02450: Introduction to Machine Learning and Data Mining

Performance evaluation, Bayes, and Naive Bayes

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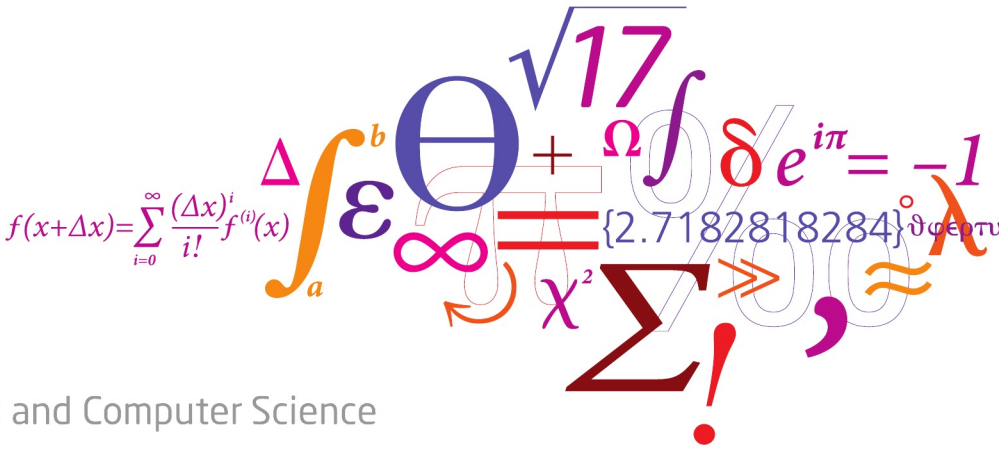


DTU Compute
Department of Applied Mathematics and Computer Science

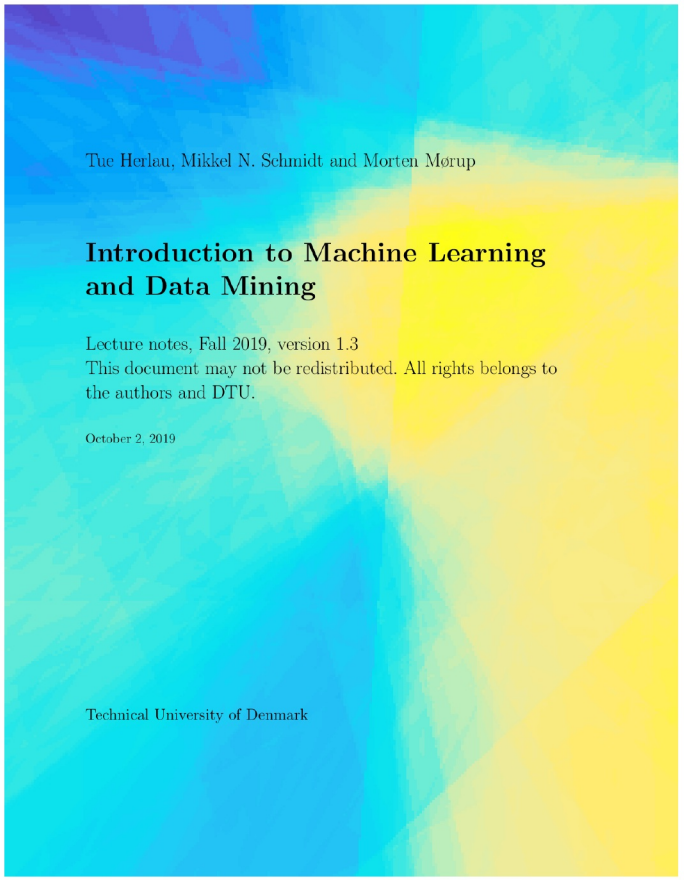
Today

Feedback Groups of the day:

Enrique Nicolas Quiroz Salazar, Sofus Albert Høgsbro Rose, Sunniva Olsrud Punsvik, Benjamin Lindegren Larsen, Arnor Ingi Palsson, Carl Nørby Mouridsen, ANTONIO Iglesias Marquez, Ditte Aarøe Jepsen, Amanda Mølgaard Sommer, Cecilie Kørner Kosack, Daryl Stephen Paul, Sylvain Ledur, Jeremy Paul Coffelt, Asger Laurits Schultz, William Diedrichsen Marstrand, Nanna Søtang Steenberg Olsen, Cecilia Duyen Thuy Cong Nguyen, Oliver Svane Olsen, Vimal Mollyn, Vimal Mollyn, Kishan Suchet Palani, Emil-August Torp, Gaétan Pierre Moisson-Franckhauser, Lilian Mehl, Tanguy Navez, Bo Simmendefeldt Schmidt, Mikkel Müller-Hansen, Camilla Lind Ommen, Sidsel Grabow Olesen, Jacques Daniel Pierre Michel, Rosa Ferrigno, Thomas Richard Yatman, Emil Skov Rasmussen, Jan Olsen, Anna Schrøder Lassen, Malene Nørregaard Nielsen, Natasja Kaas Lund, Manon Tania Hélène Petit, Yann Larré, Christian Mathias Jedermann Pilgaard, Henriette Becker Kristiansen, Sebastian Seedorff Larsson, Lasse Hassel-Pflugh, Luka Kovac, Arnhold Simonsen, Johanne Schjødt-Hansen, Moein Jahanbani Veshareh, Asger Ulf Jensen, Ryan Jørgensen, Jonas Juhler-Nøttrup, Erik Nicolas Klemt, Edgars Kipans

Reading material:

Chapter 11, Chapter 13



Lecture Schedule

1. Introduction
   3 September: C1

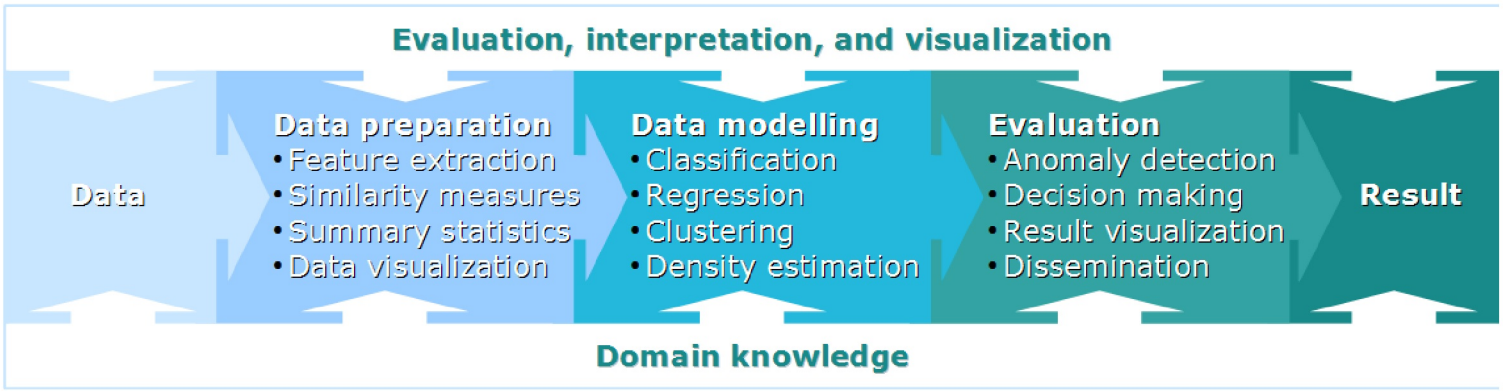
   Data: Feature extraction, and visualization
2. Data, feature extraction and PCA
   10 September: C2, C3
3. Measures of similarity, summary statistics and probabilities
   17 September: C4, C5
4. Probability densities and data Visualization
   24 September: C6, C7

   Supervised learning: Classification and regression
5. Decision trees and linear regression
   1 October: C8, C9 **(Project 1 due before 13:00)**
6. Overfitting, cross-validation and Nearest Neighbor
   8 October: C10, C12
7. **Performance evaluation, Bayes, and Naive Bayes**
   22 October: C11, C13
8. Artificial Neural Networks and Bias/Variance
   29 October: C14, C15
9. AUC and ensemble methods
   5 November: C16, C17

   Unsupervised learning: Clustering and density estimation
10. K-means and hierarchical clustering
    12 November: C18 **(Project 2 due before 13:00)**
11. Mixture models and density estimation
    19 November: C19, C20
12. Association mining
    26 November: C21

    Recap
13. Recap and discussion of the exam
    3 December: C1-C21 **(Project 3 due before 13:00)**

Piazza online help: `https://piazza.com/dtu.dk/fall2019/02450`
Videos/streaming of lectures: `https://video.dtu.dk`



Learning Objectives

- Understand the two different evaluation setups
- Apply appropriate statistical tests to evaluate and compare models
- Account for the assumptions made in Naïve Bayes
- Apply Bayes Theorem to obtain the class posterior likelihood

Why test?

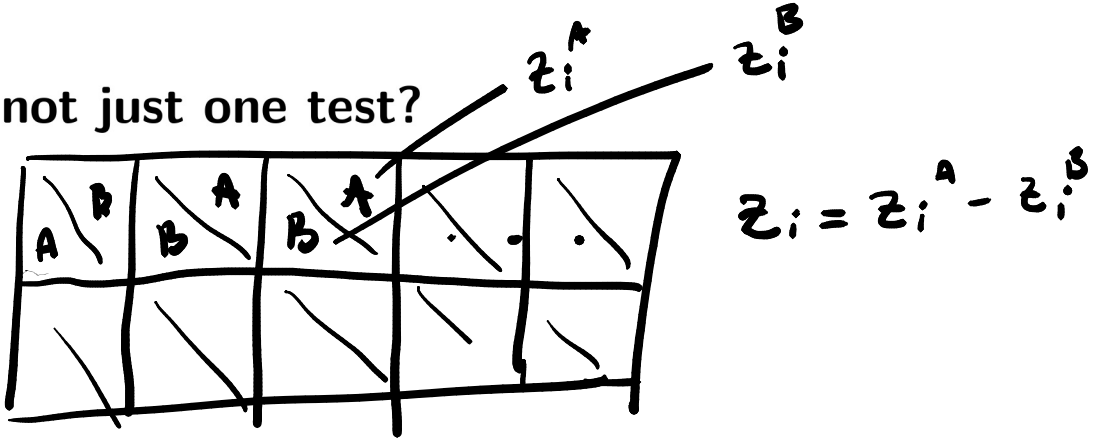
Statistical evaluation can mean a number of things:

- A social media company wish to know if introducing a new ad-placement method increases the click-through rate over another
- How many customers are likely click adds next month?
- How well can a neural network model learn to distinguish between diseased/non-diseased X-rays?
- Should I recommend that people use my neural network model over a competing method?

Tests can provide two things:

- An objective way to choose between methods
- A way to quantify model performance which takes uncertainty into account

Outline: why not just one test?



- What is our overall **objective**? What conclusions do we want?
- What is our fundamental **evaluation criteria**?
- What specific test should I use? (classification, regression, etc.)

The objective and evaluation criteria

- We compare models based on how well they **generalize to future data**
- Suppose we have data $\mathcal{D} = (\boldsymbol{X}, \boldsymbol{y})$ and two models $\mathcal{M}_A$, $\mathcal{M}_B$
- Training on $\mathcal{D}$, we obtain prediction rules

$$f_{\mathcal{D},A}, \quad \text{and} \quad f_{\mathcal{D},B}.$$

- Compared by the **difference in generalization error**:

$$z_{\mathcal{D}} = E^{\text{gen}}_{\mathcal{D},A} - E^{\text{gen}}_{\mathcal{D},B}$$

$$E^{\text{gen}}_{\mathcal{D},A} = \int p(\boldsymbol{x}, y) L(f_{\mathcal{D},A}(\boldsymbol{x}), y) d\boldsymbol{x} dy, \quad E^{\text{gen}}_{\mathcal{D},B} = \int p(\boldsymbol{x}, y) L(f_{\mathcal{D},B}(\boldsymbol{x}), y) d\boldsymbol{x} dy.$$

- If $z_{\mathcal{D}} < 0$, it means **that $\mathcal{M}_A$ is better than $\mathcal{M}_B$... ...when trained on $\mathcal{D}$**
- This is **one possible objective**:

  Setup I Statistical tests of performance considering the **specific** training set $\mathcal{D}$

A more general objective

- Compared by the difference in generalization error:

$$z_{\mathcal{D}} = E^{\text{gen}}_{\mathcal{D},A} - E^{\text{gen}}_{\mathcal{D},B}$$

- Therefore, if you prove $z_{\mathcal{D}} < 0$, you can't know if this is true for $\mathcal{D}'$ (from same distribution as $\mathcal{D}$)
- Therefore, our experiment is not independently reproducible
- To overcome this, test if $\mathcal{M}_A$ is better than $\mathcal{M}_B$ when averaging over dataset

$$z = \mathbb{E}_{\mathcal{D}}[z_{\mathcal{D}}] < 0$$

$$E^{\text{gen}} = \int \left[\int L(f_{\mathcal{D}}(\boldsymbol{x}), y) p(\boldsymbol{x}, \boldsymbol{y}) d\boldsymbol{x} dy \right] p(\mathcal{D}) d\mathcal{D}$$

- If $z < 0$, it means $\mathcal{M}_A$ **is better than** $\mathcal{M}_B$ **... on a typical training set**

Setup II *Statistical tests of performance considering a dataset of size* N

Choices, choices

Setup I Statistical tests of performance considering the **specific** training set $\mathcal{D}$?

Setup II *Statistical tests of performance considering* ***a dataset*** *of size* N

Which to choose fundamentally depends on the situation and what you want to conclude. Write the conclusion correctly!

- Setup II is a more general (impressive) conclusion
- Setup II is probably what we want in science
- Setup II requires (a lot of) cross-validation
- If you have a single train/test split, use setup I

We will consider **setup I** here

Statistical goals

Hypothesis testing Determine whether there is an effect, i.e. choose between $H_0 : z = 0$ vs. $H_1 : z \neq 0$

Estimation Determine (likely) value $z \approx \hat{z}$ and an interval $[z_L, z_U]$ that likely contains z

- Focus should be on estimation: No two models are equal and a difference of 1% is often of little interest
- Use hypothesis testing as a decision rule or to color entries in a table

Connecting objective to numbers

- We want to draw conclusions about the difference in performance:

$$z_{\mathcal{D}} = E^{\text{gen}}_{\mathcal{D},A} - E^{\text{gen}}_{\mathcal{D},B}$$

$$E^{\text{gen}}_{\mathcal{D},A} = \int p(\boldsymbol{x}, y) L(f_{\mathcal{D},A}(\boldsymbol{x}), y) d\boldsymbol{x} dy, \quad E^{\text{gen}}_{\mathcal{D},B} = \int p(\boldsymbol{x}, y) L(f_{\mathcal{D},B}(\boldsymbol{x}), y) d\boldsymbol{x} dy.$$

- We can be estimated as

$$\hat{z}_{\mathcal{D}} = \frac{1}{N^{\text{test}}} \sum_{i=1}^{N^{\text{test}}} [L(f_{\mathcal{D},A}(\boldsymbol{x}_i), y_i) - L(f_{\mathcal{D},B}(\boldsymbol{x}_i), y_i)]$$

$$= \frac{1}{N^{\text{test}}} \sum_{i=1}^{N^{\text{test}}} z_i, \quad \text{where:} \quad z_i = L(f_{\mathcal{D},A}(\boldsymbol{x}_i), y_i) - L(f_{\mathcal{D},B}(\boldsymbol{x}_i), y_i).$$

Abstracting to a statistical question

Consider data as the n numbers

$$D = (z_1, \ldots, z_n). \tag{1}$$

General form of the problem: Draw conclusions about

$$\theta = E^{\text{gen}}_{A,\mathcal{D}} - E^{\text{gen}}_{B,\mathcal{D}}$$

Based on D and the estimate:

$$\hat{\theta} = \frac{1}{n} \sum_{i=1}^{n} z_i. \tag{2}$$

Statistical tools: Parameter

- We assume z_i is a realization of a random variable Z_i
- It has density

$$p(Z_i = z_i|\theta) = p_\theta(z_i)$$

- Density of all dataset

$$p_\theta(D) = \prod_{i=1}^{n} p_\theta(z_i). \tag{3}$$

- Returning to our goals:
  - **estimating plausible ranges of θ**
  - **hypothesis testing such as whether θ takes a particular value** $\theta = 0$
- Let's look at the statistical tools to accomplish this

Statistical tools: Statistic and estimator

Statistic A statistic is a function of the data D and will be denoted t.
For instance, the mean and variance are both statistics:

$$t_0(D) = \frac{1}{n}\sum_{i=1}^{n} Z_i, \text{ or } t_1(D) = \frac{1}{n}\sum_{i=1}^{n}(Z_i - t_0(D))^2.$$

Estimator An estimator is a statistic t of D such that $t(D)$ is close to θ.
In the examples we will consider the mean

$$t_0(D) = \frac{1}{n}\sum_{i=1}^{n} Z_i$$

Statistical tools: Confidence interval

- A **confidence interval** (CI) is an interval $[\theta_L, \theta_U]$ which likely contains θ
- The CI is a function of the data D. θ_L and θ_U are two statistics and for a concrete dataset the interval is computed to be

$$[\theta_L(D), \theta_U(D)]. \tag{4}$$

- With probability $1 - \alpha$, the true value θ should fall within the confidence interval $[\theta_L(D), \theta_U(D)]$ as we randomize over different datasets

$$P_\theta(\theta \in [\theta_L, \theta_U]) = 1 - \alpha. \tag{5}$$

Statistical tools: Null hypothesis testing and p-value

- Determining whether a hypothesis H_0 about the parameters (the **null hypothesis**) is true or false

$$H_0 : \theta = 0 \quad \text{vs.} \quad H_1 : \theta \neq 0$$

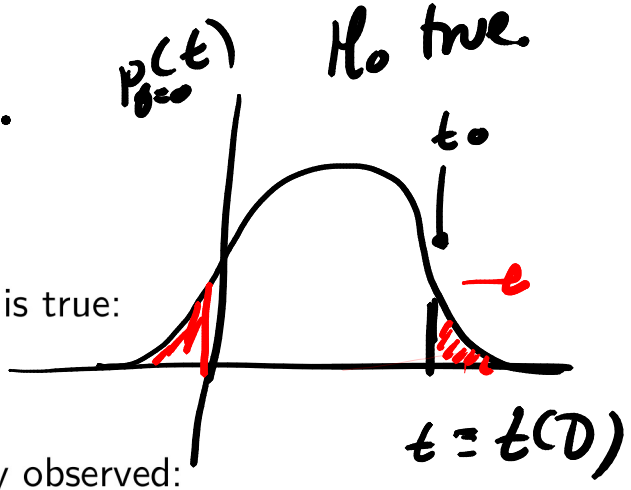
- Intuitively, if H_0 is true, the data should behave in a certain way. **We test if the data is implausible assuming H_0**
- Specifically, let t be a statistic, for our purpose

$$t(D) = \frac{1}{n}\sum_{i=1}^{n} Z_i$$

On our dataset it has a particular value $t_0 = \frac{1}{n}\sum_{i=1}^{n} z_i$

- We can compute the density $t(D)$ takes a particular value given H_0 is true:

$$p(t(D) = t|H_0) = p_{\theta=\theta_0}(t(D) = t)$$



- p-value is the chance $t(D)$ is at least as extreme as what we actually observed:

$$\textit{p-value}: \quad p = P\left(t(D) > |t_0| \mid H_0\right) = P_{\theta=\theta_0}(t(D) \geq |t_0|). \qquad (6)$$

Setup I: Fixed training set

Suppose we carry out cross-validation to obtain:

$$(\mathcal{D}_1^{\text{train}}, \mathcal{D}_1^{\text{test}}), \ldots, (\mathcal{D}_K^{\text{train}}, \mathcal{D}_K^{\text{test}}). \tag{7}$$

We collect these into (paired) vectors of predictions and true values:

$$\hat{\boldsymbol{y}} = \begin{bmatrix} \hat{\boldsymbol{y}}_1^{A} \\ \hat{\boldsymbol{y}}_2^{A} \\ \vdots \\ \hat{\boldsymbol{y}}_K^{A} \end{bmatrix}, \quad \boldsymbol{y} = \begin{bmatrix} \boldsymbol{y}_1^{\text{train}} \\ \boldsymbol{y}_2^{\text{train}} \\ \vdots \\ \boldsymbol{y}_K^{\text{train}} \end{bmatrix} \begin{matrix} \text{test} \\ \text{test} \\ \\ \text{test} \end{matrix}. \tag{8}$$

$\hat{y}_i = f_{\mathcal{D},A}(x_i^{\text{test}})$,

$\mathcal{D} = (\hat{y}, y)$

Evaluation of a single classifier

- Define:

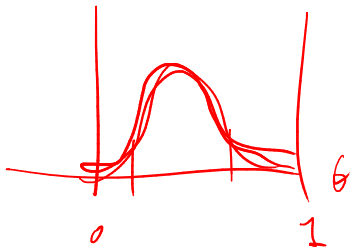
$$c_i = \begin{cases} 1 & \text{if } \hat{y}_i = y_i \\ 0 & \text{if otherwise.} \end{cases}$$

- Number of accurate guesses:

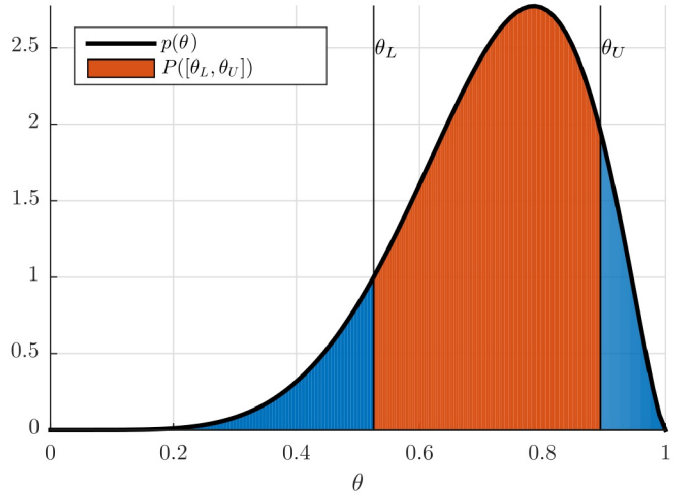
$$m = \sum_{i=1}^{n} c_i.$$

- Let the chance the classifier is correct be θ. Then, from **Lecture 4**, we know

$$p(\theta|m,n) = \text{Beta}(\theta|a,b), \quad a = m + \frac{1}{2}, \text{ and } b = n - m + \frac{1}{2}. \tag{9}$$



Intermezzo: cummulative densities



- Consider a general probability density $p(\theta)$ of a parameter θ
- Recall that by the definition of p, then

$$p(\theta \text{ in the interval } [\theta_L, \theta_U]) = p([\theta_L, \theta_U]) = \int_{\theta_L}^{\theta_U} p(\theta) d\theta$$

- Suppose $p([\theta_L, \theta_U]) = 0.95$. $= 1 - \alpha$.
  The interpretation is **we are nearly certain that θ is in $[\theta_L, \theta_U]$**.
- We can use this to define intervals that likely contain the true parameter

Credibility interval

- We define the cummulative density function cdf as

$$\mathrm{cdf}(\theta) = P([-\infty, \theta]) = \int_{-\infty}^{\theta} p(\theta')d\theta'$$

- The blue area is therefore $P(A) = \mathrm{cdf}(\theta)$
- We can define the inverse of the cdf

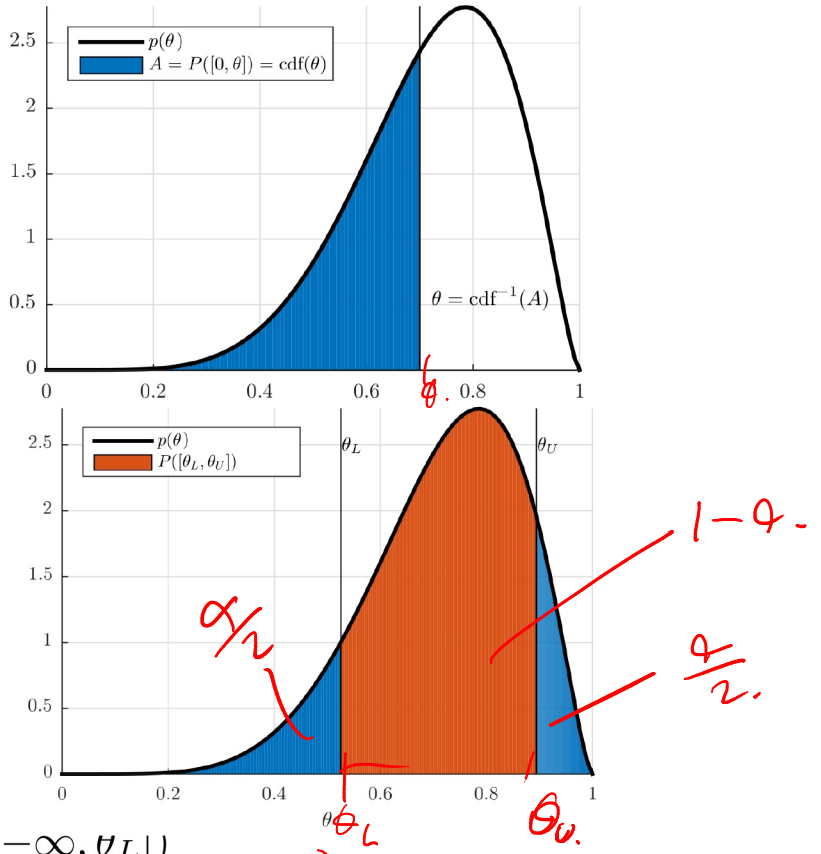
$$\theta = \mathrm{cdf}^{-1}(x), \quad x = p([-\infty, \theta])$$

- Therefore, the $1-\alpha$ candidate confidence interval

$$\theta_L = \mathrm{cdf}^{-1}\left(\frac{\alpha}{2}\right), \ \mathrm{cdf}^{-1}\left(1-\frac{\alpha}{2}\right)$$

In which case

$$\begin{aligned} P([\theta_L, \theta_U]) &= P([-\infty, \theta_U]) - P([-\infty, \theta_L]) \\ &= \mathrm{cdf}(\theta_U) - \mathrm{cdf}(\theta_L) \\ &= 1-\alpha \end{aligned}$$



Evaluating a single classifier

- If m is the number of accurate guesses, then

$$p(\theta|m,n) = \text{Beta}(\theta|a,b), \quad a = m + \frac{1}{2}, \text{ and } b = n - m + \frac{1}{2}.$$

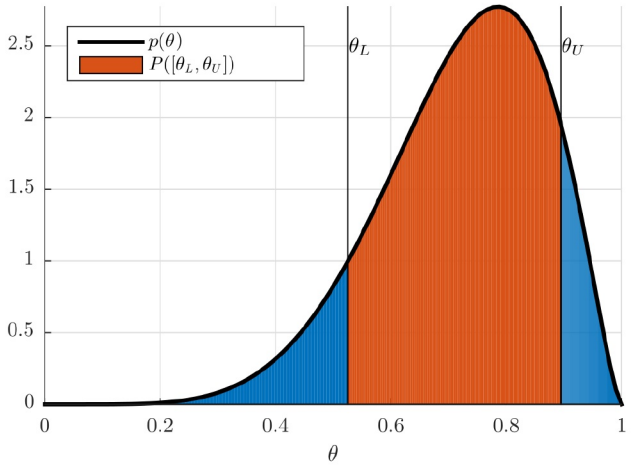
- The $1-\alpha$ confidence interval is given as $[\theta_L, \theta_U]$:

$$\theta_L = \text{cdf}_B^{-1}\left(\frac{\alpha}{2}|a,b\right) \text{ if } m > 0 \text{ otherwise } \theta_L = 0$$

$$\theta_U = \text{cdf}_B^{-1}\left(1-\frac{\alpha}{2}|a,b\right) \text{ if } m < n \text{ otherwise } \theta_U = 1$$

$$\hat{\theta} = \mathbb{E}[\theta] = \frac{a}{a+b}$$

$= \int_0^1 \theta \, \text{Bet}(\theta|a,b) =$



Comparing two classifiers

- Assume we have predictions from both classifiers:

$$\hat{\boldsymbol{y}}^A = \hat{y}_1^A, \ldots, \hat{y}_n^A, \quad \hat{\boldsymbol{y}}^B = \hat{y}_1^B, \ldots, \hat{y}_n^B.$$

- As before, we want to know if the classifiers are correct or not:

$$c_i^A = \begin{cases} 1 & \text{if } \hat{y}_i^A = y_i \\ 0 & \text{if otherwise.} \end{cases} \quad \text{and} \quad c_i^B = \begin{cases} 1 & \text{if } \hat{y}_i^B = y_i \\ 0 & \text{if otherwise.} \end{cases}$$

- The relevant information is the contingency table:

$$\begin{aligned} n_{11} &= \sum_{i=1}^{n} c_i^A c_i^B && = \{\text{Both classifiers are correct}\} \\ n_{12} &= \sum_{k=1}^{n} c_i^A (1 - c_i^B) && = \{A \text{ is correct, } B \text{ is wrong}\} \\ n_{21} &= \sum_{k=1}^{n} (1 - c_i^A) c_i^B && = \{A \text{ is wrong, } B \text{ is correct}\} \\ n_{22} &= \sum_{k=1}^{n} (1 - c_i^A)(1 - c_i^B) && = \{\text{Both classifiers are wrong}\} \end{aligned}$$

Comparing two classifiers: McNemars test

- We want to compare the accuracy difference:

$$\theta = \theta_A - \theta_B$$

- It is possible to show (approximately)

$$p(\theta|\boldsymbol{n}) = \frac{1}{2}\text{Beta}\left(\frac{\theta+1}{2}\,\middle|\,\alpha = p, \beta = q\right)$$

$$\theta_L = 2\text{cdf}_B^{-1}\left(\frac{\alpha}{2}\,\middle|\,\alpha = p, \beta = q\right) - 1$$

$$\theta_U = 2\text{cdf}_B^{-1}\left(1 - \frac{\alpha}{2}\,\middle|\,\alpha = p, \beta = q\right) - 1$$

- For a p-value, note that A is better than B if $n_{12} > n_{21}$
- Chance of a particular value n_{12} given H_0 is $p_{\text{binom}}(n_{12}|\theta = \frac{1}{2}, N = n_{12} + n_{21})$
- The probability of obtaining as extreme value as the one observed is:

$$\begin{aligned} p &= P(N_{12} \leq m) + P(N_{21} \geq N - m) \\ &= 2\text{cdf}_{\text{binom}}\left(m = \min\{n_{12}, n_{21}\}\,\middle|\,\theta = \frac{1}{2}, N = n_{12} + n_{21}\right) \end{aligned}$$

Confidence interval for a regression model

- Use cross-validation to obtain predictions $\hat{y}_i$ and true values y_i. Select loss

$$z_i = |\hat{y}_i - y_i| \quad \text{or} \quad z_i = (\hat{y}_i - y_i)^2 \tag{10}$$

- Estimated error is: $\hat{z} = \frac{1}{n}\sum_{i=1}^{n} z_i$.
- Assume each error is normally distributed (**warning!**)

$$p(D|u, \sigma^2) = \prod_{i=1}^{n} \mathcal{N}(z_i|u, \sigma^2)$$

- It is possible to show u follows a generalized Student's t-distribution:

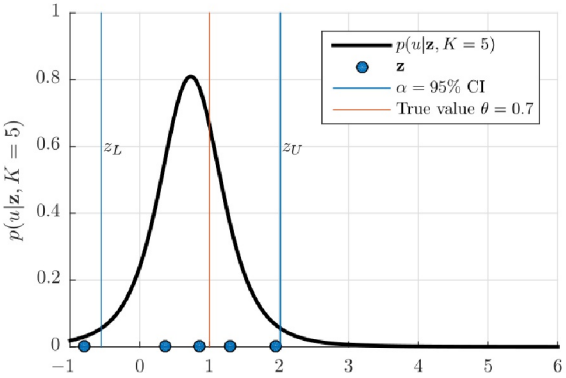
$$p(u|D) = p_{\mathcal{T}}(u|\nu = n-1, \mu = \hat{z}, \sigma = \tilde{\sigma})$$

with parameters $\hat{z} = \frac{1}{n}\sum_{i=1}^{n} z_i$ and $\tilde{\sigma} = \sqrt{\sum_{i=1}^{n} \frac{(z_i - \hat{z})^2}{n(n-1)}}$.

- The Student's t-distribution has density

$$\textit{Student } t\textit{-distribution} \quad p_{\mathcal{T}}(x|\nu, \mu, \sigma) = \frac{\Gamma\left(\frac{\nu+1}{2}\right)}{\Gamma\left(\frac{\nu}{2}\right)\sqrt{\pi\nu\sigma^2}} \left(1 + \frac{1}{\nu}\left[\frac{x-\mu}{\sigma}\right]^2\right)^{-\frac{\nu+1}{2}}.$$

Confidence interval for a regression model



- Step back: Assuming $z_i = L(y_i, \hat{y}_i)$ and

$$z_i \sim \mathcal{N}(z_i|\mu = u, \sigma^2)$$

- In this case u is the average error rate. Since we have shown:

$$p(u|D) = p_{\mathcal{T}}(u|\nu = n-1, \mu = \hat{z}, \sigma = \tilde{\sigma})$$

- An approximate $1-\alpha$ confidence interval is:

$$z_L = \mathrm{cdf}_{\mathcal{T}}^{-1}\left(\frac{\alpha}{2} \,\middle|\, \nu, \hat{z}, \tilde{\sigma}\right), \; z_U = \mathrm{cdf}_{\mathcal{T}}^{-1}\left(1-\frac{\alpha}{2} \,\middle|\, \nu, \hat{z}, \tilde{\sigma}\right). \tag{11}$$

Comparing two regression models

- Use cross-validation to obtain (paired) predictions along with true values y_i

$$\hat{y}_1^A, \ldots, \hat{y}_n^A, \quad \text{and} \quad \hat{y}_1^B, \ldots, \hat{y}_n^B. \tag{12}$$

- Select a loss-function to compute the per-observation losses as in

$$z_1^A, \ldots, z_n^A, \quad \text{and} \quad z_1^B, \ldots, z_n^B.$$

- Note that $z_i^A = |y_i - \hat{y}_i^A|$

$$z = E_{A,\mathcal{D}}^{\text{gen}} - E_{B,\mathcal{D}}^{\text{gen}} \approx \hat{z} = \left(\frac{1}{n}\sum_{i=1}^{n} z_i^A\right) - \left(\frac{1}{n}\sum_{i=1}^{n} z_i^B\right)$$

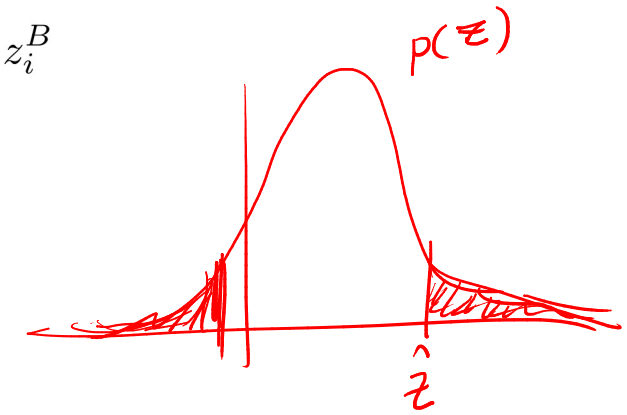
$$= \frac{1}{n}\sum_{i=1}^{n} z_i, \quad \text{where } z_i = z_i^A - z_i^B$$

Compute a $1-\alpha$ CI using methods on previous slide

Comparing two regression models: p-values

- Still using

$$z = E_A^{\text{gen}} - E_B^{\text{gen}} \approx \hat{z} = \frac{1}{n}\sum_{i=1}^{n} z_i, \qquad \text{where } z_i = z_i^A - z_i^B$$



- Assuming

$$z_i \sim \mathcal{N}(z_i|\mu = u, \sigma^2)$$

- where u is the true difference in error function we have shown:

$$p(u|D) = p_{\mathcal{T}}(u|\nu = n-1, \mu = \hat{z}, \sigma = \tilde{\sigma})$$

- Therefore, we can test the hypothesis

$$H_0 : \text{Model } \mathcal{M}_A \text{ and } \mathcal{M}_B \text{ have the same performance, } u = 0 \qquad (13)$$

$$H_1 : \text{Model } \mathcal{M}_A \text{ and } \mathcal{M}_B \text{ have different performance, } u \neq 0. \qquad (14)$$

- A p-value can be computed as

$$p = P\left(|Z| \geq |\hat{z}| \mid H_0\right) = 2\int_{-\infty}^{-|\hat{z}|} p_{\mathcal{T}}\left(z \mid \nu = n-1, \mu = 0, \sigma = \tilde{\sigma}\right) dz$$

$$= 2\text{cdf}_{\mathcal{T}}\left(-|\hat{z}| \mid \nu = n-1, \mu = 0, \sigma = \tilde{\sigma}\right). \qquad (15)$$

Example: Real datasets

Classification data: Presence of breast cancer and Forrest cover type

	N	M	Classes
Fisher Iris	150.0	4.0	3.0
Breast Cancer	569.0	30.0	2.0
Covertype	1000.0	54.0	7.0

Regression data: Price of houses

	N	M
Boston	506.0	13.0
Diabetes	442.0	10.0
California Housing	1000.0	8.0

Setup: Use 2-layer CV to tune parameters and $K_1 = 10$ outer folds to obtain predictions $\hat{y}$. Splits are re-used across methods.

Performance evaluation

Using Jeffreys interval and the t-test to obtain confidence intervals.

	Fisher Iris	Breast Cancer	Covertype
Decision Tree	0.950 (0.911 to 0.979)	0.920 (0.897 to 0.941)	0.669 (0.660 to 0.679)
Logistic Regression	nan	0.955 (0.937 to 0.971)	nan
KNN	0.937 (0.893 to 0.970)	0.966 (0.949 to 0.979)	0.744 (0.735 to 0.752)
Baseline	0.334 (0.262 to 0.411)	0.627 (0.587 to 0.666)	0.489 (0.479 to 0.498)

	Boston	Diabetes	California Housing
Decision Tree	0.399 (0.363 to 0.436)	0.858 (0.795 to 0.921)	0.565 (0.556 to 0.575)
Linear Regression	0.368 (0.335 to 0.400)	0.578 (0.538 to 0.617)	0.460 (0.452 to 0.469)
KNN	0.313 (0.279 to 0.347)	0.755 (0.693 to 0.817)	0.483 (0.472 to 0.493)
Baseline	0.725 (0.665 to 0.785)	0.857 (0.808 to 0.905)	0.790 (0.778 to 0.802)

Pairwise evaluation (McNemera)

Fisher Iris $M_A - M_B$	M_B: Decision Tree	M_B: Logistic Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		nan	0.013 (−0.009 to 0.036)	**0.620 (0.564 to 0.673)**
M_A: Logistic Regression	nan	nan	nan	nan
M_A: KNN	−0.013 (−0.036 to 0.009)	nan		**0.607 (0.549 to 0.662)**
M_A: Baseline	**−0.620 (−0.673 to −0.564)**	nan	**−0.607 (−0.662 to −0.549)**	

Breast Cancer $M_A - M_B$	M_B: Decision Tree	M_B: Logistic Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		**−0.035 (−0.054 to −0.017)**	**−0.046 (−0.060 to −0.032)**	**0.293 (0.263 to 0.324)**
M_A: Logistic Regression	**0.035 (0.017 to 0.054)**		−0.011 (−0.024 to 0.003)	**0.329 (0.298 to 0.359)**
M_A: KNN	**0.046 (0.032 to 0.060)**	0.011 (−0.003 to 0.024)		**0.339 (0.311 to 0.367)**
M_A: Baseline	**−0.293 (−0.324 to −0.263)**	**−0.329 (−0.359 to −0.298)**	**−0.339 (−0.367 to −0.311)**	

Covertype $M_A - M_B$	M_B: Decision Tree	M_B: Logistic Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		nan	**−0.074 (−0.082 to −0.067)**	**0.181 (0.172 to 0.190)**
M_A: Logistic Regression	**0.035 (0.017 to 0.054)**		−0.011 (−0.024 to 0.003)	**0.329 (0.298 to 0.359)**
M_A: KNN	**0.074 (0.067 to 0.082)**	nan		**0.255 (0.247 to 0.263)**
M_A: Baseline	**−0.181 (−0.190 to −0.172)**	nan	**−0.255 (−0.263 to −0.247)**	

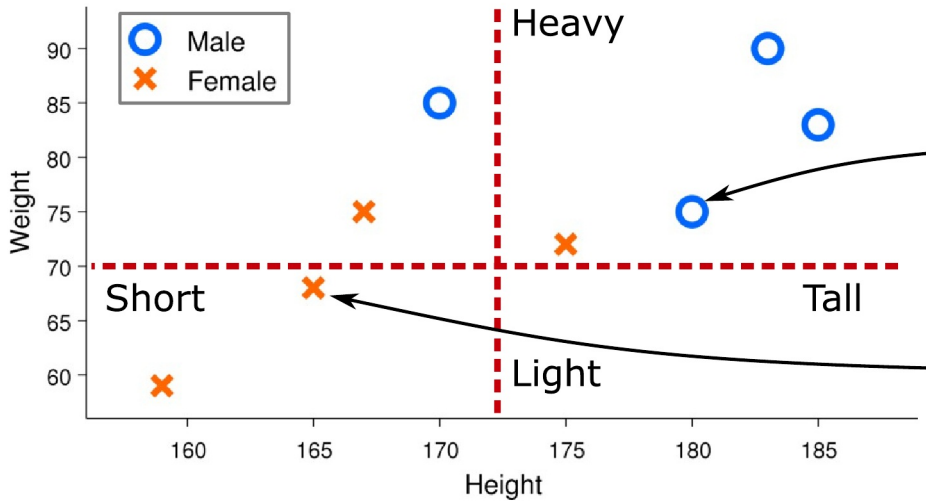
Pairwise evaluation (t-test)

Boston $M_A - M_B$	M_B: Decision Tree	M_B: Linear Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		**0.032 (−0.006 to 0.070)**	**0.086 (0.049 to 0.124)**	**−0.326 (−0.386 to −0.266)**
M_A: Linear Regression	**−0.032 (−0.070 to 0.006)**		**0.054 (0.023 to 0.086)**	**−0.358 (−0.411 to −0.304)**
M_A: KNN	**−0.086 (−0.124 to −0.049)**	**−0.054 (−0.086 to −0.023)**		**−0.412 (−0.471 to −0.353)**
M_A: Baseline	**0.326 (0.266 to 0.386)**	**0.358 (0.304 to 0.411)**	**0.412 (0.353 to 0.471)**	

Diabetes $M_A - M_B$	M_B: Decision Tree	M_B: Linear Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		**0.281 (0.224 to 0.337)**	**0.103 (0.033 to 0.174)**	0.002 (−0.075 to 0.078)
M_A: Linear Regression	**−0.281 (−0.337 to −0.224)**		**−0.177 (−0.235 to −0.119)**	**−0.279 (−0.331 to −0.227)**
M_A: KNN	**−0.103 (−0.174 to −0.033)**	**0.177 (0.119 to 0.235)**		**−0.102 (−0.176 to −0.027)**
M_A: Baseline	−0.002 (−0.078 to 0.075)	**0.279 (0.227 to 0.331)**	**0.102 (0.027 to 0.176)**	

California Housing $M_A - M_B$	M_B: Decision Tree	M_B: Linear Regression	M_B: KNN	M_B: Baseline
M_A: Decision Tree		**0.105 (0.099 to 0.112)**	**0.083 (0.072 to 0.094)**	**−0.224 (−0.235 to −0.214)**
M_A: Linear Regression	**−0.105 (−0.112 to −0.099)**		**−0.022 (−0.033 to −0.012)**	**−0.330 (−0.340 to −0.319)**
M_A: KNN	**−0.083 (−0.094 to −0.072)**	**0.022 (0.012 to 0.033)**		**−0.307 (−0.322 to −0.293)**
M_A: Baseline	**0.224 (0.214 to 0.235)**	**0.330 (0.319 to 0.340)**	**0.307 (0.293 to 0.322)**	

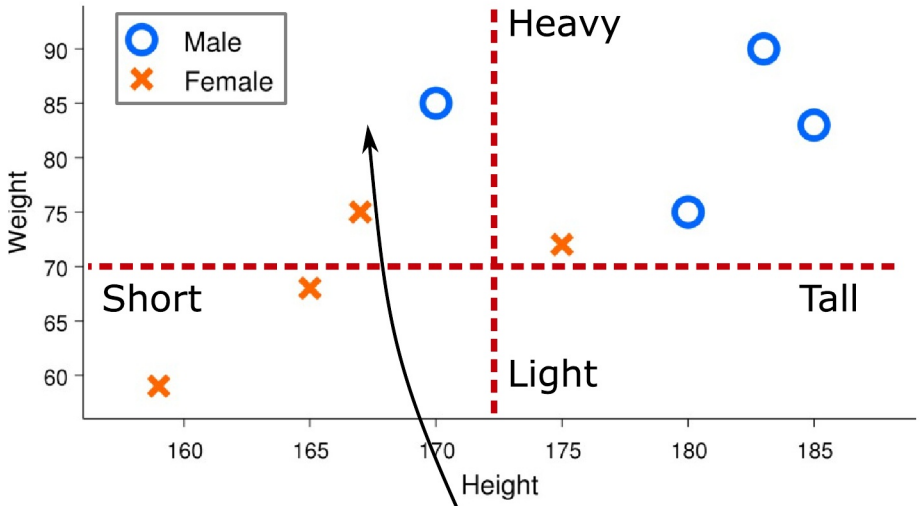
Bayes and Naive-Bayes



Gender y	Tall x_1	Heavy x_2
0	1	1
0	1	1
0	1	1
0	0	1
1	1	1
1	0	1
1	0	0
1	0	0

$$p(y|x_1, x_2) = \frac{p(x_1, x_2|y)p(y)}{\sum_{k=0}^{1} p(x_1, x_2|y = k)p(y = k)}$$

Example 1: Normal Bayes



Gender y	Tall x_1	Heavy x_2
0	1	1
0	1	1
0	1	1
0	0	1
1	1	1
1	0	1
1	0	0
1	0	0

Probability a short, heavy person is male:

$$P(y=0|x_1=0,x_2=1) = \frac{p(x_1=0,x_2=1|y=0)p(y=0)}{\sum_{k=0}^{1} p(x_1=0,x_2=1|y=k)p(y=k)}$$

Example 1: Solution

Probability a short, heavy person is male:

$$P(y=0|x_1=0,x_2=1) = \frac{p(x_1=0,x_2=1|y=0)p(y=0)}{\sum_{k=0}^{1} p(x_1=0,x_2=1|y=k)p(y=k)}$$
$$= \frac{\frac{1}{4}\frac{4}{8}}{\frac{1}{4}\frac{4}{8}+\frac{1}{4}\frac{4}{8}} = \frac{1}{2}$$

A practical problem with Bayesian classifier

- In general:

$$p(y|x_1, x_2, \ldots, x_M) = \frac{p(x_1, x_2, \ldots, x_M|y)p(y)}{\sum_{k=0}^{K-1} p(x_1, x_2, \ldots, x_M|y=k)p(y=k)}$$

$$p(x_1, \ldots, x_M|y=k) = \frac{\text{Nr. obs where } y=k \text{ and we measure } x_1, \ldots, x_M}{\text{Observations where } y=k}$$

A practical problem with Bayesian classifier

- In general:

$$p(y|x_1, x_2, \ldots, x_M) = \frac{p(x_1, x_2, \ldots, x_M|y)p(y)}{\sum_{k=0}^{K-1} p(x_1, x_2, \ldots, x_M|y = k)p(y = k)}$$

$$p(x_1, \ldots, x_M|y = k) = \frac{\text{Nr. obs where } y = k \text{ and we measure } x_1, \ldots, x_M}{\text{Observations where } y = k}$$

- Naive Bayes assumption

assume!

$$p(x_1, x_2, \ldots, x_M|y) = p(x_1|y)p(x_2|y) \times \cdots \times p(x_M|y)$$

$p(x_1, x_1|y) = p(x_1|y)^2$
$= p(x_1|y)$

A practical problem with Bayesian classifier

- In general:

$$p(y|x_1, x_2, \ldots, x_M) = \frac{p(x_1, x_2, \ldots, x_M|y)p(y)}{\sum_{k=0}^{K-1} p(x_1, x_2, \ldots, x_M|y = k)p(y = k)}$$

$$p(x_1, \ldots, x_M|y = k) = \frac{\text{Nr. obs where } y = k \text{ and we measure } x_1, \ldots, x_M}{\text{Observations where } y = k}$$

- Naive Bayes assumption

$$p(x_1, x_2, \ldots, x_M|y) = p(x_1|y)p(x_2|y) \times \cdots \times p(x_M|y)$$

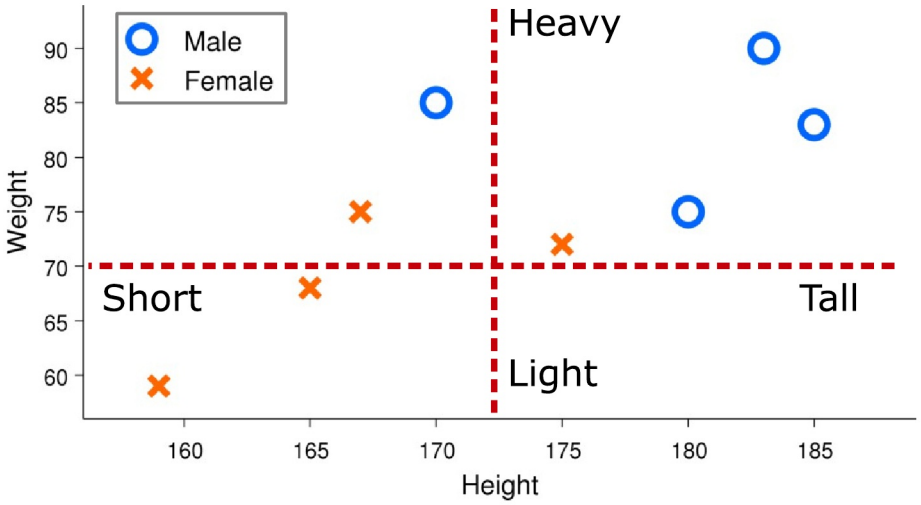
- Naive Bayes classifier

$$\begin{aligned} p(y|x_1, x_2, \ldots, x_M) &= \frac{p(x_1, x_2, \ldots, x_M|y)p(y)}{\sum_{k=0}^{1} p(x_1, x_2, \ldots, x_M|y = k)p(y = k)} \\ &= \frac{p(x_1|y)p(x_2|y) \times \cdots \times p(x_M|y)p(y)}{\sum_{k=0}^{1} p(x_1|y = k)p(x_2|y = k) \times \cdots \times p(x_M|y = k)p(y = k)} \end{aligned}$$

Example 2:

- Naive Bayes classifier (Probability someone is a female given they are heavy and tall)

$$p(y=1|x_1=1,x_2=1)=\frac{p(x_1|y)p(x_2|y)p(y)}{\sum_{k=0}^{1}p(x_1|y=k)p(x_2|y=k)p(y=k)}$$



Gender y	Tall x_1	Heavy x_2
0	1	1
0	1	1
0	1	1
0	0	1
1	1	1
1	0	1
1	0	0
1	0	0

Example 2: Solution

- Naive Bayes classifier (Probability someone is a female given they are heavy and tall)

$$p(y=1|x_1=1,x_2=1) = \frac{p(x_1|y)p(x_2|y)p(y)}{\sum_{k=0}^{1} p(x_1|y=k)p(x_2|y=k)p(y=k)}$$
$$= \frac{\frac{1}{4}\frac{2}{4}\frac{1}{2}}{\frac{1}{4}\frac{2}{4}\frac{1}{2} + \frac{3}{4}\frac{4}{4}\frac{1}{2}} = \frac{2}{2+12} = \frac{1}{7}$$

Quiz 1, Naive-Bayes (Spring 2012)

	S1	S2	S3	S4	S5	S6	S7	S8	S9	S10
P1	1	0	0	0	1	1	0	0	1	1
P2	1	0	1	0	0	1	1	1	0	0
P3	0	1	0	1	0	1	0	1	1	1
P4	0	1	1	1	0	0	1	0	0	0
P5	1	0	0	1	1	0	0	1	0	1
P6	1	0	1	1	1	1	1	0	1	0

Table 1: Table indicating whether 10 songs denoted S1–S10 are downloaded to 6 different phones denoted P1–P6. P1 and P2 given in red are phones that belong to females whereas P3, P4, P5, and P6 given in blue belong to males.

The phones P1 and P2 are owned by females whereas P3, P4, P5 and P6 are owned by males (this is indicated in red and blue respectively in Table 1). We would like to predict whether a phone is owned by a male based on whether or not the songs S1, S2 and S3 have been downloaded. We will therefore classify whether the phone belongs to a male or female considering only the attributes S1, S2 and S3 and the data in Table 1. We will apply a Naïve Bayes classifier that assumes independence between these attributes. Given that a phone has installed songs 1, 2 and 3 (i.e., S1=1, S2=1 and S3=1) What is the probability that the phone is owned by a male according to the Naïve Bayes classifier?

A. 1/12

B. 1/6

C. 2/3

D. 1

E. Don't know.

$$p(y|x_1, x_2, \ldots, x_M) = \frac{p(x_1|y) \times \cdots \times p(x_M|y)p(y)}{\sum_{k=0}^{1} p(x_1|y=k) \times \cdots \times p(x_M|y=k)p(y=k)}$$

According to the Naïve Bayes classifier we have

$$P(Male|S1=1,S2=1,S3=1) =$$

$$\frac{\begin{pmatrix} P(S1=1|Male)\times \\ P(S2=1|Male)\times \\ P(S3=1|Male)\times \\ P(Male) \end{pmatrix}}{\begin{pmatrix} P(S1=1|Female)\times \\ P(S2=1|Female)\times \\ P(S3=1|Female)\times \\ P(Female) \end{pmatrix} + \begin{pmatrix} P(S1=1|Male)\times \\ P(S2=1|Male)\times \\ P(S3=1|Male)\times \\ P(Male) \end{pmatrix}}$$

$$= \frac{2/4 \cdot 2/4 \cdot 2/4 \cdot 4/6}{2/2 \cdot 0/2 \cdot 1/2 \cdot 2/6 + 2/4 \cdot 2/4 \cdot 2/4 \cdot 4/6} = 1.$$

robust estimation and non-binary data

Assume

$$p(x_1, \ldots, x_M|y) = \prod_{k=1}^{M} p(x_k|y)$$

Defining $n_k = \sum_{i=1}^{N} \delta_{X_{ij},k}\delta_{y,c}$ we have more generally:

Binary case: $$p(x_j = 1|y = c) = \frac{n_1 + \alpha}{N_c + 2\alpha}.$$

Categorical case: $$p(x_j = k|y = c) = \frac{n_k + \alpha}{N_c + K\alpha}.$$

Continious case: $$p(x_j = x|y = c) = \mathcal{N}(x|\mu = \mu_c, \sigma^2 = (\sigma_c + \alpha)^2)$$

$$\mu_c = \mathbb{E}_{y=c}[x_j] = \frac{1}{N_c}\sum_{i=1}^{N} \delta_{y,c} X_{ij},$$

$$\sigma_c = \hat{\text{std}}_{y=c}[x_j] = \sqrt{\frac{1}{N_c - 1}\sum_{i=1}^{N} \delta_{y,c}(X_{ij} - \mu_c)^2}$$

Select these parameters using cross-validation.

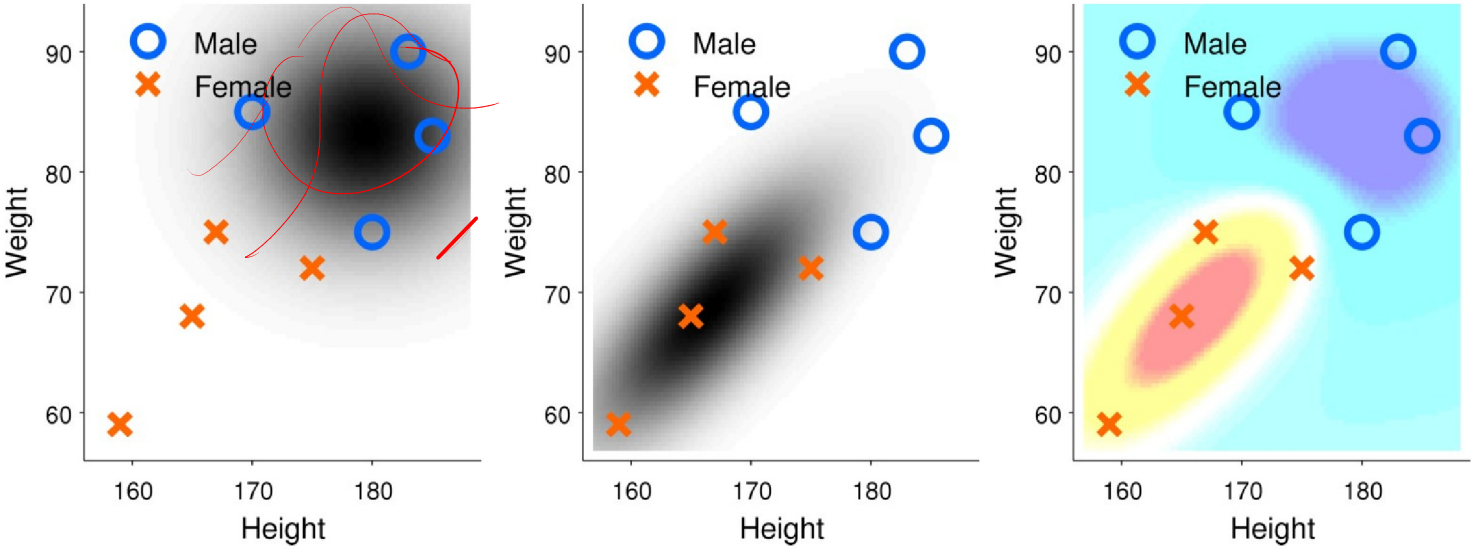
Bayesian classification by the multivariate normal distribution

Continuous density estimation

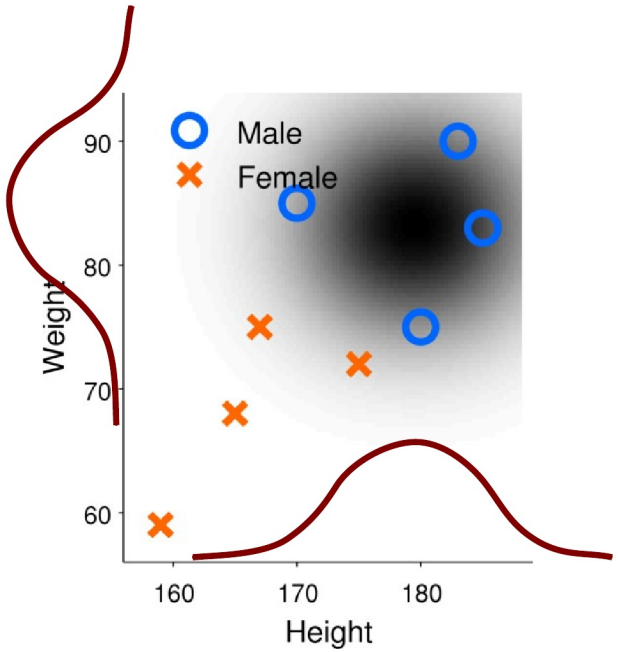
- Fit a Normal distribution to each class
  - Compute class mean and covariance
- Classify using Bayes rule as before

$$P(\boldsymbol{x}|y=c) = \frac{1}{(2\pi)^{M/2} det(\boldsymbol{\Sigma}_c)^{\frac{1}{2}}} \exp\left(-\frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_c)^\top \boldsymbol{\Sigma}_c^{-1}(\boldsymbol{x}-\boldsymbol{\mu}_c) \right)$$

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



- What does the Naive Bayes assumption of independence of the attributes correspond to in terms of the parameters of the multivariate normal distribution?



Midterm practice test

Look at the test on campusnet (under assignments). Note the test is not part of your evaluation.

Resources

https://www.youtube.com Video explaining Naive Bayes

(https://www.youtube.com/watch?v=8yvBqhm92xA)

https://machinelearningmastery.com Statistical comparison of the cross-validation estimate of the generalization error is not a solved problem. This reference provides an overview of various issues and proposed solutions. Note no simple solution exists.

(https://machinelearningmastery.com/

statistical-significance-tests-for-comparing-machine-learning-algorithms/)