AI6102: Machine Learning Methodologies & Applications

L9: Evaluation & Density Estimation

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Outline

- Other evaluation metrics for classification
  - Imbalance classification problems
- Density estimation
  - Estimate unknown probability density function
    - Parametric & Non-parametric

Metrics for Classification

Confusion Matrix

		Predicted Class	
		Class = 1	Class = 0
Actual Class	Class = 1	f_{11}	f_{10}
	Class = 0	f_{01}	f_{00}

f_{11}: TP (true positive)

f_{10}: FN (false negative)

f_{01}: FP (false positive)

f_{00}: TN (true negative)

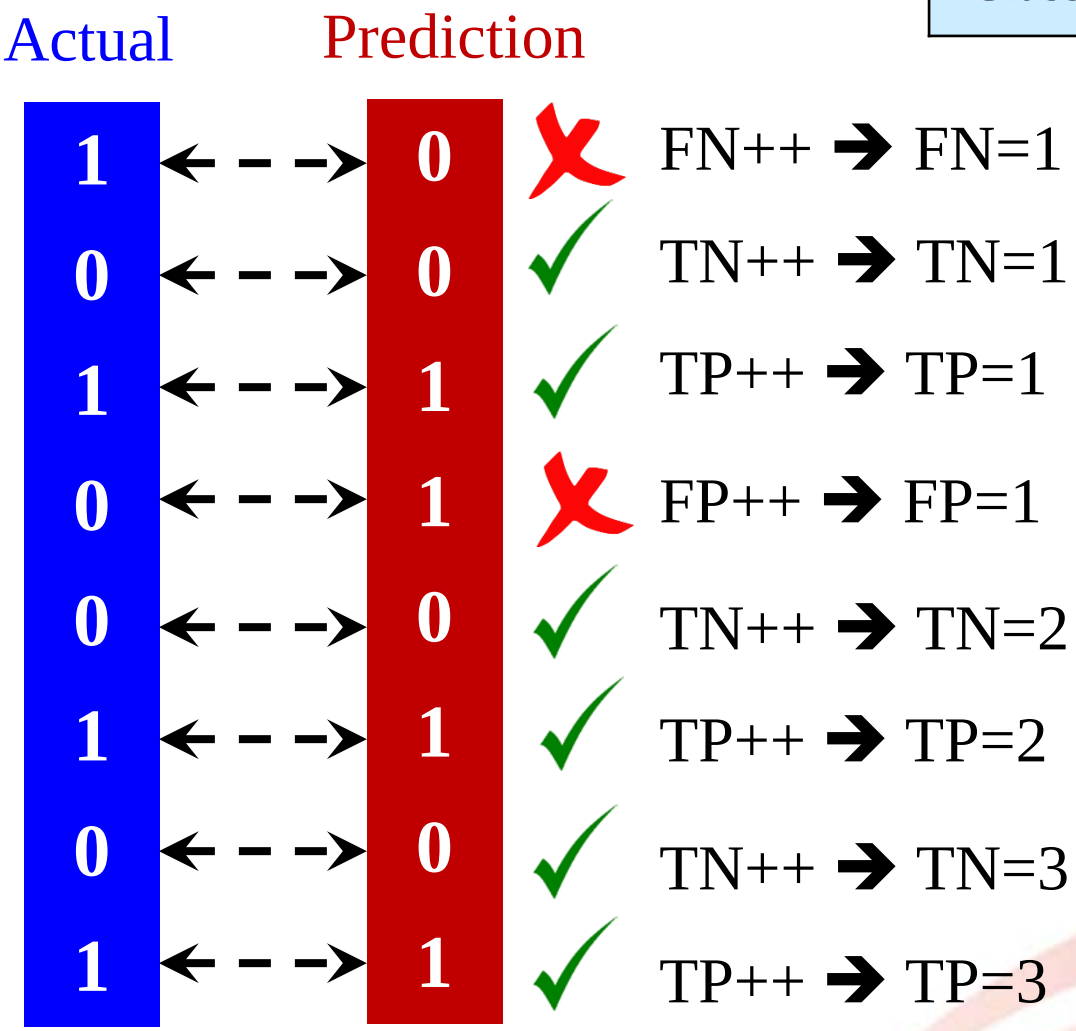
Most widely-used metric:

$$\text{Accuracy} = \frac{\text{\# correct predictions}}{\text{\# predictions}} = \frac{f_{11} + f_{00}}{f_{11} + f_{10} + f_{01} + f_{00}}$$

$$\text{Error rate} = \frac{\text{\# incorrect predictions}}{\text{\# predictions}} = 1 - \text{accuracy}$$

Initialization:
TP = 0, FN = 0, FP = 0, TN = 0

		Predicted Class	
		Class = 1	Class = 0
Actual Class	Class = 1	f_{11} (TP)	f_{10} (FN)
	Class = 0	f_{01} (FP)	f_{00} (TN)



		Predicted Class	
		1	0
Actual Class	1	3	1
	0	1	3

$$\text{Acc} = \frac{\text{TP} + \text{TN}}{\#} = \frac{3+3}{8} = 0.75$$

Potential Issue of Accuracy

- Consider a 2-class classification problem
  - Number of Class 0 data instances = 99
  - Number of Class 1 data instances = 1
- If model predicts every data instance to be class 0, accuracy is $99/100 = 99\%$
  - Accuracy is misleading because model does not detect any class 1 data instance

Class Imbalance Problem

- In many real-world applications, data sets may have imbalanced class distributions
  - In medical domain, to diagnose whether a patient has cancer or not, the number of patients without cancer is much larger than that with cancer
  - In software engineering, to predict whether a source file has potential defect, the number of non-defective source files is much larger than that of defective files
  - In information retrieval, among all the retrieved webpages, the number of relevant webpages is much smaller than that of irrelevant webpages

Alternative Metrics

- Accuracy measure treats every class as equally important
- It is not suitable for analyzing imbalance data sets, where the rare class is considered more interesting than the majority class
  - e.g., the patients who really have cancer
- For binary classification, the rare class is often denoted as the positive class, while the majority class is denoted as the negative class
  - i.e., f_{11} (TP) is more important

		Predicted Class	
		Class = 1	Class = 0
Actual Class	Class = 1	f_{11} (TP)	f_{10} (FN)
	Class = 0	f_{01} (FP)	f_{00} (TN)

Recall and Precision

- Recall and precision are two widely used metrics employed in applications where successful detection of one of the classes is considered more significant than detection of the other classes.
- Precision:

$$p = \frac{TP}{TP + FP}$$

instances predicted as positive

Precision is to measure among all the predicted positive instances, how many are true positive.

- Recall:

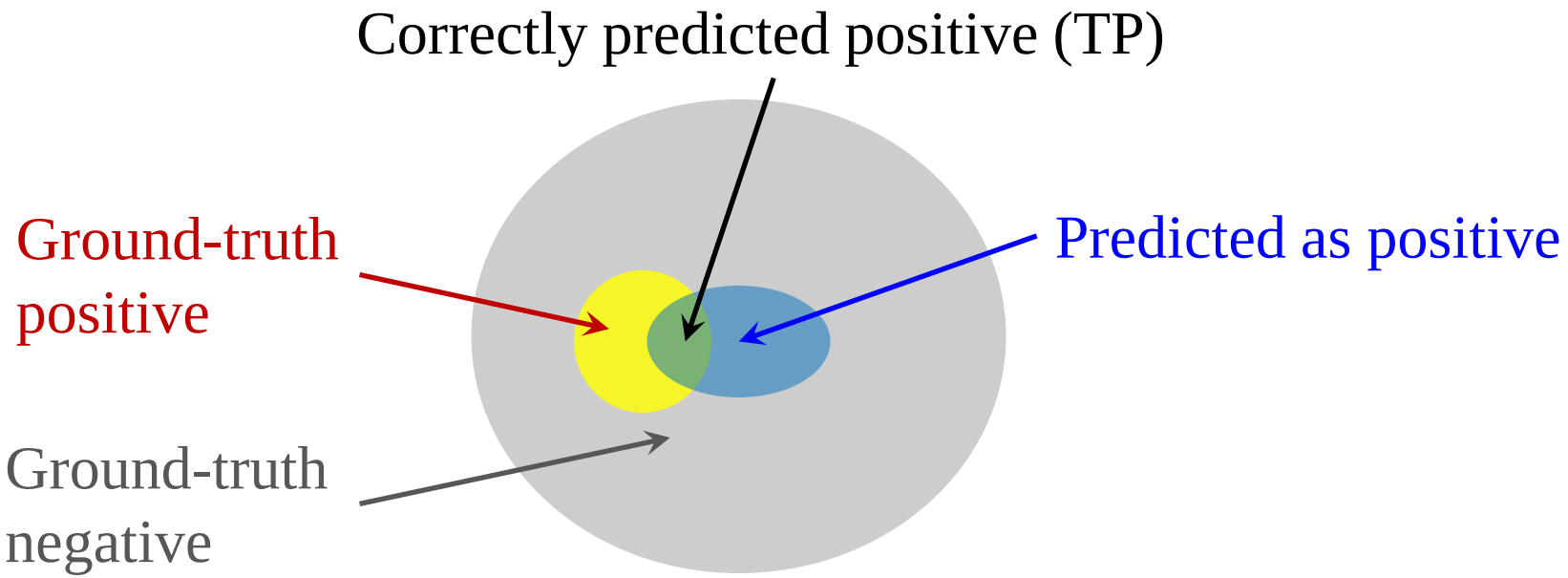
true positive instances

$$r = \frac{TP}{TP + FN}$$

Recall is to measure among all true positive instances, how many are predicted correctly by the classifier

- A good model should have both high precision and recall

Recall and Precision (cont.)



Precision: $p = \frac{\text{TP}}{\text{TP} + \text{FP}}$

The area of the overlapping region between yellow and blue divided by the area of the blue region

Recall: $r = \frac{\text{TP}}{\text{TP} + \text{FN}}$

The area of the overlapping region between yellow and blue divided by the area of the yellow region

F_1 Measure

- Recall and precision can be summarized into another metric known as F_1 measure

$$F_1 = \frac{2rp}{r + p}$$

- A high value of F_1-measure ensures that precision and recall are reasonably high

ROC

- ROC (Receiver Operating Characteristic) is a graphical approach to displaying the trade-off between true positive rate and false positive rate of a classifier

		Predicted Class	
		Class = 1	Class = 0
Actual Class	Class = 1	f_{11}	f_{10}
	Class = 0	f_{01}	f_{00}

f_{11}: TP (true positive)

f_{10}: FN (false negative)

f_{01}: FP (false positive)

f_{00}: TN (true negative)

True positive rate: $\mathrm{TPR} = \frac{\mathrm{TP}}{\mathrm{TP} + \mathrm{FN}} = \frac{\mathrm{TP}}{\#\mathrm{POS}}$ Recall

False positive rate: $\mathrm{FPR} = \frac{\mathrm{FP}}{\mathrm{TN} + \mathrm{FP}} = \frac{\mathrm{FP}}{\#\mathrm{NEG}}$

Some Special Points

- (FPR, TPR):
  - $\left(\text{FPR}=\frac{\text{FP}}{\#\text{NEG}}, \text{TPR}=\frac{\text{TP}}{\#\text{POS}}\right)$
  - (0,0): to predict every data instance to be negative class
  - (1,1): to predict every data instance to be positive class
  - (0,1): ideal

Varying Decision Threshold

- For balanced classification problem, the decision threshold is usually 0.5
- For imbalanced problem, as there are only a few positive instances, the threshold is set to be a larger values, e.g., 0.8
  - The best threshold can be tuned via cross-validation
  - For each threshold, generate a 2D point (FPR, TPR)
  - By connecting this points, we can construct a curve

			0.5	0.8
ID	$P(+\|\mathbf{X})$	Truth	Pred	Pred
1	0.95	+	+	+
2	0.93	+	+	+
3	0.87	−	+	+
4	0.85	−	+	+
5	0.85	−	+	+
6	0.85	+	+	+
7	0.76	−	+	−
8	0.53	+	+	−
9	0.43	−	−	−
10	0.25	+	−	−

How to Draw ROC Curve?

- Sort the instances according to $P(+|\mathbf{X})$ in decreasing order
- Apply threshold at each unique value of $P(+|\mathbf{X})$
- Count the number of TP, FP, TN, FN based on each threshold
  - TP Rate, $\text{TPR} = \frac{\text{TP}}{\text{TP+FN}}$
  - FP Rate, $\text{FPR} = \frac{\text{FP}}{\text{TN+FP}}$

Not efficient

ID	$P(+|\mathbf{X})$	Truth
1	0.95	+
2	0.93	+
3	0.87	-
4	0.85	-
5	0.85	-
6	0.85	+
7	0.76	-
8	0.53	+
9	0.43	-
10	0.25	+

random

An Efficient Approach

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5										
FP	5										
TN	0										
FN	0										
TPR	1										
FPR	1										

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4									
FP	5	5									
TN	0	0									
FN	0	1									
TPR	1	0.8									
FPR	1	1									

An Efficient Approach (cont.)

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4								
FP	5	5	4								
TN	0	0	1								
FN	0	1	1								
TPR	1	0.8	0.8								
FPR	1	1	0.8								

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3							
FP	5	5	4	4							
TN	0	0	1	1							
FN	0	1	1	2							
TPR	1	0.8	0.8	0.6							
FPR	1	1	0.8	0.8							

An Efficient Approach (cont.)

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3						
FP	5	5	4	4	3						
TN	0	0	1	1	2						
FN	0	1	1	2	2						
TPR	1	0.8	0.8	0.6	0.6						
FPR	1	1	0.8	0.8	0.6						

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3					
FP	5	5	4	4	3	2					
TN	0	0	1	1	2	3					
FN	0	1	1	2	2	2					
TPR	1	0.8	0.8	0.6	0.6	0.6					
FPR	1	1	0.8	0.8	0.6	0.4					

An Efficient Approach (cont.)

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3				
FP	5	5	4	4	3	2	1				
TN	0	0	1	1	2	3	4				
FN	0	1	1	2	2	2	2				
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6				
FPR	1	1	0.8	0.8	0.6	0.4	0.2				

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2			
FP	5	5	4	4	3	2	1	1			
TN	0	0	1	1	2	3	4	4			
FN	0	1	1	2	2	2	2	3			
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4			
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2			

An Efficient Approach (cont.)

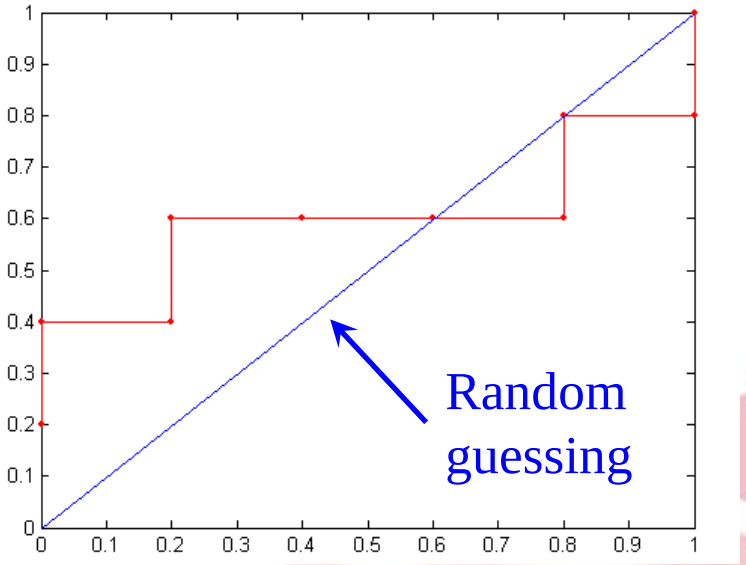
Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2		
FP	5	5	4	4	3	2	1	1	0		
TN	0	0	1	1	2	3	4	4	5		
FN	0	1	1	2	2	2	2	3	3		
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4		
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0		

Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2	1	
FP	5	5	4	4	3	2	1	1	0	0	
TN	0	0	1	1	2	3	4	4	5	5	
FN	0	1	1	2	2	2	2	3	3	4	
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	

An Efficient Approach (cont.)

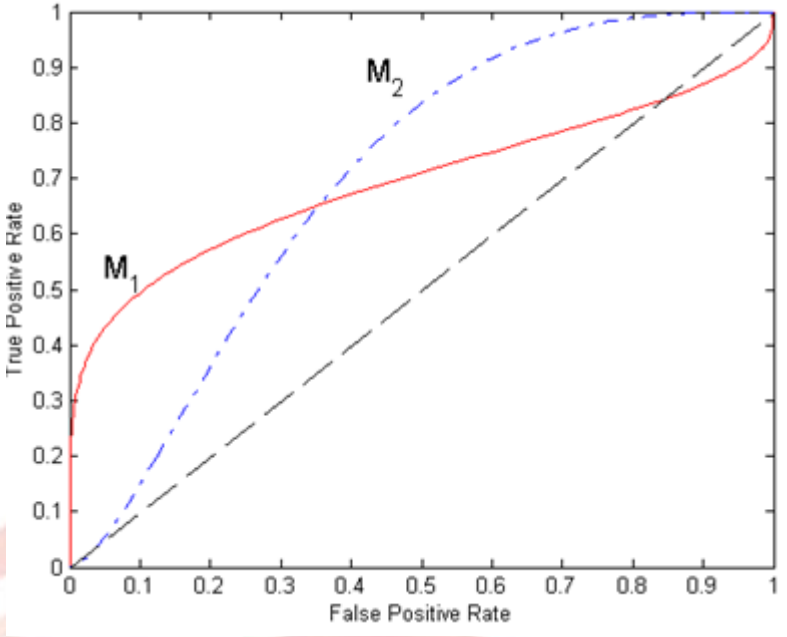
Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=	0.25	0.43	0.53	0.76	0.85	0.85	0.85	0.87	0.93	0.95	1.00
TP	5	4	4	3	3	3	3	2	2	1	0
FP	5	5	4	4	3	2	1	1	0	0	0
TN	0	0	1	1	2	3	4	4	5	5	5
FN	0	1	1	2	2	2	2	3	3	4	5
TPR	1	0.8	0.8	0.6	0.6	0.6	0.6	0.4	0.4	0.2	0
FPR	1	1	0.8	0.8	0.6	0.4	0.2	0.2	0	0	0

ROC Curve:



AUC for Classifiers Comparison

- In practice, on a specific dataset, a classifier may not consistently outperform the other with all the thresholds
  - M_1 is better for small FPR
  - M_2 is better for large FPR
- Area Under the ROC Curve (AUC)
  - Ideal: AUC = 1
    Random guess: AUC = 0.5



Implementation using scikit-learn

- API: sklearn.metrics
  https://scikit-learn.org/stable/modules/classes.html#module-sklearn.metrics

Classification metrics

See the Classification metrics section of the user guide for further details.

metrics.accuracy_score(y_true, y_pred, *[, ...])	Accuracy classification score.
metrics.auc(x, y)	Compute Area Under the Curve (AUC) using the trapezoidal rule
metrics.average_precision_score(y_true, ...)	Compute average precision (AP) from prediction scores
metrics.balanced_accuracy_score(y_true, ...)	Compute the balanced accuracy
metrics.brier_score_loss(y_true, y_prob, *)	Compute the Brier score.
metrics.classification_report(y_true, y_pred, *)	Build a text report showing the main classification metrics.
metrics.cohen_kappa_score(y1, y2, *[, ...])	Cohen's kappa: a statistic that measures inter-annotator agreement.
metrics.confusion_matrix(y_true, y_pred, *)	Compute confusion matrix to evaluate the accuracy of a classification.
metrics.dcg_score(y_true, y_score, *[, k, ...])	Compute Discounted Cumulative Gain.
metrics.f1_score(y_true, y_pred, *[, ...])	Compute the F1 score, also known as balanced F-score or F-measure
metrics.fbeta_score(y_true, y_pred, *, beta)	Compute the F-beta score
metrics.hamming_loss(y_true, y_pred, *[, ...])	Compute the average Hamming loss.
metrics.hinge_loss(y_true, pred_decision, *)	Average hinge loss (non-regularized)
metrics.jaccard_score(y_true, y_pred, *[, ...])	Jaccard similarity coefficient score
metrics.log_loss(y_true, y_pred, *[, eps, ...])	Log loss, aka logistic loss or cross-entropy loss.
metrics.matthews_corrcoef(y_true, y_pred, *)	Compute the Matthews correlation coefficient (MCC)
metrics.multilabel_confusion_matrix(y_true, ...)	Compute a confusion matrix for each class or sample
metrics.ndcg_score(y_true, y_score, *[, k, ...])	Compute Normalized Discounted Cumulative Gain.
metrics.precision_recall_curve(y_true, ...)	Compute precision-recall pairs for different probability thresholds
metrics.precision_recall_fscore_support(...)	Compute precision, recall, F-measure and support for each class
metrics.precision_score(y_true, y_pred, *[, ...])	Compute the precision
metrics.recall_score(y_true, y_pred, *[, ...])	Compute the recall
metrics.roc_auc_score(y_true, y_score, *[, ...])	Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.
metrics.roc_curve(y_true, y_score, *[, ...])	Compute Receiver operating characteristic (ROC)
metrics.zero_one_loss(y_true, y_pred, *[, ...])	Zero-one classification loss.

Outline

- Other evaluation metrics for classification
  - Imbalance classification problems
- Density estimation
  - Estimate unknown probability density function
    - Parametric & Non-parametric

Density Estimation

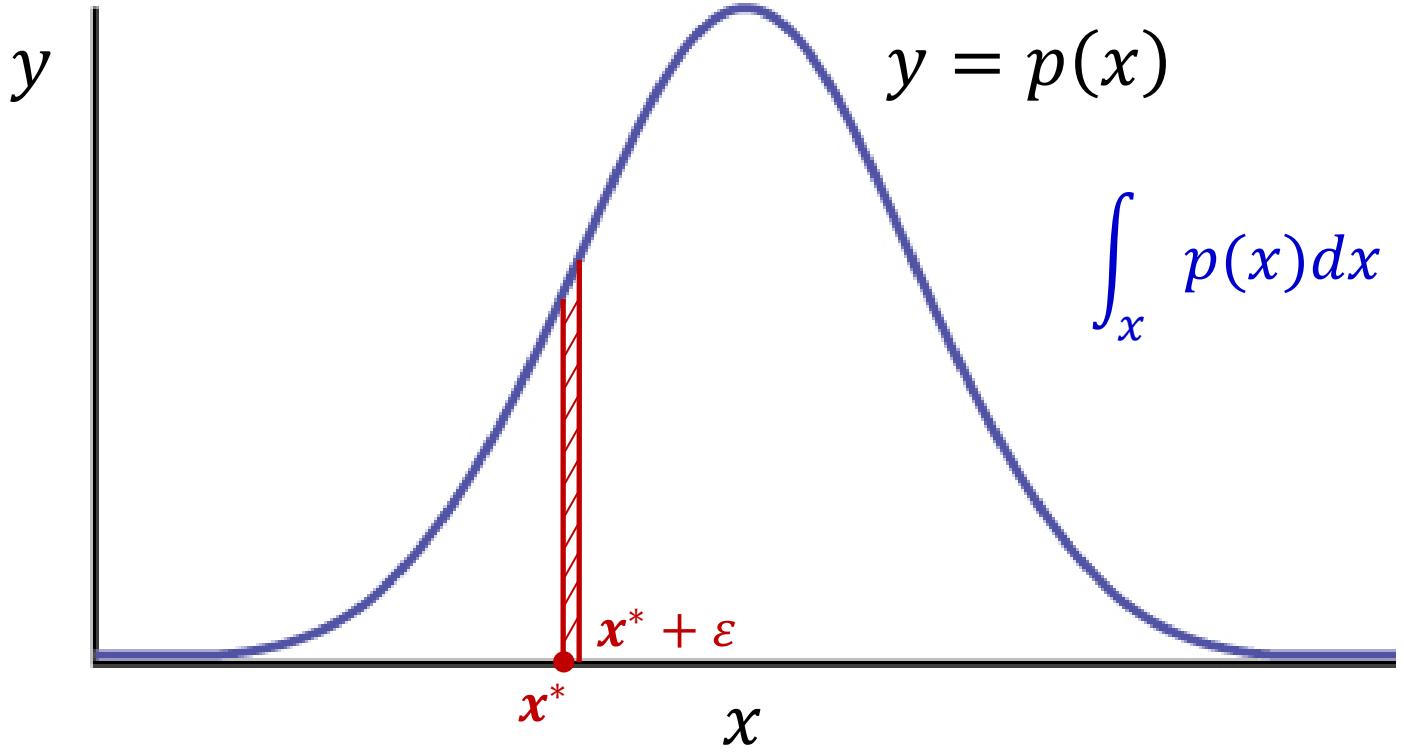
- Density estimation aims to estimate an unobservable underlying probability density function based on observed data
- Denote by $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ the set of observed data points, drawn from an unknown $p(\boldsymbol{x})$,

$$\boldsymbol{x}_i \sim p(\boldsymbol{x}), \text{for } i = 1, 2, \ldots, N$$

- The goal is to estimate the probability density function $p(\boldsymbol{x})$

$$\int_x p(x)dx = 1$$

Probability Density Function



$$\int_x p(x)dx = 1$$

$$P(\boldsymbol{x}^*) = \int_{\boldsymbol{x}^*}^{\boldsymbol{x}^*+\varepsilon} p(x)dx \approx p(\boldsymbol{x}^*) \times \varepsilon$$

Approaches

- Parametric density estimation
  - Assume a form for $p(\boldsymbol{x};\boldsymbol{\theta})$, defined up to parameters, $\boldsymbol{\theta}$
    - E.g., Guassian distribution $\mathcal{N}(\mu,\sigma^2)$, $\boldsymbol{\theta}=\{\mu,\sigma^2\}$
  - Estimate $\boldsymbol{\theta}$ from the observed data points
    - Maximum Likelihood Estimation
      - To find $\boldsymbol{\theta}$ that makes sampling $\boldsymbol{x}_i$ from $p(\boldsymbol{x};\boldsymbol{\theta})$ as likely as possible
- Nonparametric density estimation

Maximum Likelihood Estimation

- Likelihood of parameter $\boldsymbol{\theta}$ given sample $\mathcal{D}$:

$$l(\boldsymbol{\theta}|\mathcal{D}) \triangleq p(\mathcal{D};\boldsymbol{\theta})$$

- Suppose $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \dots, \boldsymbol{x}_N\}$ are i.i.d., the above likelihood is the product of the likelihoods of the individual data points

$$l(\boldsymbol{\theta}|\mathcal{D}) \triangleq p(\mathcal{D};\boldsymbol{\theta}) = \prod_{i=1}^{N} p(\boldsymbol{x}_i;\boldsymbol{\theta})$$

- In MLE, we aim to find $\boldsymbol{\theta}$ that makes $\mathcal{D}$ the most likely to be drawn. Mathematically, we aim to search for $\widehat{\boldsymbol{\theta}}$ such that

$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}|\mathcal{D})$$

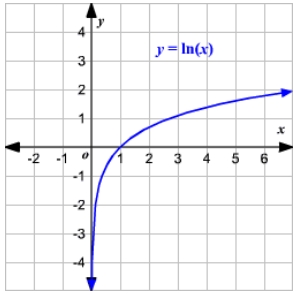
MLE (cont.)

- Recall that we maximize the log-likelihood:

$$\mathcal{L}(\boldsymbol{\theta}|\mathcal{D}) \triangleq \ln l(\boldsymbol{\theta}|\mathcal{D})$$

- Why (refer to logistic regression)?

1. The $\ln(\cdot)$ function is a strictly increasing function, one can maximize the likelilood without changing the value where it takes its maximum



$$\widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} l(\boldsymbol{\theta}|\mathcal{D}) \Leftrightarrow \widehat{\boldsymbol{\theta}} = \arg\max_{\boldsymbol{\theta}} \ln l(\boldsymbol{\theta}|\mathcal{D})$$

2. The $\ln(\cdot)$ function converts the product into a sum

$$\ln l(\boldsymbol{\theta}|\mathcal{D}) = \ln p(\mathcal{D};\boldsymbol{\theta}) = \ln\left(\prod_{i=1}^{N} p(\boldsymbol{x}_i;\boldsymbol{\theta})\right) = \sum_{i=1}^{N} \ln p(\boldsymbol{x}_i;\boldsymbol{\theta})$$

Solution to MLE

- As $\max_{\boldsymbol{\theta}} \ln l(\boldsymbol{\theta}|\mathcal{D})$ is an unconstrained optimization problem, to solve it, we first set to the derivative of $\ln l(\boldsymbol{\theta}|\mathcal{D})$ w.r.t. $\boldsymbol{\theta}$ to be zero

$$\nabla_{\boldsymbol{\theta}} \ln l(\boldsymbol{\theta}|\mathcal{D}) = \nabla_{\boldsymbol{\theta}} \left(\sum_{i=1}^{N} \ln p(\boldsymbol{x}_i; \boldsymbol{\theta}) \right) = \sum_{i=1}^{n} \nabla_{\boldsymbol{\theta}} \ln p(\boldsymbol{x}_i; \boldsymbol{\theta}) = \mathbf{0},$$

$$\nabla_{\boldsymbol{\theta}} = \left[\frac{\partial}{\partial \theta_1} \; \frac{\partial}{\partial \theta_2} \; \cdots \; \frac{\partial}{\partial \theta_p} \right]^T$$

- If we can obtain a closed form solution $\widehat{\boldsymbol{\theta}}$ by solving the p equations, then it is done
- Otherwise, we may use gradient descent to find $\widehat{\boldsymbol{\theta}}$

Univariate Gaussian

- Suppose $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$. Each data instance $\boldsymbol{x}_i$ is 1 dimensional, and drawn from Gaussian distribution with unknown μ and σ^2:

$$\boldsymbol{x}_i \sim p(\boldsymbol{x}; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{\left(-\frac{(\boldsymbol{x}-\mu)^2}{2\sigma^2}\right)}$$

- The log-likelihood is

$$\ln l(\boldsymbol{\theta}|\mathcal{D}) = \sum_{i=1}^{N} \ln p(\boldsymbol{x}_i; \mu, \sigma^2) = \sum_{i=1}^{N} \ln\left(\exp\left(-\frac{(\boldsymbol{x}_i - \mu)^2}{2\sigma^2}\right)\right) - \sum_{i=1}^{N} \ln(\sqrt{2\pi\sigma^2})$$

$$= -\frac{\sum_{i=1}^{N}(\boldsymbol{x}_i - \mu)^2}{2\sigma^2} - \sum_{i=1}^{N} \frac{1}{2} \ln(2\pi\sigma^2)$$

$$= -\frac{\sum_{i=1}^{N}(\boldsymbol{x}_i - \mu)^2}{2\sigma^2} - \frac{N}{2} \ln(2\pi) - \frac{N}{2} \ln \sigma^2$$

Univariate Gaussian (cont.)

- The log-likelihood:

$$\ln l(\boldsymbol{\theta}|\mathcal{D}) = -\frac{\sum_{i=1}^{N}(\boldsymbol{x}_i - \mu)^2}{2\sigma^2} - \frac{N}{2}\ln(2\pi) - \frac{N}{2}\ln\sigma^2$$

- The derivative of the log-likelihood:

$$\nabla_{\boldsymbol{\theta}} \ln l(\boldsymbol{\theta}|\mathcal{D}) = \begin{bmatrix} \nabla_{\mu} \ln l(\boldsymbol{\theta}|\mathcal{D}) \\ \\ \nabla_{\sigma^2} \ln l(\boldsymbol{\theta}|\mathcal{D}) \end{bmatrix} = \begin{bmatrix} \frac{1}{\sigma^2}\sum_{i=1}^{N}(\boldsymbol{x}_i - \mu) \\ \frac{\sum_{i=1}^{N}(\boldsymbol{x}_i - \mu)^2}{2(\sigma^2)^2} - \frac{N}{2\sigma^2} \end{bmatrix}$$

Univariate Gaussian (cont.)

- By setting the derivative to be zero:

$$\begin{cases} \frac{1}{\sigma^2}\sum_{i=1}^{N}(\boldsymbol{x}_i-\mu)=0 \\ \frac{\sum_{i=1}^{N}(\boldsymbol{x}_i-\mu)^2}{2(\sigma^2)^2}-\frac{N}{2\sigma^2}=0 \end{cases}$$

- We have

$$\begin{cases} \hat{\mu}=\frac{1}{N}\sum_{i=1}^{N}\boldsymbol{x}_i \\ \hat{\sigma}^2=\frac{1}{N}\sum_{i=1}^{N}(\boldsymbol{x}_i-\hat{\mu})^2 \end{cases}$$

Unbiased estimation

$\mathbb{E}[\hat{\mu}]=\mu$ ← True

$\mathbb{E}[\hat{\sigma}^2]=\frac{N-1}{N}\sigma^2$

Biased estimation

To correct bias

$$\tilde{\sigma}^2=\frac{N}{N-1}\hat{\sigma}^2$$

$$=\frac{1}{N-1}\sum_{i=1}^{N}(\boldsymbol{x}_i-\hat{\mu})^2$$

Multivariate Gaussian

- Suppose $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$, and each data instance $\boldsymbol{x}_i$ is m-dimensional, and drawn from Guassian distribution with unknown $\boldsymbol{\mu}$ and $\boldsymbol{\Sigma}$:

$m \times m$ covariance matrix

m-dimensional mean vector

$$\boldsymbol{x}_i \sim p(\boldsymbol{x}; \boldsymbol{\mu}, \boldsymbol{\Sigma}) = \frac{1}{(2\pi)^{m/2}} \frac{1}{|\boldsymbol{\Sigma}|^{1/2}} \exp\left(-\frac{1}{2}(\boldsymbol{x} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right)$$

The determinant of $\boldsymbol{\Sigma}$

- By using MLE

$$\hat{\boldsymbol{\mu}} = \frac{1}{N} \sum_{i=1}^{N} \boldsymbol{x}_i$$

$$\hat{\boldsymbol{\Sigma}} = \frac{1}{N} \sum_{i=1}^{N} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})^T \qquad \mathbb{E}[\hat{\boldsymbol{\Sigma}}] = \frac{N-1}{N} \boldsymbol{\Sigma}$$

Unbiased estimation:

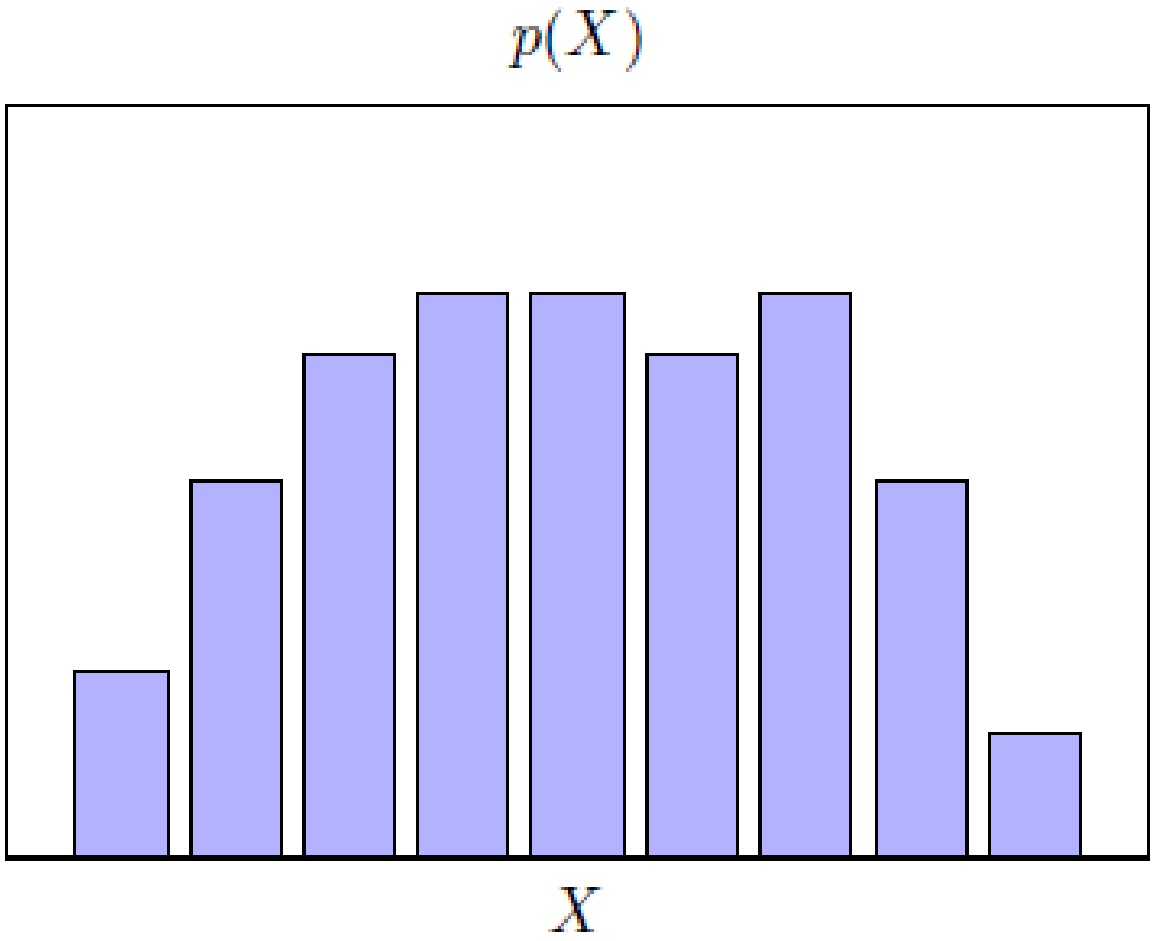
$$\mathbb{E}[\hat{\boldsymbol{\mu}}] = \boldsymbol{\mu}$$

$$\tilde{\boldsymbol{\Sigma}} = \frac{1}{N-1} \sum_{i=1}^{N} (\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})(\boldsymbol{x}_i - \hat{\boldsymbol{\mu}})^T$$ Unbiased estimation

Non-Parametric Density Estimation

- Assume that $\mathcal{D} = \{\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots, \boldsymbol{x}_N\}$ are drawn from some unknown probability density $p(\boldsymbol{x})$
  - Without assuming any forms for the underlying density
- To learn the estimator $\hat{p}(\boldsymbol{x})$ for $p(\boldsymbol{x})$
  - Assume that similar inputs have similar outputs: if $\boldsymbol{x}_i$ and $\boldsymbol{x}_j$ are similar, then $p(\boldsymbol{x}_i)$ and $p(\boldsymbol{x}_j)$ are similar
- Approaches
    - Histogram Estimator
    - Naïve Estimator / Parzen Windows / Kernel Estimator

Histogram Estimator



Histogram Estimator (cont.)

- Simply partition $\boldsymbol{x}$ (suppose 1-dimensional for simplicity) into distinct bins of width Δ_t
- Count the number N_t of data instances falling into bin t
- Turn this count into a normalized probability density via dividing by the total number of observed data points N and by the width Δ_t of the bins:

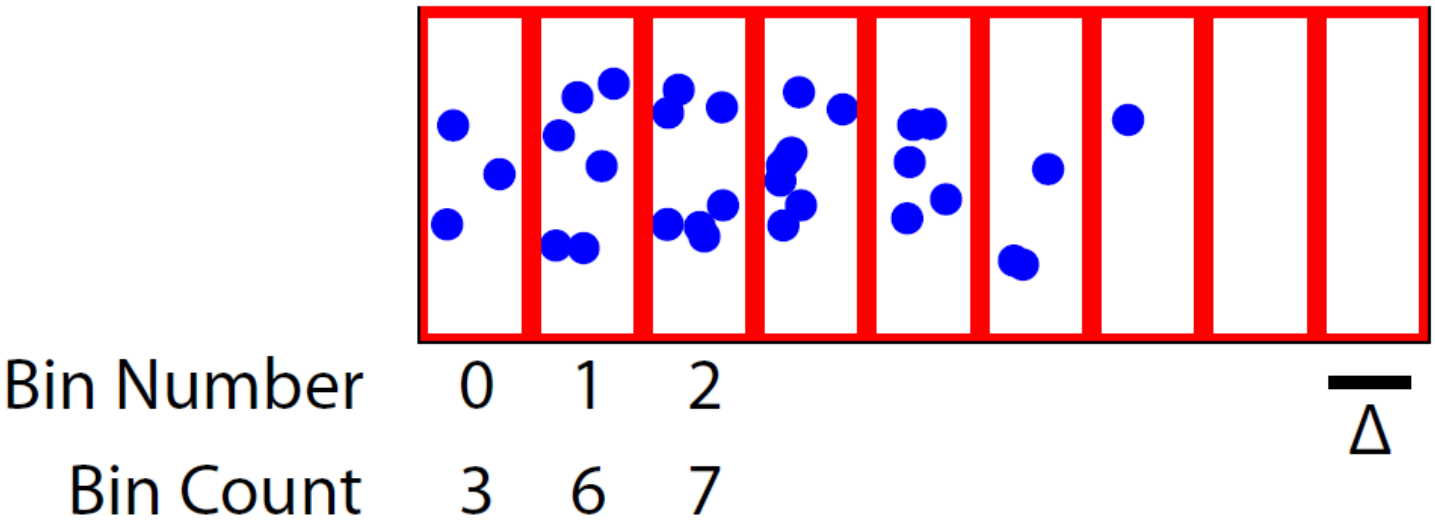
$$p_t = \frac{N_t}{N\Delta_t} \xrightarrow{\text{Suppose all the bins have the same width } \Delta_t = \Delta} p_t = \frac{N_t}{N\Delta}$$

- The model for the density $p(\boldsymbol{x})$ is constant over the width of each bin: find the bin where $\boldsymbol{x}$ is in (e.g., bin t), then

$$\hat{p}(\boldsymbol{x}) = \frac{\#\{\boldsymbol{x}_i \text{ in the same bin as } \boldsymbol{x}\}}{N\Delta} = p_t$$

Histogram Estimator (cont.)

- Typically, the bins are chosen to have the same width $\Delta_t = \Delta$



$$p_t = \frac{N_t}{N\Delta}$$

Why divided by Δ?

Histogram Estimator (cont.)

- For a specific bin denoted by t, the probability that a data instance $\boldsymbol{x}$ falls into the bin (e.g., $\left(x^{(t)}, x^{(t)} + \Delta\right]$) is

The start value of the bin t

$$P = \int_{x^{(t)}}^{x^{(t)}+\Delta} p(\boldsymbol{x}')d\boldsymbol{x}' = p(\boldsymbol{x})\Delta$$

- On the other hand,

$$P = \frac{\#\{\boldsymbol{x}_i \text{ in the bin } i\}}{N} = \frac{N_t}{N}$$

- Therefore:

$$p(\boldsymbol{x}) = \frac{N_t}{N\Delta}$$

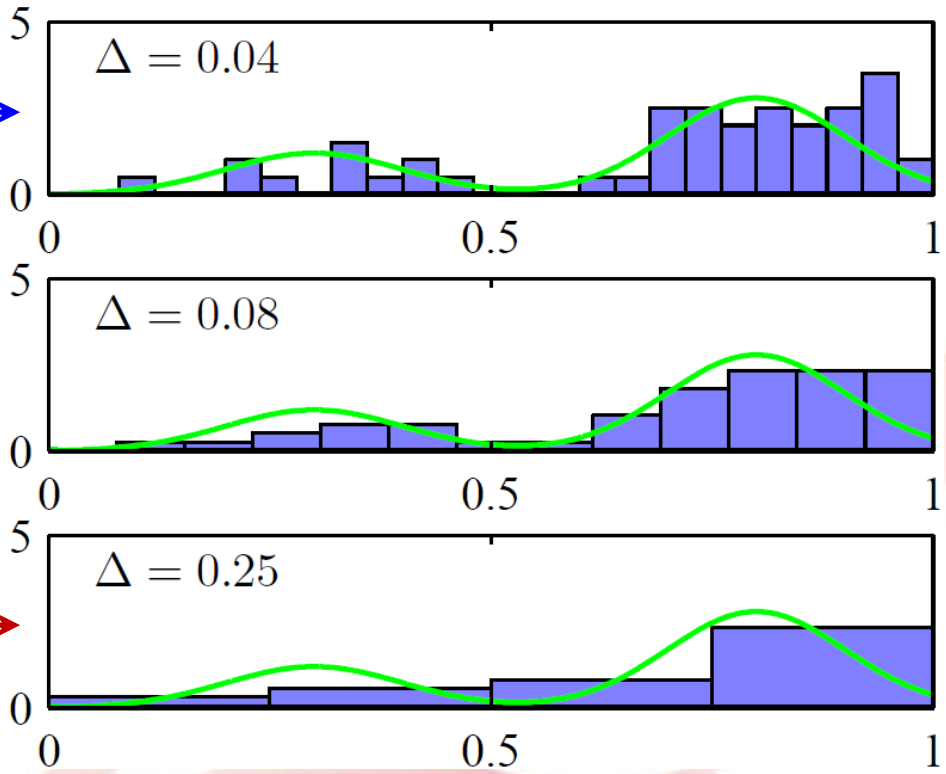
Histogram Estimator (cont.)

- Histogram density as a function of bin width Δ

The green curve is the underlying true density from which the data points were drawn

When Δ is very small, the resulting density is quite spiky and hallucinates a lot of structure not present in the true density →

When Δ is very big, the resulting density is quite smooth and consequently fails to capture the bimodality of the true density →



Discussion

- Advantages:
  - Simple to evaluate and simple to use
  - One can throw away $\mathcal{D}$ once the histogram is computed
  - Can be updated incrementally
- Disadvantages:
  - The estimated density has discontinuities due to the bin edges rather than any property of the underlying density
  - Scales poorly to multivariate cases: we would have L^m bins if we divided each variable in a m-dimensional space into L bins

Naïve Estimator: An Alternative

- In Histogram Estimator, besides Δ, we have to choose an origin x_0 as well, the bins are the intervals defined as

$$(\boldsymbol{x}_0 + t\Delta, \boldsymbol{x}_0 + (t+1)\Delta]$$

0, positive or negative integers

- The Naïve Estimator does no need to set on origin

$$\hat{p}(\boldsymbol{x}) = \frac{\#\{\boldsymbol{x}_i \text{ in the same bin as } \boldsymbol{x}\}}{N\Delta}$$

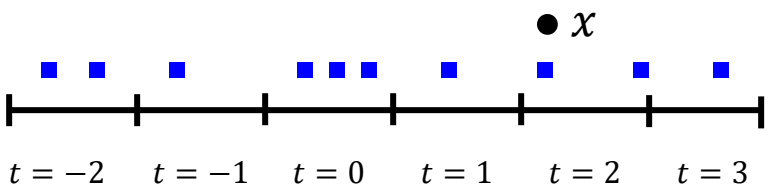
$$\hat{p}(\boldsymbol{x}) = \frac{\#\left\{\boldsymbol{x} - \frac{\Delta}{2} < x_i \leq \boldsymbol{x} + \frac{\Delta}{2}\right\}}{N\Delta}$$

$(\xleftrightarrow{\frac{\Delta}{2}} \boldsymbol{x} \xleftrightarrow{\frac{\Delta}{2}}]$

Histogram v.s. Naïve Estimator

Histogram Estimator

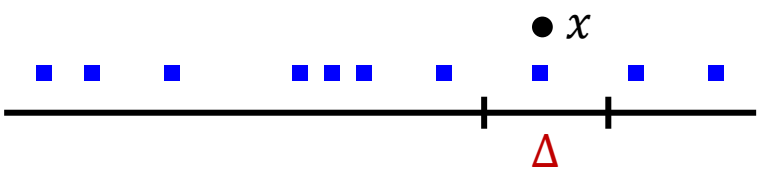
$$p(x) = \frac{2}{10 \times \Delta}$$



Count: 2 1 3 1 2 1

Naïve Estimator

$$p(x) = \frac{1}{10 \times \Delta}$$



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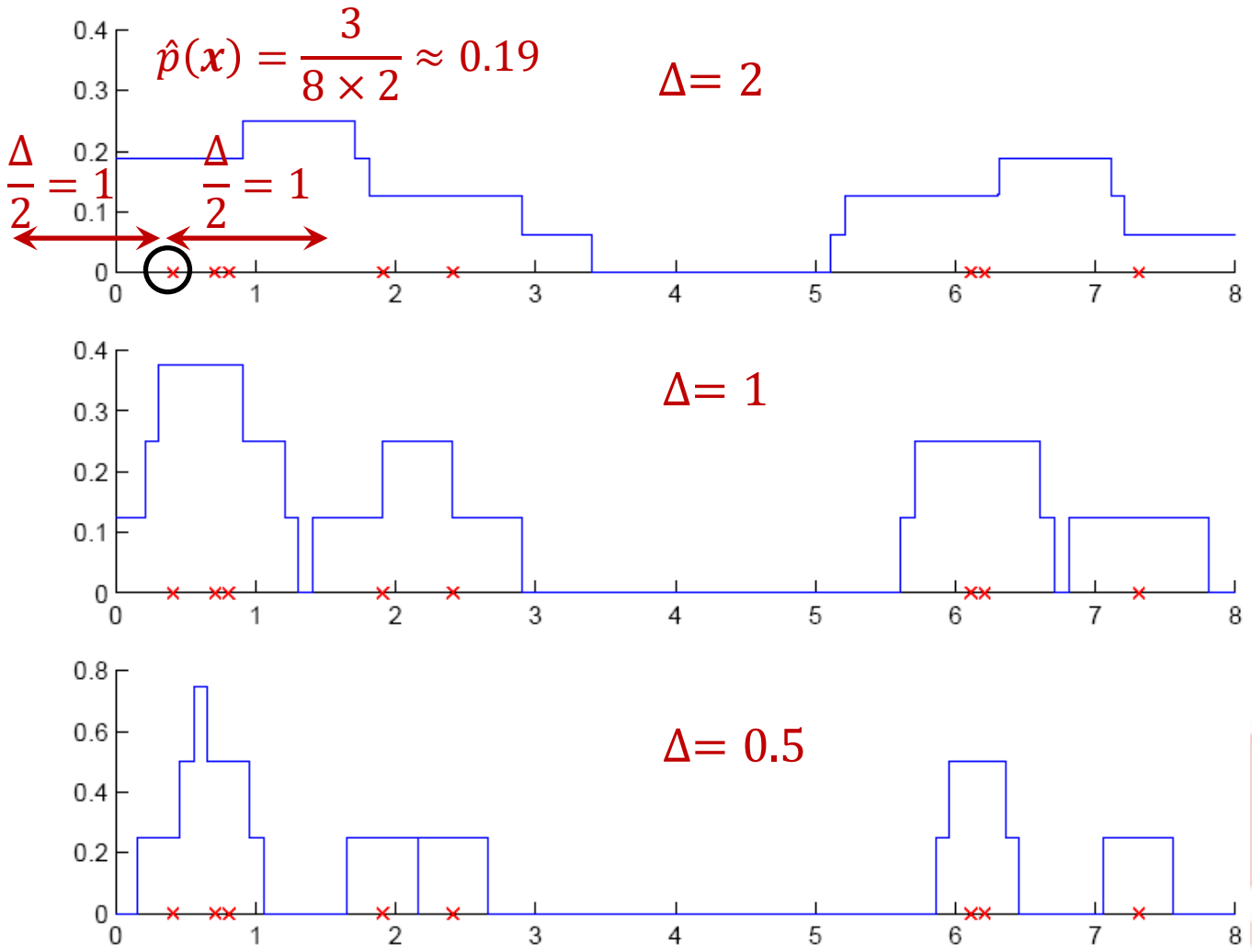
Naïve Estimator: Example



Parzen Windows

- The Naïve Estimator can also be written as

$$\hat{p}(x) = \frac{\#\left\{x - \frac{\Delta}{2} < x_i \leq x + \frac{\Delta}{2}\right\}}{N\Delta}$$

x_i is in the bin with width Δ centered at x

$$\hat{p}(x) = \frac{1}{N\Delta}\sum_{i=1}^{N} w\left(\frac{x - x_i}{\Delta}\right)$$

$$-\frac{1}{2} \leq \frac{x - x_i}{\Delta} < \frac{1}{2}$$

$$u = \frac{x - x_i}{\Delta}$$

Windowing function $w(u) = \begin{cases} 1 & \text{if } -\frac{1}{2} \leq u < \frac{1}{2} \\ 0 & \text{otherwise} \end{cases}$

Parzen windows

Multiple Dimensions Case

- Given $\mathcal{D} = \{\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N\}$, each data instance is m-dimensional
- We define $\mathcal{R}$ is a m-dimensional hypercube with h being the length of each edge. The volume of the hypercube is given by

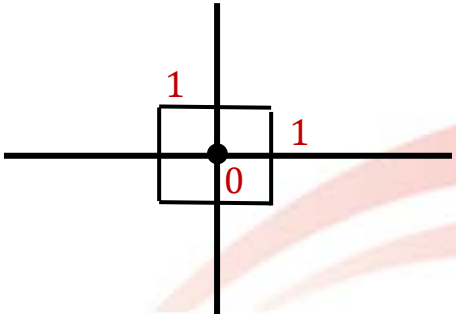
$$V = h^m$$

- The window function can be defined as

$$w(\boldsymbol{u}) = \begin{cases} 1 & \text{if } -\frac{1}{2} \leq u_i < \frac{1}{2} \text{ for all } i \in \{1, \ldots, m\} \\ 0 & \text{otherwise} \end{cases}$$

This window function defines a unit hypercube centered at the origin

E.g., $d = 2$

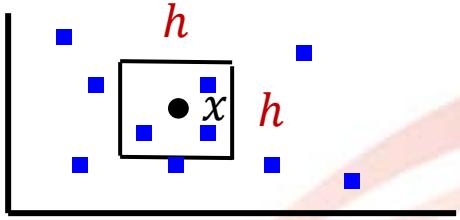


Multiple Dimensions Case (cont.)

- Hence, $w\left(\frac{\boldsymbol{x}-\boldsymbol{x}_i}{h}\right)$ is equal to unity if $\boldsymbol{x}_i$ falls within the hypercube of volume V centered at $\boldsymbol{x}$, and is zero otherwise
- The density estimator can be written as

$$\hat{p}(\boldsymbol{x}) = \frac{\#\{\boldsymbol{x}_i \text{ in the same hypercube as } \boldsymbol{x}\}}{NV}$$

$$\hat{p}(\boldsymbol{x}) = \frac{1}{NV}\sum_{i=1}^{N} w\left(\frac{\boldsymbol{x}-\boldsymbol{x}_i}{h}\right)$$



$$\hat{p}(\boldsymbol{x}) = \frac{3}{10h^2}$$

Kernel Estimator

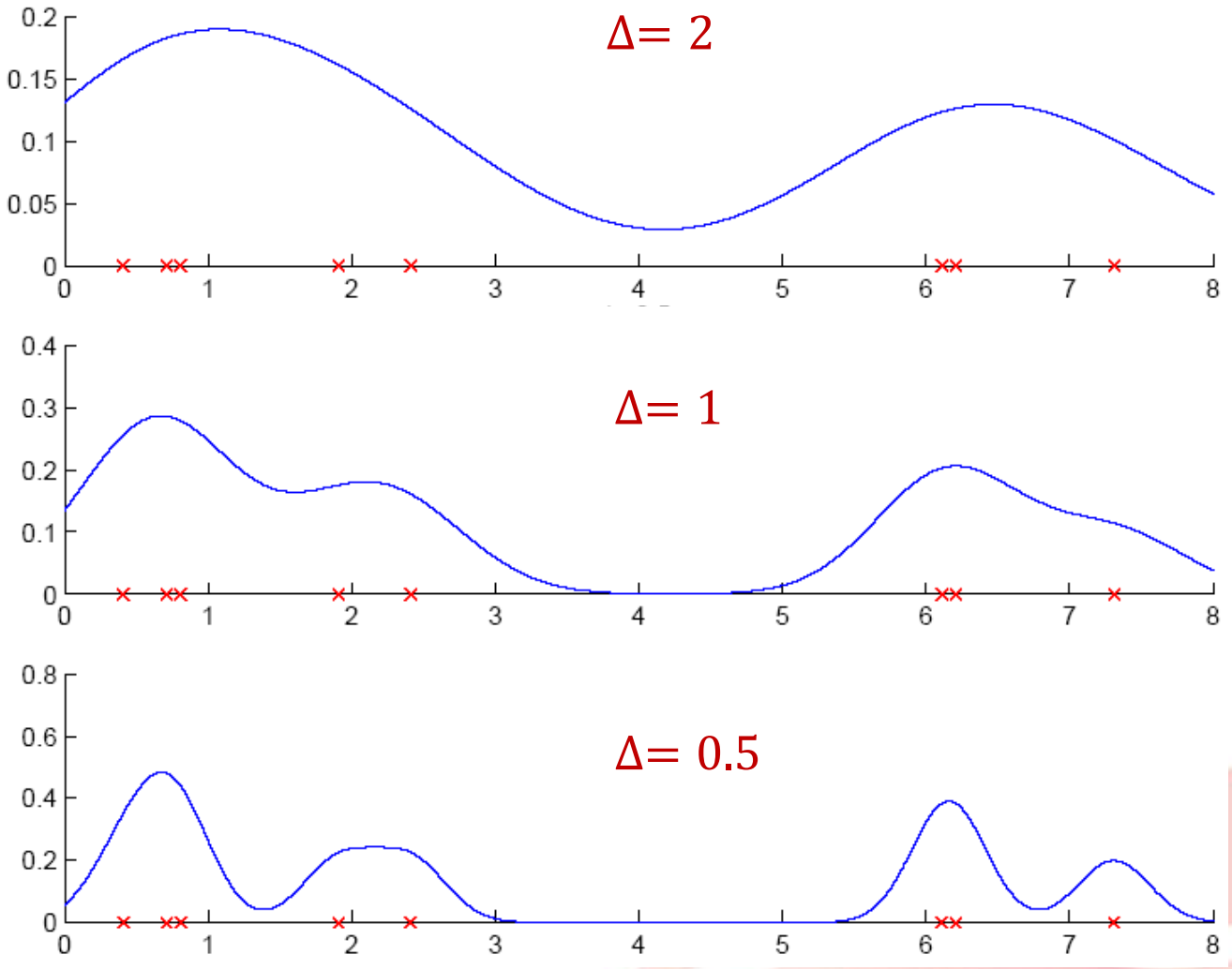
- To get a smooth estimate, we use a smooth weight function, kernel function, e.g., the Gaussian kernel
- For the univariate case, i.e., each data point is 1-dimensional, the Gaussian kernel is defined as

$$k(u) = \frac{1}{\sqrt{2\pi}} \exp\left(-\frac{u^2}{2}\right)$$

- The Kernel Estimator is computed via

$$\hat{p}(x) = \frac{1}{N\Delta} \sum_{i=1}^{N} k\left(\frac{x - x_i}{\Delta}\right)$$

Kernel Estimator: An Example



Kernel Estimator (cont.)

- For the multivariate case, i.e., each data instance is m-dimensional, the Gaussian kernel is defined as

$$k(\boldsymbol{u}) = \frac{1}{(2\pi)^{m/2}} \exp\left(-\frac{\|\boldsymbol{u}\|_2^2}{2}\right)$$

- The Kernel Estimator is computed via

$$\hat{p}(\boldsymbol{x}) = \frac{1}{NV} \sum_{i=1}^{N} k\left(\frac{\boldsymbol{x} - \boldsymbol{x}_i}{h}\right)$$

Implementation using scikit-learn

- API: sklearn.neighbors.KernelDensity
  https://scikit-learn.org/stable/modules/generated/sklearn.neighbors.KernelDensity.html#sklearn.neighbors.KernelDensity

sklearn.neighbors.KernelDensity

class sklearn.neighbors.**KernelDensity**(*, *bandwidth=1.0, algorithm='auto', kernel='gaussian', metric='euclidean', atol=0, rtol=0, breadth_first=True, leaf_size=40, metric_params=None*) [source]

Kernel Density Estimation.

Read more in the User Guide.

Parameters:

bandwidth : *float*
The bandwidth of the kernel.

algorithm : *str*
The tree algorithm to use. Valid options are ['kd_tree'|'ball_tree'|'auto']. Default is 'auto'.

kernel : *str*
The kernel to use. Valid kernels are ['gaussian'|'tophat'|'epanechnikov'|'exponential'|'linear'|'cosine'] Default is 'gaussian'.

Example

```
>>> from sklearn.neighbors import KernelDensity
>>> import numpy as np

>>> n_samples, n_features = 10, 5
>>> rng = np.random.RandomState(0)
>>> X = rng.randn(n_samples, n_features)

>>> kde = KernelDensity( kernel='gaussian', bandwidth=0.5 )
>>> kde.fit(X)
>>> log_den_X= kde.score_samples(X)
```

Return log density of X

Thank you!