# Chapter ML:VII (continued)

#### VII. Bayesian Learning

- □ Approaches to Probability
- □ Conditional Probability
- Bayes Classifier
- □ Exploitation of Data
- □ Frequentist versus Subjectivist

ML:VII-96 Bayesian Learning ©STEIN/VÖLSKE 2022

#### **Data Events**

#### Data from a "predictor-response" setting:

```
D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\} (regression) D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\} (classification)
```

- D is the result of n <u>i.i.d.</u> trials. I.e., n objects are sampled independently and from the same probability distribution. All objects are characterized by a "response" variable that is either quantitative (a number y) or categorical (a class label c), and by p "predictors" (a feature vector  $\mathbf{x}$ ).
- $p(\mathbf{x}_i, c_i), p(\mathbf{x}_i, c_i) := P(\mathbf{X}_i = \mathbf{x}_i, \mathbf{C}_i = c_i)$ , is the probability of the joint event  $\{\mathbf{X}_i = \mathbf{x}_i, \mathbf{C}_i = c_i\}$ , i.e., (1) to get the vector  $\mathbf{x}_i$ , and, (2) that the respective object belongs to class  $c_i$ . The  $p(\mathbf{x}_i, y_i)$  are defined analogously.
- The  $Y_i$ ,  $C_i$ , and  $\mathbf{X}_i$  are i.i.d. (multivariate) random variables. Typically, the  $Y_i$  are of continuous type, the  $C_i$  of discrete type, and the variables of the random vector  $\mathbf{X}_i$ ,  $\mathbf{X}_i := (X_{1,i}, \dots, X_{n,i})^T$ , of continuous type.

ML:VII-97 Bayesian Learning © STEIN/VÖLSKE 2022

#### **Data Events**

#### Data from a "predictor-response" setting:

```
D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\} (regression) D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\} (classification)
```

- $\square$  *D* is the result of n <u>i.i.d.</u> trials. I.e., n objects are sampled independently and from the same probability distribution. All objects are characterized by a "response" variable that is either quantitative (a number y) or categorical (a class label c), and by p "predictors" (a feature vector  $\mathbf{x}$ ).
- $p(\mathbf{x}_i, c_i), p(\mathbf{x}_i, c_i) := P(\mathbf{X}_i = \mathbf{x}_i, C_i = c_i)$ , is the probability of the joint event  $\{\mathbf{X}_i = \mathbf{x}_i, C_i = c_i\}$ , i.e., (1) to get the vector  $\mathbf{x}_i$ , and, (2) that the respective object belongs to class  $c_i$ . The  $p(\mathbf{x}_i, y_i)$  are defined analogously.
- The  $Y_i$ ,  $C_i$ , and  $\mathbf{X}_i$  are i.i.d. (multivariate) <u>random variables</u>. Typically, the  $Y_i$  are of continuous type, the  $C_i$  of discrete type, and the variables of the random vector  $\mathbf{X}_i$ ,  $\mathbf{X}_i := (X_{1,i}, \dots, X_{p,i})^T$ , of continuous type.

ML:VII-98 Bayesian Learning © STEIN/VÖLSKE 2022

Data Events (continued)

#### Data from an "outcome-only" setting:

- $D = \{y_1, \dots, y_n\}$  (quantitative)  $D = \{c_1, \dots, c_n\}$  (categorical)
  - $extbf{ iny } D$  is the result of n <u>i.i.d.</u> trials. I.e., n outcomes are sampled independently and from the same probability distribution. All outcomes are characterized by either a number y or a class label c.
  - $p(y_i), p(y_i) := P(Y_i = y_i),$  is the probability of the event  $Y_i = y_i$ .  $p(c_i), p(c_i) := P(C_i = c_i),$  is the probability of the event  $C_i = c_i$ .
  - □ The  $Y_i$ , and  $C_i$  are i.i.d. random variables. Typically, the  $Y_i$  are of continuous type and the  $C_i$  of discrete type.

ML:VII-99 Bayesian Learning © STEIN/VÖLSKE 2022

Data Events (continued)

#### Data from an "outcome-only" setting:

```
D = \{y_1, \dots, y_n\} (quantitative) D = \{c_1, \dots, c_n\} (categorical)
```

- $\square$  *D* is the result of n <u>i.i.d.</u> trials. I.e., n outcomes are sampled independently and from the same probability distribution. All outcomes are characterized by either a number y or a class label c.
- $p(y_i), p(y_i) := P(Y_i = y_i),$  is the probability of the event  $Y_i = y_i$ .  $p(c_i), p(c_i) := P(C_i = c_i),$  is the probability of the event  $C_i = c_i$ .
- $\Box$  The  $Y_i$ , and  $C_i$  are i.i.d. <u>random variables</u>. Typically, the  $Y_i$  are of continuous type and the  $C_i$  of discrete type.

ML:VII-100 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks:

- $\Box$  The following remarks on the predictor-response setting are detailed for a categorical response variable c; they apply to a quantitative response variable y as well.
- $\Box$  By experiment design, the n joint events,  $\{\mathbf{X}_1 = \mathbf{x}_1, C_1 = c_1\}, \ldots, \{\mathbf{X}_n = \mathbf{x}_n, C_n = c_n\}$ , generating the data D are mutually independent:

$$p(D) = p\left(\{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}\right) = \prod_{i=1,\dots,n} p(\mathbf{x}_i, c_i)$$

$$\stackrel{(1)}{=} \prod_{i=1,\dots,n} \left(p(c_i \mid \mathbf{x}_i) \cdot p(\mathbf{x}_i)\right)$$

$$= \prod_{i=1,\dots,n} p(\mathbf{x}_i) \cdot \prod_{i=1,\dots,n} p(c_i \mid \mathbf{x}_i)$$

(1) Usually *not* independent are any two events  $\mathbf{X}_i = \mathbf{x}_i$  and  $C_i = c_i$ , i = 1, ..., n:  $p(\mathbf{x}_i, c_i) \neq p(\mathbf{x}_i) \cdot p(c_i)$ 

For maximizing p(D), see the maximum likelihood derivation of the logistic loss  $L_{\sigma}(\mathbf{w})$ .

- By experiment design, the probabilities,  $p(\mathbf{x}_i)$ , i = 1, ..., n, are independent, i.e., the probability of the joint event  $\{\mathbf{X}_1 = \mathbf{x}_1, ..., \mathbf{X}_n = \mathbf{x}_n\}$  is equal to the product of the singleton events:  $p(\mathbf{x}_1, ..., \mathbf{x}_n) = \prod_{i=1,...,n} p(\mathbf{x}_i)$ .
  - A consistent and unbiased estimate for  $p(\mathbf{x})$  is  $\hat{p}(\mathbf{x}) = |\{(\mathbf{x}, \cdot) \in D\}| \cdot \frac{1}{|D|}$ .
- By experiment design, the conditional probabilities,  $p(c_i | \mathbf{x}_i)$ , i = 1, ..., n, are *invariant under covariate shift*, i.e., invariant under a change of  $p(\mathbf{x}_i)$ . That is, the classification procedure, "determination of  $c_i$  given some  $\mathbf{x}_i$ ", always runs the same way, regardless of how often  $\mathbf{x}_i$  is encountered.

ML:VII-101 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks: (continued)

The invariance of  $p(c_i \mid \mathbf{x}_i)$  under a covariate shift can also be understood as the fact that any two events  $\mathbf{X}_i = \mathbf{x}_i$  and  $(C_i = c_i \mid \mathbf{X}_i = \mathbf{x}_i)$ , i = 1, ..., n are independent:

"
$$p(\mathbf{x}, (c \mid \mathbf{x}))$$
" =  $p(\mathbf{x}) \cdot p(c \mid \mathbf{x}) = p(\mathbf{x}, c)$ 

However, this interpretation is problematic since standard probability theory does not allow a conditional event being combined with other events. See section Probability Basics of this part, conditional event algebra, and Lewis's triviality result for details.

- Within an outcome-only setting such as "flipping a coin", the object features (coin diameter, coin age, etc.) are not used as predictors. I.e., one does not model the relationship between a response variable and predictors  $\mathbf{x}$  but models (the probability of) a sequence of outcomes  $D = \{y_1, \dots, y_n\}$  or  $D = \{c_1, \dots, c_n\}$ .
- ☐ The type of setting, be it predictor-response or outcome-only, is independent of data exploitation aspects such as
  - discriminative versus generative,
  - non-probabilistic versus probabilistic,
  - maximum likelihood versus Bayes, or
  - frequentist versus subjectivist.

ML:VII-102 Bayesian Learning © STEIN/VÖLSKE 2022

# Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$ 

(1) RSS(w): 
$$\sum_{(\mathbf{x},y)\in D} (y)$$

$$(y - \mathbf{w}^T \mathbf{x})^T$$

$$\mathbf{I}_{n(c \mid \mathbf{x} \cdot \mathbf{w})}$$

$$(c) \cdot p(c)$$







$$D = \{a, a\}$$

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

$$D = \{c_1, \dots, c_n\}$$

$$D = \{c_1, \dots, c_n\}$$

$$\binom{n}{\cdot \theta^k \cdot (1-\theta)^n}$$

$$\binom{n}{k} \cdot \theta^k \cdot (1 - \theta)$$

$$\binom{k}{k} \cdot 0 \cdot (1 = 0)$$

 $D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$ 

### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

$$(\mathbf{R}^T\mathbf{x})^2$$
 RSS for  $D$  u

(1) 
$$BSS(\mathbf{w})$$
  $\sum (\mathbf{u} - \mathbf{w}^T \mathbf{x})^2$  RSS for  $D$   $\mathbf{u}$ 

RSS for 
$$D$$
 under a linear model, parameterized by  $\mathbf{w}$ .

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$  us Least square

$$\mathbf{w}^T\mathbf{x})^2$$
 RSS for  $D$  u

$$(y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$  u

ASS for 
$$D$$
 under each course.

HSS for 
$$D$$
 unde  
Least squares  $f e$ 

RSS for 
$$D$$
 under east squares as

RSS for 
$$D$$
 und  
east squares

Least squares estimate: 
$$\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \mathsf{RSS}(\mathbf{w})$$

bability of 
$$D$$
 und

$$v$$
 w. Maximum likelihood esti

$$v_{\mathsf{ML}} =$$

$$_{ extsf{ iny L}} = \operatorname{argmax}_{\mathrm{w} \in \mathrm{R}}$$

© STEIN/VÖLSKE 2022 ML:VII-104 Bayesian Learning

### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$ 

RSS for D under a linear model, parameterized by  $\mathbf{w}$ . Least squares estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \operatorname{RSS}(\mathbf{w})$ 

(2) 
$$p(D; \mathbf{w})$$
: 
$$\prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$

Probability of D under a logistic model, parameterized by  $\mathbf{w}$ . Maximum likelihood estimate:  $\mathbf{w}_{\mathsf{ML}} = \mathsf{argmax}_{\mathbf{w} \in \mathbf{R}^{p+1}} \, p(D; \mathbf{w})$ 

(3) 
$$L(\mathbf{w})$$
: 
$$\sum l_{\sigma}(c, \sigma(\mathbf{w}^T \mathbf{x}))$$

loss for D under a logistic model, parameterized by  $\mathbf{w}$ . Minimum loss (= maximum likelihood) estimate:  $\mathbf{w} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} L(\mathbf{w})$ 

$$\frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$

Probability of c given  $\mathbf x$  via Bayes's rule. Maximum a posteriori class for  $\mathbf x$ :  $c_{\mathsf{MAP}} = \mathsf{argmax}_{c \in \{\oplus, \ominus\}} \, p(c \mid \mathbf x)$ 

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

$$p(D;\theta)$$
: Probability of  $D$  under the parameterized by  $\theta$ . Maximum

parameterized by  $\theta$ . Maximum likelihood estimate:  $\theta_{\rm ML} = \operatorname{argmax}_{\theta \in [0;1]} p(D;\theta)$ 

(6) 
$$p(\theta \mid D)$$
: 
$$\frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$$

Probability of  $\theta$  given D via Bayes's rule. Maximum a posteriori hypothesis:  $\theta_{\mathsf{MAP}} = \mathsf{argmax}_{\theta \in \{\theta_1, \theta_2\}} \, p(\theta \mid D)$ 

### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$ 

RSS for D under a linear model, parameterized by  $\mathbf{w}$ . Least squares estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \operatorname{RSS}(\mathbf{w})$ 

(2) 
$$p(D; \mathbf{w})$$
: 
$$\prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$

Probability of D under a logistic model, parameterized by  $\mathbf{w}$ . Maximum likelihood estimate:  $\mathbf{w}_{\mathsf{ML}} = \mathsf{argmax}_{\mathbf{w} \in \mathbf{R}^{p+1}} \, p(D; \mathbf{w})$ 

(3) 
$$L(\mathbf{w})$$
: 
$$\sum_{(\mathbf{x}.c) \in D} l_{\sigma}(c, \sigma(\mathbf{w}^T \mathbf{x}))$$

Loss for D under a logistic model, parameterized by  $\mathbf{w}$ . Minimum loss (= maximum likelihood) estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} L(\mathbf{w})$ 

(4) 
$$p(c \mid \mathbf{x})$$
: 
$$\frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$

Probability of c given  $\mathbf x$  via Bayes's rule. Maximum a posteriori class for  $\mathbf x$ :  $c_{\mathsf{MAP}} = \mathsf{argmax}_{c \in \{\oplus,\ominus\}} \, p(c \mid \mathbf x)$ 

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

Probability of 
$$D$$
 under the binomial distribution, parameterized by  $\theta$ . Maximum likelihood estimates  $\theta_{\text{ML}} = \operatorname{argmax}_{\theta \in [0:1]} p(D; \theta)$ 

6) 
$$p(\theta \mid D)$$
:  $\frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$  Probability of  $\theta$  given  $D$  via Bayes's rule. Maximum a posteriori hypothesis:  $\theta_{\mathsf{MAP}} = \operatorname{argmax}_{\theta \in \{\theta_1, \theta_2\}} p(\theta \mid D)$ 

### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$ 

RSS for 
$$D$$
 under a linear model, parameterized by  $\mathbf{w}$ .  
Least squares estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \operatorname{RSS}(\mathbf{w})$ 

(2) 
$$p(D; \mathbf{w})$$
: 
$$\prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$

Probability of 
$$D$$
 under a logistic model, parameterized by  $\mathbf{w}$ . Maximum likelihood estimate:  $\mathbf{w}_{\mathsf{ML}} = \mathsf{argmax}_{\mathbf{w} \in \mathbf{R}^{p+1}} \, p(D; \mathbf{w})$ 

(3) 
$$L(\mathbf{w})$$
: 
$$\sum_{(\mathbf{x},c)\in D} l_{\sigma}(c,\sigma(\mathbf{w}^T\mathbf{x}))$$

Loss for 
$$D$$
 under a logistic model, parameterized by  $\mathbf{w}$ . Minimum loss (= maximum likelihood) estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} L(\mathbf{w})$ 

(4) 
$$p(c \mid \mathbf{x})$$
: 
$$\frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$

Probability of 
$$c$$
 given  $\mathbf x$  via Bayes's rule. Maximum a posteriori class for  $\mathbf x$ :  $c_{\mathsf{MAP}} = \mathsf{argmax}_{c \in \{\oplus,\ominus\}} \, p(c \mid \mathbf x)$ 

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

Probability of 
$$D$$
 under the bin parameterized by  $\theta$ . Maximum  $\theta$  argument  $\theta$  ar

(6) 
$$p(\theta \mid D)$$
: 
$$\frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$$

Probability of 
$$\theta$$
 given  $D$  via Bayes's rule. Maximum a posteriori hypothesis:  $\theta_{\mathsf{MAP}} = \mathrm{argmax}_{\theta \in \{\theta_1, \theta_2\}} \, p(\theta \mid L)$ 

#### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$

RSS for D under a linear model, parameterized by  $\mathbf{w}$ . Least squares estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \operatorname{RSS}(\mathbf{w})$ 

(2) 
$$p(D; \mathbf{w})$$
: 
$$\prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$

Probability of D under a logistic model, parameterized by  $\mathbf{w}$ . Maximum likelihood estimate:  $\mathbf{w}_{\mathsf{ML}} = \mathsf{argmax}_{\mathbf{w} \in \mathbf{R}^{p+1}} p(D; \mathbf{w})$ 

(3) 
$$L(\mathbf{w})$$
: 
$$\sum_{(\mathbf{x}.c)\in D} l_{\sigma}(c, \sigma(\mathbf{w}^T\mathbf{x}))$$

Loss for D under a logistic model, parameterized by  $\mathbf{w}$ . Minimum loss (= maximum likelihood) estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} L(\mathbf{w})$ 

(4) 
$$p(c \mid \mathbf{x})$$
: 
$$\frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$

Probability of c given  $\mathbf x$  via Bayes's rule. Maximum a posteriori class for  $\mathbf x$ :  $c_{\mathsf{MAP}} = \mathsf{argmax}_{c \in \{\oplus,\ominus\}} \, p(c \mid \mathbf x)$ 

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

(5) 
$$p(D;\theta)$$
: 
$$\binom{n}{k} \cdot \theta^k \cdot (1-\theta)^{n-k}$$

Probability of D under the binomial distribution, parameterized by  $\theta$ . Maximum likelihood estimate:  $\theta_{\text{ML}} = \operatorname{argmax}_{\theta \in [0;1]} p(D;\theta)$ 

(6) 
$$p(\theta \mid D)$$
: 
$$\frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$$

Probability of  $\theta$  given D via Bayes's rule. Maximum a posteriori hypothesis:  $\theta_{\mathsf{MAP}} = \mathrm{argmax}_{\theta \in \{\theta_1, \theta_2\}} \ p(\theta \mid D)$ 

### Typical Learning Settings

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

(1) RSS(w): 
$$\sum (y - \mathbf{w}^T \mathbf{x})^2$$
 RSS for  $D$  Least square

RSS for D under a linear model, parameterized by  $\mathbf{w}$ . Least squares estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} \operatorname{RSS}(\mathbf{w})$ 

(2) 
$$p(D; \mathbf{w})$$
:  $\prod p(c \mid \mathbf{x}; \mathbf{w})$ 

Probability of D under a logistic model, parameterized by  $\mathbf{w}$ . Maximum likelihood estimate:  $\mathbf{w}_{\mathsf{ML}} = \mathsf{argmax}_{\mathbf{w} \in \mathbf{R}^{p+1}} \, p(D; \mathbf{w})$ 

$$\sum_{\mathbf{k}} l_{\sigma}(c, \sigma(\mathbf{w}^T \mathbf{x}))$$

Loss for D under a logistic model, parameterized by  $\mathbf{w}$ . Minimum loss (= maximum likelihood) estimate:  $\hat{\mathbf{w}} = \operatorname{argmin}_{\mathbf{w} \in \mathbf{R}^{p+1}} L(\mathbf{w})$ 

$$p(\mathbf{x} \mid c) \cdot p(c)$$

Probability of c given  $\mathbf x$  via Bayes's rule. Maximum a posteriori class for  $\mathbf x$ :  $c_{\mathsf{MAP}} = \mathsf{argmax}_{c \in \{\oplus,\ominus\}} \, p(c \mid \mathbf x)$ 

(4) 
$$p(c \mid \mathbf{x})$$
: 
$$\frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

(5) 
$$p(D;\theta)$$
: Probability of  $D$  under the binomial distribution, parameterized by  $\theta$ . Maximum likelihood estimate:  $\theta_{\mathsf{ML}} = \operatorname{argmax}_{\theta \in [0:1]} p(D;\theta)$ 

(6) 
$$p(\theta \mid D)$$
: 
$$\frac{p(D \mid \theta) \cdot p(\theta)}{p(D)}$$
 Probability of  $\theta$  given  $D$  via Bayes's rule. Maximum a posteriori hypothesis:  $\theta_{\mathsf{MAP}} = \mathrm{argmax}_{\theta \in \{\theta_1, \theta_2\}} \, p(\theta \mid D)$ 

(3)  $L(\mathbf{w})$ :

Remarks (predictor-response vs. outcome-only setting):

- Predictor-response setting,  $\mathbf{x} \to y$  or  $\mathbf{x} \to c$ . The relation between  $\mathbf{x}$  and y or c is captured by a model function  $y(\mathbf{x})$ . The data D is exploited to fit  $y(\mathbf{x})$ , which in turn means to determine a parameter w or parameter vector  $\mathbf{w}$  for  $y(\mathbf{x})$ . Modeling and predicting a quantitative response variable y is a regression task; modeling and predicting a categorical response variable c is a classification task.
  - An example for a categorical predictor-response setting is the classification of an email as spam  $(c = \oplus)$  or ham  $(c = \ominus)$ , given a vector  $\mathbf{x}$  of linguistic features for that email.
  - Outcome-only setting,  $y_1, \ldots, y_n$  or  $c_1, \ldots, c_n$ . Modeling a sole outcome variable means to fit the data D using a suited distribution function, which in turn means to determine the distribution parameter  $\theta$  or distribution parameters  $\theta$ . Again, one can distinguish between different measurement scales, such as quantitative (y) or categorical (c).
    - An example for a categorical outcome-only setting is a coin flip experiment where one has to fit the observations (number of heads and tails) under the binomial distribution, which in turn means to determine the distribution parameter  $\theta$ .
- Depending on the experiment setting, i.e., fitting of a model function vs. fitting of a distribution, either the symbol w (or w), or the symbol  $\theta$  (or  $\theta$ ) may be used to denote the parameter (or parameter vector).

ML:VII-110 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks (discriminative vs. generative approach):

- (1), (2), (3) Discriminative approach to classification. Exploit the data to determine a decision boundary. Typically, "discriminative" implies "frequentist".
  - The optimization (argmin, argmax) considers  $p(\mathbf{x})$ , the distribution of the independent variables  $\mathbf{x}$ , implicitly via the multiplicity of  $\mathbf{x}$  in the data D. Recall that D is a multiset of examples.
- (2), (3), (5) Maximum likelihood (ML) principle to parameter estimation.
  - (2) Recall the identities from the maximum likelihood derivation of the logistic loss  $L_{\sigma}(\mathbf{w})$ :

$$p(D; \mathbf{w}) = \prod_{(\mathbf{x}, c) \in D} p(\mathbf{x}, c; \mathbf{w}), \quad \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\operatorname{argmax}} \ p(D; \mathbf{w}) = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\operatorname{argmax}} \ \prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$

- (1), (2) If the data comes from an exponential family and mild conditions are satisfied, least-squares estimates and maximum-likelihood estimates are identical.
- (2), (3) Probabilistic model. The conditional class probability function (CCPF),  $p(c \mid \mathbf{x})$ , is estimated for all feature vectors (= at all quantiles). The model is not generative since the distribution of the independent variable,  $p(\mathbf{x})$ , is not modeled (but of course exploited implicitly via D).

Maximizing the probability under a logistic model is equivalent to minimizing the logistic loss  $L_{\sigma}$ . Hence,  $\mathbf{w}_{\mathsf{ML}} = \hat{\mathbf{w}}$ .

ML:VII-111 Bayesian Learning © STEIN/VÖLSKE 2022

Remarks (discriminative vs. generative approach): (continued)

- Generative approach to classification. Exploit the data D (here: estimate  $p(\mathbf{x} \mid c)$  and p(c) for all  $\mathbf{x}$  and c) to provide a model for the joint probability distribution,  $p(\mathbf{x}, c)$ , from which D is sampled.
- Generative approach. Assuming the conditions of the binomial data model, exploit the data D (here: estimate the parameter  $\theta$ ) to provide a model for the binomial probability distribution, p(c), from which D is sampled.
- Generative or discriminative approach.  $p(\theta \mid D)$  can be estimated by either providing ( $\rightarrow$  generative) or by *not* providing ( $\rightarrow$  discriminative) a model for the probability distribution from which D is sampled.

ML:VII-112 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks (ML principle vs. Bayes method):

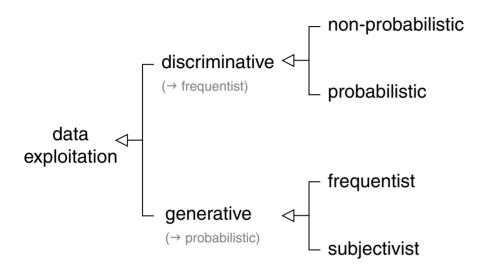
- (1), (2), (3)  $\mathbf{w}$  (as well as  $\theta$ ) is not the realization of a random variable—which would come along with a distribution—but an *exogenous parameter*, which is varied in order to find the maximum probability  $p(D; \mathbf{w})$  (or  $p(D; \theta)$ ) or the minimum loss  $L(\mathbf{w})$ .
  - The fact that  $\mathbf{w}$  (or  $\theta$ ) is an exogenous parameter and not a realization of a random variable is reflected by the notation, which uses a  $\mathbf{w}$ ;  $\mathbf{w}$  instead of a  $\mathbf{w}$  |  $\mathbf{w}$  in the argument of  $\mathbf{p}$ ().
  - (4) Application of Bayes's rule, presupposing that one can estimate the likelihoods  $p(\mathbf{x} \mid \cdot)$  ( $p(x_j \mid \cdot)$  in case of Naive Bayes) at higher fidelity than the conditional class probabilities,  $p(\cdot \mid \mathbf{x})$ , from the data.
    - Under the Naive Bayes Assumption,  $p(\mathbf{x} \mid c)$  is modeled as  $\prod_{j=1}^{p} p(x_j \mid c)$ .
  - (4), (6) Likelihoods,  $p(\mathbf{x} \mid \cdot)$ ,  $p(D \mid \cdot)$ , are computed for events under alternative classes c or parameters  $\theta$ . The settings differ in that an event in (4) is about a feature vector  $\mathbf{x}$ , while an event in (6) is about a sequence D. (4) may (but not need to) apply the Naive Bayes assumption to compute the likelihood  $p(\mathbf{x} \mid c)$ , which is a common approximation for a nominal feature space and if data are sparse. For (6), if the data originate from a coin flip experiment, the likelihood  $p(D \mid \theta)$  is computed via the binomial distribution.

If the prior probabilities, p(c) or  $p(\theta)$ , are estimated also from D, we follow the frequentist paradigm; if the priors rely on subjective assessments we follow the subjectivist paradigm.

If we assume uniform priors, i.e., the p(c) or the  $p(\theta)$  are equally probable, MAP estimates and ML estimates are equal since  $p(c \mid \mathbf{x}) \propto p(\mathbf{x} \mid c)$  or  $p(\theta \mid D) \propto p(D \mid \theta)$ , where » $\propto$ « means "is proportional to".

ML:VII-113 Bayesian Learning © STEIN/VÖLSKE 2022

#### Learning Approaches Overview



Support vector machine

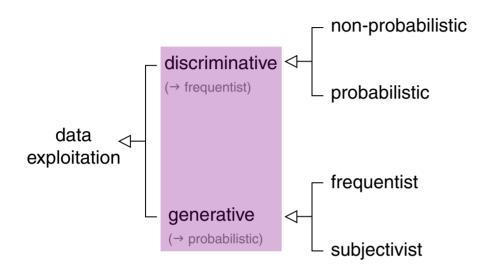
- (1) Linear regression with least square estimates from D
- 2) Logistic regression via p() with ML estimates from D
- (3) Logistic regression via L() with ML estimates from D
- (4) Bayes with ML estimates from D as priors
  - (5) Probability model with ML estimate from D
  - (6) Bayes with subjective priors
- (4) Bayes with subjective priors

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

ML:VII-114 Bayesian Learning © STEIN/VÖLSKE 2022

#### Learning Approaches Overview (continued)



Support vector machine

- (1) Linear regression with least square estimates from D
- 2) Logistic regression via p() with ML estimates from D
- (3) Logistic regression via L() with ML estimates from D
- (4) Bayes with ML estimates from D as priors
  - (5) Probability model with ML estimate from D
  - (6) Bayes with subjective priors
- (4) Bayes with subjective priors

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

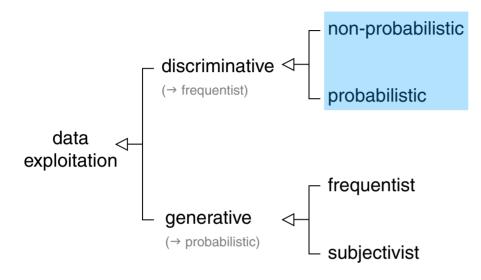
$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

discriminative: Determine a boundary to split  $D. \rightarrow No$  model for the distribution of D.

generative: Provide a model for the probability distribution from which D is sampled.

ML:VII-115 Bayesian Learning © STEIN/VÖLSKE 2022

Learning Approaches Overview (continued)



Support vector machine

- (1) Linear regression with least square estimates from D
- 2) Logistic regression via p() with ML estimates from D
- (3) Logistic regression via L() with ML estimates from D
- (4) Bayes with ML estimates from D as priors
  - (5) Probability model with ML estimate from D
  - (6) Bayes with subjective priors
- (4) Bayes with subjective priors

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

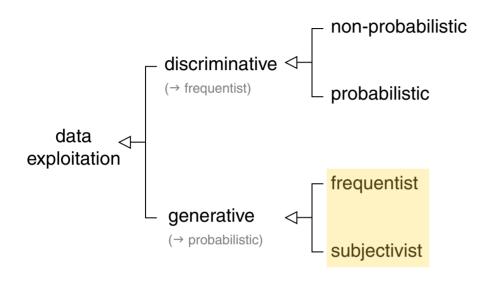
$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

non-probabilistic: Threshold some model function (typically at zero). ightarrow Classification, Labeling

probabilistic: Estimate  $p(c \mid \mathbf{x})$  at all quantiles.  $\rightarrow$  Class probability estimation, CCPF

ML:VII-116 Bayesian Learning © STEIN/VÖLSKE 2022

#### Learning Approaches Overview (continued)



Support vector machine

- (1) Linear regression with least square estimates from D
- (2) Logistic regression via p() with ML estimates from D
- (3) Logistic regression via L() with ML estimates from D
- (4) Bayes with ML estimates from D as priors
  - (5) Probability model with ML estimate from D
  - (6) Bayes with subjective priors
- (4) Bayes with subjective priors

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

frequentist: Consider a unique mechanism that generated the data D.

subjectivist: Specify beliefs for alternative mechanisms one of which generated *D*.

ML:VII-117 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks:

- We call a data exploitation approach "generative" if it provides us with a model for the probability distribution from which D is sampled. With such a model we are able to generate arbitrary samples from the population where D is sampled from.
- □ The overview does not show all but common combinations. In particular:
  - Typically, "discriminative" implies "frequentist". The inverse does not apply: consider a Bayes classifier with priors estimated from the data.
  - Typically, "generative" implies "probabilistic". The inverse does not apply: logistic regression provides a probabilistic model to classification.
- □ Discriminative approaches are further distinguished as "non-probabilistic" or "probabilistic".
- Generative approaches are further distinguished as "frequentist" or "subjectivist".

ML:VII-118 Bayesian Learning © STEIN/VÖLSKE 2022

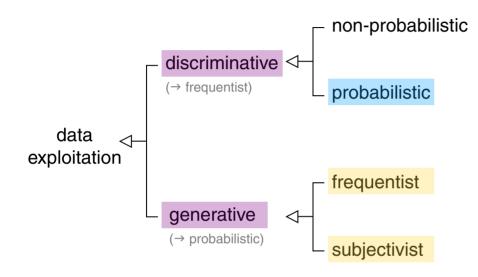
# Chapter ML:VII (continued)

#### VII. Bayesian Learning

- □ Approaches to Probability
- □ Conditional Probability
- Bayes Classifier
- □ Exploitation of Data
- □ Frequentist versus Subjectivist

ML:VII-119 Bayesian Learning ©STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples]



Support vector machine

- (1) Linear regression with least square estimates from D
- (2) Logistic regression via p() with ML estimates from D
- (3) Logistic regression via L() with ML estimates from D
- (4) Bayes with ML estimates from D as priors
  - 5) Probability model with ML estimate from D
  - (6) Bayes with subjective priors
- (4) Bayes with subjective priors

$$D = \{(\mathbf{x}_1, y_1), \dots, (\mathbf{x}_n, y_n)\}, D = \{(\mathbf{x}_1, c_1), \dots, (\mathbf{x}_n, c_n)\}$$

$$D = \{y_1, \dots, y_n\}, D = \{c_1, \dots, c_n\}$$

ML:VII-120 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \ \prod_{(\mathbf{x},c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \underset{c \in \{\oplus,\ominus\}}{\mathsf{argmax}} \ p(c \mid \mathbf{x})$$

#### Observation 1. Both approaches maximize p(D)

- (2), the "ML principle", determines the parameters  $\mathbf{w}$  of the logistic model function such that  $\prod_D p(c \mid \mathbf{x})$  becomes maximum. Note that a parameter vector  $\mathbf{w}$  that maximizes  $\prod_D p(c \mid \mathbf{x})$  will also maximize  $\prod_D p(\mathbf{x}, c)$ , and thus p(D) (under the i.i.d. assumption).
- $\Box$  (4), the "Bayes method", determines for a given  $\mathbf{x}$  its most probable class. By choosing  $c_{\mathsf{MAP}}$  for each  $\mathbf{x}$ , Bayes maximizes p(D) by maximizing each factor of  $\prod_D p(c \mid \mathbf{x})$ . Note that  $p(\mathbf{x})$  is constant per factor. Recall that Naive Bayes approximates  $p(\mathbf{x} \mid c)$  with  $\prod_{i=1}^p p(x_i \mid c)$ .

ML:VII-121 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \prod_{(\mathbf{x},c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \underset{c \in \{\oplus, \ominus\}}{\mathsf{argmax}} \quad \frac{p(\mathbf{x} \mid c) \cdot p(c)}{p(\mathbf{x})}$$
 (Bayes)

#### Observation 1. Both approaches maximize p(D)

- (2), the "ML principle", determines the parameters  $\mathbf{w}$  of the logistic model function such that  $\prod_D p(c \mid \mathbf{x})$  becomes maximum. Note that a parameter vector  $\mathbf{w}$  that maximizes  $\prod_D p(c \mid \mathbf{x})$  will also maximize  $\prod_D p(\mathbf{x}, c)$ , and thus p(D) (under the i.i.d. assumption).
- Quantum (4), the "Bayes method", determines for a given  $\mathbf{x}$  its most probable class. By choosing  $c_{\mathsf{MAP}}$  for each  $\mathbf{x}$ , Bayes maximizes p(D) by maximizing each factor of  $\prod_D p(c \mid \mathbf{x})$ . Note that  $p(\mathbf{x})$  is constant per factor. Recall that Naive Bayes approximates  $p(\mathbf{x} \mid c)$  with  $\prod_{i=1}^p p(x_i \mid c)$ .

ML:VII-122 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \prod_{(\mathbf{x},c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \operatorname*{argmax}_{c \in \{\oplus,\ominus\}} \ \frac{\prod_{j=1}^p p(x_j \mid c) \cdot p(c)}{p(\mathbf{x})}$$
 (Naive Bayes)

#### Observation 1. Both approaches maximize p(D)

- (2), the "ML principle", determines the parameters  $\mathbf{w}$  of the logistic model function such that  $\prod_D p(c \mid \mathbf{x})$  becomes maximum. Note that a parameter vector  $\mathbf{w}$  that maximizes  $\prod_D p(c \mid \mathbf{x})$  will also maximize  $\prod_D p(\mathbf{x}, c)$ , and thus p(D) (under the i.i.d. assumption).
- $\Box$  (4), the "Bayes method", determines for a given  $\mathbf{x}$  its most probable class. By choosing  $c_{\mathsf{MAP}}$  for each  $\mathbf{x}$ , Bayes maximizes p(D) by maximizing each factor of  $\prod_D p(c \mid \mathbf{x})$ . Note that  $p(\mathbf{x})$  is constant per factor. Recall that Naive Bayes approximates  $p(\mathbf{x} \mid c)$  with  $\prod_{i=1}^p p(x_i \mid c)$ .

ML:VII-123 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \prod_{(\mathbf{x},c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \underset{c \in \{\oplus,\ominus\}}{\mathsf{argmax}} \quad \prod_{j=1}^p p(x_j \mid c) \cdot p(c)$$
 (Naive Bayes)

#### Observation 1. Both approaches maximize p(D):

- (2), the "ML principle", determines the parameters  $\mathbf{w}$  of the logistic model function such that  $\prod_D p(c \mid \mathbf{x})$  becomes maximum. Note that a parameter vector  $\mathbf{w}$  that maximizes  $\prod_D p(c \mid \mathbf{x})$  will also maximize  $\prod_D p(\mathbf{x}, c)$ , and thus p(D) (under the i.i.d. assumption).
- $\Box$  (4), the "Bayes method", determines for a given  $\mathbf{x}$  its most probable class. By choosing  $c_{\mathsf{MAP}}$  for each  $\mathbf{x}$ , Bayes maximizes p(D) by maximizing each factor of  $\prod_D p(c \mid \mathbf{x})$ . Note that  $p(\mathbf{x})$  is constant per factor. Recall that Naive Bayes approximates  $p(\mathbf{x} \mid c)$  with  $\prod_{i=1}^p p(x_i \mid c)$ .

ML:VII-124 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \prod_{(\mathbf{x}, \mathbf{c}) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \underset{c \in \{\oplus,\ominus\}}{\mathsf{argmax}} \quad \prod_{j=1}^p p(x_j \mid c) \cdot p(c)$$
 (Naive Bayes)

#### Observation 1. Both approaches maximize p(D):

- $\Box$  (2), the "ML principle", determines the parameters  $\mathbf{w}$  of the logistic model function such that  $\prod_D p(c \mid \mathbf{x})$  becomes maximum. Note that a parameter vector  $\mathbf{w}$  that maximizes  $\prod_D p(c \mid \mathbf{x})$  will also maximize  $\prod_D p(\mathbf{x}, c)$ , and thus p(D) (under the i.i.d. assumption).
- Use (4), the "Bayes method", determines for a given  $\mathbf{x}$  its most probable class. By choosing  $c_{\mathsf{MAP}}$  for each  $\mathbf{x}$ , Bayes maximizes p(D) by maximizing each factor of  $\prod_D p(c \mid \mathbf{x})$ . Note that  $p(\mathbf{x})$  is constant per factor. Recall that Naive Bayes approximates  $p(\mathbf{x} \mid c)$  with  $\prod_{j=1}^p p(x_j \mid c)$ .

ML:VII-125 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes [data exploitation examples] (continued)

(2) 
$$\mathbf{w}_{\mathsf{ML}} = \underset{\mathbf{w} \in \mathbf{R}^{p+1}}{\mathsf{argmax}} \prod_{(\mathbf{x}, c) \in D} p(c \mid \mathbf{x}; \mathbf{w})$$
 (logistic regression)

(4) 
$$c_{\mathsf{MAP}} = \underset{c \in \{\oplus,\ominus\}}{\mathsf{argmax}} \quad \prod_{j=1}^p p(x_j \mid c) \cdot p(c)$$
 (Naive Bayes)

#### Observation 2 (corollary). Both approaches model the covariate distribution:

- $\Box$  (2), the "ML principle", considers  $p(\mathbf{x})$ , the distribution of the independent variables  $\mathbf{x}$ , implicitly via the multiplicity of  $\mathbf{x}$  in the data D. Recall that D is a multiset of examples.
- (4), the "Bayes method", as a generative approach, models  $p(\mathbf{x} \mid c)$  and p(c), and hence also  $p(\mathbf{x}, c)$ ,  $p(\mathbf{x})$ , and  $p(c \mid \mathbf{x})$ . The likelihoods,  $p(\mathbf{x} \mid c)$  (or  $p(x_j \mid c)$  under Naive Bayes), are estimated from D; the priors, p(c), may be estimated by subjective assessments.

ML:VII-126 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks:

- Both approaches maximize p(D) by maximizing  $\prod_D p(c \mid \mathbf{x})$ . Estimating  $p(c \mid \mathbf{x})$  is usually significantly easier than estimating  $p(\mathbf{x}, c)$ .
- Naive Bayes models  $p(\mathbf{x} \mid c)$  as  $\prod_{j=1}^p p(x_j \mid c)$ , where  $p(x_j \mid c)$  is estimated as  $\hat{p}(x_j \mid c)$ ,  $\hat{p}(x_j \mid c) = |\{(\mathbf{x}, c) \in D : \mathbf{x}|_j = x_j\}| / |\{(\cdot, c) \in D\}|$ . Similarly, p(c) can estimated as  $\hat{p}(c)$ ,  $\hat{p}(c) = |\{(\cdot, c) \in D\}|$ ; but, also a dedicated (and subjective) prior probability model can be stated.
  - $p(\mathbf{x})$  can be computed with the Law of Total Probability,  $p(\mathbf{x}) = \sum_{c \in \{\oplus,\ominus\}} p(\mathbf{x} \mid c) \cdot p(c)$ . Note, however, that  $p(\mathbf{x})$  is not required to compute  $c_{\mathsf{MAP}}$  for  $\mathbf{x}$ .
- If for the Bayes method—aside from the likelihoods  $p(x_j \mid c)$  also the class priors, p(c), are computed from D, we follow the frequentist paradigm, similar to the ML principle. Only if the values for p(c) (= the prior probability model) rely on subjective assessments, the Bayes method can be considered as subjectivist.
- □ Whether to apply the ML principle or the Bayes method is not a free choice; it depends on
  - the availability of data D,
  - the conditional strengths of the likelihoods,  $p(\mathbf{x} \mid c)$ ,
  - the reliability of the assessments for the prior probabilities, p(c), and,
  - whether or not subjective assessments shall be considered to estimate the priors p(c).

Synonymous: covariate, independent, predictor [variable / distribution].

ML:VII-127 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks: (continued)

- Observe the subtle distinction between "Bayes rule" and "Bayes method" made here. With the former we refer to the identity that connects the posterior probability,  $P(A \mid B)$ , and the likelihood,  $P(B \mid A)$  (the "reversal of condition and consequence"). With the latter we refer to the *parameter estimation principle* where the maximum a posteriori probability is determined.
- Note that a class-conditional event " $\mathbf{X}=\mathbf{x}\mid C=c$ " does not necessarily model a cause-effect relation: the event "C=c" may cause—but does not need to cause—the event " $\mathbf{X}=\mathbf{x}$ ". Examples:
  - A disease c will cause the symptoms  $\mathbf{x}$  (but not vice versa).
  - Weather conditions x will cause the decision "*EnjoySurfing*=yes" (but not vice versa).

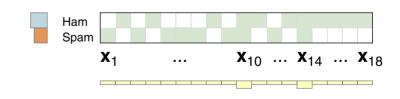
Similarly, also if  $\mathbf{x}$  is the independent variable of a function  $y(\mathbf{x})$  that maps features to classes c, the cause-effect direction is not necessarily  $\mathbf{x} \to c$ , but can also be the other way around: Consider  $y(\mathbf{x}) = c$  with "disease c"  $\to$  "symptoms  $\mathbf{x}$ ".

ML:VII-128 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Example

#### A multiset of examples *D*:

	URLs	Spelling errors	Spam
1	5	3	yes
2	4	1	no
3	4	3	yes
÷	:	÷	:
10	1	0	no
11	1	0	yes
÷	÷	:	:
15	1	4	no
16	1	4	yes
÷	:	:	:
20	0	4	no



#### Learning task:

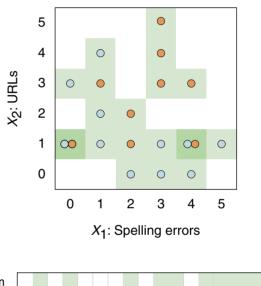
 $\Box$  Fit *D* to compute a classifier for feature vectors  $\mathbf{x}$ ,  $\mathbf{x} \notin D$ .

ML:VII-129 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Example (continued)

#### A multiset of examples *D*:

	URLs	Spelling errors	Spam
1	5	3	yes
2	4	1	no
3	4	3	yes
÷	:	:	:
10	1	0	no
11	1	0	yes
:	:	:	:
15	1	4	no
16	1	4	yes
:	:	:	:
20	0	4	no





#### Learning task:

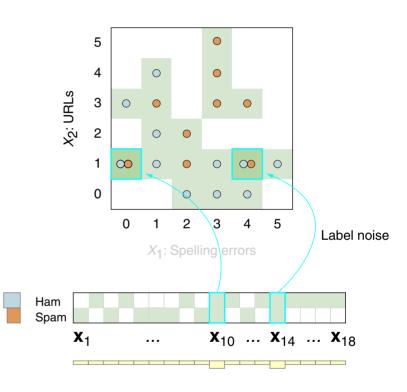
 $\Box$  Fit D to compute a classifier for feature vectors  $\mathbf{x}$ ,  $\mathbf{x} \notin D$ .

ML:VII-130 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Example (continued)

#### A multiset of examples *D*:

URLs	Spelling errors	Spam
5	3	yes
4	1	no
4	3	yes
:	:	:
1	0	no
1	0	yes
:	:	:
1	4	no
1	4	yes
:	:	:
0	4	no
	5 4 4 : 1 1 :	5 3 4 1 4 3 1 0 1 0 1 4 1 4



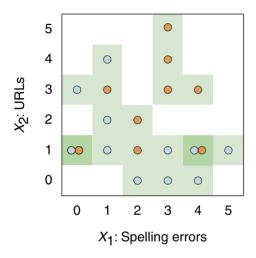
#### Learning task:

 $\Box$  Fit *D* to compute a classifier for feature vectors  $\mathbf{x}$ ,  $\mathbf{x} \notin D$ .

ML:VII-131 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Conditional Class Probabilities

#### Logistic regression:

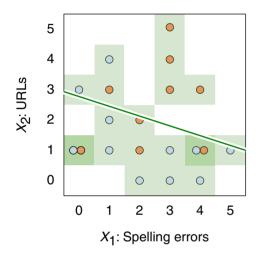


 $\Box$  Distribution of D.

ML:VII-132 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:

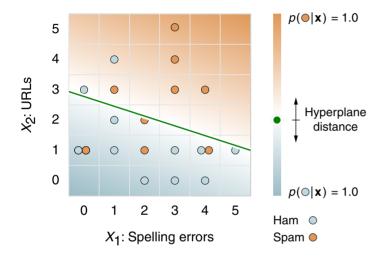


 $\Box$  Hyperplane  $\langle \mathbf{w}_{\mathsf{ML}}, \mathbf{x} \rangle = 0$ .

ML:VII-133 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:

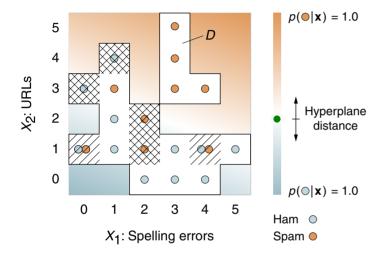


 $exttt{ o}$  Conditional class probabilities computed with  $w_{\text{ML}}$ , the ML estimate for w given D.

ML:VII-134 Bayesian Learning © STEIN/VÖLSKE 2022

Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:

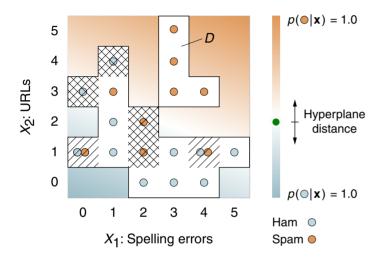


Training error.

ML:VII-135 Bayesian Learning © STEIN/VÖLSKE 2022

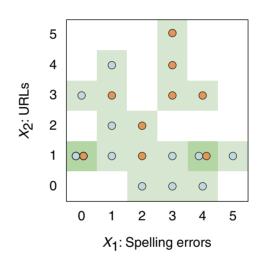
Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:



Training error.

#### Naive Bayes:

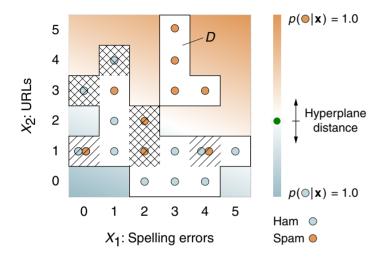


 $\Box$  Distribution of D.

ML:VII-136 Bayesian Learning © STEIN/VÖLSKE 2022

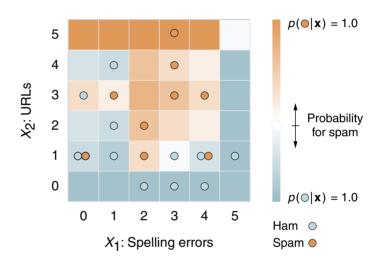
Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:



Training error.

#### Naive Bayes:

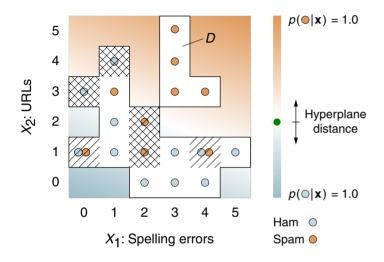


 $\Box$  Conditional class probabilities computed for the respective MAP class, using p(c) estimates from D.

ML:VII-137 Bayesian Learning © STEIN/VÖLSKE 2022

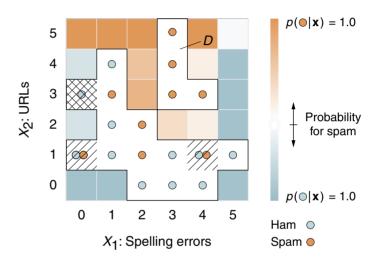
Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:



Training error.

#### Naive Bayes:

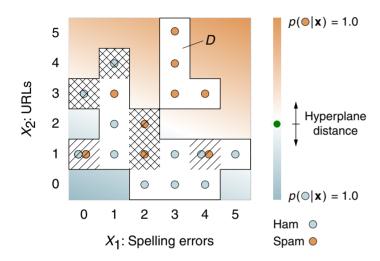


Training error.

ML:VII-138 Bayesian Learning © STEIN/VÖLSKE 2022

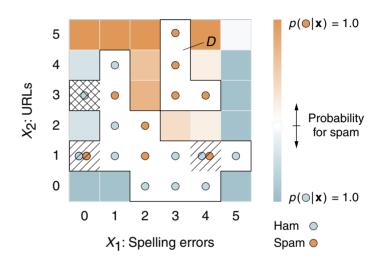
Logistic Regression versus Naive Bayes: Conditional Class Probabilities (continued)

#### Logistic regression:



- Computation of a hyperplane.
- Approach: minimization of accumulated "misclassification distances" for examples in D.
- Discriminative and probabilistic.

#### Naive Bayes:



- Computation of a probability distribution.
- □ Basis: class-conditional feature and class frequencies in D.
- Generative (implies probabilistic).

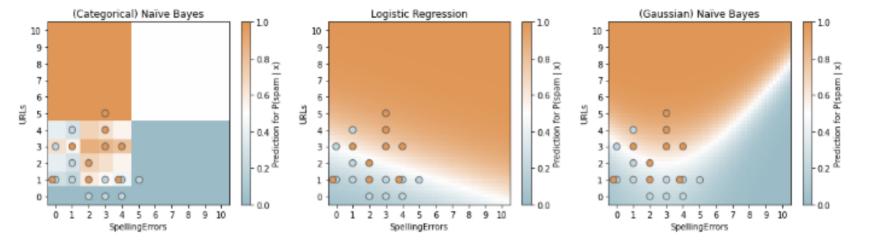
ML:VII-139 Bayesian Learning © STEIN/VÖLSKE 2022

#### Remarks:

- Both approaches, logistic regression and Naive Bayes, estimate the conditional class probability function,  $p(\text{Spam} \mid \mathbf{x})$  or  $p(\text{Ham} \mid \mathbf{x}) = 1 p(\text{Spam} \mid \mathbf{x})$ . However, the two estimation approaches follow very different concepts.
- Generalization characteristic:
  - The conditional class probability function as computed via logistic regression decides not only the feature space  $\{0, 1, 2, 3, 4, 5\}^2$  but the entire  $\mathbf{R}^2$ . (Whether that makes sense is another matter.)
  - The conditional class probability function as computed via Naive Bayes provides class probability estimates for  $\mathbf{x} \in \{0,1,2,3,4,5\}^2$ . The probabilities are estimated from the class-conditional feature frequencies (likelihood estimates) and class frequencies,  $\hat{p}(x_1 \mid c)$ ,  $\hat{p}(x_2 \mid c)$ , and  $\hat{p}(c)$ , as found in D. Note that a vector  $\mathbf{x} = (x_1, x_2)^T$  gets the probability of zero for class c, if  $x_1$  or  $x_2$  does not occur in some feature vector with class label c in D.
- □ Handling of class imbalance and covariate distribution:
  - Logistic regression considers the p(c) and the  $p(\mathbf{x})$  implicitly via their multiplicity in D. I.e., the learned parameter vector  $\mathbf{w}$  has the class imbalance as well as the covariate distribution "compiled in".
  - Naive Bayes, again, estimates the p(c) and the  $p(\mathbf{x})$  from the frequencies in D. More specifically,  $p(\mathbf{x})$  can be estimated from  $\hat{p}(x_1 \mid c)$ ,  $\hat{p}(x_2 \mid c)$ , and  $\hat{p}(c)$  with the Law of Total Probability. Note that the computation of  $p(\mathbf{x})$  is not necessary for a ranking (= classification without class membership probability).

ML:VII-140 Bayesian Learning © STEIN/VÖLSKE 2022

#### Naive Bayes: Smoothing and Continuous Likelihoods

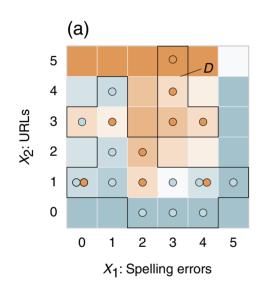


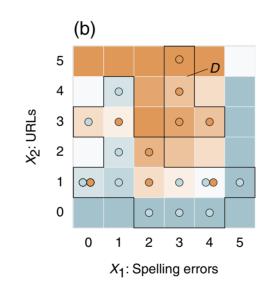
 $\sim$  BOARD

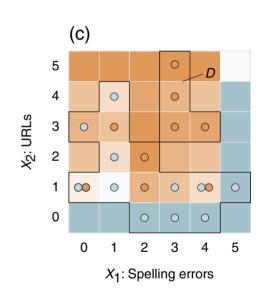
ML:VII-141 Bayesian Learning © STEIN/VÖLSKE 2022

Naive Bayes: Prior Probability Models

Comparison of the conditional class probability function,  $p(c \mid \mathbf{x})$ , under Naive Bayes for three different prior probability models (= assessments of class priors), p(c).







p(c) estimates from D

$$P_a(\mathbf{C} = \mathbf{Spam}) = \hat{p}(\mathbf{Spam}) = 0.45$$

$$P_a(\mathbf{C} = \mathsf{Ham}) = \hat{p}(\mathsf{Ham}) = 0.55$$

Subjective assessments for p(c)

$$P_b(C = \text{Spam}) = 0.6$$

$$P_b(C=Ham) = 0.4$$

$$P_c(C=Spam) = 0.8$$

$$P_c(C=Ham) = 0.2$$

Classification: Bayes Optimum versus MAP versus Ensemble

 $\sim \mathcal{BOARD}$ 

ML:VII-143 Bayesian Learning ©STEIN/VÖLSKE 2022

Advanced Bayesian Decision Making

Recall the Bayes rule,

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)},$$

with A and B in the role of a "hypothesis event", H=h, and a "data event",  $\mathbf{D}=D$ ,

$$P(H=h \mid \mathbf{D}=D) = \frac{P(\mathbf{D}=D \mid H=h) \cdot P(H=h)}{P(\mathbf{D}=D)}$$

ML:VII-144 Bayesian Learning © STEIN/VÖLSKE 2022

Advanced Bayesian Decision Making (continued)

Recall the Bayes rule,

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)},$$

with A and B in the role of a "hypothesis event", H=h, and a "data event", D=D,

$$P(H=h \mid \mathbf{D}=D) = \frac{P(\mathbf{D}=D \mid H=h) \cdot P(H=h)}{P(\mathbf{D}=D)}$$

$$p(h \mid D) = \frac{p(D \mid h) \cdot p(h)}{p(D)}$$

- $\square$  Likelihood: How well does h explain (= entail, induce, evoke) the data D?
- $\square$  Prior: How probable is the hypothesis h a priori (= in principle)?
- $\square$  Normalization: How probable is the observation of the data D?
- $\Box$  Posterior: How probable is the hypothesis h when observing the data D?

Advanced Bayesian Decision Making (continued)

Recall the Bayes rule,

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)},$$

with A and B in the role of a "hypothesis event", H=h, and a "data event", D=D,

$$P(H=h \mid \mathbf{D}=D) = \frac{P(\mathbf{D}=D \mid H=h) \cdot P(H=h)}{P(\mathbf{D}=D)}$$

$$p(h \mid D) = \frac{p(D \mid h) \cdot p(h)}{p(D)}$$

- $\Box$  Likelihood: How well does h explain (= entail, induce, evoke) the data D?
- $\Box$  Prior: How probable is the hypothesis h a priori (= in principle)?
- $\square$  Normalization: How probable is the observation of the data D?
- $lue{}$  Posterior: How probable is the hypothesis h when observing the data D?

Advanced Bayesian Decision Making (continued)

Recall the Bayes rule,

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)},$$

with A and B in the role of a "hypothesis event", H=h, and a "data event", D=D,

$$P(H=h \mid \mathbf{D}=D) = \frac{P(\mathbf{D}=D \mid H=h) \cdot P(H=h)}{P(\mathbf{D}=D)}$$

$$p(h \mid D) = \frac{p(D \mid h) \cdot p(h)}{p(D)}$$

- $\square$  Likelihood: How well does h explain (= entail, induce, evoke) the data D?
- $\square$  Prior: How probable is the hypothesis h a priori (= in principle)?
- $\square$  Normalization: How probable is the observation of the data D?
- $\square$  Posterior: How probable is the hypothesis h when observing the data D'

Advanced Bayesian Decision Making (continued)

Recall the Bayes rule,

$$P(A \mid B) = \frac{P(B \mid A) \cdot P(A)}{P(B)},$$

with A and B in the role of a "hypothesis event", H=h, and a "data event", D=D,

$$P(H=h \mid \mathbf{D}=D) = \frac{P(\mathbf{D}=D \mid H=h) \cdot P(H=h)}{P(\mathbf{D}=D)}$$

$$p(h \mid D) = \frac{p(D \mid h) \cdot p(h)}{p(D)}$$

- $\square$  Likelihood: How well does h explain (= entail, induce, evoke) the data D?
- $\square$  Prior: How probable is the hypothesis h a priori (= in principle)?
- $\square$  Normalization: How probable is the observation of the data D?
- $\Box$  Posterior: How probable is the hypothesis h when observing the data D?

#### Remarks:

- When using the Bayes method for a predictor-response setting, then p(D),  $p(D) := P(\mathbf{D} = D)$ , is the probability of the data  $D = \mathbf{x}$ . I.e.,  $\mathbf{D}$  is a random vector whose domain is the feature space  $\mathbf{X}$ .
- When using the Bayes method for an outcome-only setting, then p(D),  $p(D) := P(\mathbf{D} = D)$ , is the probability of the data  $D = \{y_1, \dots, y_n\}$  or  $D = \{c_1, \dots, c_n\}$ . I.e.,  $\mathbf{D}$  is a random vector whose domain is  $\mathbf{R}^n$  or  $C^n$ , where C is the set of possible classes or class labels.
- p(h) := P(H=h) (also  $p(\mathbf{w})$ ,  $p(\theta)$ , or similar) is the probability of choosing a certain h, a parameter vector  $\mathbf{w}$ , or some model function as hypothesis. I.e., H is a random variable whose domain is the set H of possible hypotheses.
- $\square$  Recall that p() is defined via P() and that the two notations can be used interchangeably, arguing about realizations of random variables and events respectively.

ML:VII-149 Bayesian Learning © STEIN/VÖLSKE 2022