Foundations of Machine Learning
Classification: decisions and discriminants

Srinandan (“Sri”) Dasmahapatra

2-class classification: determine which class a given input $X=x$ belongs to

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decision boundary at equal posterior probability for either class, which are:

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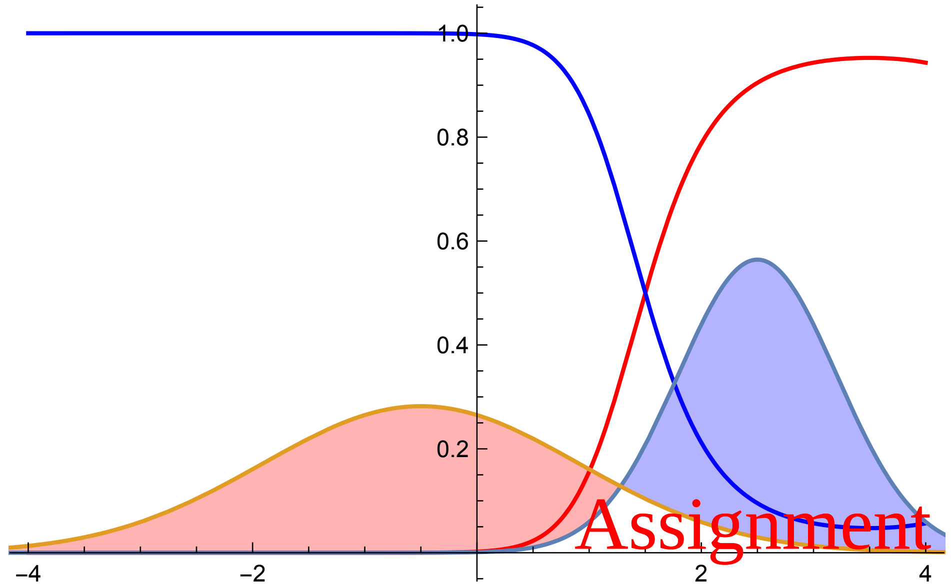

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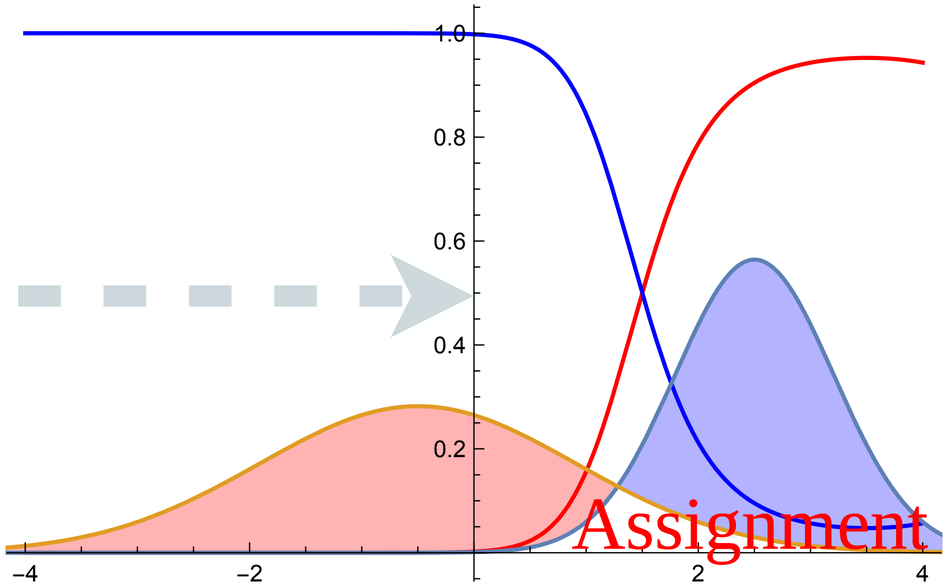

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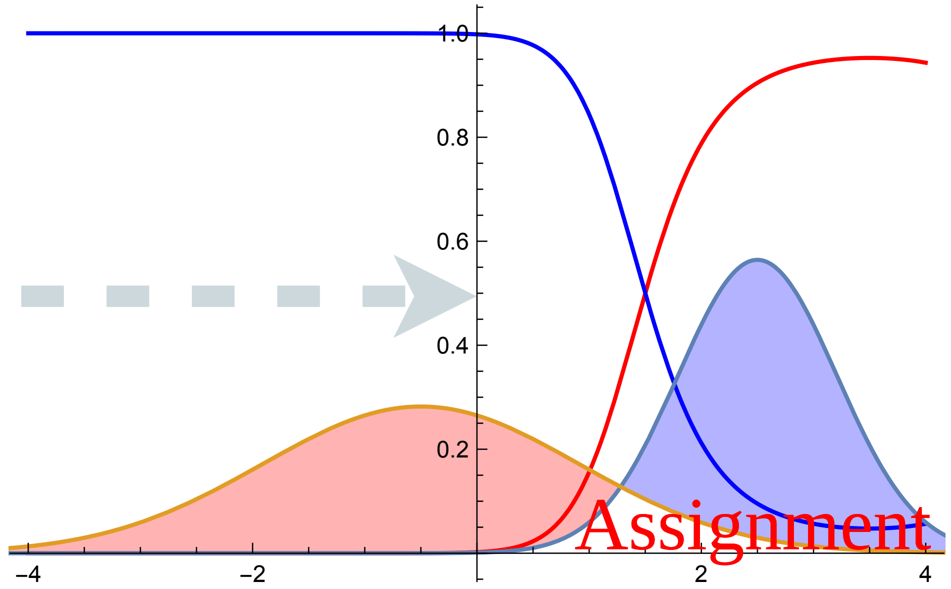

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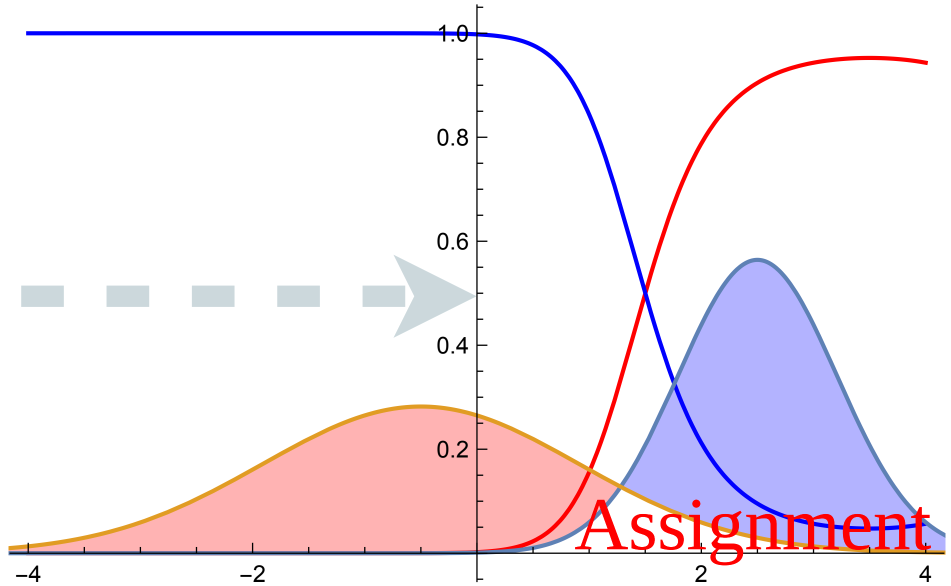

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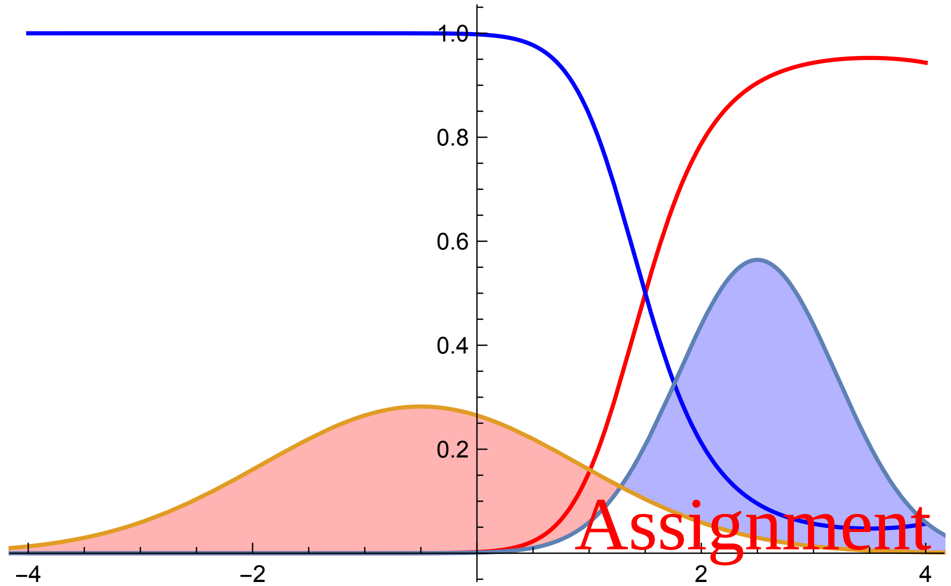

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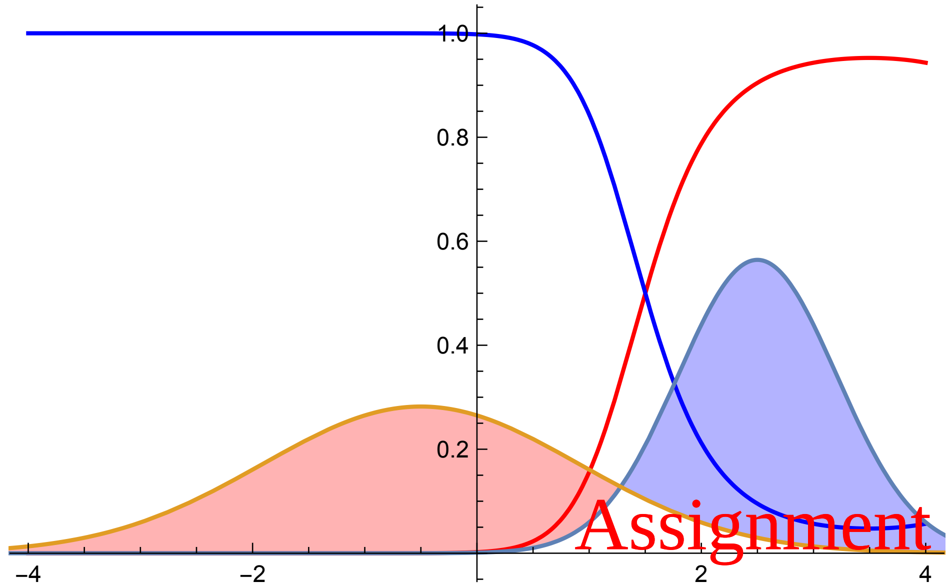

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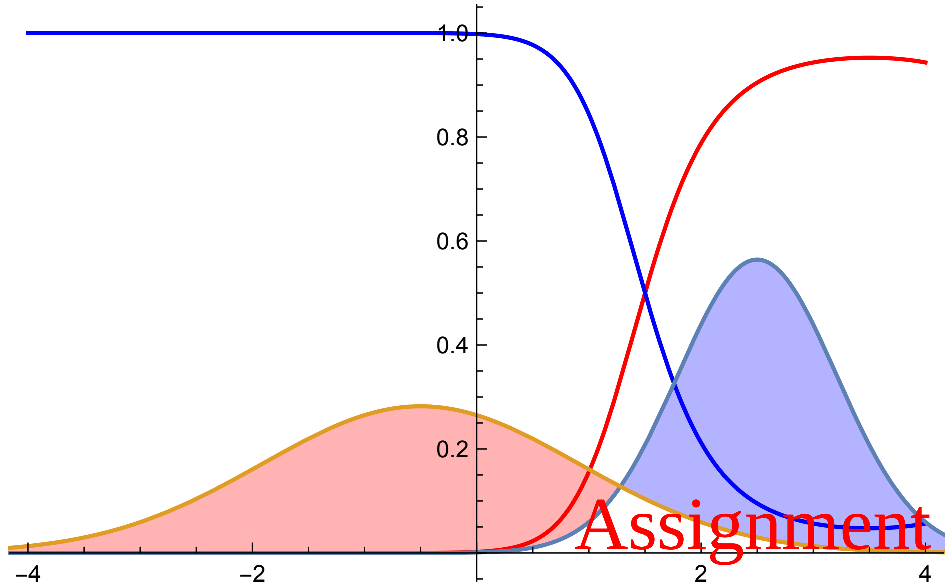

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$$\text{log-odds} = \ln\left(\frac{P(X=x|C=+)}{P(X=x|C=-)}\right) + \ln\left(\frac{P(C=+)}{P(C=-)}\right)$$

data dependent (likelihood)

data independent (prior)

Decision boundaries from probability distributions: zero log-odds: $0 = g_+(\mathbf{x}) - g_-(\mathbf{x}) = f(\mathbf{x}; \theta) + \theta_0$

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- This is 2-class softmax (logistic) regression

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- Did not seek a decision boundary, just an argmax

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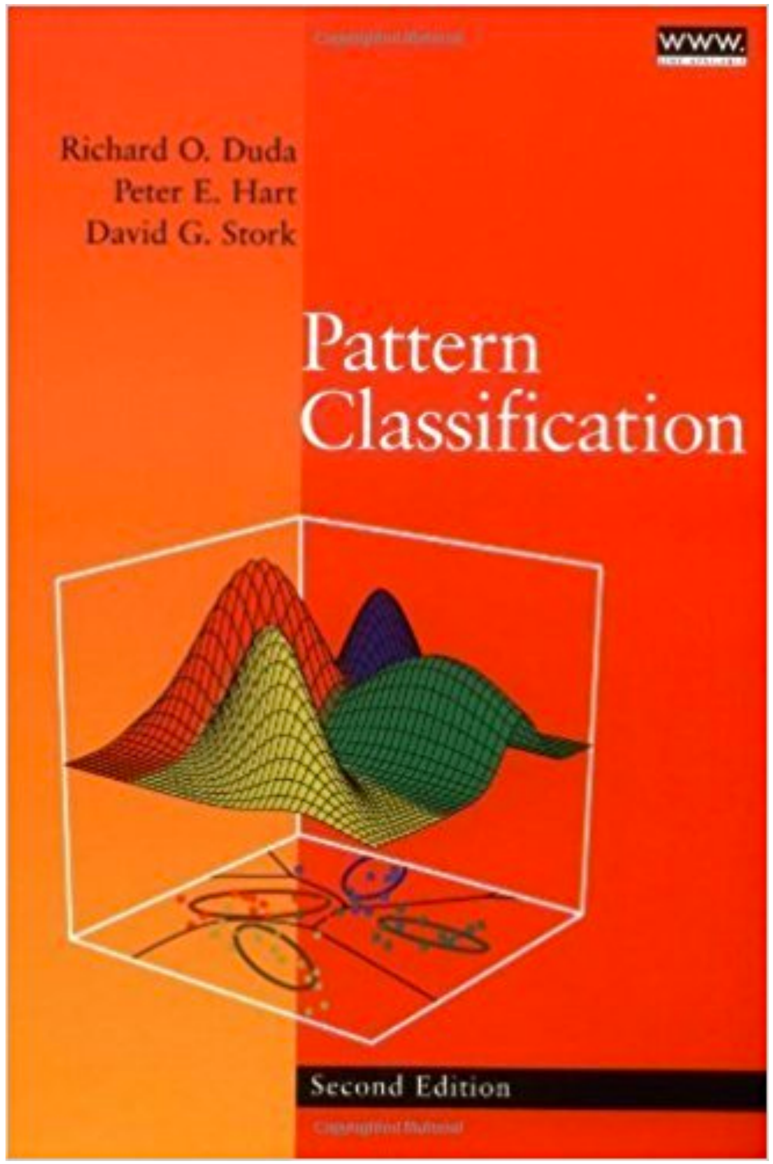

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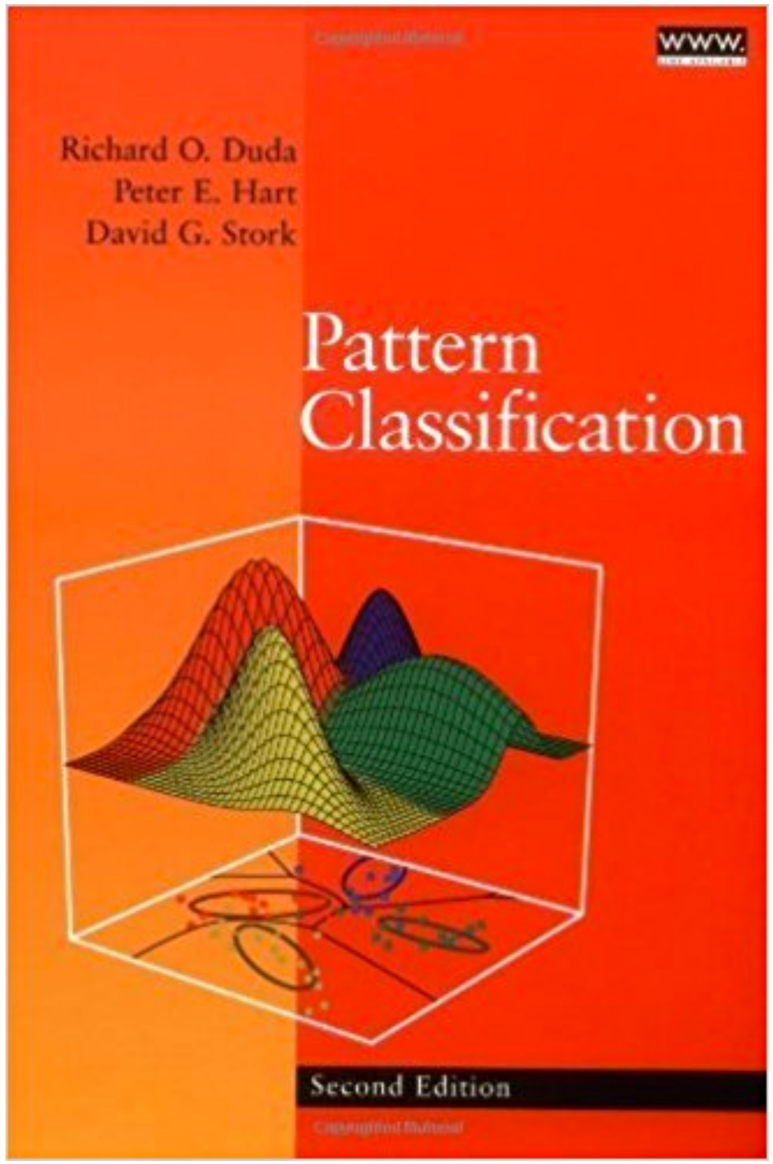

Notice the contours and line segments at the bottom of the cover graphic

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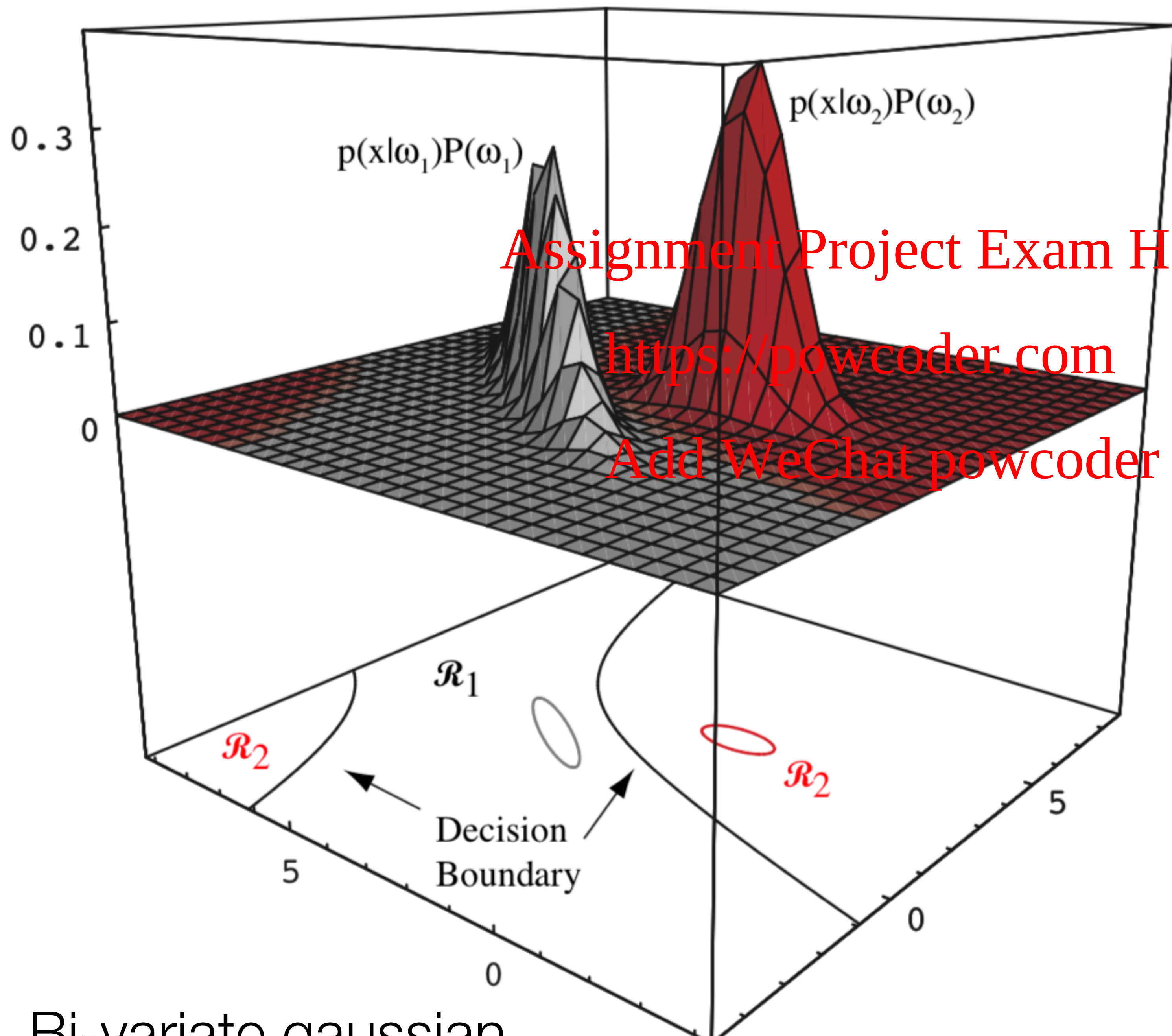
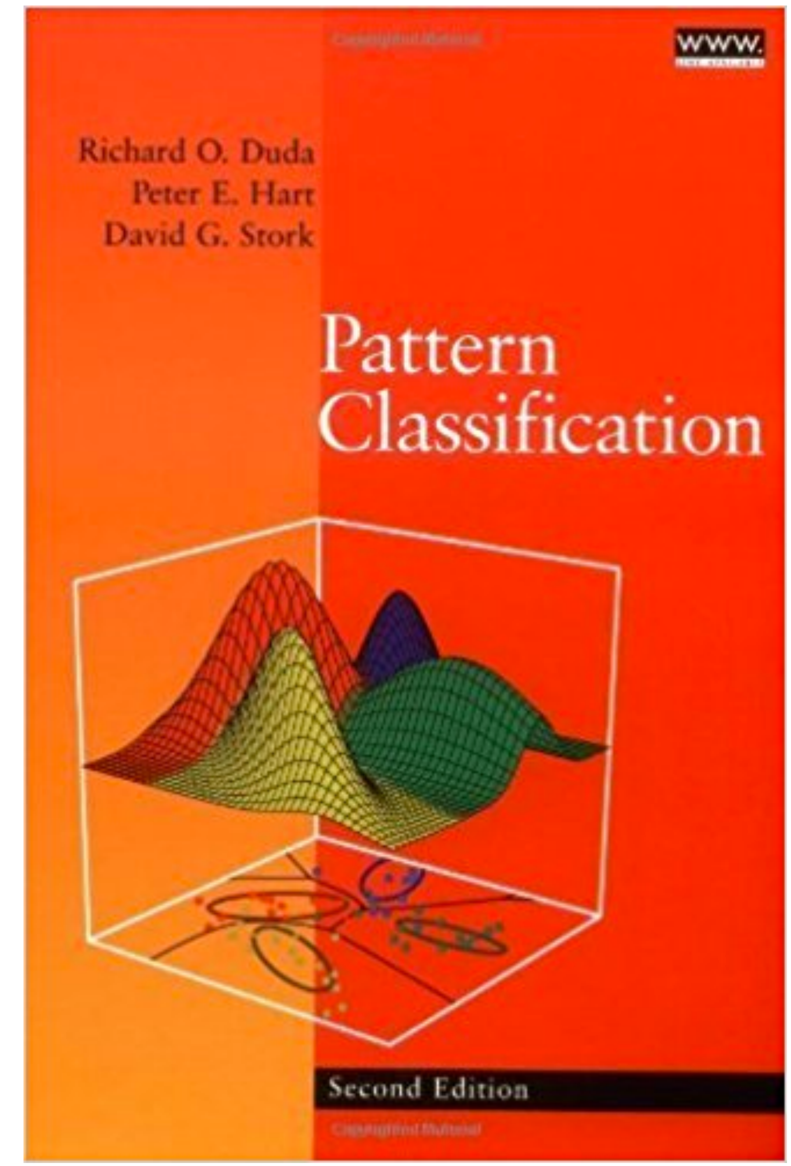


Bi-variate gaussian



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Log of ratio of two multi-dimensional Gaussians

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For 2D features

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Log-odds (no prior) for 2-class classification

$$\ln\left(\frac{p(\boldsymbol{x}|C_+)}{p(\boldsymbol{x}|C_-)}\right) = \ln\left(\frac{|\Lambda_+|}{|\Lambda_-|}\right) + \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_-)^T\Lambda_-(\boldsymbol{x}-\boldsymbol{\mu}_-) - \frac{1}{2}(\boldsymbol{x}-\boldsymbol{\mu}_+)^T\Lambda_+(\boldsymbol{x}-\boldsymbol{\mu}_+)$$

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Your turn: derive the linear equation

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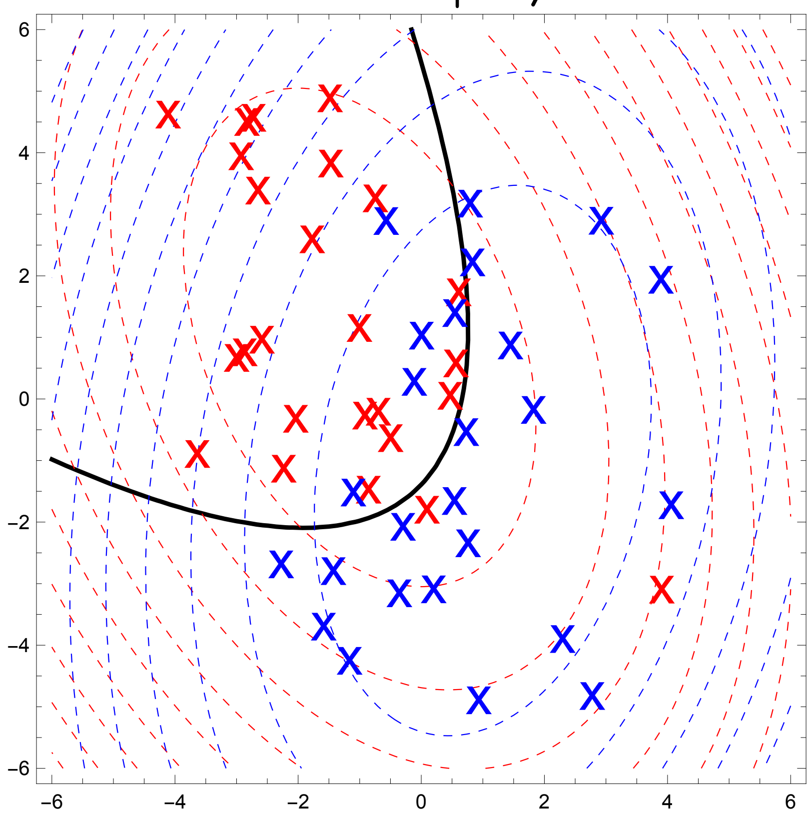

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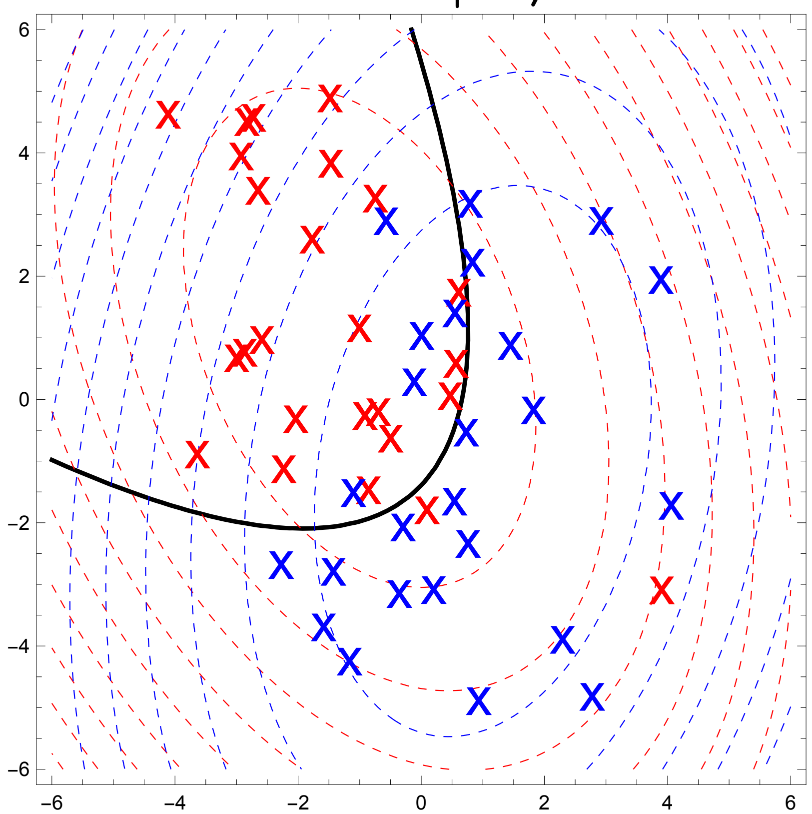

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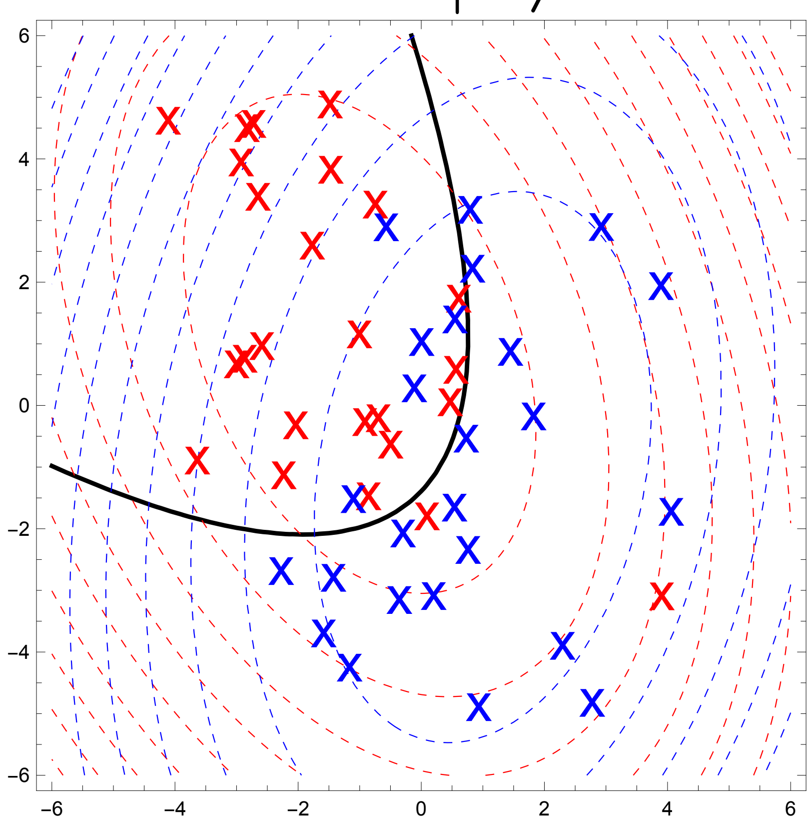

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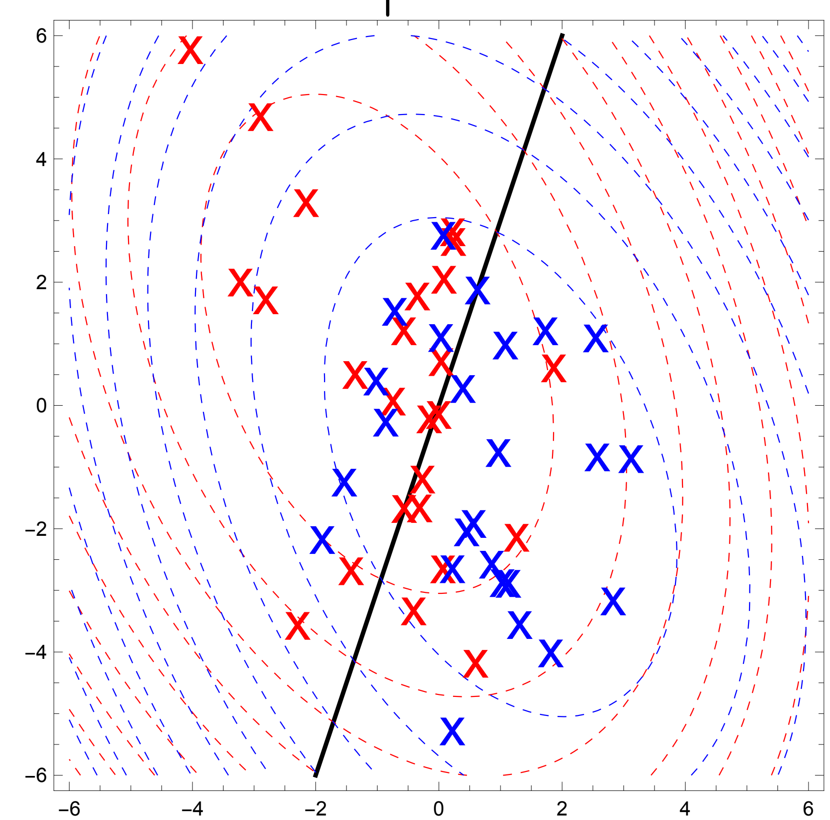
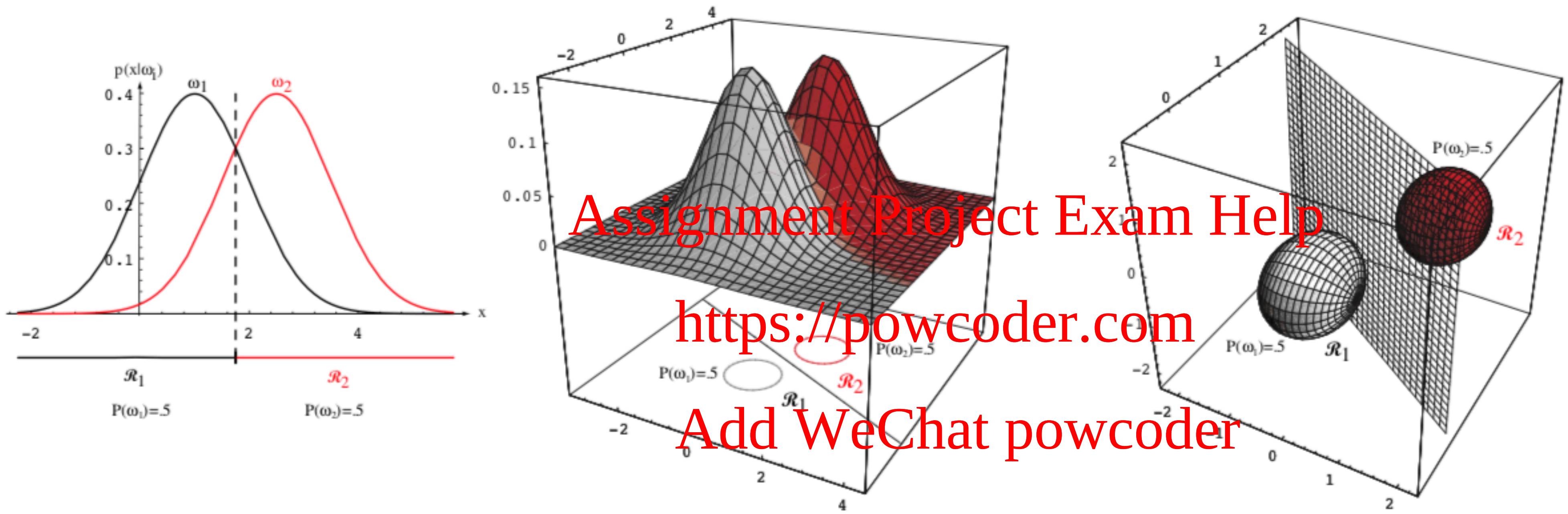
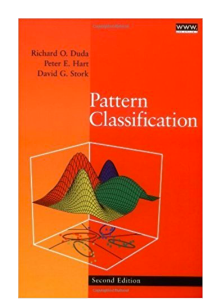


Discriminants for Gaussians for equal priors: data distribution equally divided

1-dim 2-dim 3-dim

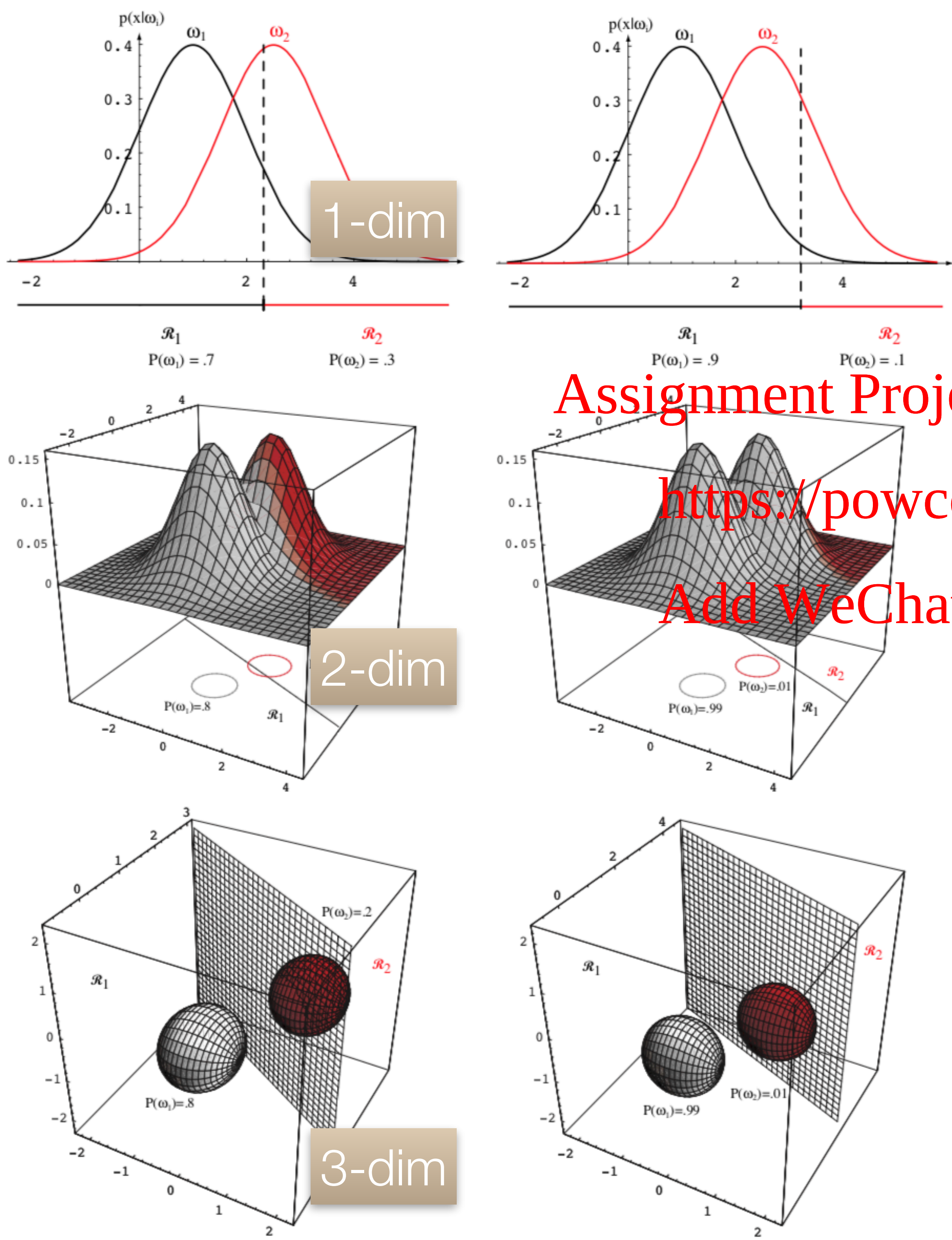


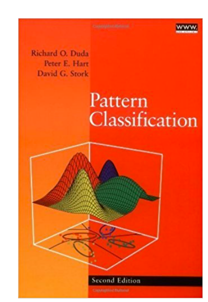
Equal priors: $\log(P_a/P_b) = 0$



From Duda and Hart

Discriminants for Gaussians: unequal priors shifts decision boundary by $\log(P_a/P_b)$





From Duda and Hart

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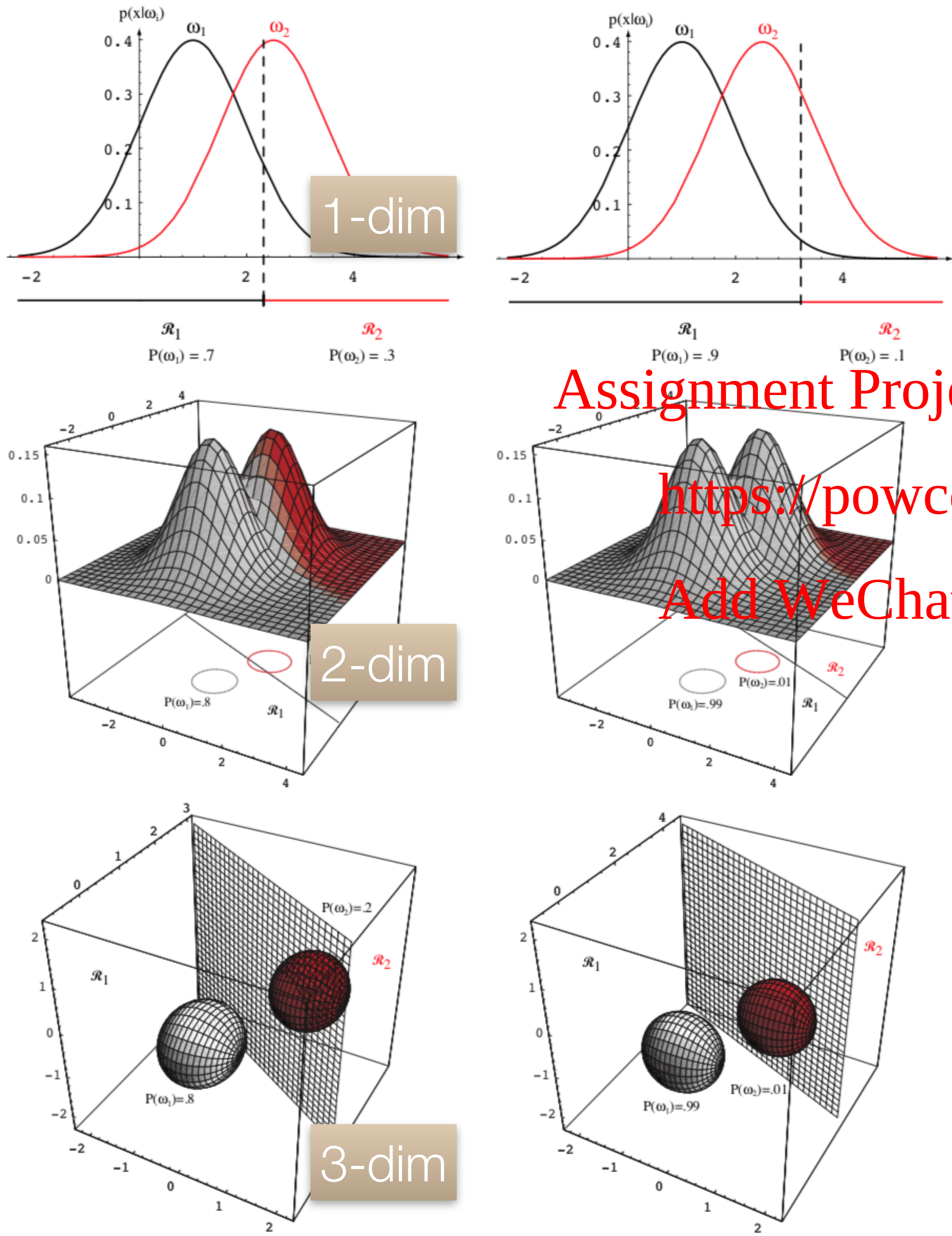
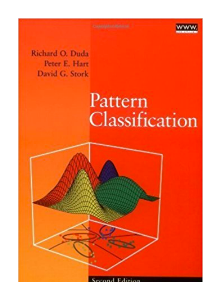


Prior overrides data distributions



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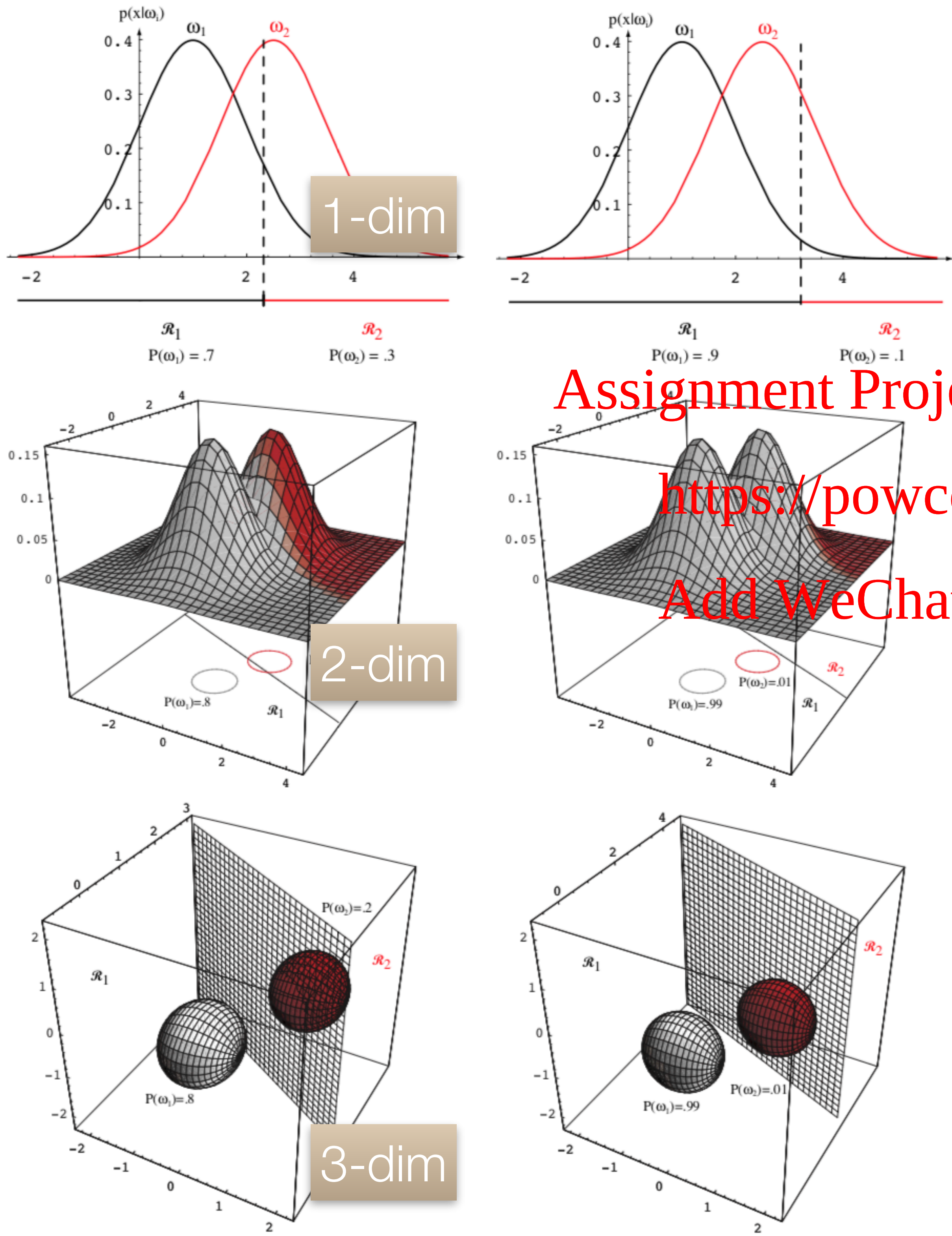
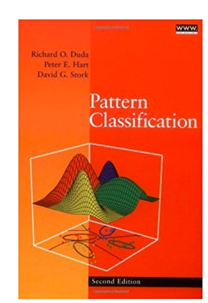


Prior overrides data distributions

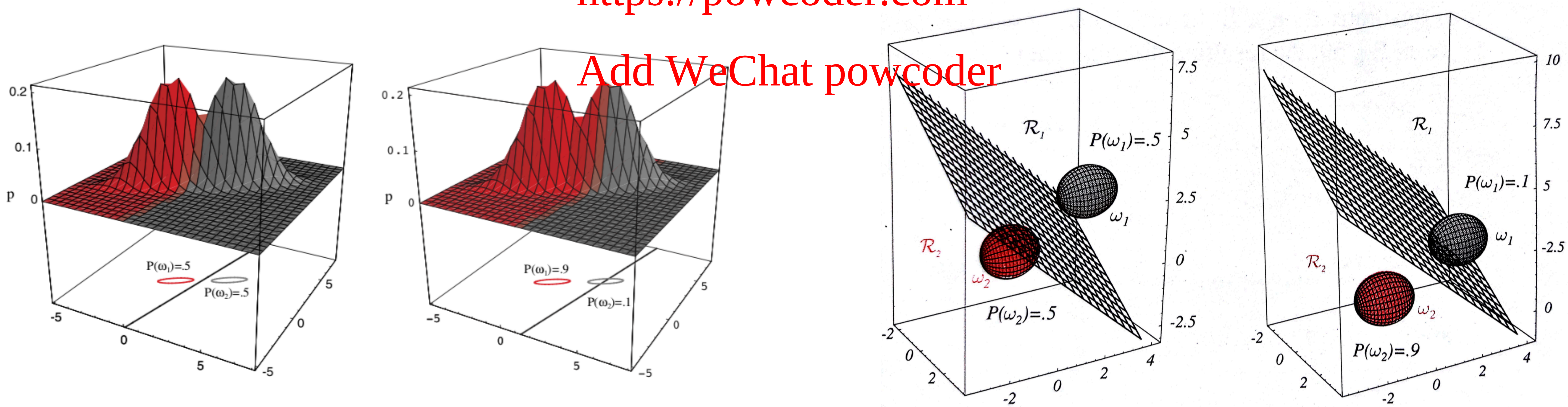
Notice how far boundary shifts

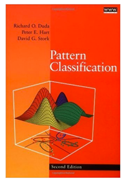


From Duda and Hart

Decision boundaries not perpendicular to line joining means if covariance matrix not proportional to the identity matrix

$$\boldsymbol{w} = \Sigma^{-1}(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)$$





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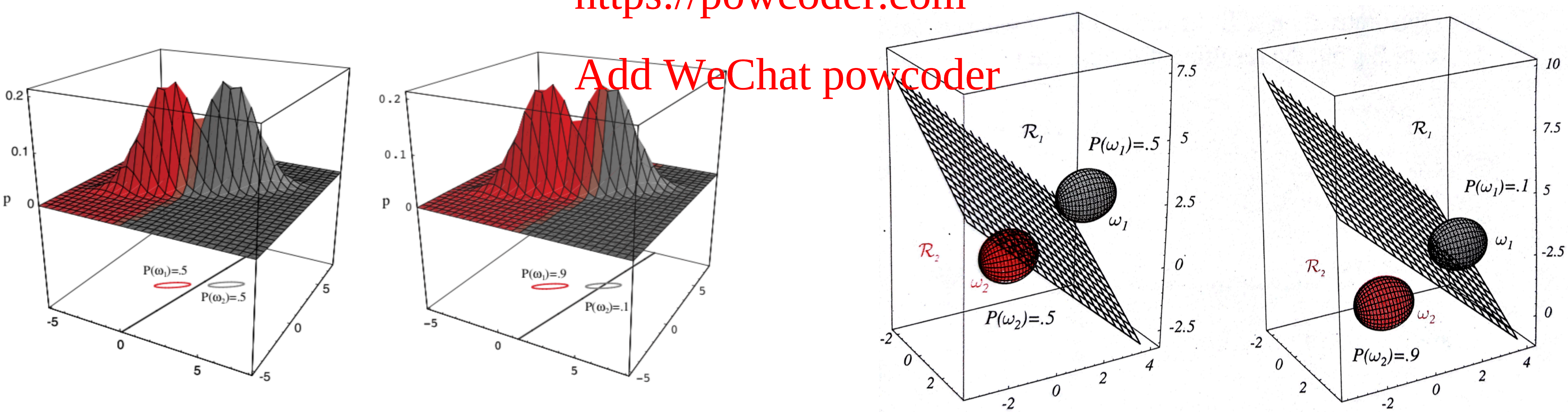
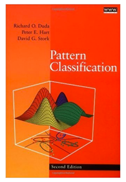
Decision boundaries not perpendicular to line joining means if covariance matrix not proportional to the identity matrix

$$g_+(\boldsymbol{x}) - g_-(\boldsymbol{x}) \quad = \quad \ln \frac{P(C_+)}{P(C_-)} + (\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)^T \Lambda \boldsymbol{x} + \boldsymbol{x}\text{-independent term}$$

$$\boldsymbol{w} = \Sigma^{-1}(\boldsymbol{\mu}_+ - \boldsymbol{\mu}_-)$$





From Duda and Hart

Distinctiveness relative to natural variation measured by distance between class means scaled by standard deviation:

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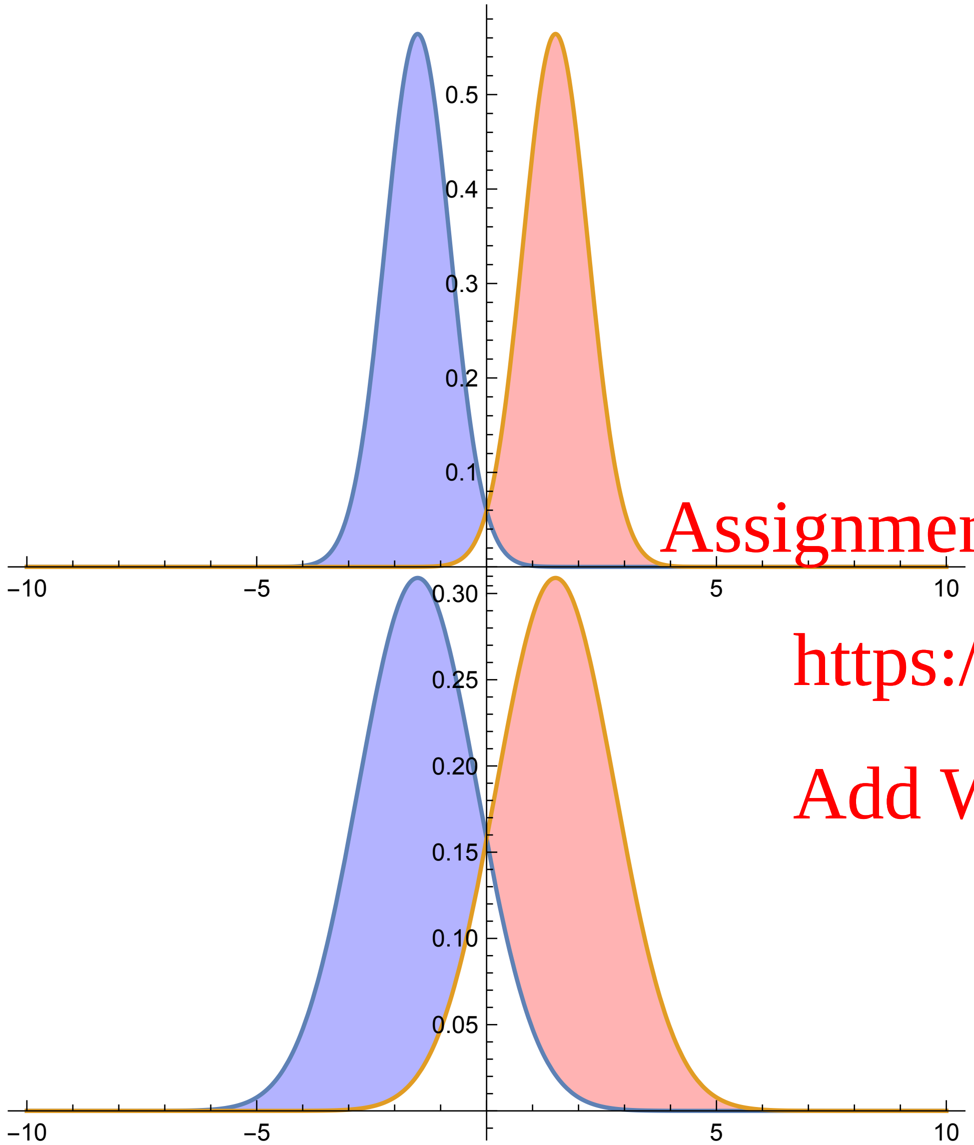

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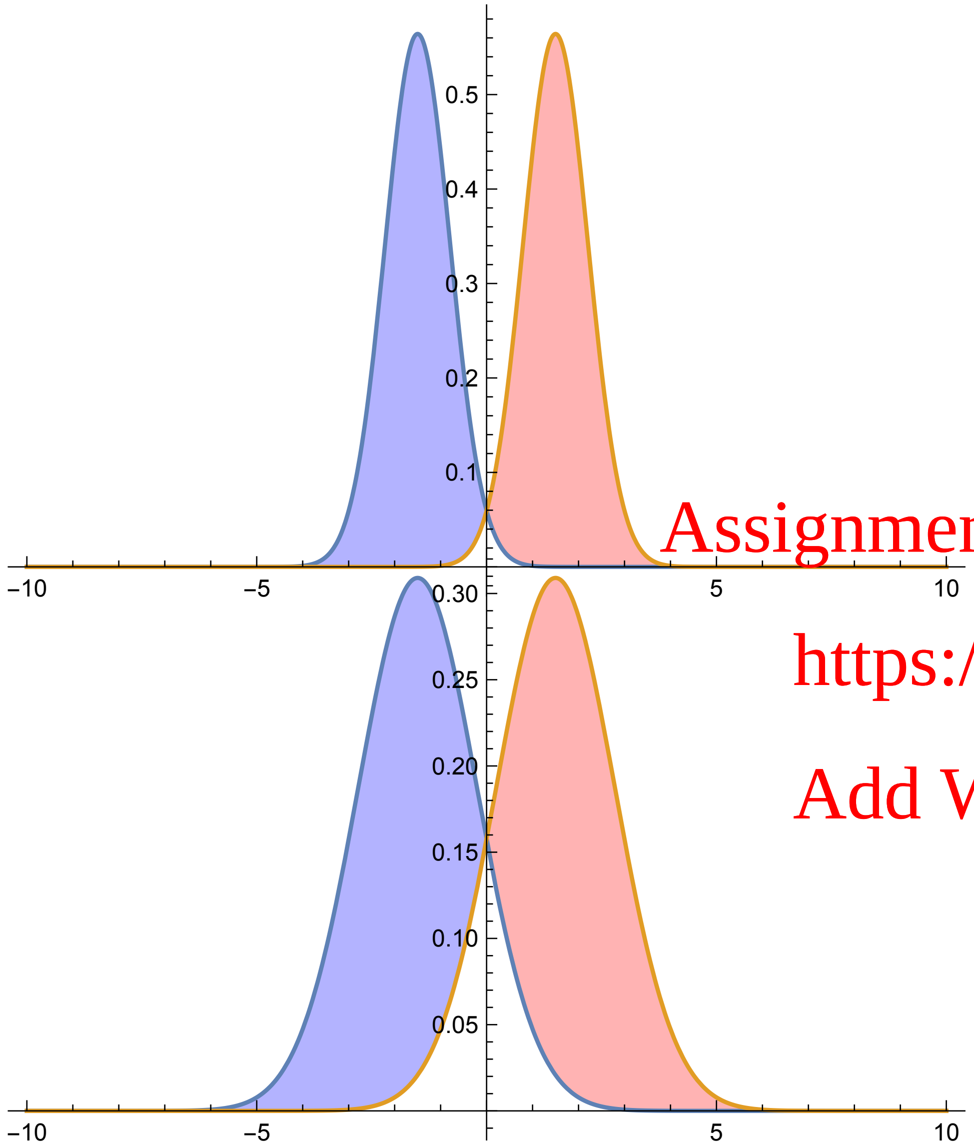

$$d = \frac{\mu_1 - \mu_2}{\sigma}$$

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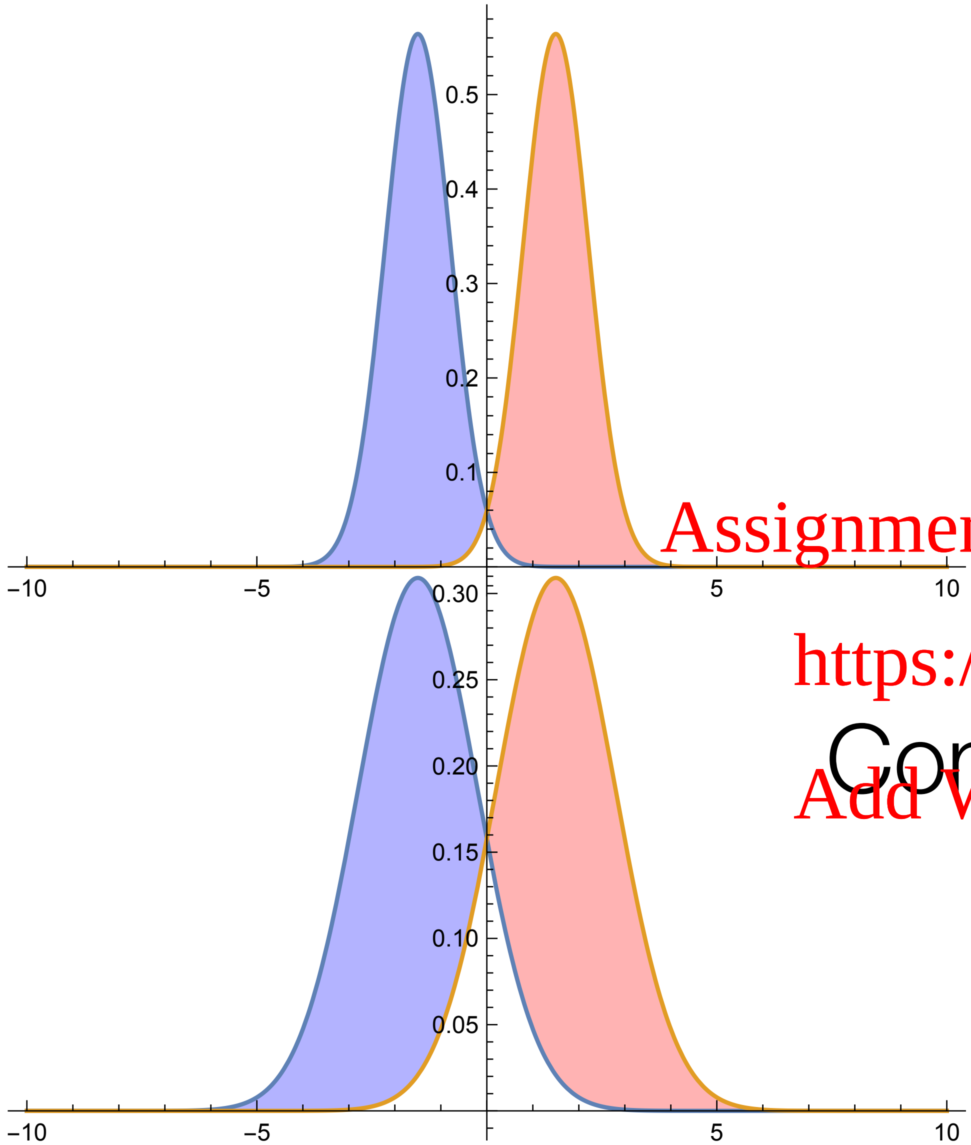

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Controls for overlap between classes

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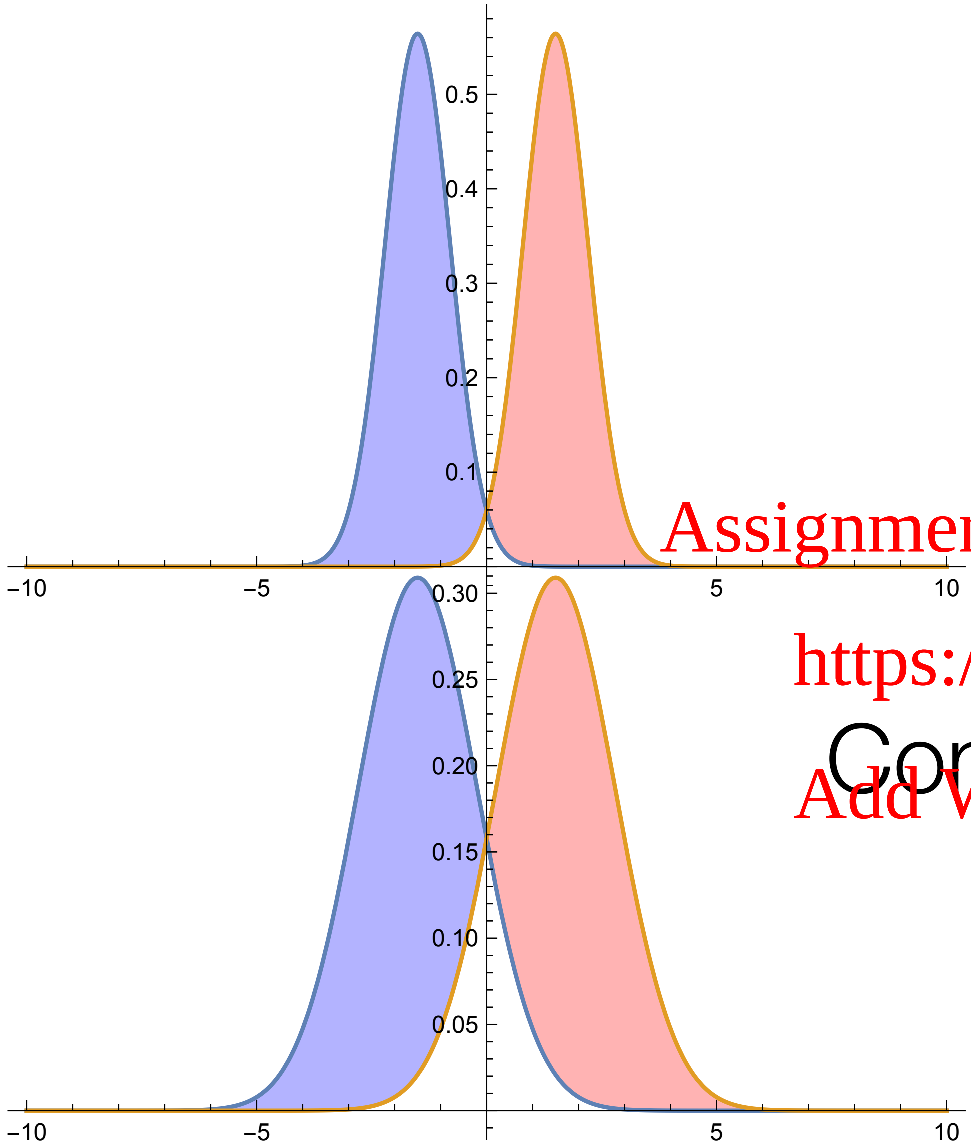


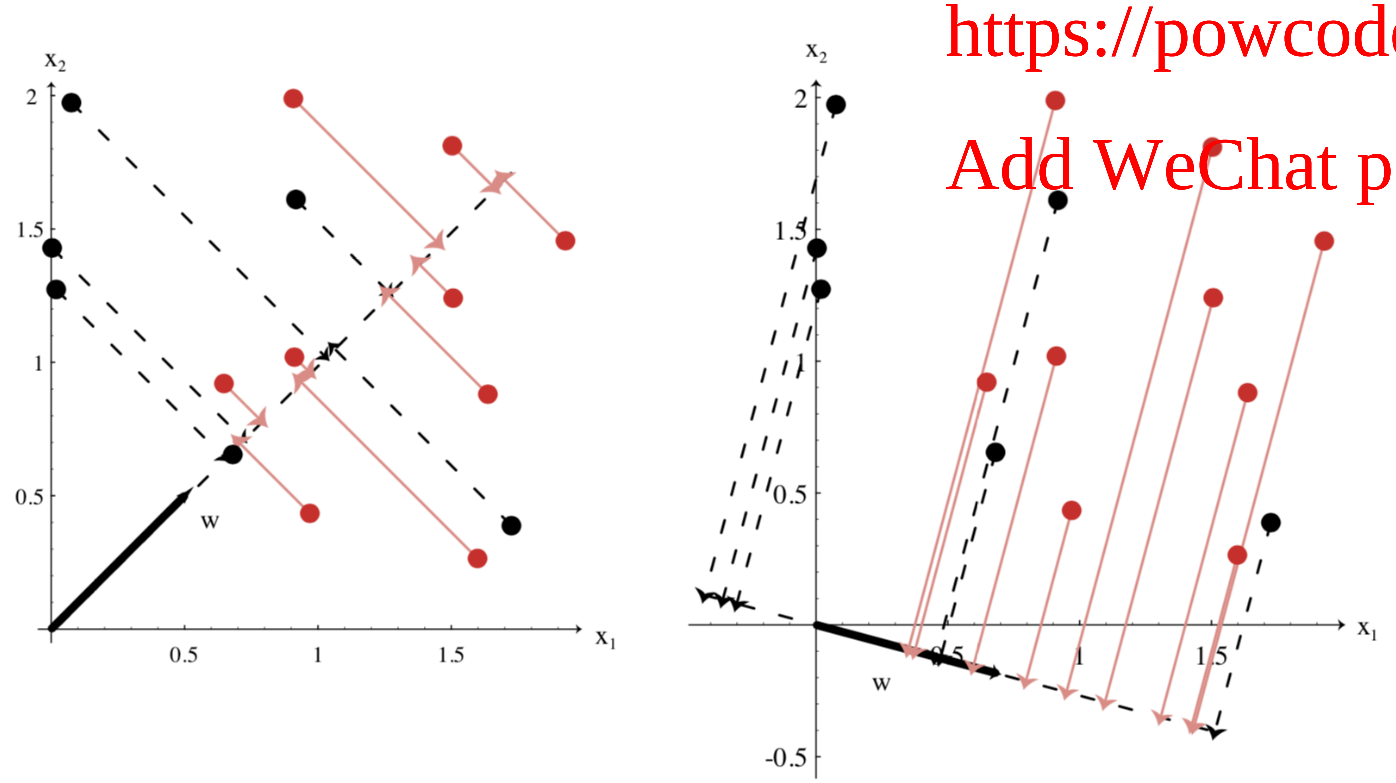
$$d = \frac{\mu_1 - \mu_2}{\sigma}$$

Controls for overlap between classes

Mahalanobis distance

$$d(\boldsymbol{x}_1, \boldsymbol{x}_2) = \sqrt{(\boldsymbol{x}_1 - \boldsymbol{x}_2)^T \Sigma^{-1} (\boldsymbol{x}_1 - \boldsymbol{x}_2)}$$

Fisher Linear Discriminant Analysis: projections along discriminative directions



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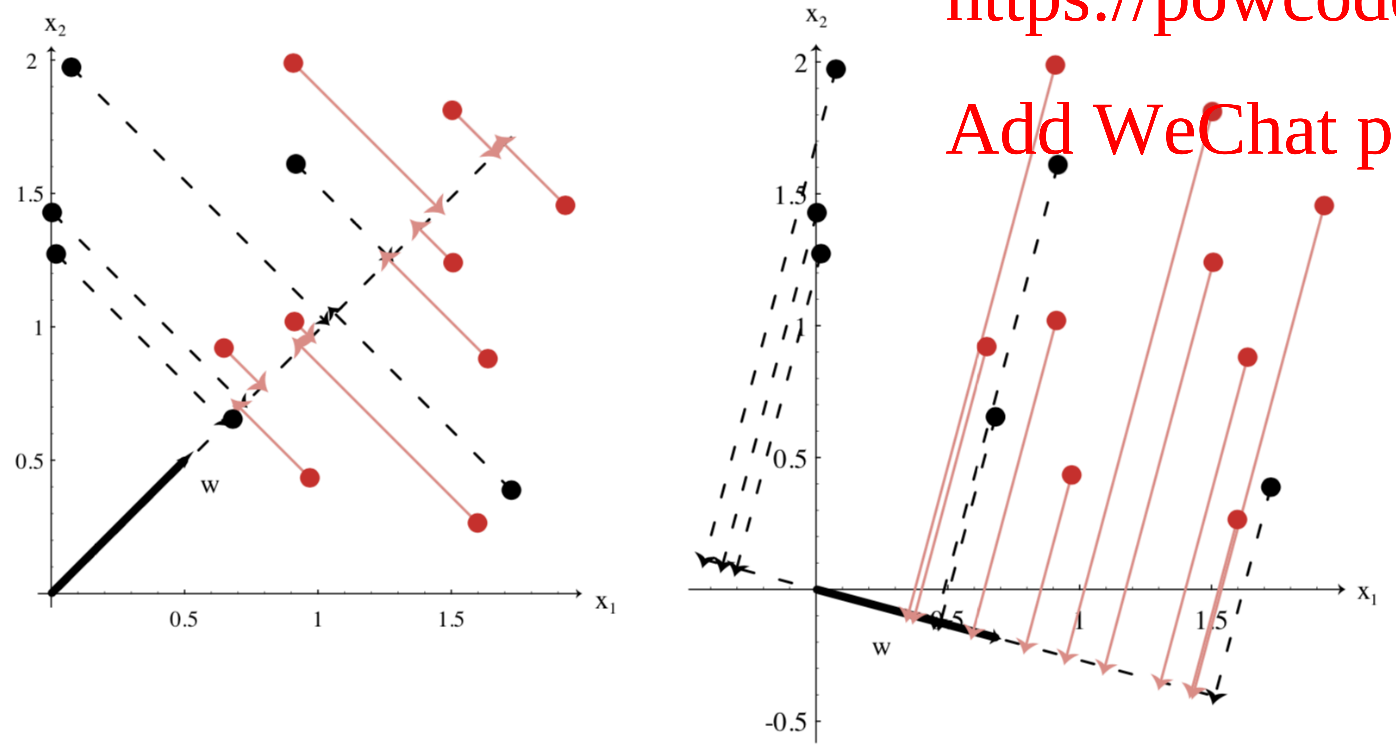
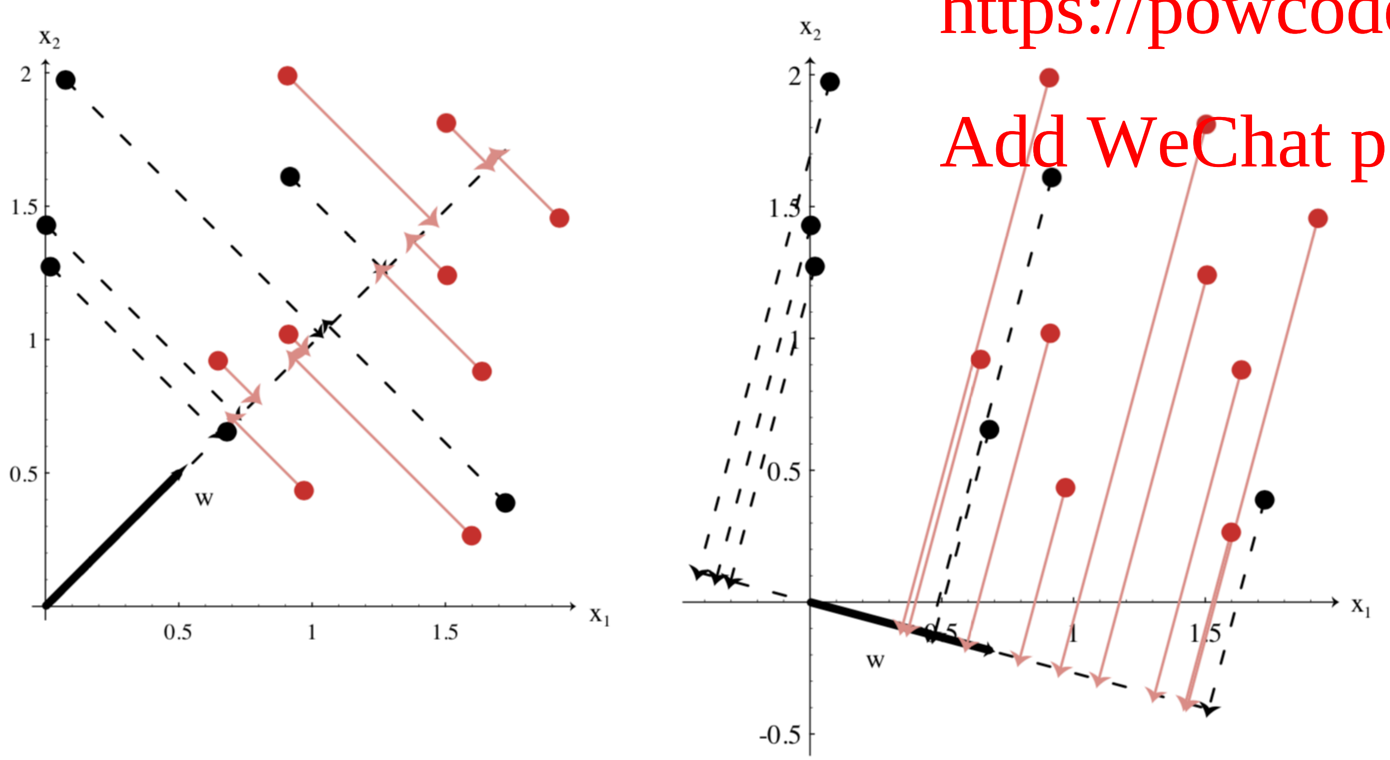


Fisher Linear Discriminant Analysis: projections along discriminative directions

$$\boldsymbol{\mu}_c = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} \boldsymbol{x}^n$$



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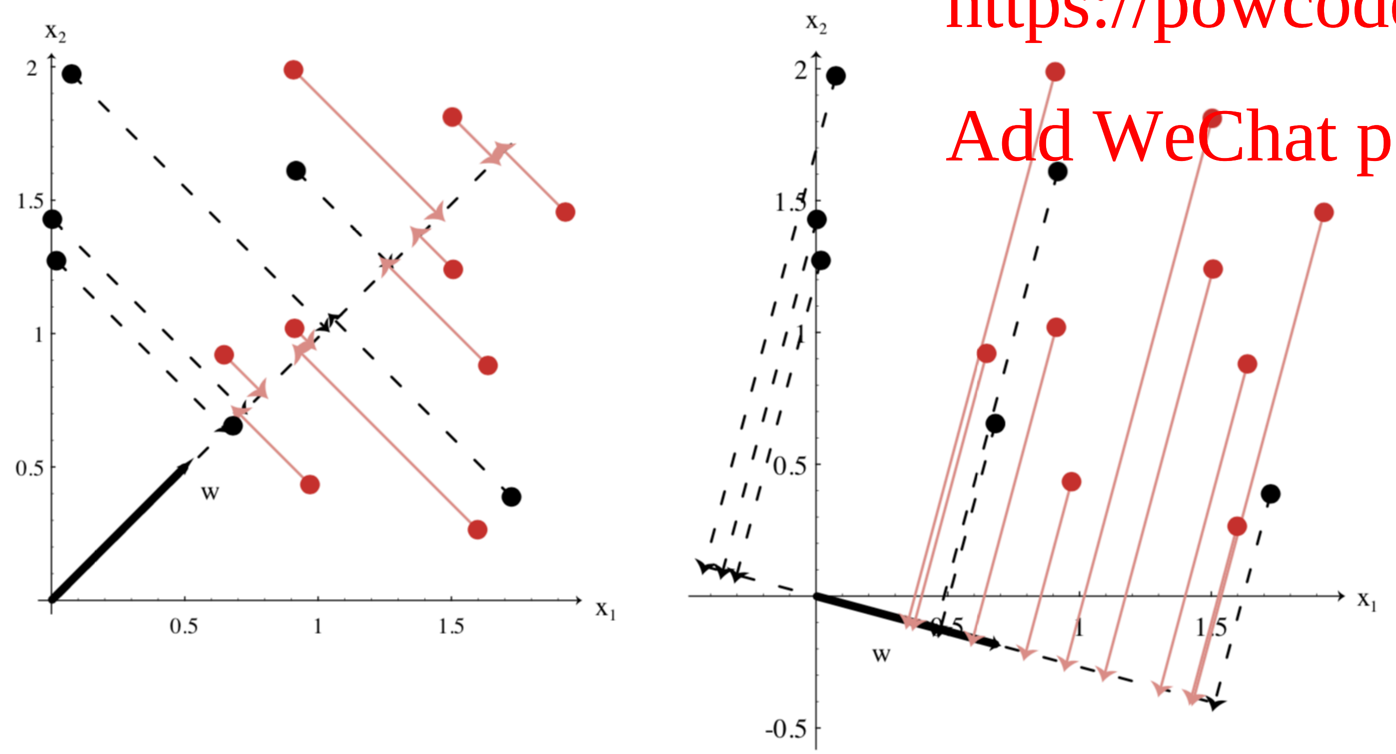
$$\boldsymbol{\mu}_c = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} \boldsymbol{x}^n \qquad m_c = \boldsymbol{w}^T \boldsymbol{\mu}_c = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} \boldsymbol{w}^T \boldsymbol{x}^n$$



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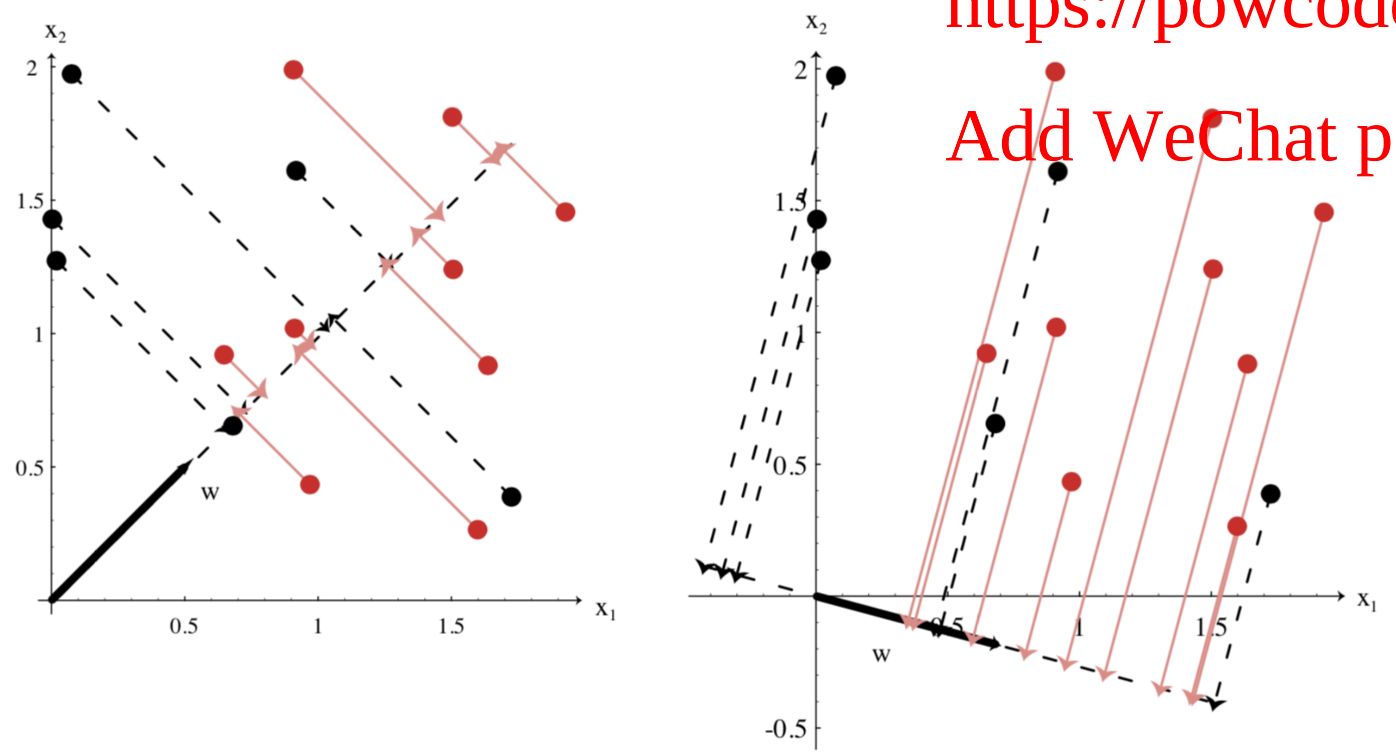
$$\triangleq \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} y^n$$



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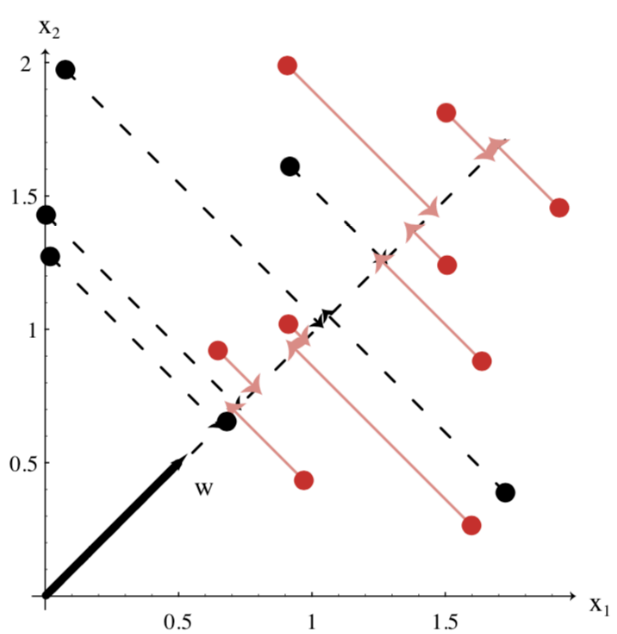
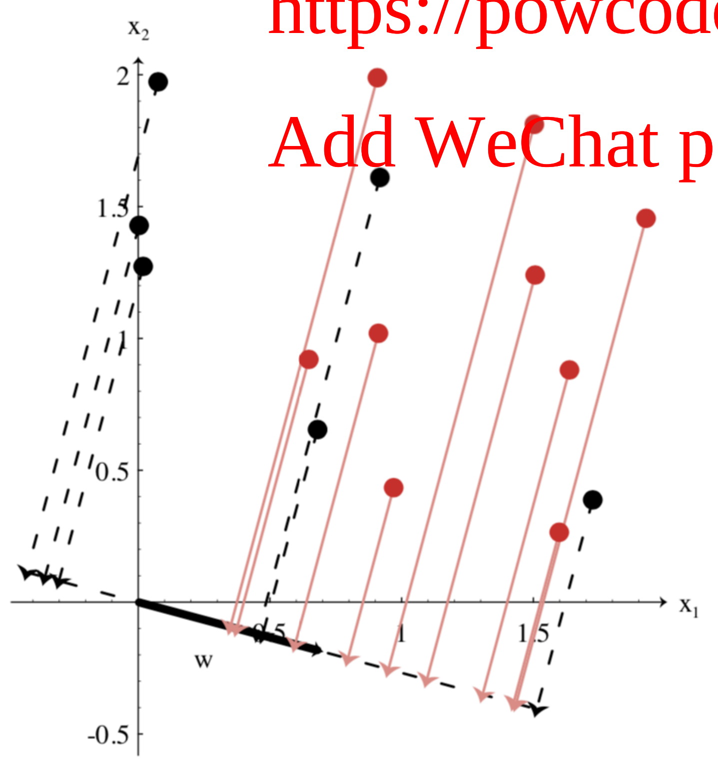
$$s_c^2 = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} (y^n - m_c)^2$$





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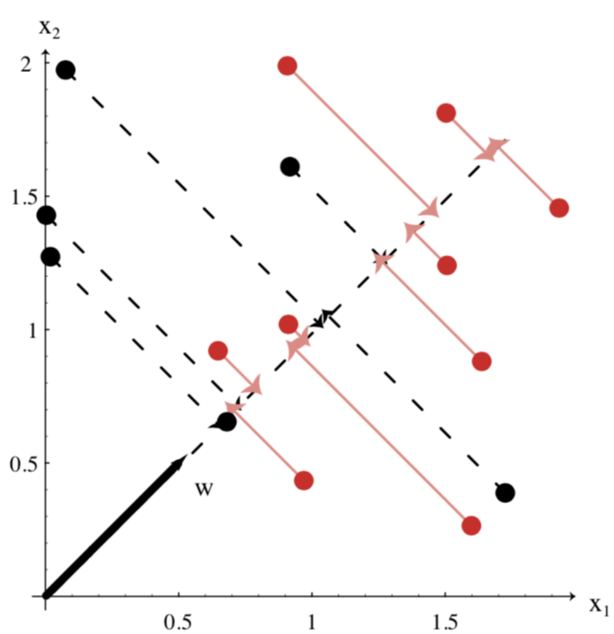

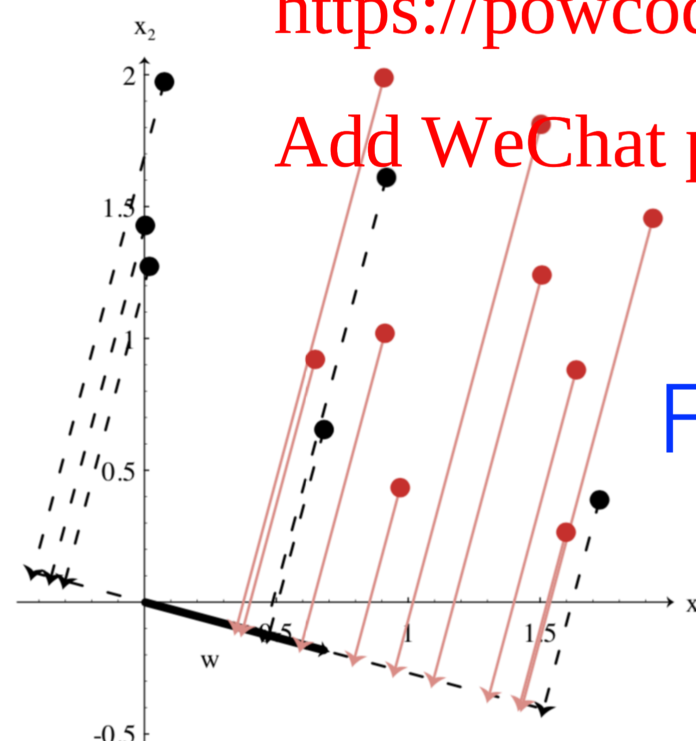

Fisher score:

$$J(\boldsymbol{w}) = \frac{(m_+ - m_-)^2}{n_+ s_+^2 + n_- s_-^2}$$

$$\text{Choose } \boldsymbol{w}^* = \operatorname{argmax}_{\boldsymbol{w}} J(\boldsymbol{w})$$

Rewrite Fisher score to make weight vector dependence explicit: between and within class scatter

$$s_c^2 = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} (y^n - m_c)^2 = \frac{1}{n_c} \sum_{\boldsymbol{x}^n \in \mathcal{D}_c} (\boldsymbol{w}^T \boldsymbol{x}^n - \boldsymbol{w}^T \boldsymbol{\mu})^2$$

denominator:
within class scatter

numerator:
between class scatter

$$J(\boldsymbol{w}) = \frac{(m_+ - m_-)^2}{n_+ s_+^2 + n_- s_-^2} \implies \boxed{J(\boldsymbol{w}) = \frac{\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}}{\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}}}$$

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$(\boldsymbol{a} \cdot \boldsymbol{b})^2 = (\boldsymbol{b}^\top \boldsymbol{a})(\boldsymbol{a}^\top \boldsymbol{b})$

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\end{aligned}
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Optimisation: find best direction, set gradients to 0

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Partial derivatives (gradient) set to 0

$$\frac{\partial J(\boldsymbol{w})}{\partial \boldsymbol{w}} = \frac{2}{(\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w})^2} \left((\boldsymbol{w}^T \boldsymbol{S}_W \boldsymbol{w}) \boldsymbol{S}_B \boldsymbol{w} - (\boldsymbol{w}^T \boldsymbol{S}_B \boldsymbol{w}) \boldsymbol{S}_W \boldsymbol{w} \right)$$

reduces to a **generalised eigenvalue problem**:

$$\boldsymbol{S}_B \boldsymbol{w} = \lambda \boldsymbol{S}_W \boldsymbol{w}$$

Optimisation: find best direction, set gradients to 0

$$\left(\frac{u}{v}\right)' = \frac{1}{v^2}\left(u'v - uv'\right)$$

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scalars

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scalars

$$\boldsymbol{S}_B\boldsymbol{w} = \underline{\lambda}\boldsymbol{S}_W\boldsymbol{w}$$

ratio

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reduces to a **generalised eigenvalue problem**:

scalars

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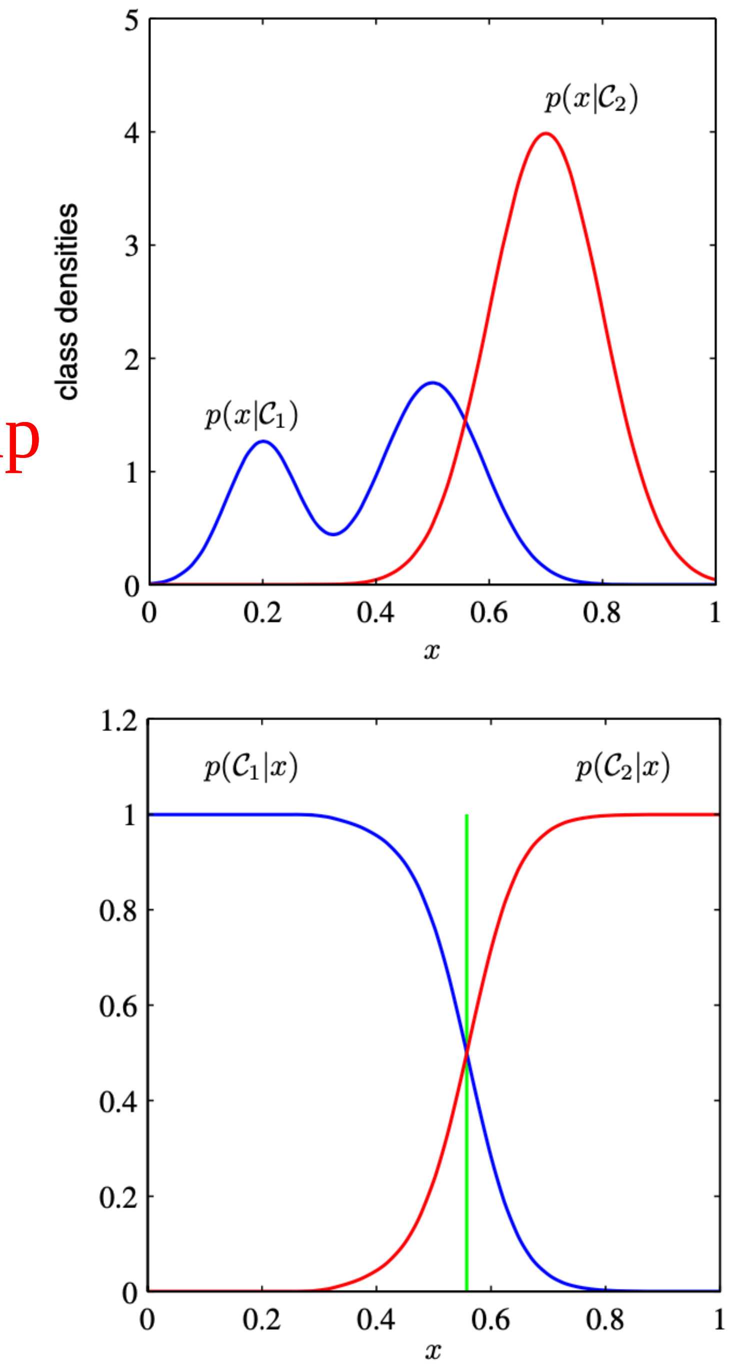
ratio

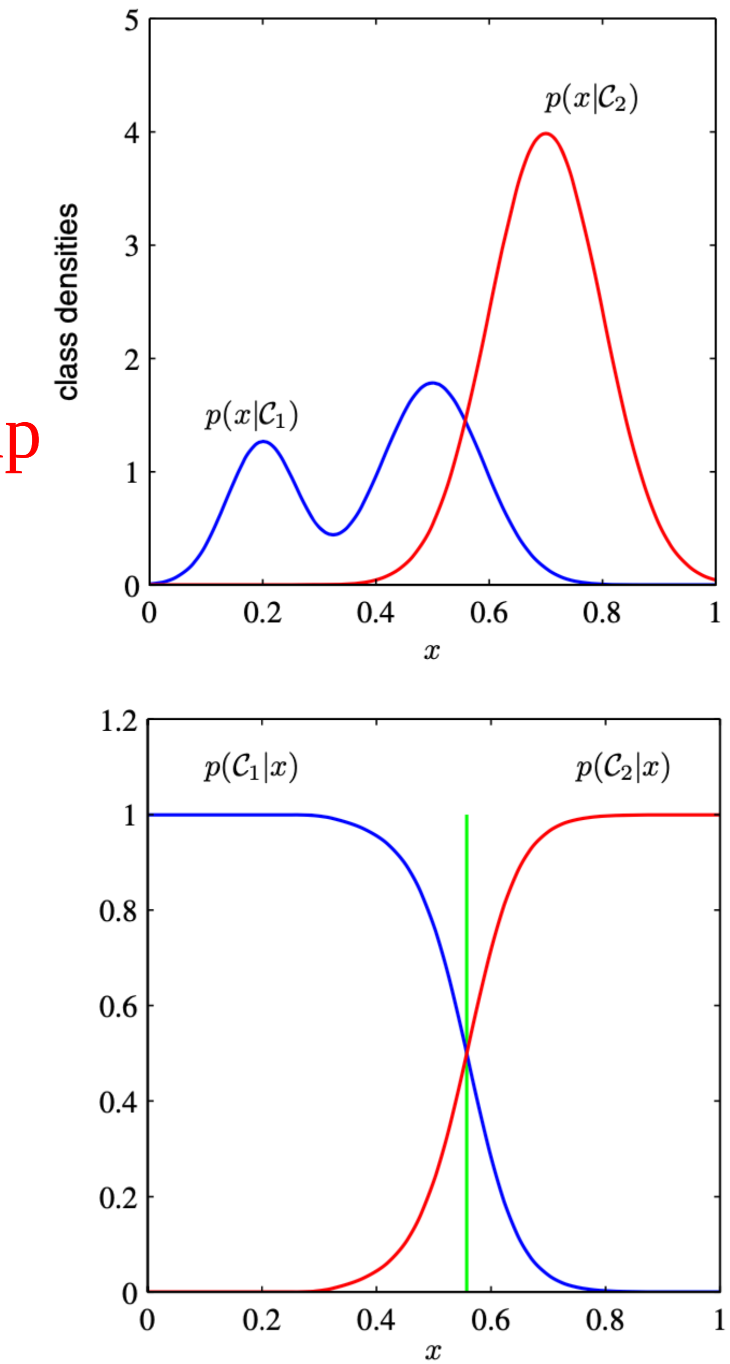
Extend to multiple classes, not just 2.

Classifiers can be generative or discriminative



Classifiers can be generative or discriminative

- Generative — class conditional probabilities can be used to simulate (generate) data



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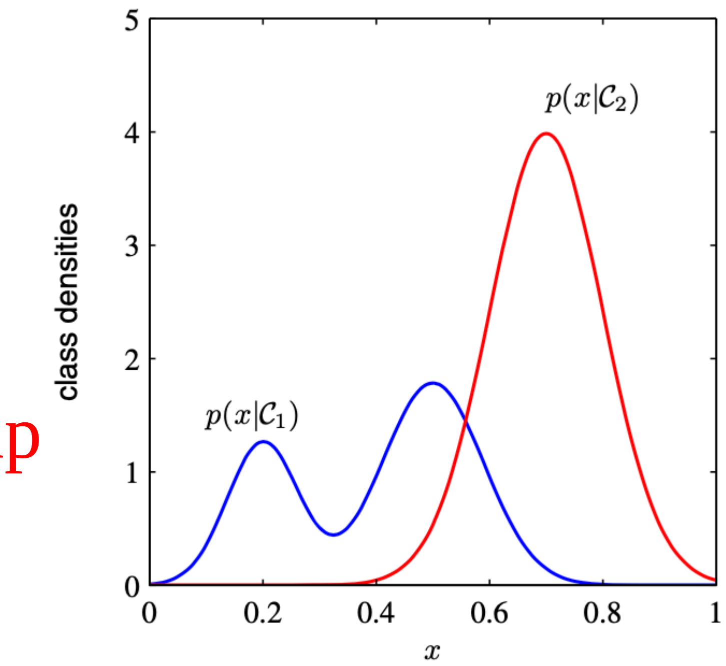
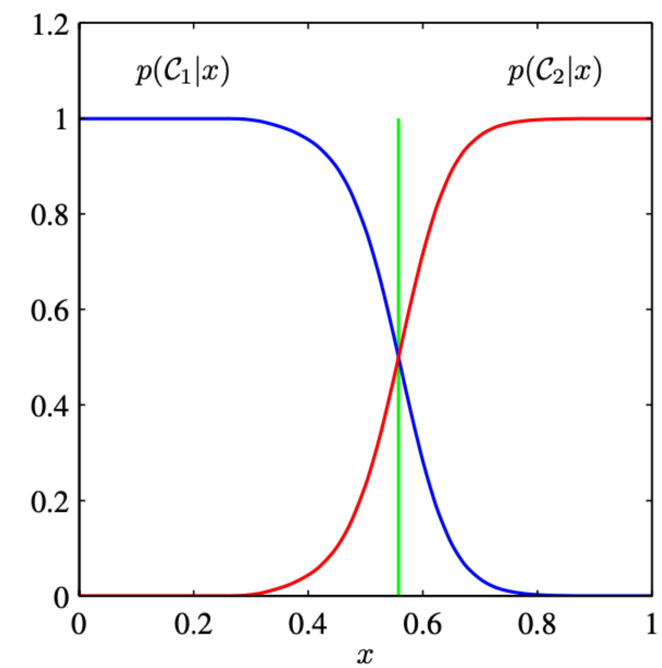
- Generative — probabilities consistent with allocation of distance from decision boundaries





Classifiers can be generative or discriminative

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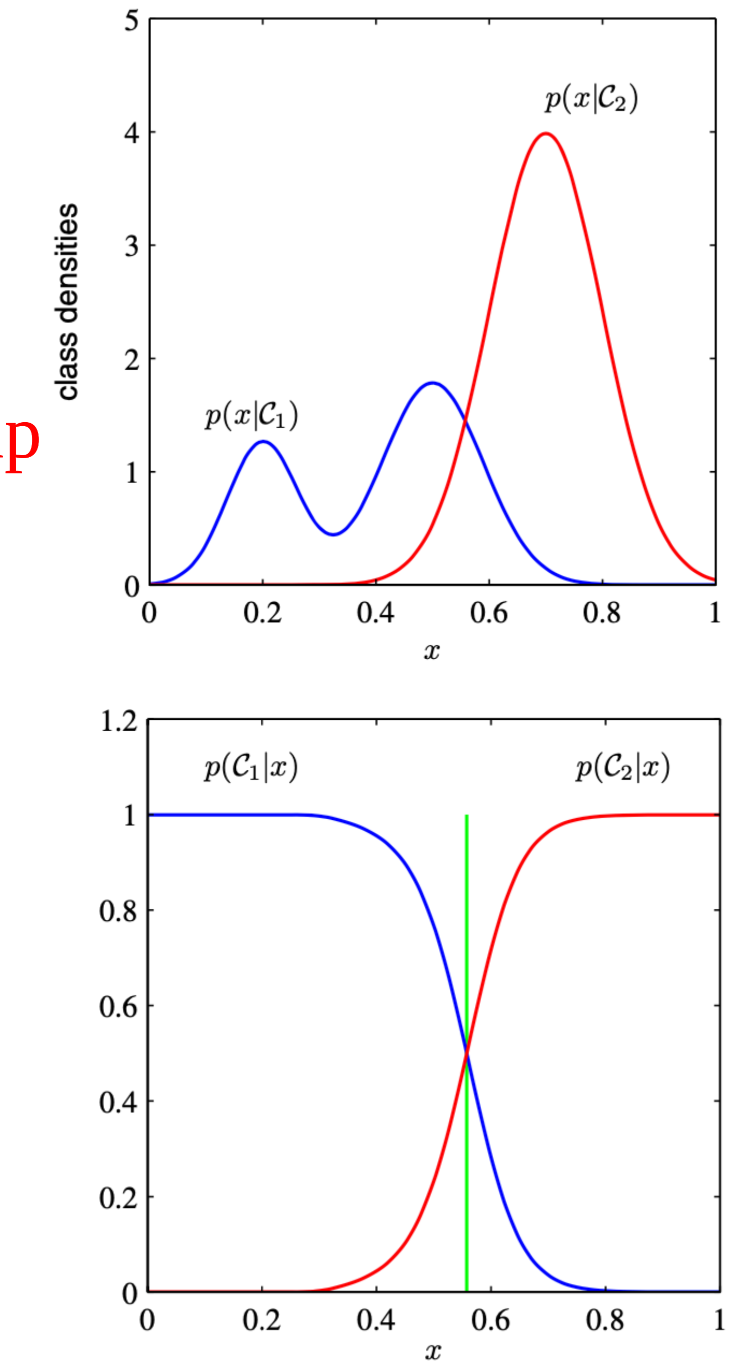
- Discriminative — does not model data within classes, only what distinguishes a class from another



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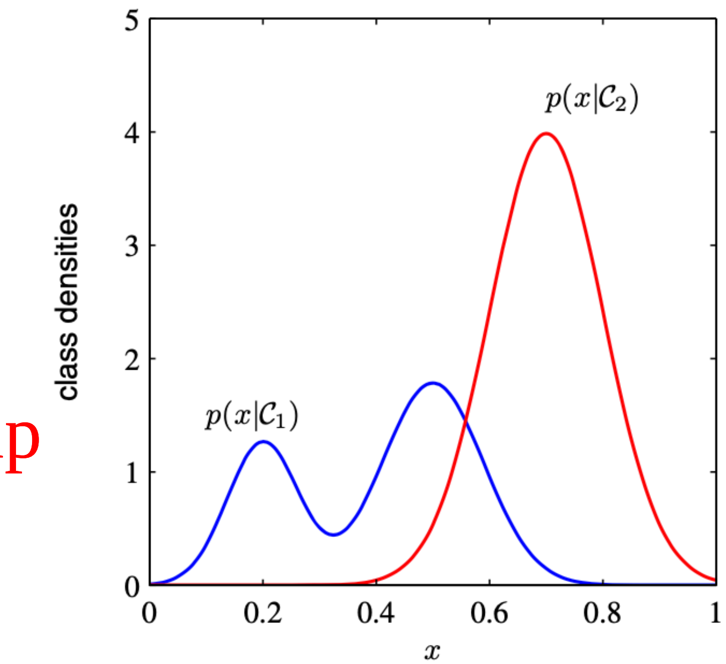
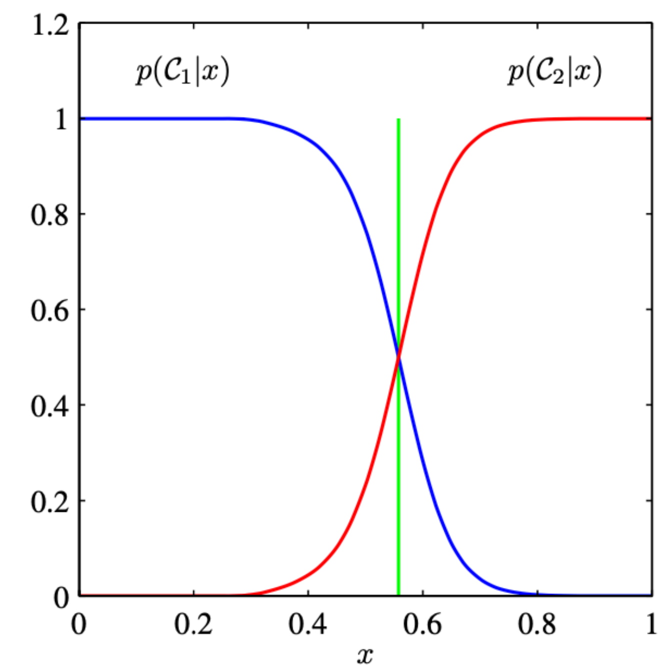
- Next time: maximum margin classifiers (Support Vector Machines)





References

- PRML, Bishop, Chapter 1, section 1.5
- PRML, Bishop, Chapter 4.
- FCML, Rogers-Girolami, Chapter 5.