

# Probabilistic Models for Supervised Learning (Contd.)

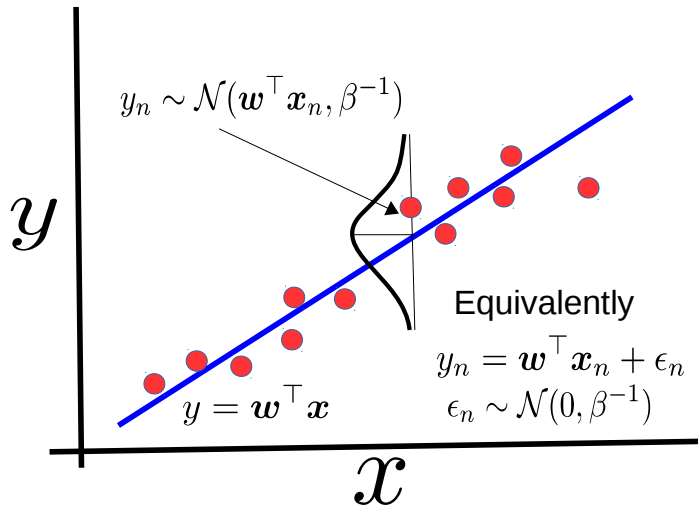
Piyush Rai

Introduction to Machine Learning (CS771A)

August 21, 2018

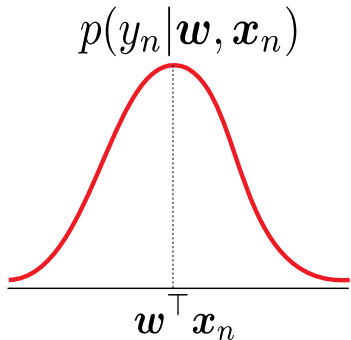


# Recap: Probabilistic Linear Regression



# Recap: Probabilistic Linear Regression

## The Likelihood



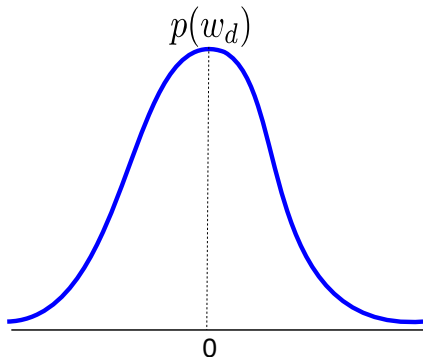
$$p(y_n | w, x_n) = \mathcal{N}(y_n | w^\top x_n, \beta^{-1}) = \sqrt{\frac{\beta}{2\pi}} \exp \left[ -\frac{\beta}{2} (y_n - w^\top x_n)^2 \right]$$

$$p(\mathbf{y} | w, \mathbf{X}) = \prod_{n=1}^N \mathcal{N}(y_n | w^\top x_n, \beta^{-1}) = \underbrace{\mathcal{N}(\mathbf{y} | \mathbf{X}w, \beta^{-1} \mathbf{I}_N)}_{\text{N-dim pdf}}$$

$$\left( \frac{\beta}{2\pi} \right)^{N/2} \exp \left[ -\frac{\beta}{2} \sum_{n=1}^N (y_n - w^\top x_n)^2 \right] = \frac{1}{\sqrt{\det(2\pi\beta^{-1}\mathbf{I}_N)}} \exp \left[ -\frac{\beta}{2} (\mathbf{y} - \mathbf{X}w)^\top (\mathbf{y} - \mathbf{X}w) \right]$$

# Recap: Probabilistic Linear Regression

## The Prior



$$p(w_d) = \mathcal{N}(w_d|0, \lambda^{-1}) = \sqrt{\frac{\lambda}{2\pi}} \exp\left[-\frac{\lambda}{2}w_d^2\right]$$

$$p(\mathbf{w}) = \prod_{d=1}^D \mathcal{N}(w_d|0, \lambda^{-1}) = \underbrace{\mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}_D)}_{D\text{-dim pdf}}$$

$$\left(\frac{\lambda}{2\pi}\right)^{D/2} \exp\left[-\frac{\lambda}{2} \sum_{d=1}^D w_d^2\right] = \frac{1}{\sqrt{\det(2\pi\lambda^{-1}\mathbf{I}_D)}} \exp\left[-\frac{\lambda}{2}\mathbf{w}^\top \mathbf{w}\right]$$

Zero-mean Gaussian prior encourages weights to be small. Precision  $\lambda$  controls how strong this prior is.

# Recap: MLE, MAP, and Bayesian Inference for Prob. Lin. Reg.

- For MLE, we **maximize the log-likelihood**. Ignoring constants w.r.t.  $\mathbf{w}$ , we have

$$\hat{\mathbf{w}}_{MLE} = \arg \max_{\mathbf{w}} \log p(\mathbf{y}|\mathbf{X}, \mathbf{w}) = \arg \min_{\mathbf{w}} \left[ \frac{\beta}{2} \sum_{n=1}^N (y_n - \mathbf{w}^\top \mathbf{x}_n)^2 \right]$$

- For MAP, we **maximize the log-posterior**. Ignoring constants w.r.t.  $\mathbf{w}$ , we have

$$\hat{\mathbf{w}}_{MAP} = \arg \max_{\mathbf{w}} \log p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \arg \min_{\mathbf{w}} \left[ \frac{\beta}{2} \sum_{n=1}^N (y_n - \mathbf{w}^\top \mathbf{x}_n)^2 + \frac{\lambda}{2} \mathbf{w}^\top \mathbf{w} \right]$$

- For Bayesian inference, we **compute the full posterior**. Easily computable (thanks to conjugacy)

$$\begin{aligned} p(\mathbf{w}|\mathbf{y}, \mathbf{X}) &= \mathcal{N}(\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N) \\ \boldsymbol{\Sigma}_N &= (\beta \mathbf{X}^\top \mathbf{X} + \lambda \mathbf{I}_D)^{-1} \\ \boldsymbol{\mu}_N &= (\mathbf{X}^\top \mathbf{X} + \frac{\lambda}{\beta} \mathbf{I}_D)^{-1} \mathbf{X}^\top \mathbf{y} \end{aligned}$$



# Recap: Predictive Distribution for Prob. Lin. Reg.

- When using MLE/MAP estimate of  $\mathbf{w}$ , we compute the “plug-in” predictive distribution

$$\begin{aligned} p(y_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) &\approx p(y_*|\mathbf{x}_*, \mathbf{w}_{MLE}) = \mathcal{N}(\mathbf{w}_{MLE}^\top \mathbf{x}_*, \beta^{-1}) \\ p(y_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) &\approx p(y_*|\mathbf{x}_*, \mathbf{w}_{MAP}) = \mathcal{N}(\mathbf{w}_{MAP}^\top \mathbf{x}_*, \beta^{-1}) \end{aligned}$$

- For MLE approach, mean of predicted output is  $\mathbf{w}_{MLE}^\top \mathbf{x}_*$ , variance is  $\beta^{-1}$
- For MAP approach, mean of predicted output is  $\mathbf{w}_{MAP}^\top \mathbf{x}_*$ , variance is  $\beta^{-1}$
- When using the fully posterior, we can compute the posterior predictive distribution

$$p(y_*|\mathbf{x}_*, \mathbf{X}, \mathbf{y}) = \int p(y_*|\mathbf{x}_*, \mathbf{w})p(\mathbf{w}|\mathbf{X}, \mathbf{y})d\mathbf{w} = \mathcal{N}(\mu_N^\top \mathbf{x}_*, \beta^{-1} + \mathbf{x}_*^\top \Sigma_N \mathbf{x}_*)$$

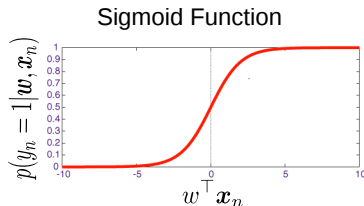
- For Bayesian approach, mean of predicted output is  $\mathbf{w}_N^\top \mathbf{x}_*$ , variance is  $\beta^{-1} + \mathbf{x}_*^\top \Sigma_N \mathbf{x}_*$  (note the different variance for each test input, unlike MLE/MAP prediction)



# Recap: Logistic Regression

- Logistic Regression models  $p(y_n = 1 | \mathbf{w}, \mathbf{x}_n)$  using the **sigmoid function**

$$p(y_n = 1 | \mathbf{w}, \mathbf{x}_n) = \mu_n = \sigma(\mathbf{w}^\top \mathbf{x}_n) = \frac{1}{1 + \exp(-\mathbf{w}^\top \mathbf{x}_n)} = \frac{\exp(\mathbf{w}^\top \mathbf{x}_n)}{1 + \exp(\mathbf{w}^\top \mathbf{x}_n)}$$



- Thus each **likelihood**  $p(y_n | \mathbf{w}, \mathbf{x}_n) = \text{Bernoulli}(y_n | \mu_n) = \mu_n^{y_n} (1 - \mu_n)^{1-y_n}$
- Assuming i.i.d. labels, likelihood is product of Bernoullis

$$p(\mathbf{y} | \mathbf{X}, \mathbf{w}) = \prod_{n=1}^N p(y_n | \mathbf{x}_n, \mathbf{w}) = \prod_{n=1}^N \mu_n^{y_n} (1 - \mu_n)^{1-y_n}$$

- Can also use a Gaussian **prior**  $p(\mathbf{w}) = \mathcal{N}(\mathbf{w} | \mathbf{0}, \lambda^{-1} \mathbf{I}_D)$  just like in probabilistic linear regression
- Can estimate  $\mathbf{w}$  via MLE, MAP, or (a somewhat hard to do) fully Bayesian inference

# Recap: Logistic Regression

- Logistic regression can be extended to more than 2 classes

$$p(y_n = k | \mathbf{x}_n, \mathbf{W}) = \frac{\exp(\mathbf{w}_k^\top \mathbf{x}_n)}{\sum_{\ell=1}^K \exp(\mathbf{w}_\ell^\top \mathbf{x}_n)} = \mu_{nk} \quad \text{and} \quad \sum_{\ell=1}^K \mu_{n\ell} = 1$$

- MLE/MAP for logistic/softmax does not have closed form solution (unlike linear regression case)
- Computing full posterior is intractable (since Bernoulli/multinoulli and Gaussian are not conjugate)
  - Laplace (Gaussian) approximation is one way to get an approximate posterior
- Predictive distribution is straightforward when using MLE/MAP
- Predictive distribution is intractable when using full posterior





# Generative Models for Supervised Learning

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

Here, we will model both inputs and outputs!



# Generative Classification

- Consider a classification problem with  $K \geq 2$  classes
- Assuming  $\theta$  to collectively denote all the params, the generative classification model is

$$p(y = k|\mathbf{x}, \theta) = \frac{p(\mathbf{x}, y = k|\theta)}{p(\mathbf{x}|\theta)}, \quad k = 1, \dots, K$$

- Note that the denominator  $p(\mathbf{x}|\theta) = \sum_{k=1}^K p(\mathbf{x}, y = k|\theta)$ , using sum rule of probability
- Can use the chain rule to re-express the above as

$$p(y = k|\mathbf{x}, \theta) = \frac{p(y = k|\theta)p(\mathbf{x}|y = k, \theta)}{p(\mathbf{x}|\theta)}$$

- This depends on two quantities
  - $p(y = k|\theta)$ : The **class-marginal distribution** (also called “class prior”)
  - $p(\mathbf{x}|y = k, \theta)$ : The **class-conditional distribution** of the inputs
- Generative classification requires first estimating the parameters  $\theta$  of these two distributions



# Generative Classification: Estimating Class-Marginal Distribution

- Estimating the class-marginal is usually straightforward in generative classification
- The class marginal distribution is (has to be!) a discrete distribution (**multinoulli**)

$$p(y|\pi) = \text{multinoulli}(y|\pi_1, \dots, \pi_K) = \prod_{k=1}^K \pi_k^{\mathbb{I}[y=k]}$$

where multinoulli parameters  $\pi = [\pi_1, \dots, \pi_K]$ ,  $\sum_{k=1}^K \pi_k = 1$ , and  $\pi_k = p(y = k)$

- Given  $N$  labeled training examples  $\{(\mathbf{x}_n, y_n)\}_{n=1}^N$ , MLE for  $\pi$  (won't depend on  $\mathbf{x}_n$ 's) will be

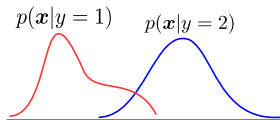
$$\pi_{MLE} = \arg \max_{\pi} \sum_{n=1}^N \log p(y_n|\pi)$$

.. which gives  $\pi_k = N_k/N$  (**exercise: verify**) where  $N_k = \sum_{n=1}^N \mathbb{I}[y_n = k]$

- Note: If MAP (or full posterior) is needed, we can use a **Dirichlet** prior distribution on  $\pi$ 
  - **Another exercise:** Try to derive the MAP estimate of  $\pi$  and also the full posterior (**good news:** multinoulli and Dirichlet are conjugate to each other, so full posterior is easy)



# Generative Classification: Estimating Class-Conditional Distr.



- We usually assume an appropriate class-conditional  $p(\mathbf{x}|y = k, \theta)$  for the inputs, e.g.,
  - If  $\mathbf{x} \in \mathbb{R}^D$ , then a  $D$ -dim Gaussian  $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$  may be appropriate (here  $\theta = (\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$ )
  - If  $\mathbf{x} \in \{0, 1\}^D$ , then a  $D$ -dim Bernoulli may be appropriate
  - Can choose more flexible distributions as well (any density estimation model for that matter)
- For the assumed class-conditional, we can do MLE/MAP estimation or learn full posterior for  $\theta$
- **An issue:** When  $D$  is large, we may need to estimate a **huge number of parameters**, e.g.,
  - A  $D$ -dim Gaussian will have  $D$  params for mean and  $O(D^2)$  params for covariance matrix
  - Some workarounds: Regularize well; assume **diagonal (or same) covariance** for all classes, which means that the **features are independent given the class** (used in “naïve” Bayes models)

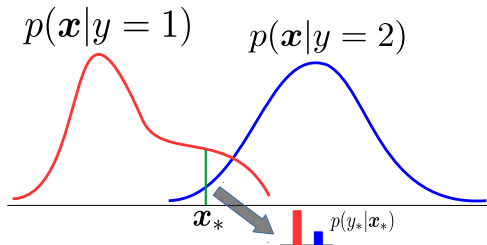


# Generative Classification: The Prediction Rule

- Suppose we've estimated the parameters of  $p(y = k|\theta)$  and  $p(\mathbf{x}|y = k, \theta)$  (assuming MLE/MAP)
- The “most likely” class for a test input  $\mathbf{x}_*$  will be (skipping  $\theta$  from the notation)

$$y_* = \arg \max_k p(y_* = k|\mathbf{x}_*) = \arg \max_k \frac{p(y_* = k)p(\mathbf{x}_*|y_* = k)}{p(\mathbf{x}_*)} = \arg \max_k p(y_* = k)p(\mathbf{x}_*|y_* = k)$$

- If  $p(y = k)$  is the same for all the classes then, we simple compare  $p(\mathbf{x}|y = k)$



# Generative Classification using Gaussian Class-conditionals

- Recall our generative classification model  $p(y = k|\mathbf{x}) = \frac{p(y=k)p(\mathbf{x}|y=k)}{p(\mathbf{x})}$
- Assume each class-conditional to be a Gaussian

$$p(\mathbf{x}|y = k) = \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k) = \frac{1}{\sqrt{(2\pi)^D |\boldsymbol{\Sigma}_k|}} \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right]$$

- Class-marginal is multinoulli (already saw):  $p(y = k) = \pi_k \in (0, 1)$ , s.t..  $\sum_{k=1}^K \pi_k = 1$
- Parameters  $\theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$  can be estimated using MLE/MAP/Bayesian approach
  - We also saw estimation of  $\pi_k$ 's.  $(\boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k)$  can be found via Gaussian parameter estimation
- If using MLE/MAP estimate of  $\theta$ , the predictive distribution will be

$$p(y_* = k|\mathbf{x}_*, \theta) = \frac{\pi_k |\boldsymbol{\Sigma}_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x}_* - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_* - \boldsymbol{\mu}_k) \right]}{\sum_{k=1}^K \pi_k |\boldsymbol{\Sigma}_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x}_* - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x}_* - \boldsymbol{\mu}_k) \right]}$$

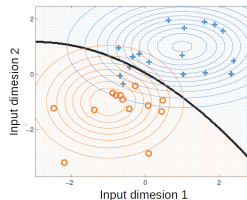


# Decision Boundaries

- The generative classification prediction rule we saw had

$$p(y = k | \mathbf{x}, \theta) = \frac{\pi_k |\Sigma_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x} - \mu_k)^\top \Sigma_k^{-1} (\mathbf{x} - \mu_k) \right]}{\sum_{k=1}^K \pi_k |\Sigma_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x} - \mu_k)^\top \Sigma_k^{-1} (\mathbf{x} - \mu_k) \right]}$$

- The decision boundary between any pair of classes will be.. a **quadratic curve**



- Reason: For any two classes  $k$  and  $k'$ , at the decision boundary  $p(y = k | \mathbf{x}) = p(y = k' | \mathbf{x})$ . Thus

$$(\mathbf{x} - \mu_k)^\top \Sigma_k^{-1} (\mathbf{x} - \mu_k) - (\mathbf{x} - \mu_{k'})^\top \Sigma_{k'}^{-1} (\mathbf{x} - \mu_{k'}) = 0 \quad (\text{ignoring terms that don't depend on } \mathbf{x})$$

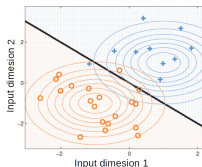
.. defines the decision boundary, which is a quadratic function of  $\mathbf{x}$  (this model is popularly known as **Quadratic Discriminant Analysis**)

# Decision Boundaries

- Let's again consider the generative classification prediction rule with Gaussian class-conditionals

$$p(y = k | \mathbf{x}, \theta) = \frac{\pi_k |\boldsymbol{\Sigma}_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right]}{\sum_{k=1}^K \pi_k |\boldsymbol{\Sigma}_k|^{-1/2} \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}_k^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right]}$$

- Let's assume all classes to have the **same covariance** (i.e., same shape/size), i.e.,  $\boldsymbol{\Sigma}_k = \boldsymbol{\Sigma}$ ,  $\forall k$
- Now the decision boundary between any pair of classes will be.. **linear**



- Reason: For any two classes  $k$  and  $k'$ , at the decision boundary  $p(y = k | \mathbf{x}) = p(y = k' | \mathbf{x})$ . Thus

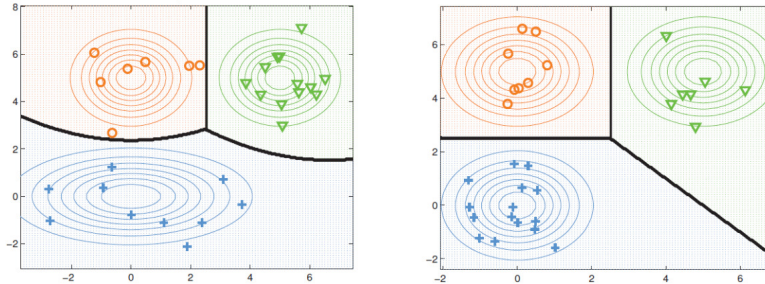
$$(\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) - (\mathbf{x} - \boldsymbol{\mu}_{k'})^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_{k'}) = 0 \quad (\text{ignoring terms that don't depend on } \mathbf{x})$$

.. terms quadratic in  $\mathbf{x}$  cancel out in this case and we get a linear function of  $\mathbf{x}$  (this model is popularly known as **Linear or “Fisher” Discriminant Analysis**)



# Decision Boundaries

- Depending on the form of the covariance matrices, the boundaries can be quadratic/linear



# A Closer Look at the Linear Case

- For the linear case (when  $\Sigma_k = \Sigma$ ), we have

$$p(y = k | \mathbf{x}, \theta) \propto \pi_k \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \Sigma^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right]$$

- Expanding further, we can write the above as

$$p(y = k | \mathbf{x}, \theta) \propto \exp \left[ \boldsymbol{\mu}_k^\top \Sigma^{-1} \mathbf{x} - \frac{1}{2} \boldsymbol{\mu}_k^\top \Sigma^{-1} \boldsymbol{\mu}_k + \log \pi_k \right] \exp \left[ \mathbf{x}^\top \Sigma^{-1} \mathbf{x} \right]$$

- Therefore, the above posterior class probability can be written as

$$p(y = k | \mathbf{x}, \theta) = \frac{\exp [\mathbf{w}_k^\top \mathbf{x} + b_k]}{\sum_{k=1}^K \exp [\mathbf{w}_k^\top \mathbf{x} + b_k]}$$

where  $\mathbf{w}_k = \Sigma^{-1} \boldsymbol{\mu}_k$  and  $b_k = -\frac{1}{2} \boldsymbol{\mu}_k^\top \Sigma^{-1} \boldsymbol{\mu}_k + \log \pi_k$

- Interestingly, this has exactly the same form as the **softmax classification** model (saw it in last class), which is a discriminative model, as opposed to a generative model.



# A Very Special Case: Prototype based Classification

- We can get a non-probabilistic analogy for the Gaussian generative classification model
- Note the decision rule when  $\Sigma_k = \Sigma$

$$\begin{aligned}\hat{y} = \arg \max_k p(y = k | \mathbf{x}) &= \arg \max_k \pi_k \exp \left[ -\frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k) \right] \\ &= \arg \max_k \log \pi_k - \frac{1}{2} (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)\end{aligned}$$

- Further, let's assume the classes to be of equal size, i.e.,  $\pi_k = 1/K$ . Then we will have

$$\hat{y} = \arg \min_k (\mathbf{x} - \boldsymbol{\mu}_k)^\top \boldsymbol{\Sigma}^{-1} (\mathbf{x} - \boldsymbol{\mu}_k)$$

- This is equivalent to assigning  $\mathbf{x}$  to the “closest” class in terms of a **Mahalanobis distance**
  - The covariance matrix “modulates” how the distances are computed



# Generative Classification: Some Comments

- A simple but powerful approach to probabilistic classification
- Especially easy to learn if class-conditionals are simple
  - E.g., Gaussian with diagonal covariances  $\Rightarrow$  Gaussian naïve Bayes
  - Another popular model is multinomial naïve Bayes (widely used for document classification)
  - The so-called “naïve” models assume features to be independent conditioned on  $y$ , i.e.,

$$p(\mathbf{x}|\theta_y) = \prod_{d=1}^D p(x_d|\theta_y) \quad (\text{significantly reduces the number of parameters to be estimated})$$

- Generative classification models work seamlessly for any number of classes
- Can choose the form of class-conditionals  $p(\mathbf{x}|y)$  based on the type of inputs  $\mathbf{x}$
- Can handle missing data (e.g., if some part of the input  $\mathbf{x}$  is missing) or missing labels
- Generative models are also useful for unsupervised and semi-supervised learning (will look at later)



# Generative Classification: Some Comments

- Estimating the class-conditional distributions  $p(\mathbf{x}|y)$  reliably is important
- In general, the class-conditional  $p(\mathbf{x}|y)$  may have **too many parameter to be estimated** (e.g., if we use **full covariance** Gaussians when the class-conditionals are Gaussians)
  - Can be difficult if we don't have enough data for each class
- Assuming shared and/or diagonal covariance for each Gaussian can reduce the number of params
  - .. or the “naïve” assumptions
- MLE for parameter estimation in these models can be prone to overfitting
  - Need to regularize the model properly to prevent that
  - A MAP or fully Bayesian approach can help (will need prior on the parameters)
- A good density estimation model is necessary for generative classification model to work well



# Probabilistic Models for Supervised Learning: Wrapping Up

- Both discriminative and generative models estimate the conditional distribution  $p(y|\mathbf{x})$
- Note that both are basically doing density estimation for learning  $p(y|\mathbf{x})$  but in different ways
- Discriminative models directly model  $p(y|\mathbf{x})$  via some parameters (say  $\mathbf{w}$  if using linear model)

$$p(y|\mathbf{w}, \mathbf{x}) = \mathcal{N}(\mathbf{w}^\top \mathbf{x}, \beta^{-1}) \quad (\text{prob. linear regression})$$

$$p(y|\mathbf{w}, \mathbf{x}) = \text{Bernoulli}[\sigma(\mathbf{w}^\top \mathbf{x})] \quad (\text{prob. linear binary classification})$$

- These parameters can then be estimated via MLE, MAP, or fully Bayesian inference
- Generative classification models define  $p(y|\mathbf{x})$  as

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

and estimate the parameters of the class-marginal and class-conditional distributions

- Note: Can use generative models for doing **regression** as well (will be an exercise)

