Special Lecture, Pattern Information Processing

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# Learning under Class-Prior Change



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#### **1. Motivating Example**

- 2. Classification and Risk
- 3. Class-prior Change
- 4. Class-prior Change Mitigation
- 5. Class-prior Change Correction
- 6. HomeWork

# **Motivating Example (1)**

- A certain medical test for a rare disease has a high accuracy:
  - If the disease is present, the test gives a positive result 90% of the time
- If the disease is not present, the test gives a negative result 90% of the time
- The disease is quite rare and only 5% of the population has the disease
- How likely is the disease if the test result is positive?
  - Around **0.9**, **0.5**, or **0.3**?

# **Motivating Example (2)**

Frequency of the disease in the population

$$P(A) = 5\% P(\bar{A}) = 1 - P(A) = 95\%$$

A Disease occurs  $ar{A}$  Disease does not occur

Frequency of a positive result when the disease is present:

P(B|A) = 90%



Frequency of a negative result when disease is not present  $P(\bar{B}|\bar{A}) = 90\%$   $P(B|\bar{A}) = 10\%$ 

Frequency that the disease occurs when the test gives a positive answer: P(A|B) 0.9, 0.5, or 0.3?

# **Motivating Example (3)**

#### This can be computed with Bayes' rule





Rev. Thomas Bayes, English statistician and minister

Substituting the values in the previous slide gives  $P(A|B) = \frac{0.9 \times 0.05}{0.9 \times 0.05 + 0.1 \times 0.95}$  = 32.13%

# **Motivating Example (4)**

- The result is counterintuitive: much lower than commonly expected
- This is due to the low class prior



P(A) = 5%

- Conclusion: When doing inference, it is important to take into account the effect of the class prior!
- In this lecture, we will discuss the effect of the class prior on classification

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  - Risk minimization for Classification
  - Risk and Class-prior
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### Classification

#### Training data: $\mathcal{X}_{\mathrm{tr}} := \{oldsymbol{x},y\}_{i=1}^n \stackrel{\mathrm{i.i.d.}}{\sim} p(oldsymbol{x},y) \quad oldsymbol{y} (\in \{-1,1\}) \text{ Class label}$ Feature i.i.d: Independently and identically distributed Goal: Learn a rule to classify the labeled and unlabeled samples Learned decision boundary applied on unlabeled samples Decision boundary learned from labeled samples 0.25 0.25 p(x, y=1)p(x) p(x, y=-1) 0.2 0.2 0.15 0.15 0.1 0.1 0.05 0.05 Labeled training data from $p(\boldsymbol{x},y)$ Unlabeled test data from $p(\boldsymbol{x})$

According to what criterion should the decision boundary be selected?

### **Risk and Classification (1)**

• f(x) is a decision boundary:

 $f(\mathbf{x}) \ge 0$ : Class 1  $f(\mathbf{x}) < 0$ : Class -1



$$\ell_{0\text{-}1}(f(oldsymbol{x})) = egin{cases} 1 & f(oldsymbol{x}) < 0, \ 0 & f(oldsymbol{x}) \geq 0. \end{cases}$$

$$\ell_{0-1}(-f({m x})) = egin{cases} 0 & f({m x}) < 0, \ 1 & f({m x}) \ge 0. \end{cases}$$



Decision boundary should minimize the risk

 $f^* = \arg\min_{f} R(f) \quad R^* = R(f^*)$ 

• When  $c_+ = c_-^{f} = 1$ , risk is the misclassification rate

• What is the optimal  $f^*$  that minimizes the risk?

#### **Optimal classifier**

• When  $c_+ = c_- = 1$ , the optimal discriminant is

$$f(\boldsymbol{x}) = \operatorname{sign} \left[ p(y=1|\boldsymbol{x}) - p(y=-1|\boldsymbol{x}) \right]$$

$$p(y|\boldsymbol{x}) = \frac{p(\boldsymbol{x}|y)p(y)}{\sum_{y'} p(\boldsymbol{x}|y')p(y')}$$

p(y) Class prior  $p(oldsymbol{x}|y)$  Class-conditional density  $p(y|oldsymbol{x})$  Posterior

f(x) is the Bayes-optimal classifier and R\* = R(f\*) is the Bayes-optimal Risk

1. Motivating Example

#### 2. Classification and Risk

Risk minimization for Classification
 Risk and Class-prior

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### **Bayes Risk vs. Class prior**

Recall, Bayes Risk is

We will use the symbol  $\pi$  to denote a class prior p(y = 1) from now on

$$R^*(\pi) = \min_f \pi R_1(f) + (1 - \pi)R_{-1}(f)$$

$$R_{1}(f) = \int \ell_{0-1}(f(\boldsymbol{x})p(\boldsymbol{x}|y=1)d\boldsymbol{x}) \left[ R_{-1}(f) = \int \ell_{0-1}(-f(\boldsymbol{x})p(\boldsymbol{x}|y=-1)d\boldsymbol{x}) \right]$$

#### **False Negative Rate**

#### **False Positive Rate**



Function is *concave* w.r.t.  $\pi$ :

 $\pi R_1(f_0) + (1-\pi)R_{-1}(f_0)$ 

 Minimum of linear functions

### Example



- The decision boundary changes when the class prior changes
- Bayes risk is dependent on the class prior

#### **Conclusion: Section 2**

- The misclassification rate is a weighted combination of the false negative and false positive rate
  - Weighted by the class priors
- The classifier that minimizes the risk is  $f(\boldsymbol{x}) = \operatorname{sign}\left[p(y=1|\boldsymbol{x}) p(y=-1|\boldsymbol{x})\right]$
- The optimal risk is a concave function of the class prior

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  - Causes of prior Change
    - Dataset shift
    - Selection Bias
    - Class-prior change and Risk
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# **Class-prior Change**

# Class prior between the training and test data differ:

$$egin{aligned} p_{ ext{te}}(oldsymbol{x},y) &= p(oldsymbol{x}|y) p_{ ext{te}}(y) \ p_{ ext{tr}}(y) 
eq p_{ ext{te}}(y) \ p(oldsymbol{x}|y) \end{aligned}$$

 $p_{\mathrm{tr}}(\boldsymbol{x}, y) = p(\boldsymbol{x}|y)p_{\mathrm{tr}}(y)$ 

Class priors differ

Same class-conditional density

#### 



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# Why may the dataset change?

#### Dataset shift

- Natural change in the dataset between training and test
- Example: Face images selected in a laboratory compared to the real world

Training dataset:



Class balance: Male: 18/20 Female: 2/20

(Olivetti dataset)

#### Selection bias (next slide)

#### **Selection bias**

- Samples drawn for the test dataset may be drawn in a biased way
- Selection bias model

$$(oldsymbol{x},y,s) \stackrel{ ext{i.i.d.}}{\sim} p(oldsymbol{x},y,s) \qquad egin{array}{c} oldsymbol{x} & ext{Feature} \ y(\in\{-1,1\}) ext{ Class label} \ s(\in\{0,1\}) & ext{ Selection of samples} \end{array}$$

- When s = 1, the sample is in the test set, when s = 0, the sample is not in the test set
- Training distribution:  $p_{tr}(\boldsymbol{x}, y) = p(\boldsymbol{x}, y)$
- Test distribution:  $p_{te}(\boldsymbol{x}, y) = p(\boldsymbol{x}, y | s = 1)$

### Selection bias (2)

Three possibilities:

**1.** No selection bias

s is independent of x and y p(s = 1|x, y) = p(s = 1)No selection bias

2. Covariate shift

s is independent of y given x p(s = 1|x, y) = p(s = 1|x)

**3.** Class-prior change

s is independent of x given y p(s = 1|x, y) = p(s = 1|y)

#### **Covariate shift**

Proof:
$$p(s = 1 | \mathbf{x}, \mathbf{y}) = p(s = 1 | \mathbf{x}) \text{ implies that}$$

$$p_{tr}(y | \mathbf{x}) = p_{te}(y | \mathbf{x})$$
Proof:
$$p_{te}(y | \mathbf{x}) = p(y | \mathbf{x}, s = 1) = \frac{p(\mathbf{x}, y, s = 1)}{p(\mathbf{x}, s = 1)}$$

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

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

$$= \frac{p(s = 1 | \mathbf{x}) p(y | \mathbf{x})}{p(s = 1 | \mathbf{x})}$$

Covariate shift occurs in practice!

Can be corrected for in the semi-supervised setup

See lecture 13

### **Class-prior Change**

$$p(s = 1 | x, y) = p(s = 1 | y) \text{ implies that}$$

$$p_{tr}(x|y) = p(s|y) = p_{te}(x|y)$$

$$Proof: \quad p_{te}(x|y) = p(x|y, s = 1) = \frac{p(x, y, s = 1)}{p(y, s = 1)}$$

$$p_{te}(x, y) = p(x, y|s = 1)$$

$$p_{tr}(x, y) = p(x, y)$$

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

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

- Class-prior change may be due to selection bias
- We discuss methods to mitigate the effect of classprior change in the <u>supervised setup</u>
- We discuss a correction for class-prior change in the <u>semi-supervised setup</u>

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#### **Effect of Class-prior Change on Risk**

- Training:  $f_{tr} = \arg\min_{r} R(f; \pi_{tr})$   $R_1(f_{tr})$   $R_{-1}(f_{tr})$
- At point  $\pi_{tr}$  this is the same as  $R^*(\pi_{tr})$
- When  $f_{tr}$  is applied to a dataset with class prior  $\pi_{te}$  the error is

 $\pi_{\text{te}}R_1(f^{\text{tr}}) + (1 - \pi_{\text{te}})R_{-1}(f^{\text{tr}}) \ge \min_f R(\pi_{\text{te}})$ 



#### **Conclusion: Section 3**

Class-prior change may occur between the training and test data:

 $\begin{aligned} p_{\text{te}}(\boldsymbol{x}, y) &= p(\boldsymbol{x}|y) p_{\text{te}}(y) \quad p_{\text{tr}}(\boldsymbol{x}, y) = p(\boldsymbol{x}|y) p_{\text{tr}}(y) \\ p_{\text{tr}}(y) &\neq p_{\text{te}}(y) \end{aligned}$ 

This may be due to dataset shift or sample selection bias

• When a classifier is selected according to  $\pi_{tr}$  and applied on a dataset with  $\pi_{te}$ , the Risk is linear and tangent to the optimal risk curve at  $\pi_{tr}$ 

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## **Class-prior change mitigation**

- Class-prior change can have an adverse effect on the classification accuracy
- In practice, the test class prior  $\pi_{te}$  is unknown
  - We can therefore not correct for the effect of classprior change

Can we mitigate the effect of class prior change?

Mitigate (definition): to make less severe

# Minimax Criterion (1)

#### Recall this figure:



- The black line is the misclassification rate according to the new class prior when trained with the old class prior
- This line is always tangent to the optimal risk  $R^*(\pi)$

## **Minimax Criterion (2)**

- Why not select this line so that it does not change w.r.t. the new class prior?
- In other words, the tangent should be 0
- Since R<sup>\*</sup>(π) is concave, this would occur at the maximum



### **Further Reading**

The minimax criterion is described in

- "Pattern Classification", 2<sup>nd</sup> Edition (Richard O. Duda, Peter E. Hart, David G. Stork), p.g. 26.
  - (Ookayama Main Lib. B1F Books 548.13/D)
- "Detection, estimation, and linear modulation theory" (Van Trees, Harry L.) 1968
  - Ookayama Main Lib. B1F ; Compact Shelving Y000998
- The minimax criterion is discussed, and an extention introduced in "*Minimax Regret Classifier for Imprecise Class Distributions*" (Alaiz-Rodríguez, Rocío, Alicia Guerrero-Curieses, and Jesús Cid-Sueiro)
  - <u>http://jmlr.org/papers/volume8/alaiz-rodriguez07a/alaiz-rodriguez07a.pdf</u>

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#### **Correction for Class-prior change**

Recall that a cost-sensitive classifier minimizes

$$R(f) = c_{+}\pi_{\rm tr}R_{1}(f) + c_{-1}\left[1 - \pi_{\rm tr}\right]R_{-1}(f)$$

False negative rate

False positive rate

Misclassification rate according to  $\pi_{te}$  can be obtained by weights:

$$c_{+} = \frac{\pi_{\rm te}}{\pi_{\rm tr}} \qquad c_{-} = \frac{1 - \pi_{\rm te}}{1 - \pi_{\rm tr}}$$

Libraries such as libSVM allows specification of cost
 Problem: Test class prior π<sub>te</sub> is often unknown

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### **Semi-supervised setup**

In many situations, unlabeled data in addition to labeled data is available

 $\mathcal{X}_{\mathrm{tr}} := \{\boldsymbol{x}, y\}_{i=1}^{n} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{tr}}(\boldsymbol{x}, y) \qquad \mathcal{X}_{\mathrm{te}} := \{\boldsymbol{x}_i\}_{i=1}^{n'} \overset{\mathrm{i.i.d.}}{\sim} p_{\mathrm{te}}(\boldsymbol{x})$ 

- In the class-prior change assumption, the two distributions shares a class-conditional density:  $p_{tr}(\boldsymbol{x}, y) = p(\boldsymbol{x}|y) p_{tr}(y) \quad p_{te}(\boldsymbol{x}, y) = p(\boldsymbol{x}|y) p_{te}(y)$ Shared Shared
- We wish to estimate the class prior of the unlabeled dataset p<sub>te</sub>(y)
- This is difficult, because no labeled samples are available

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### **Distribution matching framework**

- Lets model the test input distribution  $p_{ ext{te}}(m{x})$  in terms of:
  - The training class-conditional distribution  $p_{ ext{tr}}(oldsymbol{x}|y)$

• The test class priors  $\pi_y = p_{te}(y)$   $q_{te}(x) = \sum_{y=1}^{c} \pi_y p_{tr}(x|y)$   $p_{te}(x) = \sum_{y=1}^{c} \pi_y p_{tr}(x|y)$   $p_{te}(x) = \sum_{y=1}^{c} p_{tr}(x|y)p_{te}(y)$ • Problem: Match  $q_{te}(x)$  to  $p_{te}(x)$  under some divergence

$$p_{\mathrm{tr}}(\boldsymbol{x}|y=1)$$
  $p_{\mathrm{tr}}(\boldsymbol{x}|y=2)$   
 $p_{\mathrm{te}}(\boldsymbol{x})$ 

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#### Distribution Matching via L<sub>2</sub>-distance Minimization

The similarity between two distributions can be measured by the L<sub>2</sub>-distance:

$$L_2\left(p_{ ext{te}}, q_{ ext{te}}
ight) = rac{1}{2}\int \left[p_{ ext{te}}(oldsymbol{x}) - q_{ ext{te}}(oldsymbol{x})
ight]^2 \mathrm{d}oldsymbol{x}$$

- The class prior can therefore be selected as  $(\pi_1, \ldots, \pi_c) = \operatorname*{arg\,min}_{\pi} L_2(p_{\mathrm{te}}(\boldsymbol{x}), q_{\mathrm{te}}(\boldsymbol{x}))$
- The  $L_2$  distance can be estimated by first estimating the densities  $p_{te}(x)$  and  $q_{te}(x)$ 
  - Not good since density estimation is a difficult problem

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Expectations can be estimated via sample averages:

$$\int f(\boldsymbol{x}) p(\boldsymbol{x}) \mathrm{d}\boldsymbol{x} = \mathbb{E}_p \left[ f(\boldsymbol{x}) \right] \approx \frac{1}{n} \sum_{i=1}^n f(\boldsymbol{x}_i)$$

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$$\{\boldsymbol{x}_i\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x})$$

- Can we estimate the L<sub>2</sub>-distance in terms of sample averages?
- It is possible by obtaining a lower-bound that is linear in the densities

We use the following inequality:  $\frac{1}{2}(t-y)^2 \ge 0, \implies \frac{1}{2}t^2 \ge ty - \frac{1}{2}y^2$ 

• Applying this pointwise gives

 $w(oldsymbol{x})$  role of y

$$\frac{1}{2} \left[ p_{\text{te}}(\boldsymbol{x}) - q_{\text{te}}(\boldsymbol{x}) \right]^2 \ge w(\boldsymbol{x}) \left[ p_{\text{te}}(\boldsymbol{x}) - q_{\text{te}}(\boldsymbol{x}) \right] - \frac{1}{2} w(\boldsymbol{x})^2$$

Integrating and selecting the tightest lowerbound gives

$$egin{aligned} &rac{1}{2}\int\left[p_{ ext{te}}(oldsymbol{x})-q_{ ext{te}}(oldsymbol{x})
ight]^2\mathrm{d}oldsymbol{x}\ &\geq \sup_w\int w(oldsymbol{x})\left[p_{ ext{te}}(oldsymbol{x})-q_{ ext{te}}(oldsymbol{x})
ight]\mathrm{d}oldsymbol{x}-rac{1}{2}\int w(oldsymbol{x})^2\mathrm{d}oldsymbol{x} \end{aligned}$$

- This lower-bound can then be estimated via sample averages
- Lets model w(x) with a linear model

$$w(\boldsymbol{x}) = \sum_{\ell=1}^{b} lpha_{\ell} \varphi_{\ell}(\boldsymbol{x}) \qquad \varphi_{\ell}(\boldsymbol{x}) = \exp\left(-\frac{1}{2\sigma^{2}} \|\boldsymbol{x} - \boldsymbol{c}_{\ell}\|^{2}\right)$$

The L<sub>2</sub>-distance lower bound can be written in terms of expectations

$$L_2(p_{\text{te}}, q_{\text{te}}) \ge \sup_{w} \mathbb{E}_{p_{\text{te}}}\left[w(\boldsymbol{x})\right] - \sum_{c=1}^{n_c} \mathbb{E}_{\pi_y p_{\text{te}}}\left[w(\boldsymbol{x})\right] - \frac{1}{2} \int w(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}$$

$$L_2(p_{\text{te}}, q_{\text{te}}) \geq \sup_{w} \mathbb{E}_{p_{\text{te}}}\left[w(\boldsymbol{x})\right] - \sum_{c=1}^{n_c} \mathbb{E}_{\pi_y p_{\text{te}}}\left[w(\boldsymbol{x})\right] - \frac{1}{2}\int w(\boldsymbol{x})^2 \mathrm{d}\boldsymbol{x}$$

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The expectations can be estimated via sample averages:  $\widehat{h}_{te} = \frac{1}{n} \sum_{i=1}^{n} \varphi(\boldsymbol{x}_i) \quad \widehat{h}_c = \frac{1}{n_c} \sum_{i=1,y_i=c}^{n} \varphi(\boldsymbol{x}_i) \quad \boldsymbol{H} = \int \varphi(\boldsymbol{x}) \varphi(\boldsymbol{x})^\top d\boldsymbol{x}$   $\varphi(\boldsymbol{x}) = [\varphi_1(\boldsymbol{x}) \quad \varphi_2(\boldsymbol{x}) \quad \dots \quad \varphi_\ell(\boldsymbol{x})]$ Which gives an objective function of:

$$\widehat{L}_2(\{\pi_y\}_{y=1}^c) pprox \max_{oldsymbol{lpha}} oldsymbol{lpha}^ op \widehat{oldsymbol{h}}_{ ext{te}} - \sum_{y=1}^c heta_y oldsymbol{lpha}^ op \widehat{oldsymbol{h}}_y - rac{1}{2} oldsymbol{lpha}^ op oldsymbol{H} oldsymbol{lpha}$$

- Minimizing the  $L_2$  distance estimate w.r.t.  $\left\{\pi_y\right\}_{y=1}^c$  gives an estimate of the class prior
- This can then be used to reweight a classifier

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#### Example

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#### Example

# Samples from two Gaussians with different means:



• The true class prior is  $p_{te}(y=1) = 0.3$ 

# Example (2)

#### The L<sub>2</sub>-distance estimated from samples is given below:



Minimum of L<sub>2</sub> distance is near the true class prior
 Difference is due to estimation from a small set l

#### **Conclusion: Section 5**

- By reweighting the risk, a classifier can be trained
- The reweighting factor depends on the unknown class prior
- In a semi-supervised setup, the unknown class prior can be estimated
- Estimation is possible by matching a model of the test input density to the true test input density

### **Further Reading**

- "Adjusting the outputs of a classifier to new a priori probabilities: a simple procedure" (Saerens, M., Latinne, P., and Decaestecker, C.)
  - Neurocomputation 14 (2002)
  - Introduced estimation of the class prior for re-adjustment of the classifier
- "Semi-supervised learning of class balance under classprior change by distribution matching." (du Plessis, M. C. & Sugiyama, M.)
  - Estimation of the class prior via Pearson divergence matching
- "Density-difference estimation" (Sugiyama, M., Suzuki, T., Kanamori, T., du Plessis, M. C., Liu, S., & Takeuchi, I.)
  - Estimation of the class prior via L<sub>2</sub>-distance estimation (discussed here)

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### **Take-home Message**

- The class-prior may change between the training and test phase
- In supervised learning, the minimax approach can be used:
  - Minimizes the worst case result
- If the test class-prior is known, the classifier can be selected by reweighting
- In semi-supervised learning, the test class prior can be estimated

#### Homework

- Please hand in your reports now!
- Homework:

Write you opinion about the special lecture today. Directly submit the printed report to the lecturer next week.