

# Probabilistic Models for Supervised Learning (Contd.)

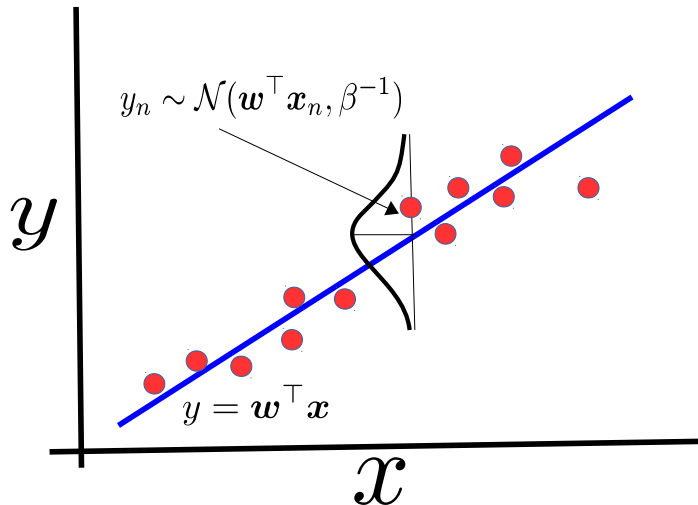
Piyush Rai

Introduction to Machine Learning (CS771A)

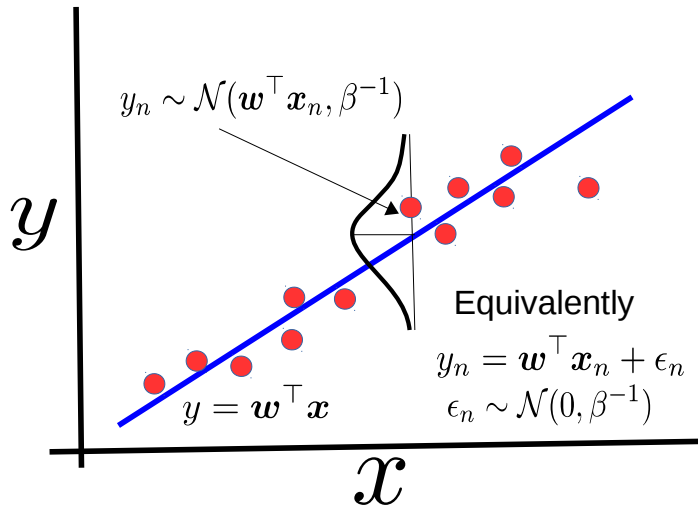
August 21, 2018



# Recap: Probabilistic Linear Regression

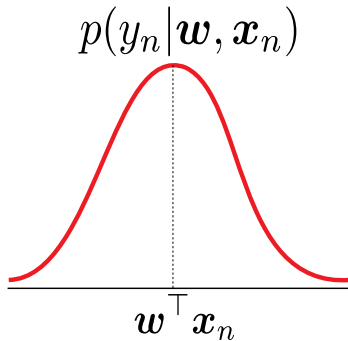


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## The Likelihood

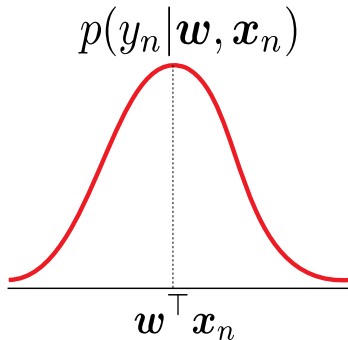


$$p(y_n | w, x_n) = \mathcal{N}(y_n | w^\top x_n, \beta^{-1}) = \sqrt{\frac{\beta}{2\pi}} \exp \left[ -\frac{\beta}{2} (y_n - w^\top x_n)^2 \right]$$



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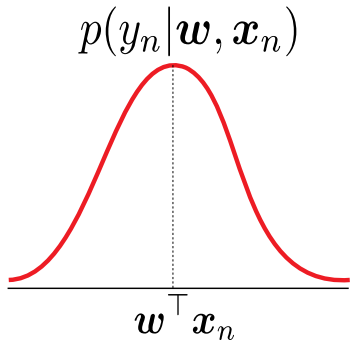


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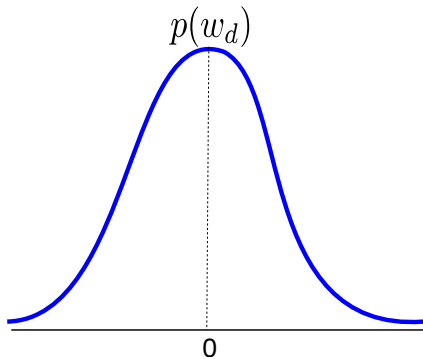
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$$\left( \frac{\beta}{2\pi} \right)^{N/2} \exp \left[ -\frac{\beta}{2} \sum_{n=1}^N (y_n - w^\top x_n)^2 \right] = \frac{1}{\sqrt{\det(2\pi\beta^{-1}\mathbf{I}_N)}} \exp \left[ -\frac{\beta}{2} (\mathbf{y} - \mathbf{X}w)^\top (\mathbf{y} - \mathbf{X}w)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

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## The Prior

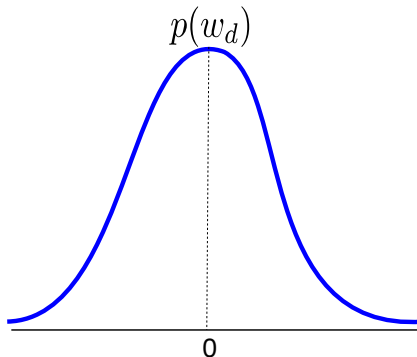


$$p(w_d) = \mathcal{N}(w_d|0, \lambda^{-1}) = \sqrt{\frac{\lambda}{2\pi}} \exp \left[ -\frac{\lambda}{2} w_d^2 \right]$$

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

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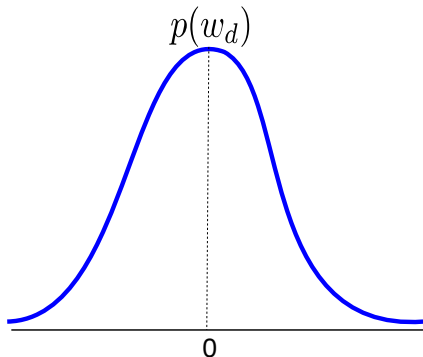
$$p(\mathbf{w}) = \prod_{d=1}^D \mathcal{N}(w_d|0, \lambda^{-1}) = \underbrace{\mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1} \mathbf{I}_D)}_{D\text{-dim pdf}}$$

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# 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

$$\hat{\mathbf{w}}_{MLE} = \arg \max_{\mathbf{w}} \log p(\mathbf{y}|\mathbf{X}, \mathbf{w})$$



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

$$p(\mathbf{w}|\mathbf{y}, \mathbf{X}) = \mathcal{N}(\boldsymbol{\mu}_N, \boldsymbol{\Sigma}_N)$$



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

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

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



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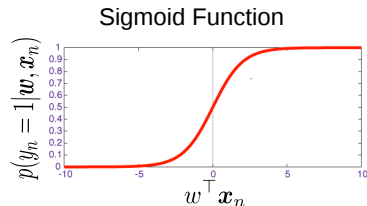
- For Bayesian approach, mean of predicted output is  $\mathbf{w}_N^\top \mathbf{x}_*$ , variance is  $\beta^{-1} + \mathbf{x}_*^\top \Sigma_N \mathbf{x}_*$  (note the different variance for each test input, unlike MLE/MAP prediction)



# Recap: Logistic Regression

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

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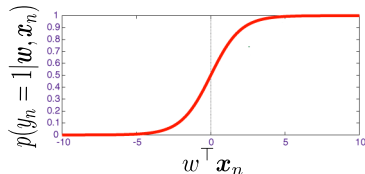


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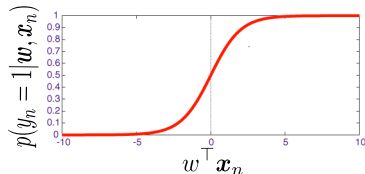


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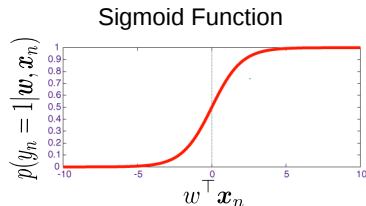
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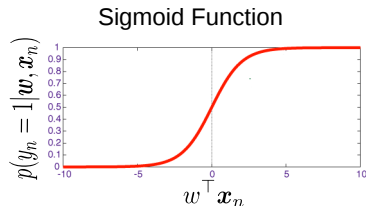
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- Can also use a Gaussian **prior**  $p(\mathbf{w}) = \mathcal{N}(\mathbf{w}|\mathbf{0}, \lambda^{-1}\mathbf{I}_D)$  just like in probabilistic linear regression
- Can estimate  $\mathbf{w}$  via MLE, MAP, or (a somewhat hard to do) fully Bayesian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

# Recap: Logistic Regression

- Logistic regression can be extended to more than 2 classes

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



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- 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)



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# 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!



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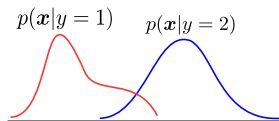
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  - **Another exercise:** Try to derive the MAP estimate of  $\pi$  and also the full posterior (**good news:** multinoulli and Dirichlet are conjugate to each other, so full posterior is easy)



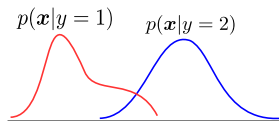
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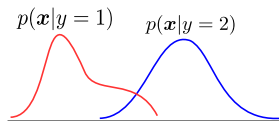


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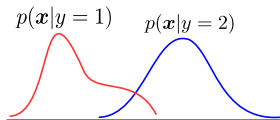
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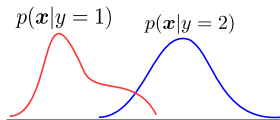
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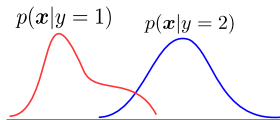


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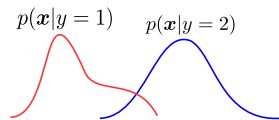
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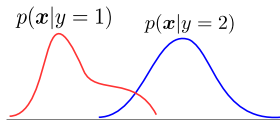


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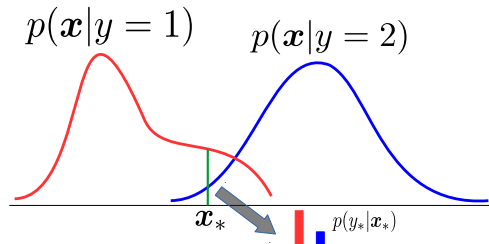


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- If  $p(y = k)$  is the same for all the classes then, we simple compare  $p(\mathbf{x}|y = k)$





# Generative Classification using Gaussian Class-conditionals

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- Parameters  $\theta = \{\pi_k, \boldsymbol{\mu}_k, \boldsymbol{\Sigma}_k\}_{k=1}^K$  can be estimated using MLE/MAP/Bayesian approach



# 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..  $\sum_{k=1}^K \pi_k = 1$
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- 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

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- The decision boundary between any pair of classes will be..

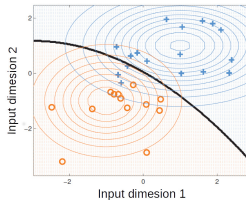


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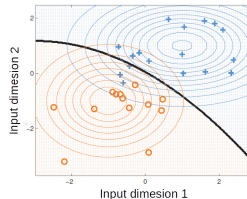


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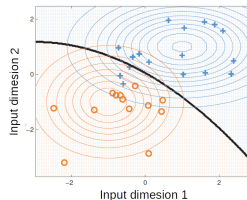


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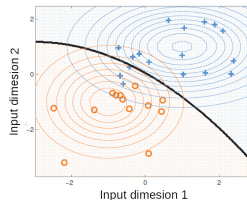


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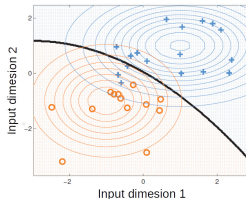


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# Decision Boundaries

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

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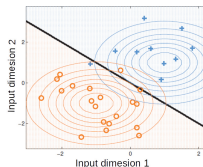


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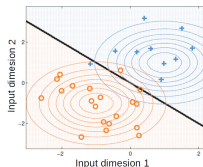


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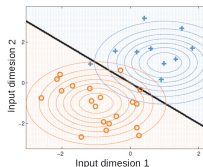


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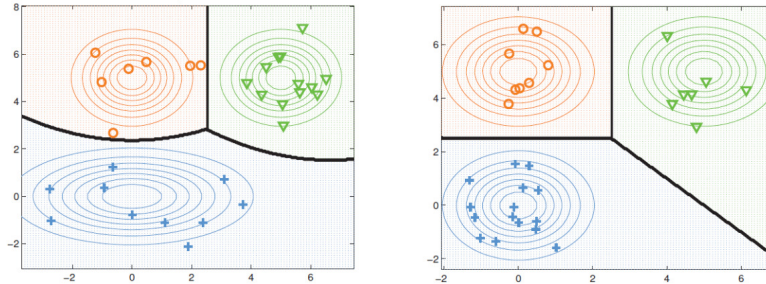
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.. terms quadratic in  $\mathbf{x}$  cancel out in this case and we get a linear function of  $\mathbf{x}$  (this model is popularly known as **Linear or “Fisher” Discriminant Analysis**)



# 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

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



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

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where  $\mathbf{w}_k = \Sigma^{-1} \boldsymbol{\mu}_k$





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- 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



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- This is equivalent to assigning  $\mathbf{x}$  to the “closest” class in terms of a [Mahalanobis distance](#)



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

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

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

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

- 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





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- Generative models are also useful for unsupervised and semi-supervised learning (will look at later)

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- A good density estimation model is necessary for generative classification model to work well



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

