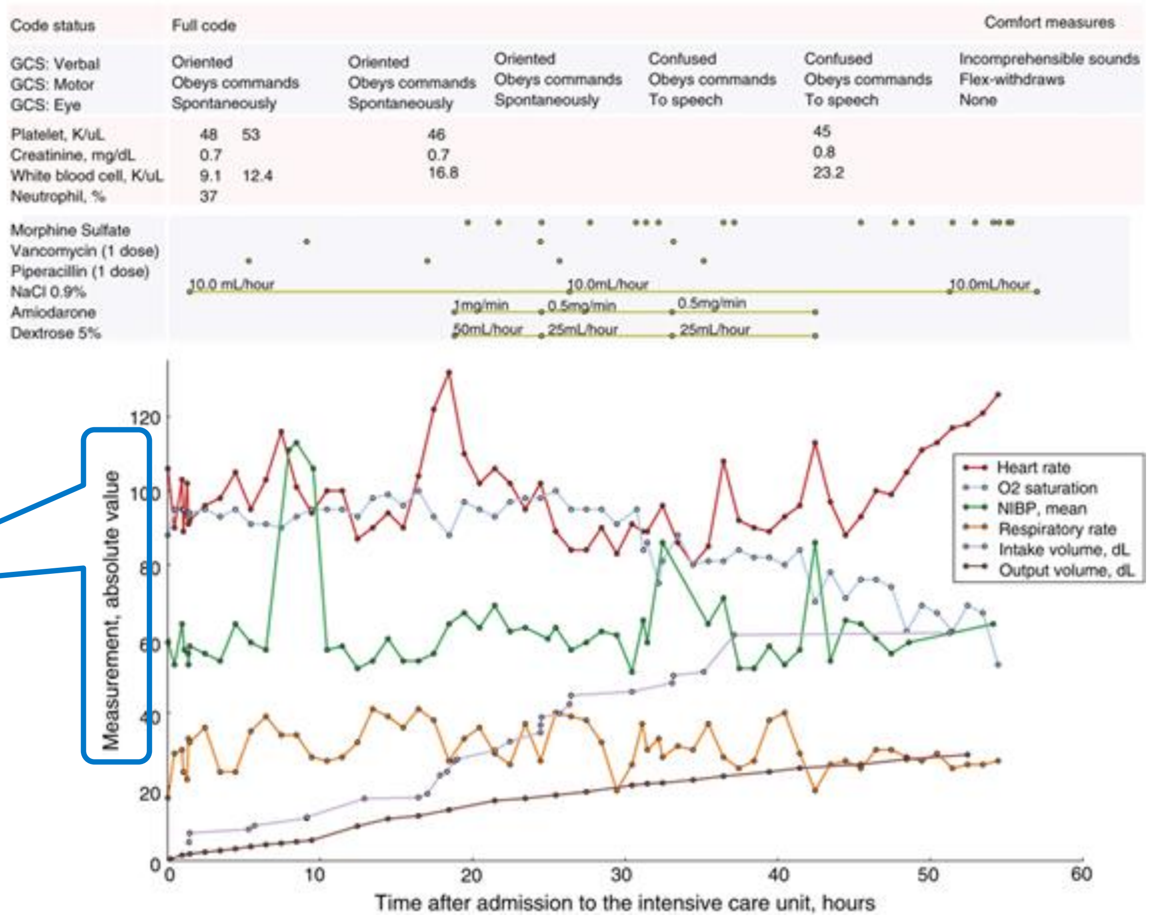

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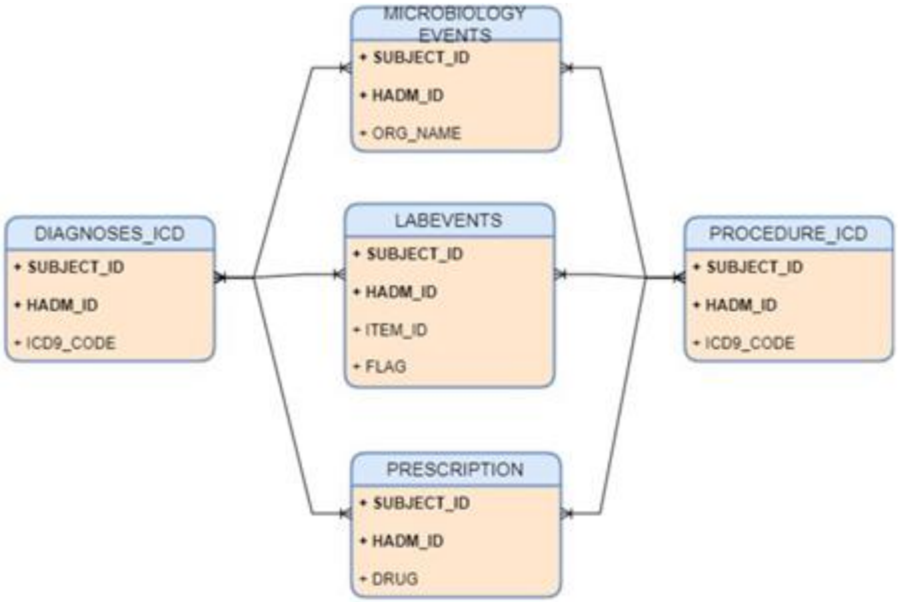

'Transfer': Physical locations for patients throughout their hospital stay

'service'(med_service_only): Lists services that a patient was admitted/transferred under.

'Callout': Provides information when a patient was READY for discharge from the ICU, and when the patient was actually discharged from the ICU.

'Patients': Defines each SUBJECT_ID in the database, i.e. defines a single patient.(demographic)

'Elixhauser': Elixhauser Comorbidity Index (ECI) is a tool used to assess the severity and number of chronic health conditions in a patient

'Diagnoses_icd': Definition table for ICD diagnoses.

'Drgcodes': Contains diagnosis related groups (DRG) codes for patients.

https://physionet.org/content/mimiciii-demo/1.4/

Separate Density Estimation

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  - Kernel Density Estimation
  - Histogram-based Method

April 18th

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d

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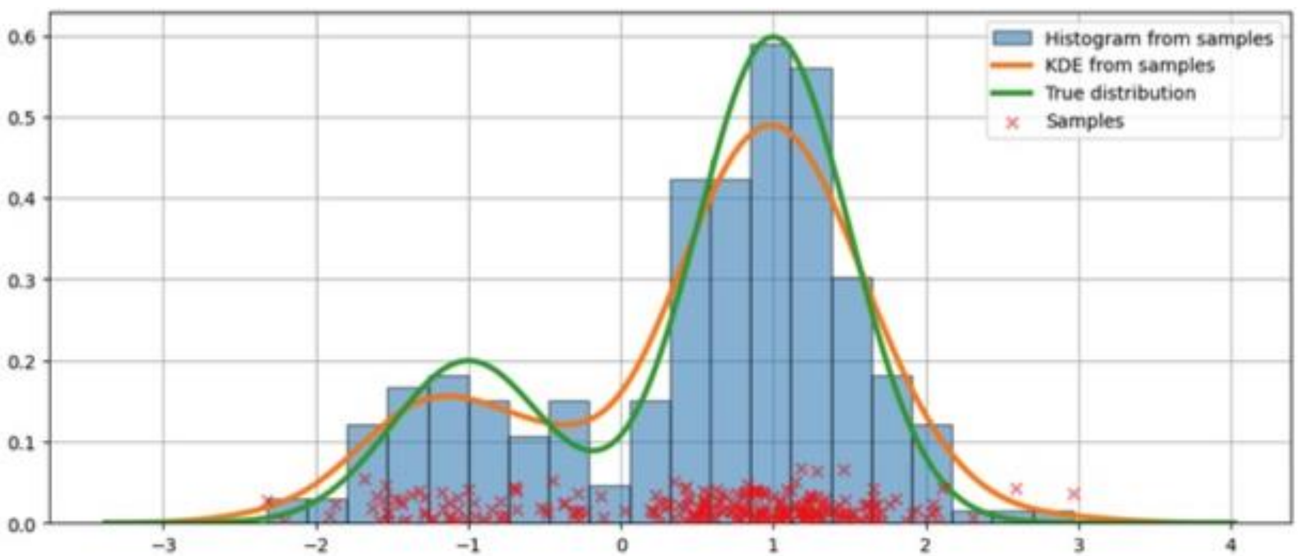
  - Optimal Transformation

$$\omega(\boldsymbol{X}) = \frac{P^{\mathcal{T}}(\boldsymbol{X})}{P^{\mathcal{S}}(\boldsymbol{X})} = \frac{f_T(\boldsymbol{X})}{f_S(\boldsymbol{X})}$$

- Parametric density estimation
- Non-parametric density estimation

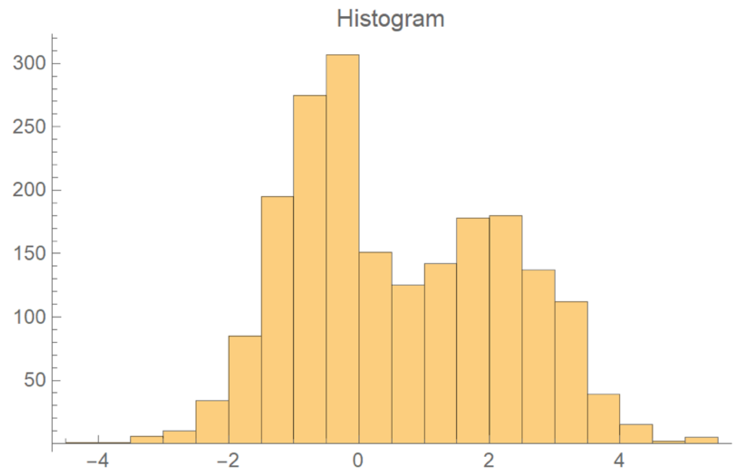


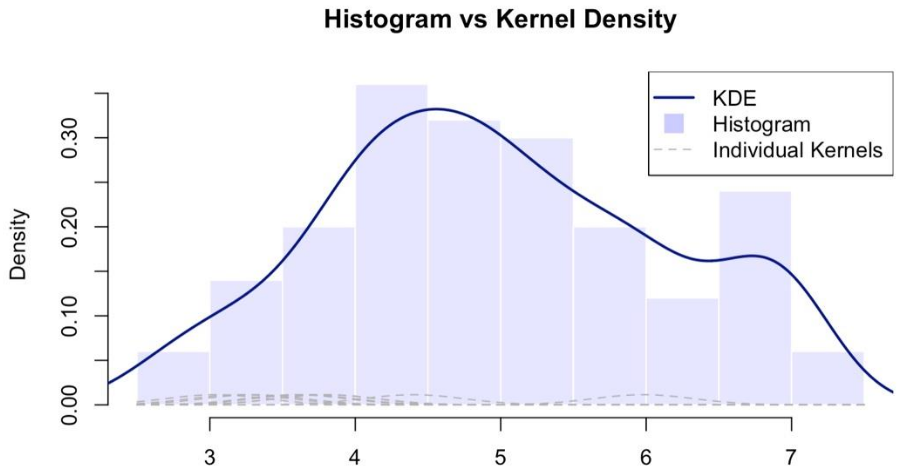
https://www.columbia.edu/~yt2661/STL/slides/Lecture-3.pdf

https://minghe4419.github.io/covariate_shift.github.io/separate_density_estimation.html

Kernel Density Estimation (KDE)

A non-parametric probability density estimation.





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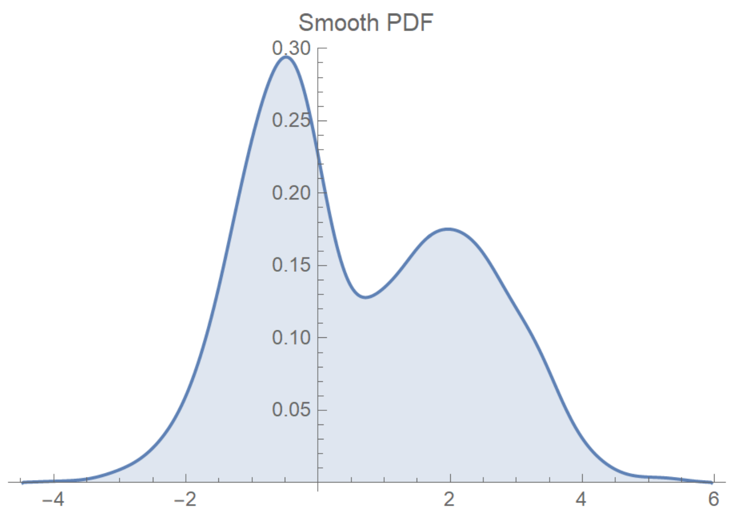
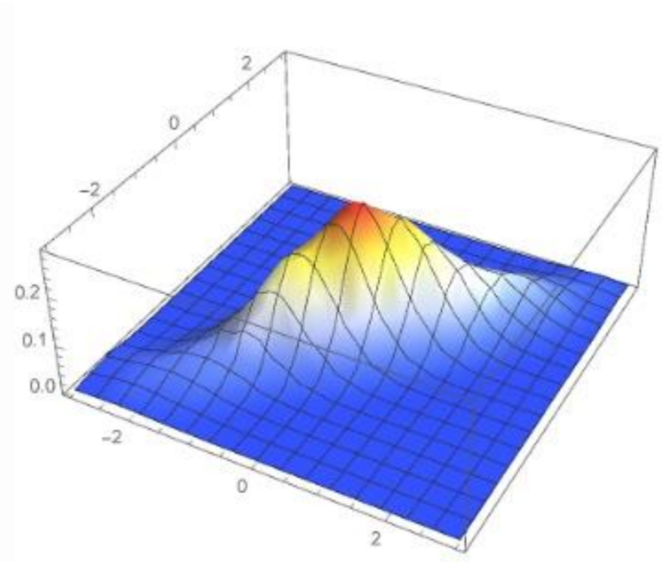




library(kdensity)

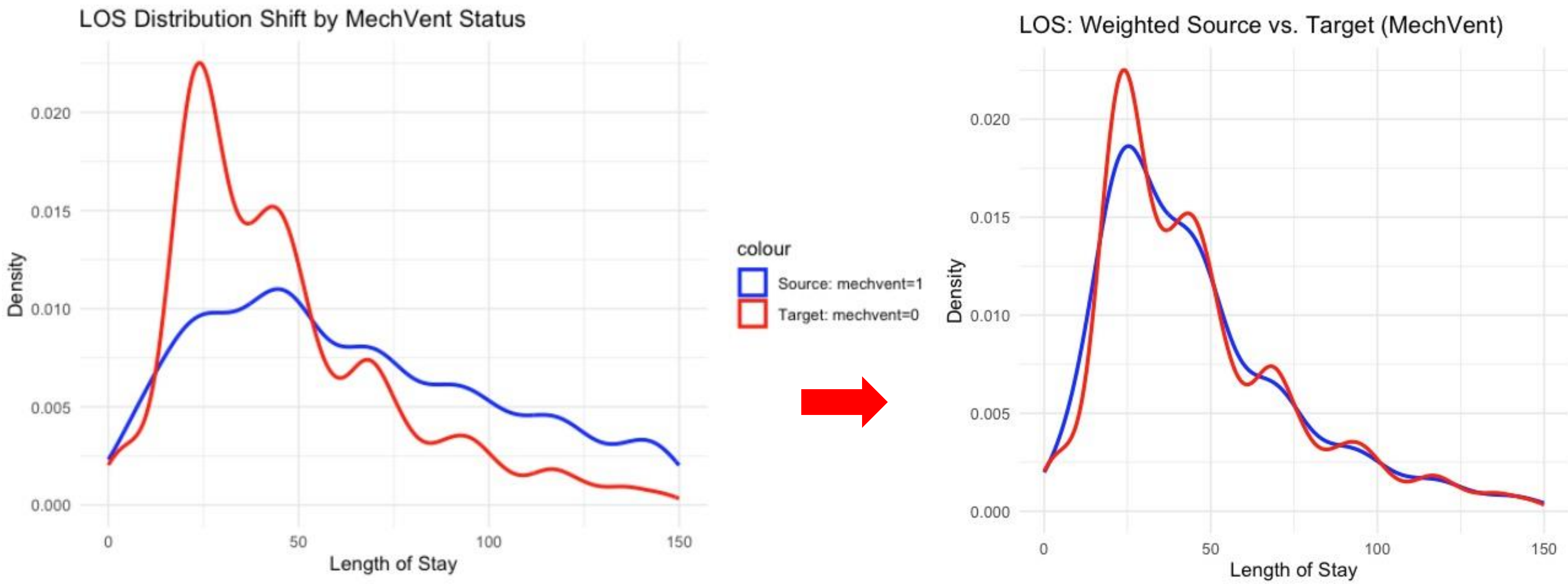
library(ks)

https://minghe4419.github.io/covariate_shift.github.io/separate_density_estimation.html

Separate KDE

Univariate Density Estimation
'library(kdensity)'

Source population: patients experienced Mechanical Ventilation
Target population: patients did NOT experience Mechanical Ventilation



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```
kde_source_hd <- kde(x = as.matrix(source_hd))
kde_target_hd <- kde(x = as.matrix(target_hd))

# 3. Evaluate densities at the source data points
p_source_hd <- predict(kde_source_hd, x = as.matrix(source_hd))
p_target_hd <- predict(kde_target_hd, x = as.matrix(source_hd))

# 4. Compute the density ratio weights: w(x) = P_T(x) / (P_S(x) + epsilon)
epsilon_val <- 1e-10
weights_hd <- p_target_hd / (p_source_hd + epsilon_val)
```

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```

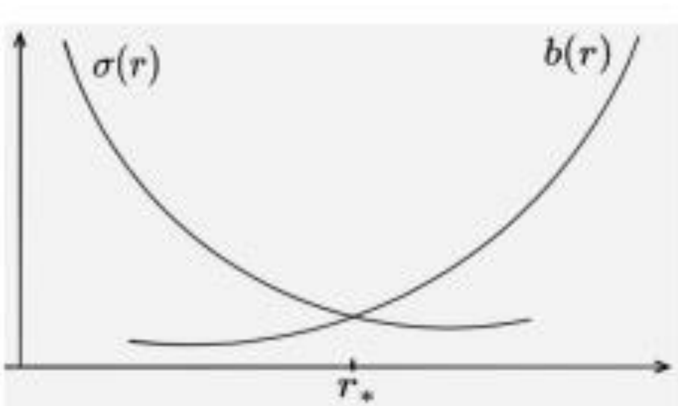
Separate Density Estimation

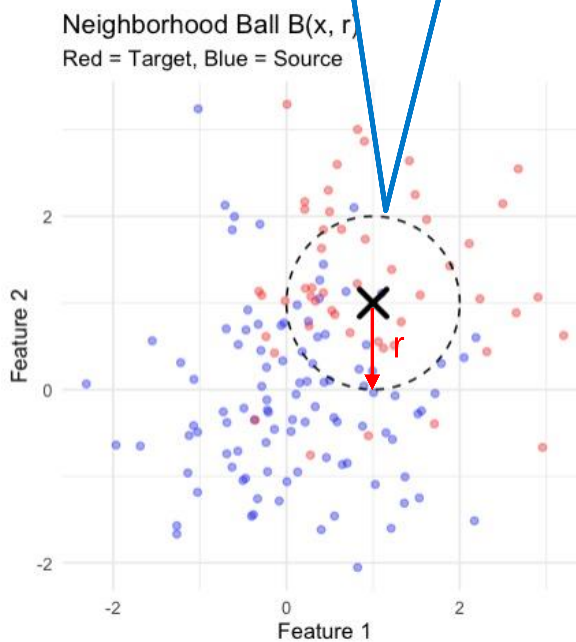
$$\omega(x) = \frac{number\ of\ target\ point\ in\ circle}{number\ of\ source\ point\ in\ circle}$$

- Histogram-based Method

$$\widetilde{\omega}(x) = \frac{P_T(B(x,r))}{P_S(B(x,r))} = \frac{n_T^{-1}\sum_{i=1}^{n_T} I(\|x - x_{T,i}\| \le r)}{n_S^{-1}\sum_{i=1}^{n_S} I(\|x - x_{S,i}\|_2 \le r)}$$

$$\widehat{\omega}(x) = \widetilde{\omega}(x) I(P_T(B(x,r)) \ge \alpha)$$

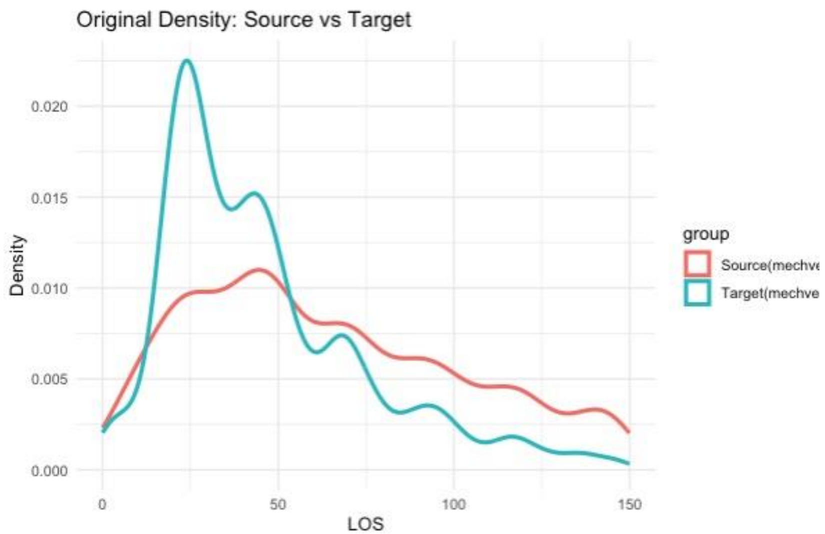


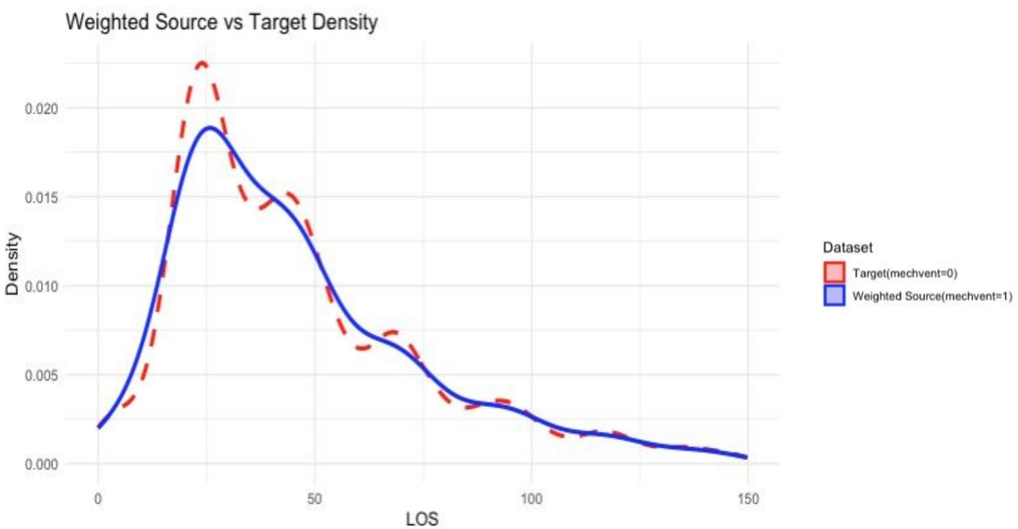


Separate Density Estimation

- Histogram-based Method

$$\widetilde{\omega}(x) = \frac{P_T(B(x,r))}{P_S(B(x,r))} = \frac{n_T^{-1}\sum_{i=1}^{n_T} I(\left\|x - x_{T,i}\right\| \le r)}{n_S^{-1}\sum_{i=1}^{n_S} I(\left\|x - x_{S,i}\right\|_2 \le r)} \qquad \widehat{\omega}(x) = \widetilde{\omega}(x) I(P_T(B(x,r)) \ge \alpha$$

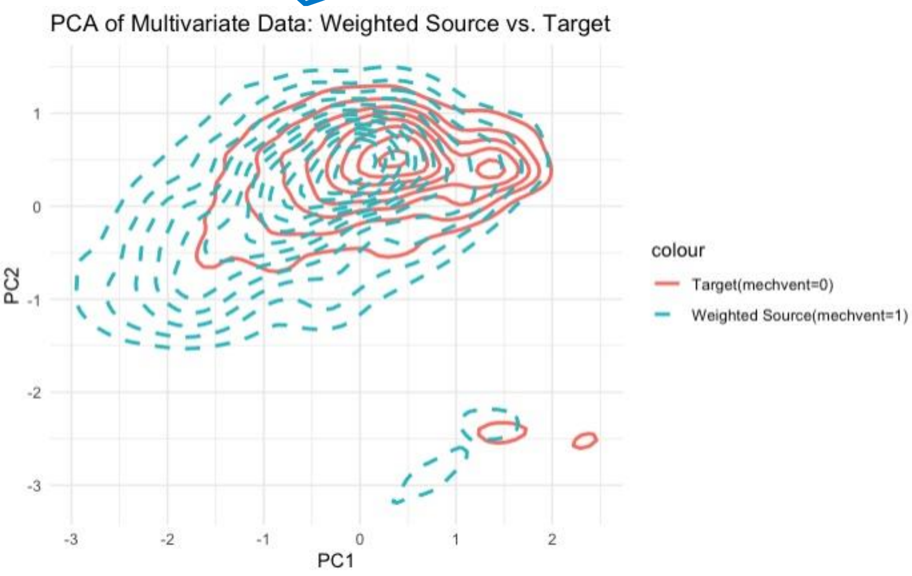




Separate Density Estimation

Multivariate Density Estimation
'library(ks)'

X = [age, length of stay, heart rate]



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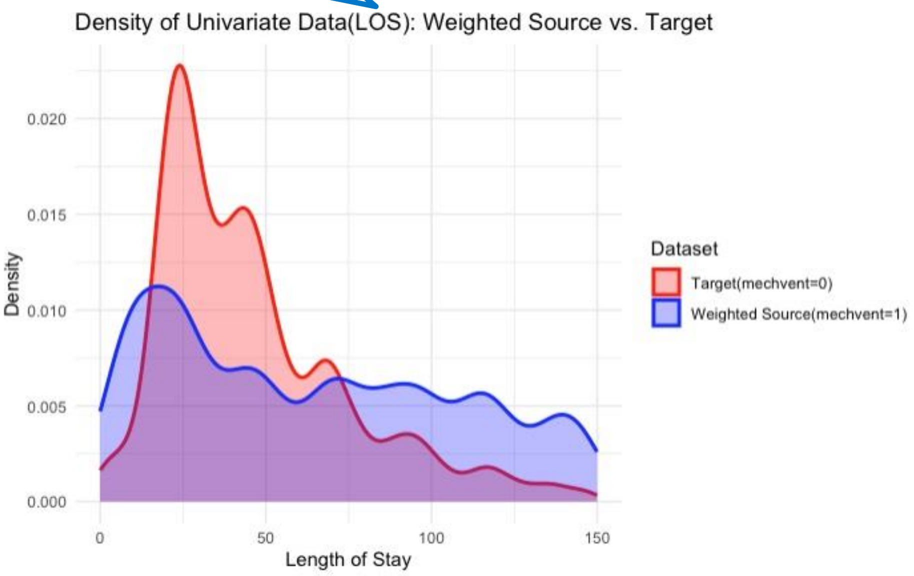
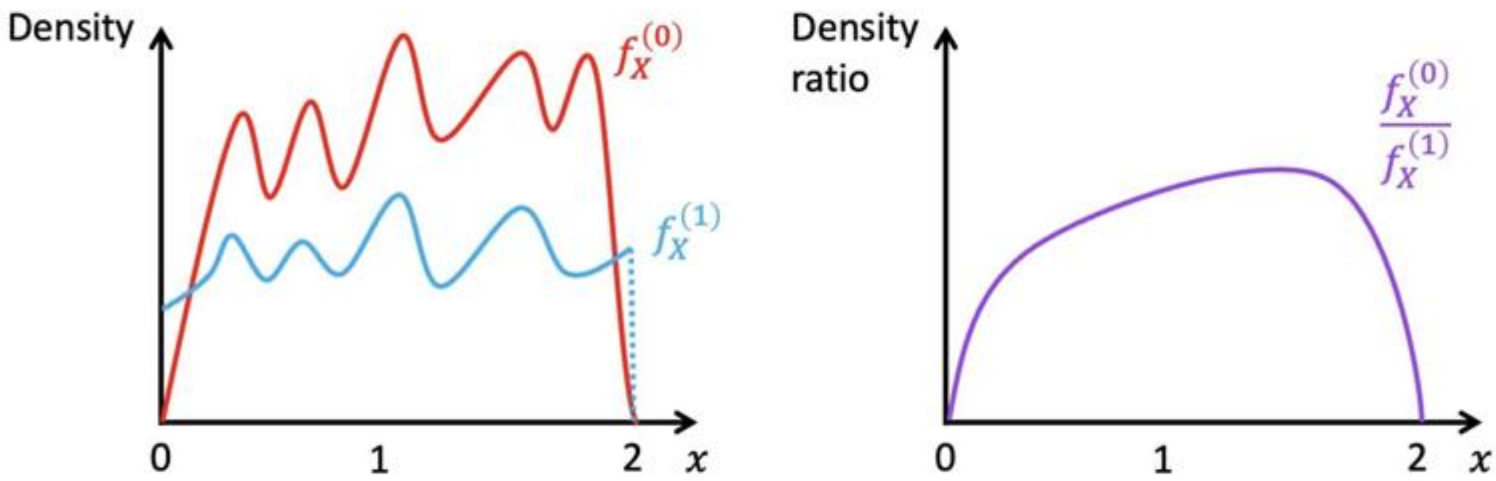


Separate Density Estimation

Issue: Worse smoothness in density ratio

- Densities are rough while the density ratio is smooth
- Resulting large variance in weights



Summary

- Transfer learning and domain adaptation
- Importance weighting framework
- Separate density estimation
  - KDE
  - Histogram-based
- Helpful sources
  - Our website about Covariate Shift: https://minghe4419.github.io/covariate_shift.github.io/index.html
    - Summary of methods to interact with more helpful resources
  - PhysioNet: https://physionet.org/
    - The Research Resource for Complex Physiologic Signals
    - Need to get credentialed and trained

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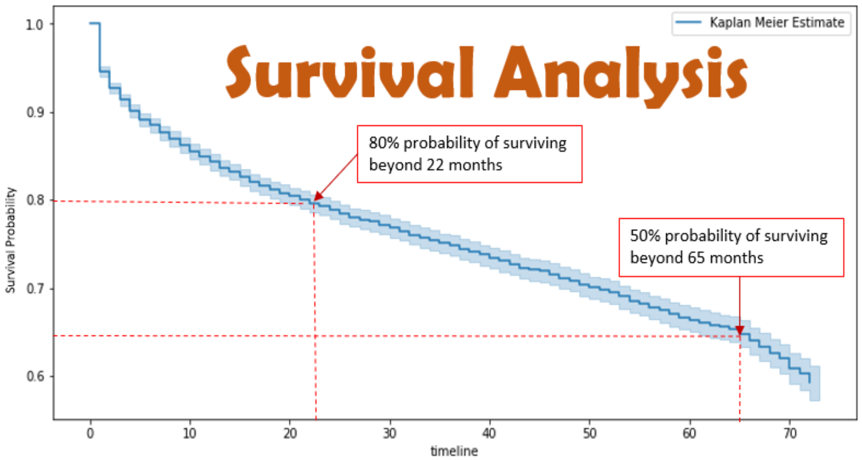
  - Profile Likelihood Method
- Beyond Reweighting Technique and Covariate Shift
  - Marginal Transfer Learning
  - Domain Invariant Method
  - Optimal Transformation

Example: Survival Analysis & Cox Model

Survival Analysis: model the time until an event of interest occurs

- Medical Research
- Finance
- Social Sciences



https://medium.com/data-science/survival-analysis-intuition-implementation-in-python-504fde4fcf8e

Example: Survival Analysis & Cox Model

$$\underbrace{\mathrm{H}(t|\boldsymbol{X})}_{\text{Hazard function at time t}} = \underbrace{h_0(t)}_{\text{Baseline Hazard}} \; \underbrace{\exp\{\boldsymbol{X}^T \overset{\text{Target parameter}}{\boldsymbol{\beta}}\}}_{\text{Scaling Factor}}$$

01 **Proportional Hazard Assumption**: The model assumes that the hazard rate is proportional across different levels of covariates

02 **Semi-parametric Nature**: The Cox model is a semi-parametric model, allowing for flexible baseline hazard functions without imposing rigid assumptions

03 **Handling Time-Dependent Covariates**: Can handle time-dependent covariates, which means that the effect of a variable on the hazard rate can change over time

04 **Identify Key Factors**: A powerful tool for identifying factors that affect the hazard rate of an event

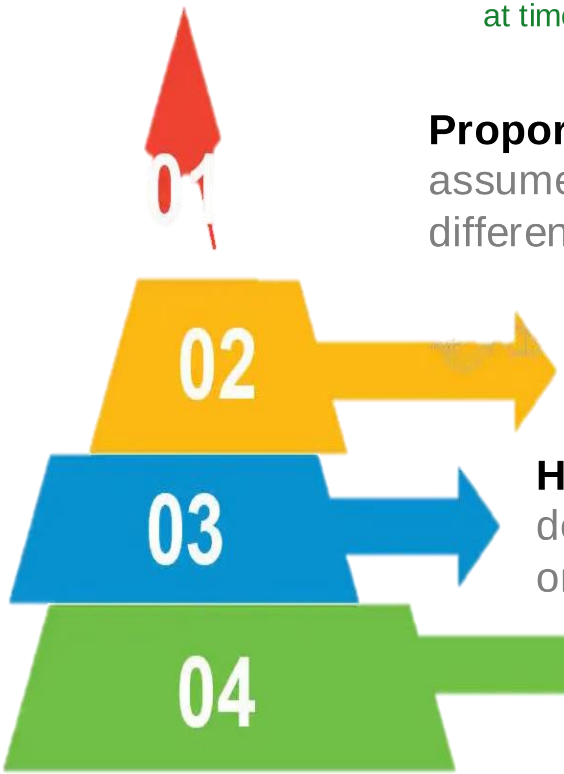
Example: Survival Analysis & Cox Model

Target parame

$$\underbrace{\mathrm{H}(t|\boldsymbol{X})}_{\text{Hazard function at time t}} = \underbrace{h_0(t)}_{\text{Baseline Hazard}} \ \underbrace{\exp\{\boldsymbol{X}^T\boldsymbol{\beta}\}}_{\text{Scaling Factor}}$$

Challenging in small-sample settings

- Rare diseases
- Subpopulations with limited representation
- Specialized clinical trials



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Handling Time-Depende dependent covariates, whi on the hazard rate can cha

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All of Us RESEARCH PROGRAM

Event of interest: end-stage-renal disease (ESRD) among high-risk patients (impaired kidney function)

→ Over ~127,000 participants
→ 203 high-risk Hispanic
→ 33 developed ESRD

https://fastercapital.com/content/Cox-proportional-hazards- tml

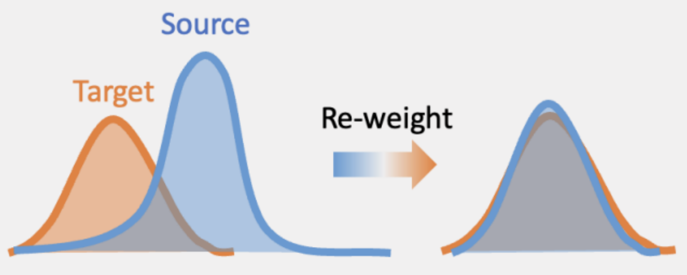
Transfer Learning in Survival Analysis
What are the gaps

- **Covariate (X) Shift:** Systematic differences between source & target datasets, which will introduce biases, reducing model robustness, especially in the Cox model when model misspecification exists
  - Cox model is used as a “working model” to analyze the relationship between covariates and the hazard rate, even when its assumptions—such as proportional hazards—do not strictly hold
- **Limited Adaptation:** Existing methods do not fully address cross-population heterogeneity, including baseline hazard variation and coefficient difference

🔍 **Our contribution**: A robust transfer learning framework that accounts for multi-level data shifts in Cox model

Proposed 2-step CoxTL

Step 1: Density Ratio Estimation $\hat{\omega}$



Step 2: Calibrate Log-likelihood for Joint Estimation

$$\boldsymbol{l}^{TL}(\boldsymbol{\beta}) = \underbrace{\boldsymbol{l}^{T}(\boldsymbol{\beta}; X_{T}, Y_{T})}_{\text{Target}} + \underbrace{\boldsymbol{\nu}}_{\text{Prevent Negative Transfer}} \hat{\boldsymbol{\omega}}\, \underbrace{\boldsymbol{l}^{S}(\boldsymbol{\beta}; X_{S}, Y_{S})}_{\text{Calibrated Source}}$$

Obtain $\boldsymbol{\beta}^{TL}$ by maximizing $\boldsymbol{l}^{TL}(\boldsymbol{\beta})$

Adjust the difference in covariate X

- Adjust the difference in parameter $\boldsymbol{\beta}$
- Prevent negative effects from heterogeneous sources