

#### Classical ML vs. Reality

- Training data and Test data share the same distribution (In classical Machine Learning)
- But that's not always the case in reality.
  - Survey data
  - Species habitat modeling based on data of only one area
  - Training and test data collected by different experiments

#### Sample selection bias

- Standard setting: data (x,y) are drawn independently from a distribution D
- If the selected samples is not a random samples of D, then the samples are biased.
- Usually, training data are biased, but we want to apply the classifier to unbiased samples.

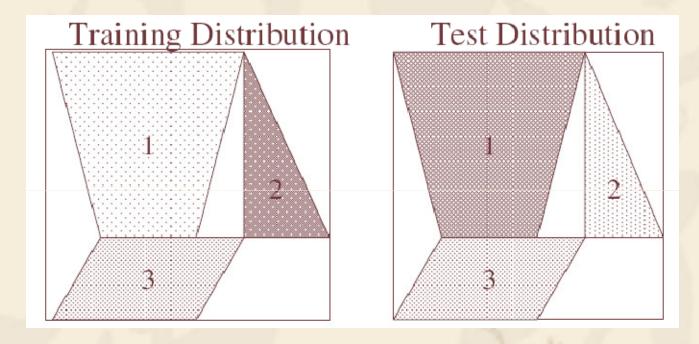
#### Four cases of Bias(1)

- Let s denote whether or not a sample is selected.
- P(s=1|x,y) = P(s=1) (not biased)
- ❖ P(s=1|x,y) = P(s=1|x) (depending only on the feature vector)
- ❖ P(s=1|x,y) = P(s=1|y) (depending only on the class label)
- P(s=1|x,y) (depending on both x and y)

## Four cases of Bias(2)

- ❖ P(s=1|x, y)= P(s=1|y): learning from imbalanced data. Can alleviate the bias by changing the class prior.
- ❖ P(s=1|x,y) = P(s=1|x) imply P(y|x) remain unchanged. This is mostly studied.
- If the bias depends on both x and y, lack information to analyze.

#### An intuitive Example



P(s=1|x,y) = P(s=1|x) => s and y are independent. So P(y|x, s=1) = P(y|x).

Does it really matter as P(y|x) remain unchanged??

# Bias Analysis for Classifiers(1)

Logistic Regression

$$P(y = 1|x, s = 1) = \frac{1}{1 + \exp(\beta_0 + \beta_1 x_1 + \dots + \beta_n x_n)}$$

Any classifiers directly models P(y|x) won't be affected by bias

Bayesian Classifier

$$\frac{P(x|y,s=1)P(y|s=1)}{P(x|s=1)} = P(y|x,s=1) = P(y|x)$$

But for naïve Bayesian classifier

$$\frac{P(x_1|y, s = 1) \dots P(x_n|y, s = 1)P(y|s = 1)}{P(x|s = 1)},$$

# Bias Analysis for Classifiers(2)

- Hard margin SVM: no bias effect. Soft margin SVM: has bias effect as the cost of misclassification might change.
- Decision Tree usually results in a different classifier if the bias is presented
- In sum, most classifiers are still sensitive to the sample bias.
- This is in asymptotic analysis assuming the samples are "enough"

#### Correcting Bias

Expected Risk:

$$R[\Pr, \theta, l(x, y, \theta)] = \mathbf{E}_{(x,y) \sim \Pr} [l(x, y, \theta)]$$

Suppose training set from Pr, test set from Pr'

$$R[\Pr', \theta, l(x, y, \theta)] = \mathbf{E}_{(x,y)\sim\Pr'}[l(x, y, \theta)] = \mathbf{E}_{(x,y)\sim\Pr}\left[\underbrace{\frac{\Pr'(x,y)}{\Pr(x,y)}}_{:=\beta(x,y)}l(x, y, \theta)\right]$$
$$= R[\Pr, \theta, \beta(x, y)l(x, y, \theta)],$$

So we minimize the empirical regularized risk:

$$R_{\text{reg}}[Z, \beta, l(x, y, \theta)] := \frac{1}{m} \sum_{i=1}^{m} \beta_i l(x_i, y_i, \theta) + \lambda \Omega[\theta],$$

#### Estimate the weights

- The samples which are likely to appear in the test data will gain more weight.
- But how to estimate the weight of each sample?

$$\left. \begin{array}{l} Pr(x,y) = Pr(x)Pr(y|x) \\ Pr'(x,y) = Pr'(x)Pr'(y|x) \end{array} \right\} \Longrightarrow \beta(x,y) = \frac{Pr'(x)}{Pr(x)}$$

- Brute force approach:
  - $\bowtie$  Estimate the density of Pr(x) and Pr'(x), respectively,
- Not applicable as density estimation is more difficult than classification given limited number of samples.
- Existing works use simulation experiments in which both Pr(x) and Pr'(x) are known (NOT REALISTIC)

#### Distribution Matching

The expectation in feature space:

$$\mu(\Pr) := \mathbf{E}_{x \sim \Pr(x)} \left[ \Phi(x) \right]$$

- We have  $Pr = Pr' \iff ||\mu(Pr) \mu(Pr')|| = 0$
- Hence, the problem can be formulated as

$$\underset{\beta}{\text{minimize}} \| \mu(\Pr') - \mathbf{E}_{x \sim \Pr(x)} [\beta(x) \Phi(x)] \|$$

subject to 
$$\beta(x) \geq 0$$
 and  $\mathbf{E}_{x \sim \Pr(x)} [\beta(x)] = 1$ 

**Solution is:**  $Pr'(x) = \beta(x)Pr(x)$ 

# **Empirical KMM optimization**

$$\left\| \frac{1}{m} \sum_{i=1}^{m} \beta_i \Phi(x_i) - \frac{1}{m'} \sum_{i=1}^{m'} \Phi(x_i') \right\|^2 = \frac{1}{m^2} \beta^\top K \beta - \frac{2}{m^2} \kappa^\top \beta + \text{const.}$$

where 
$$K_{ij} := k(x_i, x_j)$$
 and  $\kappa_i := \frac{m}{m'} \sum_{j=1}^{m'} k(x_i, x_j')$ 

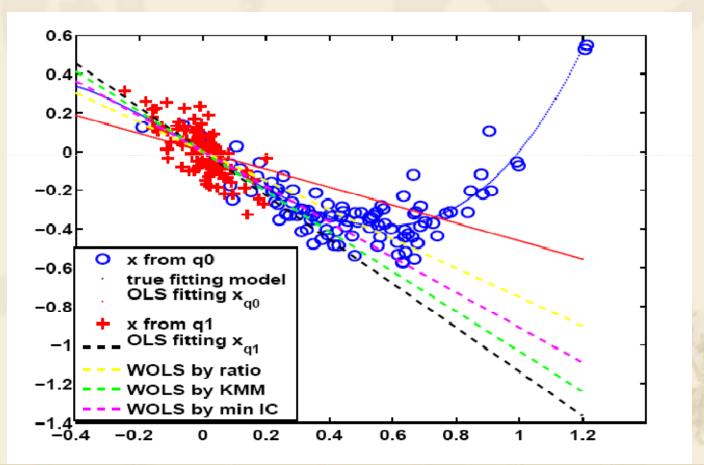
Therefore, it's equivalent to solve the QP problem:

$$\underset{\beta}{\text{minimize}} \ \frac{1}{2} \beta^\top K \beta - \kappa^\top \beta$$

subject to 
$$\beta_i \in [0, B]$$
 and  $\left| \sum_{i=1}^m \beta_i - m \right| \leq m\epsilon$ .

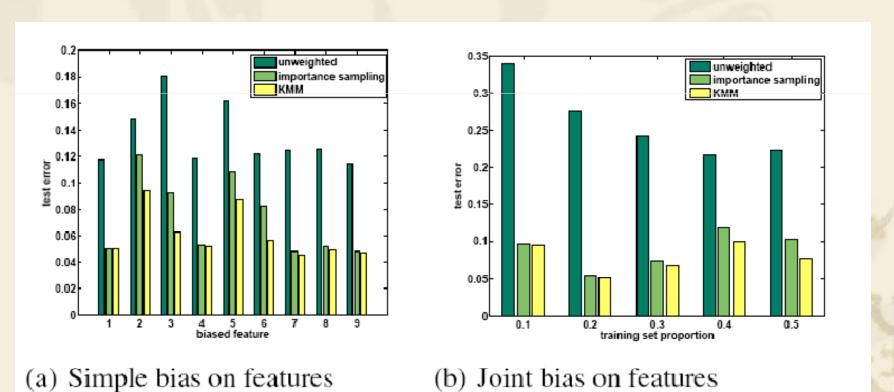
# Experiments

A Toy Regression Example

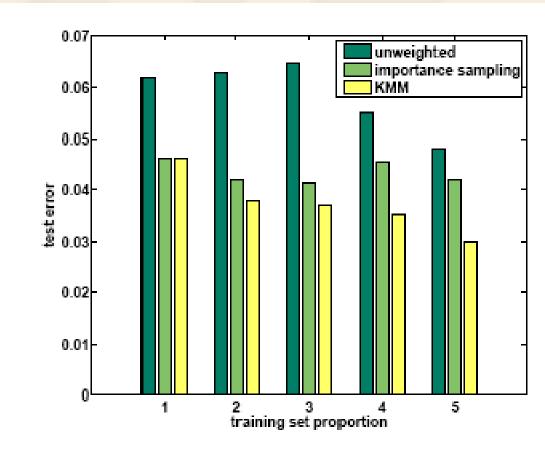


#### Simulation

Select some UCI datasets to inject some sample selection bias into training, then test on unbiased samples.



#### Bias on Labels



(c) Bias on labels

## Unexplained

- From theory, the importance sampling should be the best, why KMM performs better?
- Why kernel methods? Can we just do the matching using input features?
- Can we just perform a logistic regression to estimate \beta by treating test data as positive class, and training data as negative. Then, \beta is the odds.

#### Some Related Problems

- Semi-supervised Learning (Is it equivalent??)
- Multi-task Learning: assume P(y|x) to be different. But sample selection bias(mostly) assume P(y|x) to be the same. MTL requires training data for each task.
- Is it possible to discriminate features which introduce the bias? Or find invariant dimensionalities?

