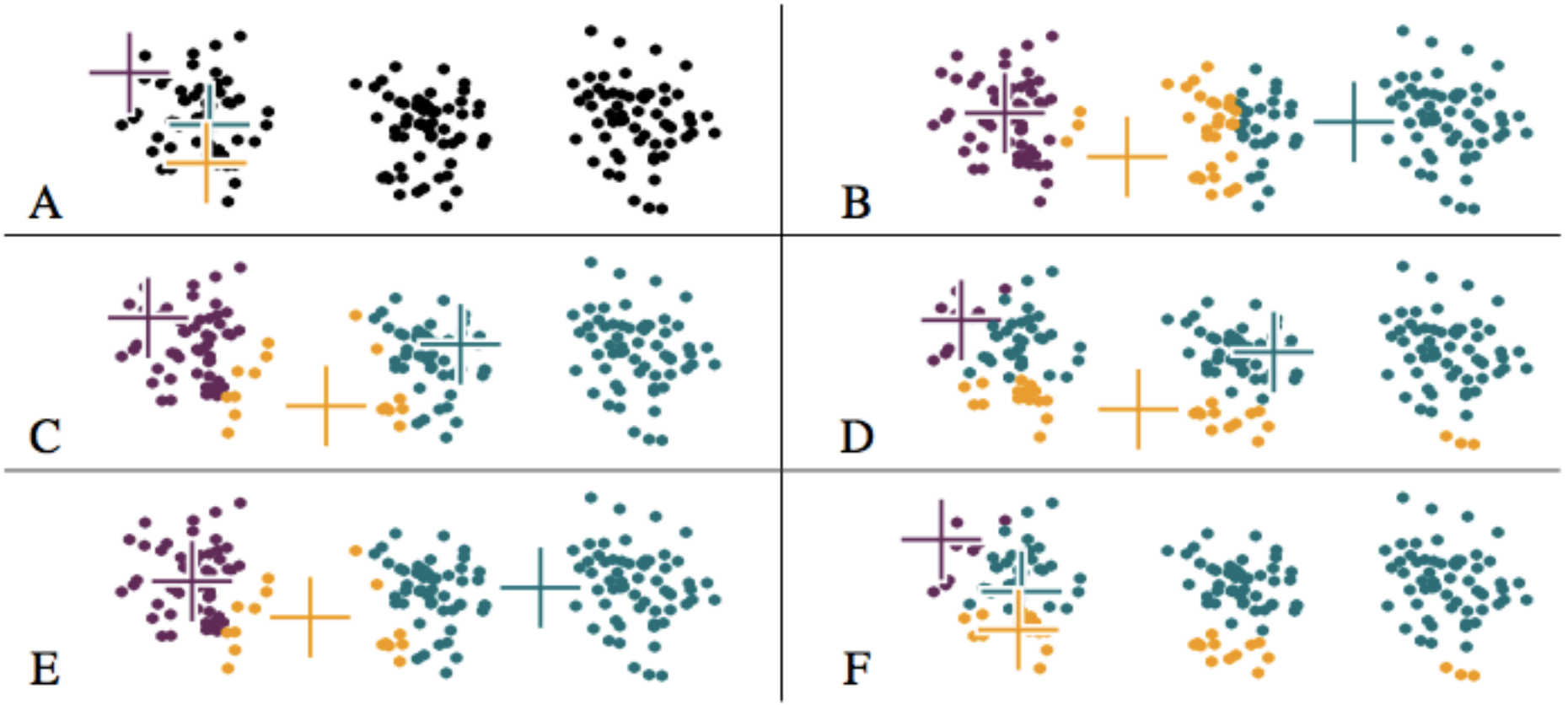
MLE, MAP, AND NAIVE BAYES

Q: Order the pictures according to the k-means algorithm (starting from A)

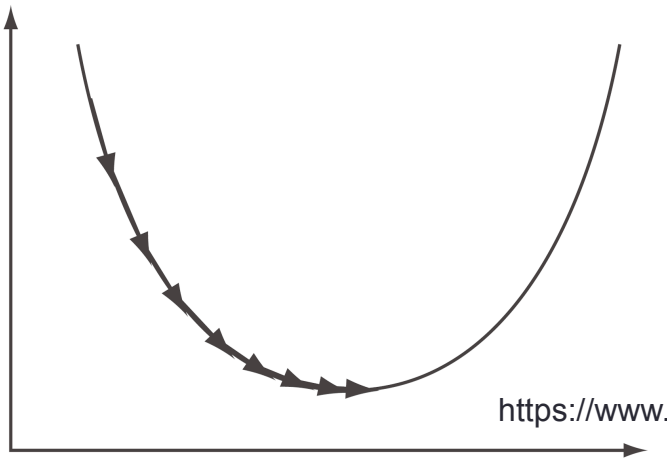


Loose Ends from HW

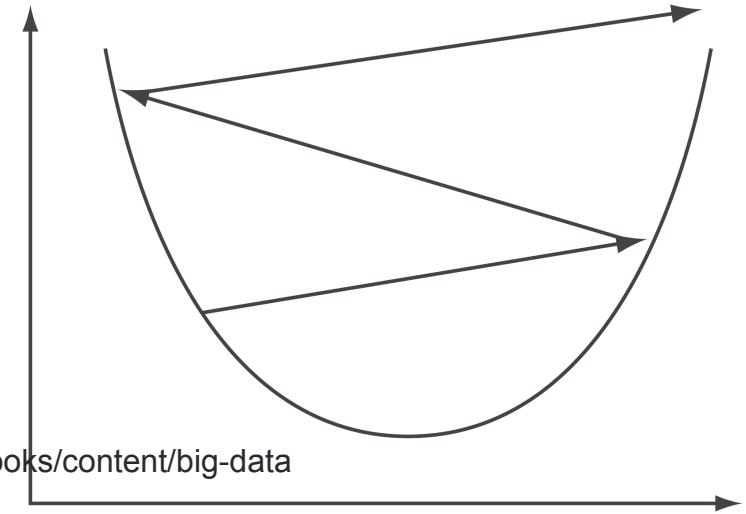
- How to select r? (The learning rate)

$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

Small learning rate



Large learning rate



https://www.packtpub.com/books/content/big-data

r too small and the model converges slowly

r too large and the model diverges

Learning rate issues

- Typically r is normalized with the amount of training examples in a mini-batch. (Divide by m)

$$\theta_j \Leftarrow \theta_j + r\Sigma_{i=1}^{m}(y_i - \theta^T \mathbf{x}_i)x_i^{(j)}$$

- Typical values are 0.1-0.001
- Usually have a decay over time

Scaling the input data

- We use age, passenger class, gender, and embark as our input.
- Age has a lot more variance (0.42 – 80) than the other data.
- This makes parameter initialization hard, and makes the learning rate selection hard.
- $h_{\theta}(x) = \theta_0 + \theta_1 x_1 + \theta_2 x_2 + \theta_3 x_3 + \theta_4 x_4$

Scaling the input data

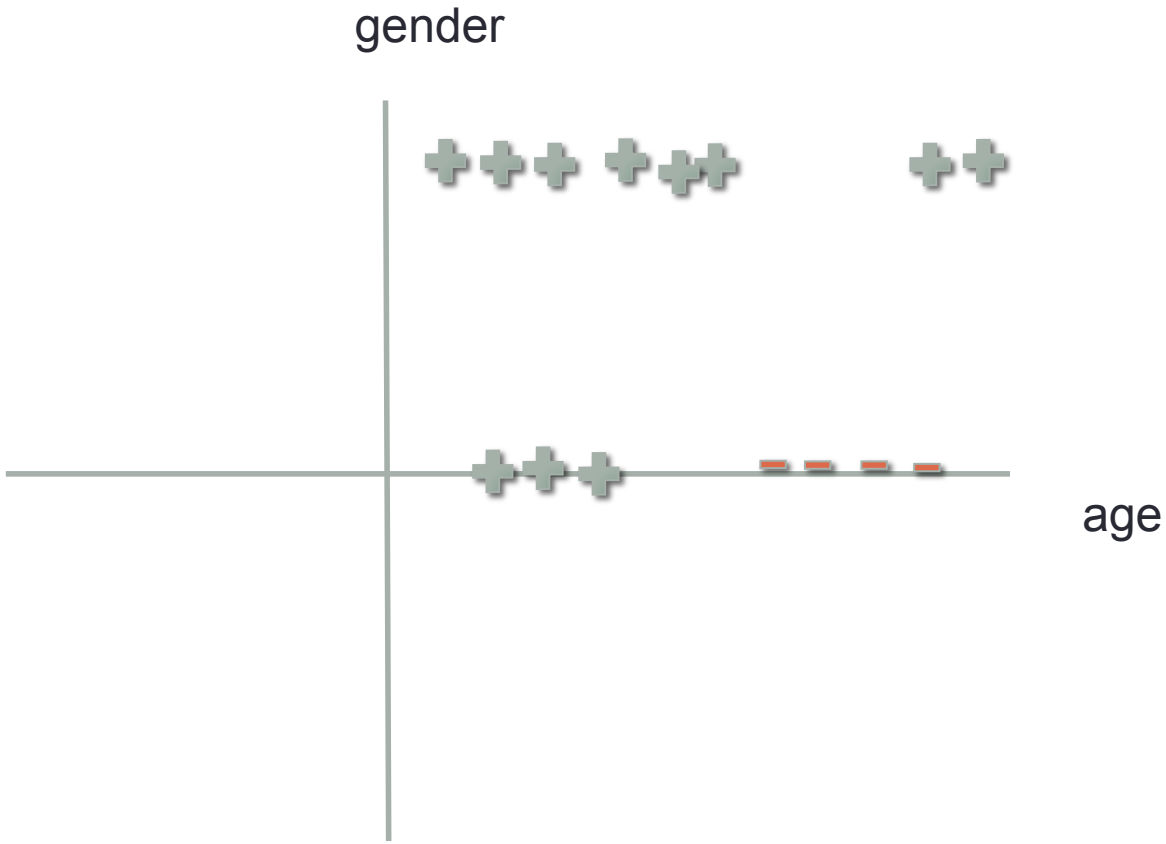
- Scale all input data to be in the same range
- Using statistics from training data
  - Scale to [-1,1]
  - Scale to [0, 1]
  - Scale to standard normal
- Don’t forget to apply the same scaling to the test data

Feature selection

- If you actually try the third optional question, most likely you will get better results with just two features.
- This is the importance of feature selection.
- Knowing what good features to select is not trivial
- Approaches for feature selection (or for not having to do feature selection)
  - Cross validation
  - Random forest
  - Boosting
  - Model averaging

Feature engineering

- Logistic regression is a linear classification

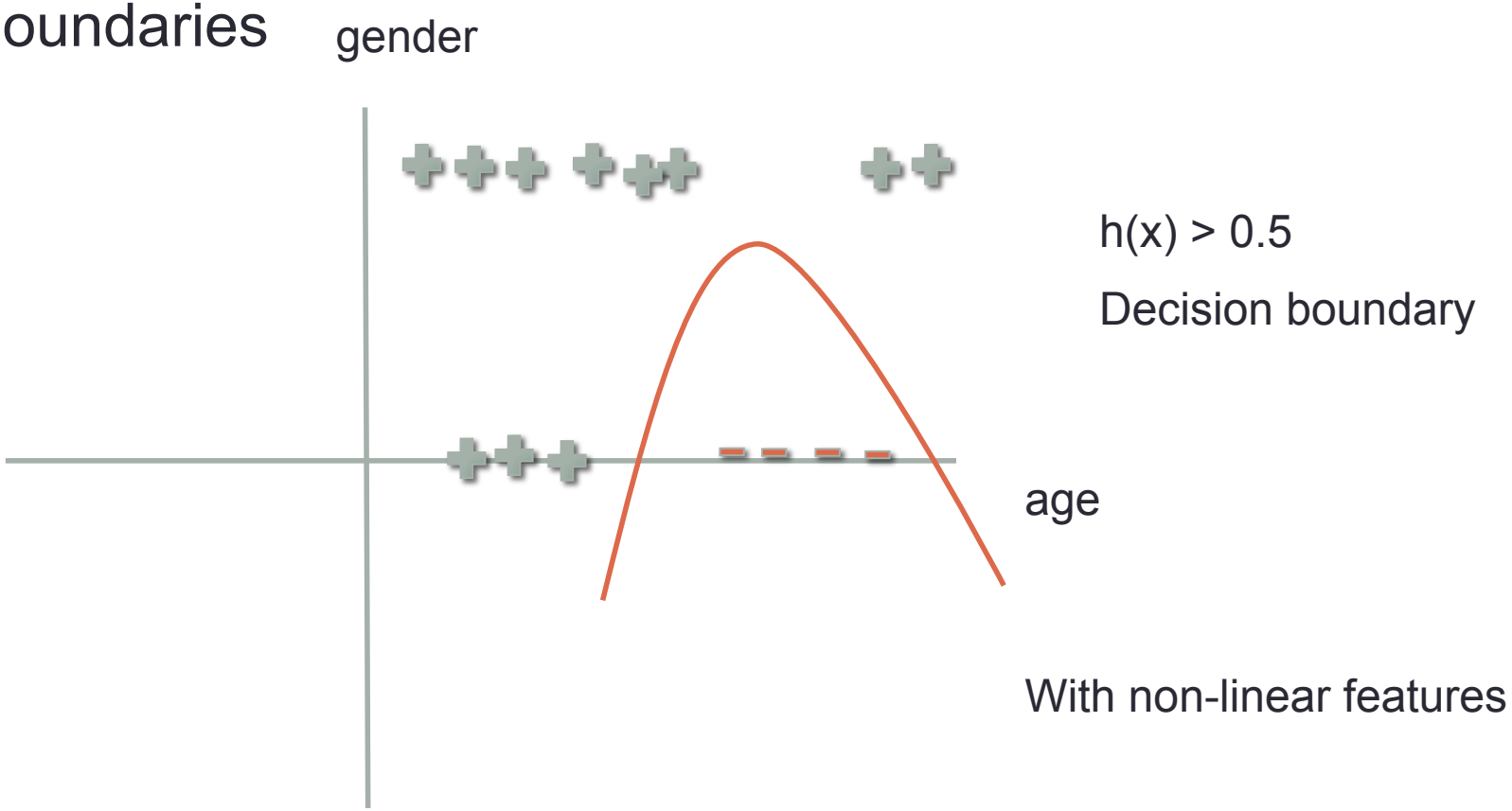


Feature engineering

- Logistic regression is a linear classification

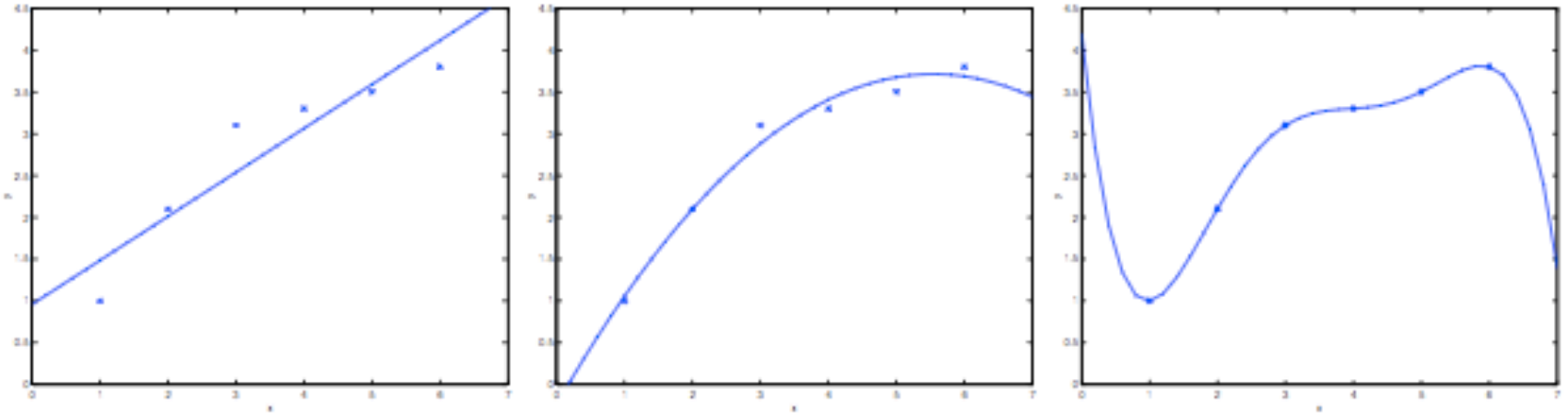
Feature engineering

- Add non-linear features to get non-linear decision boundaries



This is also a form of feature selection (more specifically feature engineering)

Overfitting Underfitting (from Lecture3)



Adding more non-linear features makes the line more curvy
(Adding more features also means more model parameters)

The curve can go directly to the outliers with enough parameters.
We call this effect overfitting
For the opposite case, having not enough parameters to model the data is called underfitting

Bias-Variance trade-off

- We will formulate overfitting and underfitting mathematically
- Using regression model

Regression with Gaussian noise

- $y = h(\mathbf{x}) + \varepsilon$
  - Where ε is normally distributed with mean zero and variance σ^2
  - The training data D = $\{(\mathbf{x_1}, y_1), (\mathbf{x_3}, y_3), (\mathbf{x_3}, y_3)\ldots\}$ is drawn from some distribution $P(\mathbf{x}, y)$ governing our universe!
  - Assume $(\mathbf{x_i}, y_i)$ is iid
- Given D we can train a regressor $h_D(x)$
- We calculate the expected error (squared error) on new $(\mathbf{x}, y)$ data with the regressor
  - $E_{(\mathbf{x},y)}[(h_D(\mathbf{x}) - y)^2] = \int_x \int_y (h_D(\mathbf{x}) - y)^2 \Pr(\mathbf{x}, y) \partial y \partial \mathbf{x}$
- But D is actually a random variable too!

Regression with Gaussian noise

- We calculate the expected error (squared error) on new (**x**,y) data with the regressor
  - $E_{(\mathbf{x},y)}[(h_D(\mathbf{x}) - y)^2] = \int_x \int_y (h_D(\mathbf{x}) - y)^2 \Pr(\mathbf{x}, y) \partial y \partial \mathbf{x}$
- Consider parallel worlds, we can receive different training data D which yields different regression $h_D(x)$
- The expectation of error over all possible new test data point (**x**,y) and different possible training data D is

$$E_{\substack{(\mathbf{x},y)\sim P \\ D\sim P^n}} \left[(h_D(\mathbf{x}) - y)^2 \right] = \int_D \int_{\mathbf{x}} \int_y (h_D(\mathbf{x}) - y)^2 \mathrm{P}(\mathbf{x}, y) \mathrm{P}(D) \partial \mathbf{x} \partial y \partial D$$

http://www.cs.cornell.edu/courses/cs4780/2017sp/lectures/lecturenote11.html

Regression with Gaussian noise

- This expression tells the expected quality of our model with random training data and a random test data

$$E_{\substack{(\mathbf{x},y)\sim P \\ D\sim P^n}}\left[(h_D(\mathbf{x})-y)^2\right] = \int_D\int_{\mathbf{x}}\int_y (h_D(\mathbf{x})-y)^2 \mathrm{P}(\mathbf{x},y)\mathrm{P}(D)\partial\mathbf{x}\partial y\partial D$$

$$\underbrace{E_{\mathbf{x},y,D}\left[(h_D(\mathbf{x})-y)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[(h_D(\mathbf{x})-\bar{h}(\mathbf{x}))^2\right]}_{\text{Variance}} + \underbrace{E_{\mathbf{x},y}\left[(\bar{y}(\mathbf{x})-y)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x}))^2\right]}_{\text{Bias}^2}$$

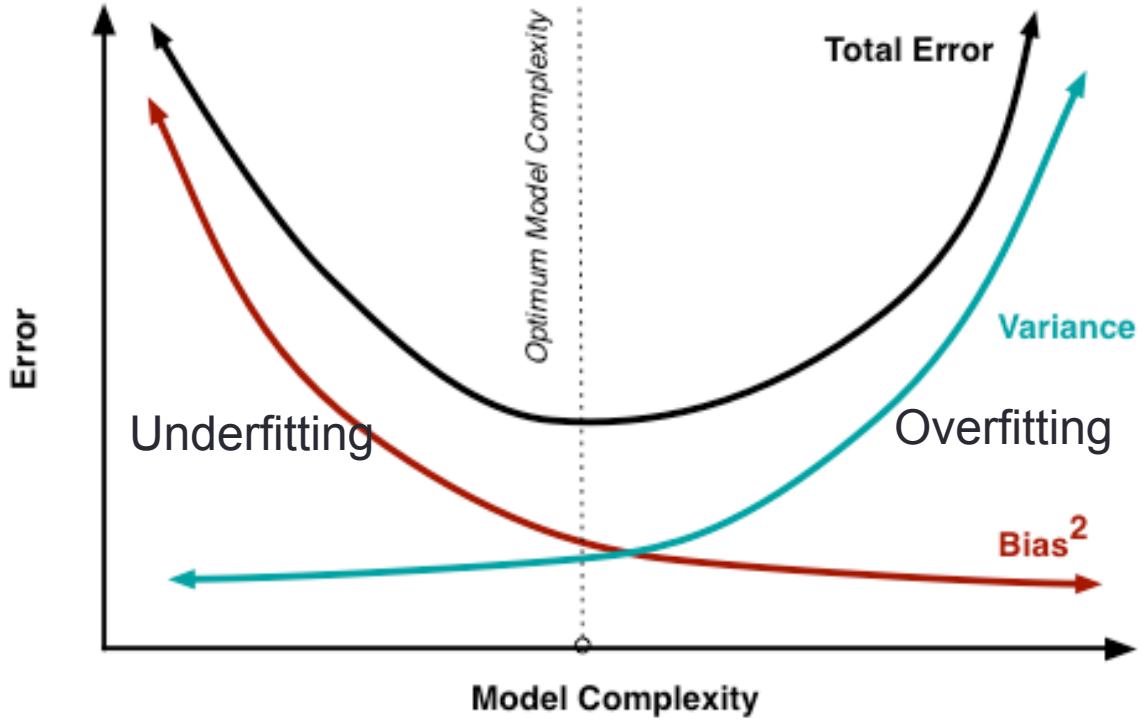
Variance, Bias, and noise

$$\underbrace{E_{\mathbf{x},y,D}\left[(h_D(\mathbf{x})-y)^2\right]}_{\text{Expected Test Error}} = \underbrace{E_{\mathbf{x},D}\left[(h_D(\mathbf{x})-\bar{h}(\mathbf{x}))^2\right]}_{\text{Variance}} + \underbrace{E_{\mathbf{x},y}\left[(\bar{y}(\mathbf{x})-y)^2\right]}_{\text{Noise}} + \underbrace{E_{\mathbf{x}}\left[(\bar{h}(\mathbf{x})-\bar{y}(\mathbf{x}))^2\right]}_{\text{Bias}^2}$$

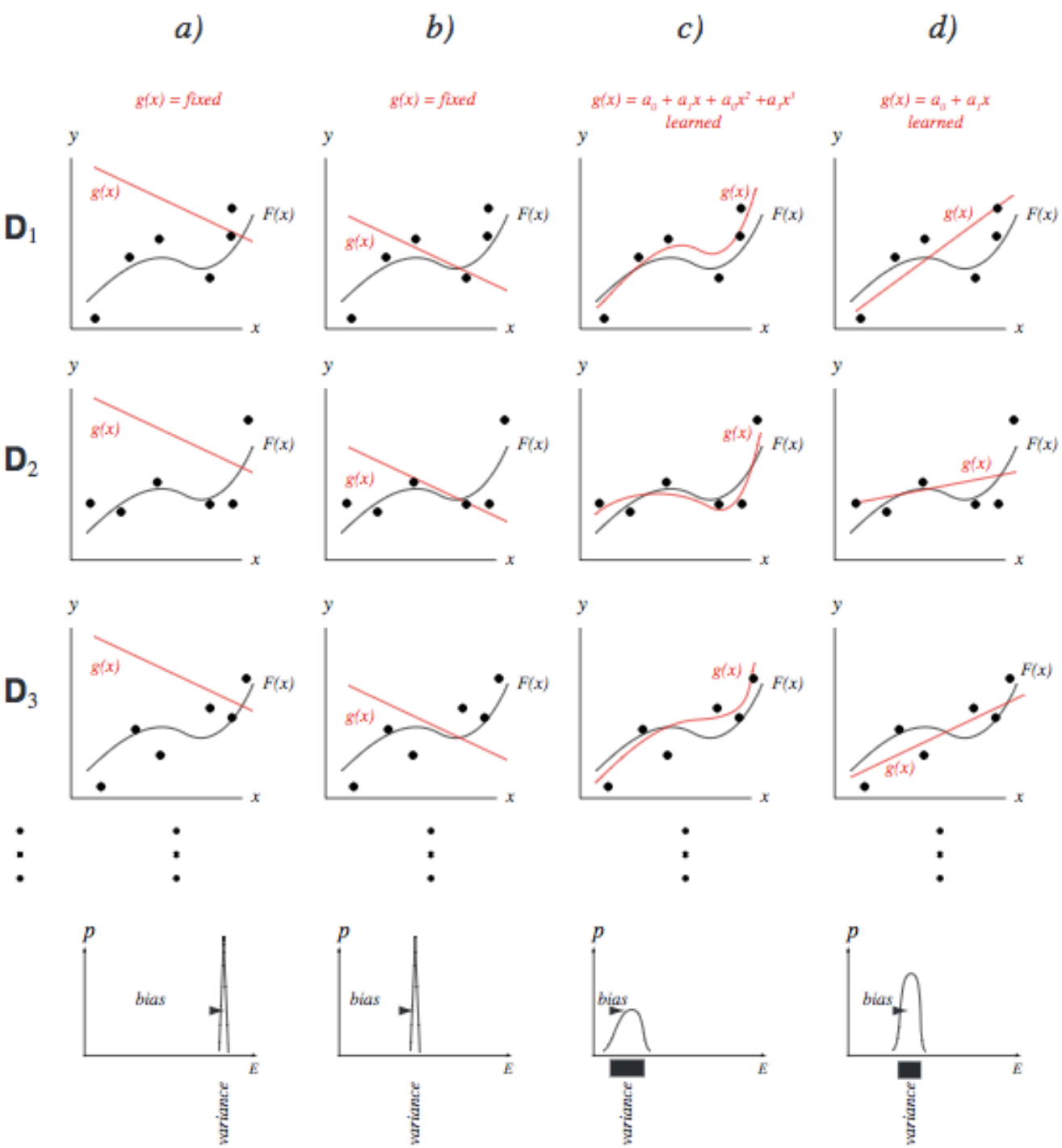
- Variance: how your classifier changes if the training data changes. Measures generalizability.
- Bias: The model's inherent error. If you have infinite training data, you will have the average classifier $\bar{h}$ and still left with this error.
  - For example, even with infinite training data, a linear classifier will still have errors if the distribution is non-linear.
- Noise: data-intrinsic noise. Noise from measurement, noise from feature extraction, etc. Regardless of your model this remains.

Bias-Variance Underfitting-Overfitting

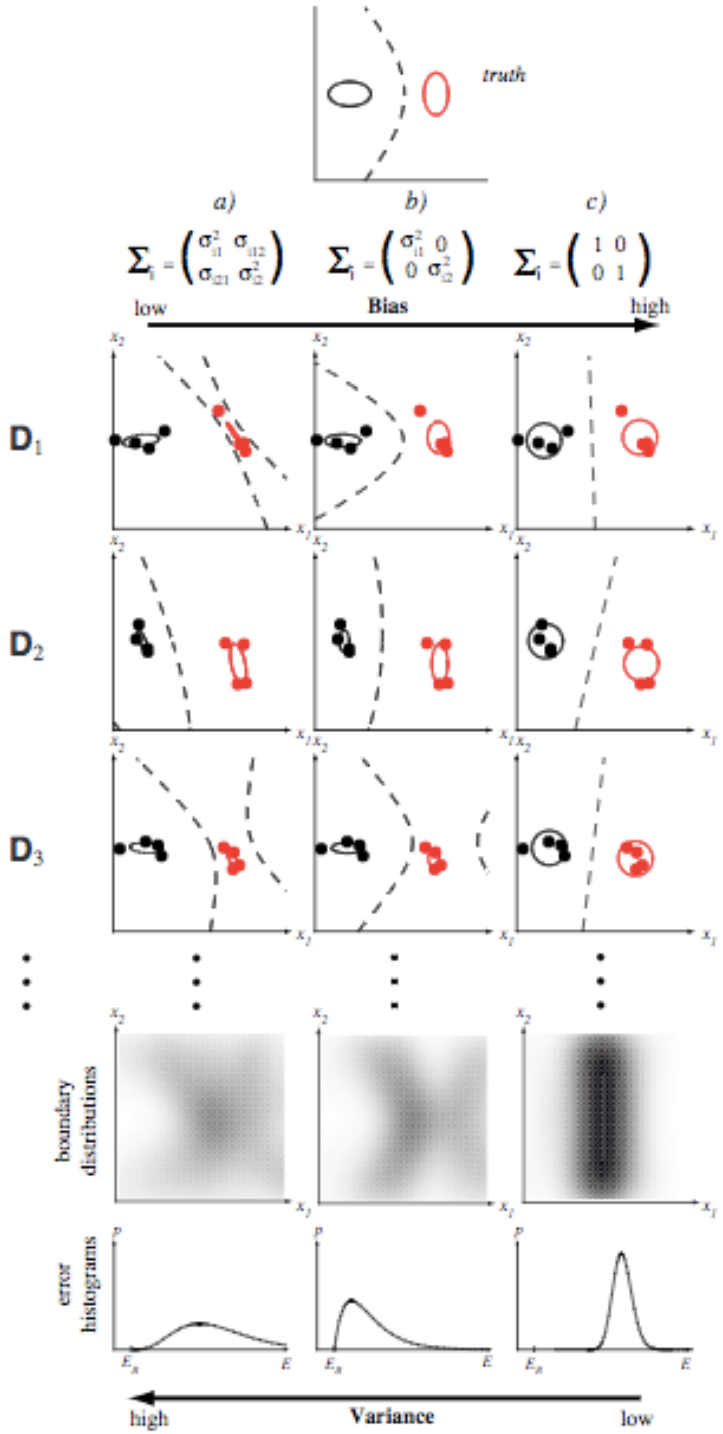
- Usually if you try to reduce the bias of your model, the variance will increase, and vice versa.
- Called the bias-variance trade-off



http://www.cs.cornell.edu/courses/cs4780/2017sp/lectures/lecturenote11.html



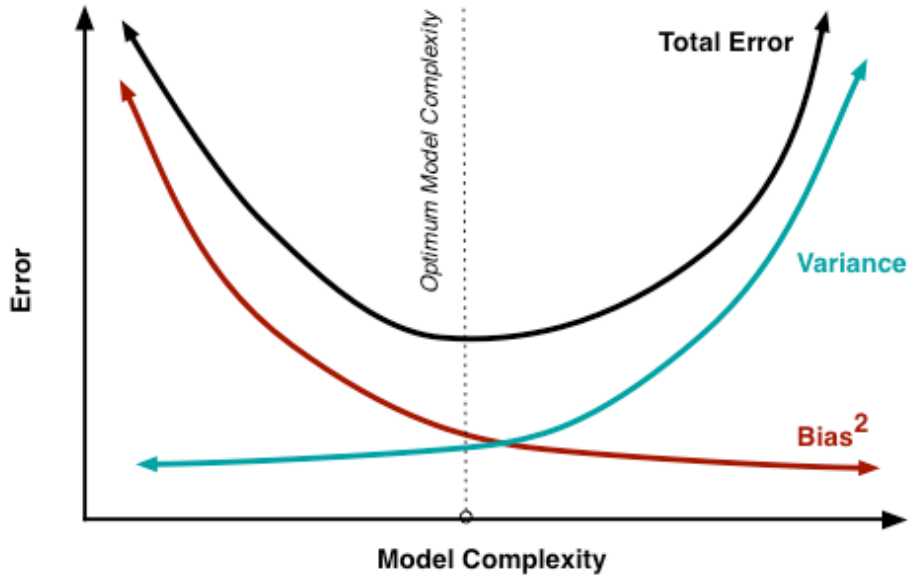
Duda et al. Pattern Classification



Duda et al. Pattern Classification

When to stop the update?

- Consider the updates of Logistic regression as trying to reduce the bias of the model
  - As we keep updating, the model overfits more to the training data
- We want to stop when the error on the validation set increases*
  - More on this later
- Validation test: a separate set that is use to measure overfitting
  - Training set
  - Validation set
  - Test set



Best submissions

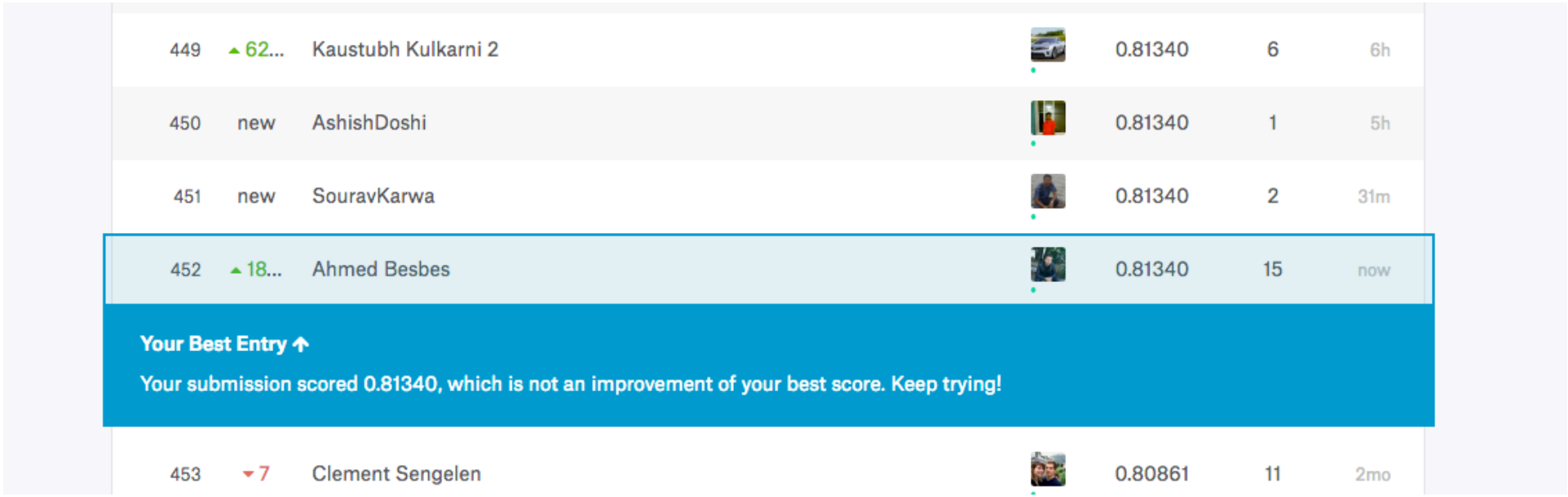
- Accuracy 77.990

- Use scaling to [0,1]
- Learning rate decay

- Use scaling to unit normal for age, [0,1] for the rest

More tricks?

- http://ahmedbesbes.com/how-to-score-08134-in-titanic-kaggle-challenge.html
- Feature Engineering/selection
- Parameter tuning
- Try different models



The Bayes Lecture

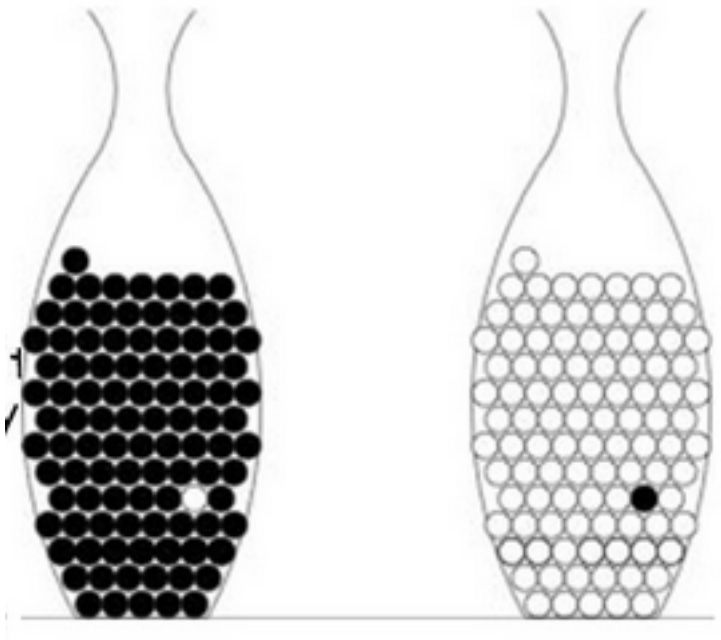
- MLE vs MAP
- Bayes Decision Rule
- Naïve Bayes

Bayes Rule & Learning theory

- x – observed data
- w_i – probability that x comes from class i

$$p(w_i|x) = \frac{p(x|w_i)p(w_i)}{p(x)}$$

$$\text{Posterior} = \frac{\text{likelihood} * \text{prior}}{\text{evidence}}$$

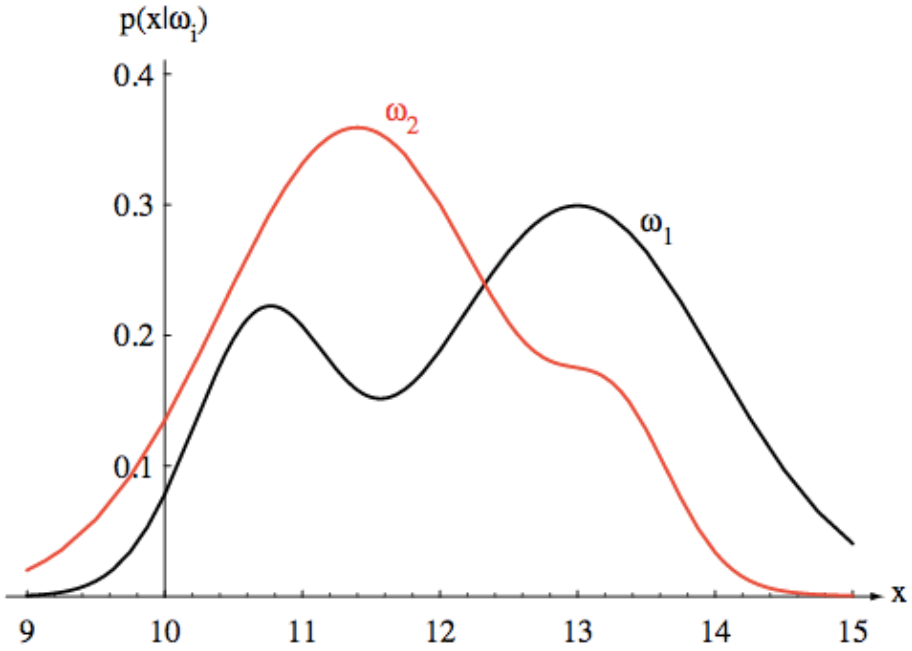


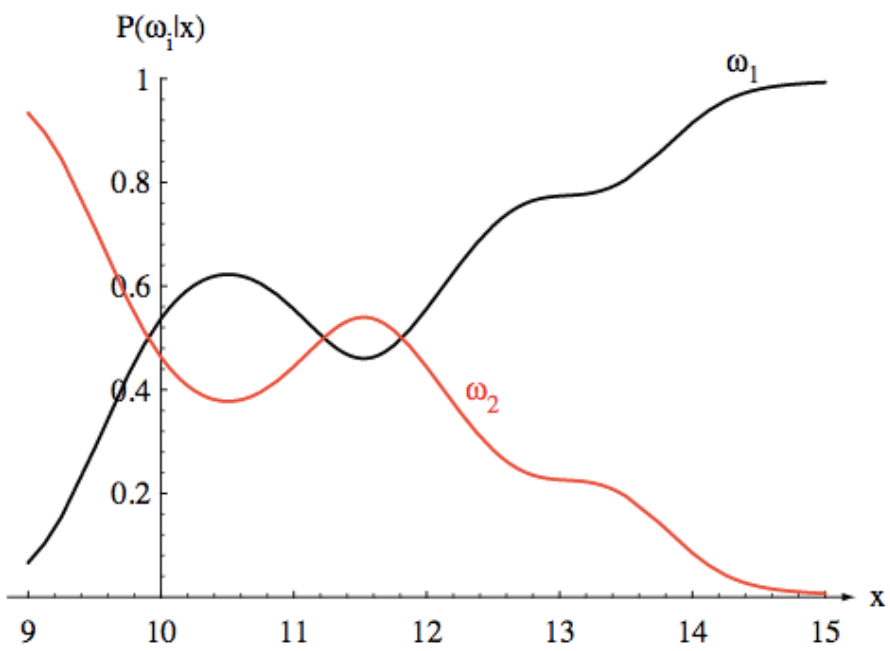
http://slideplayer.com/slide/8845876/

This relationship between the likelihood and the posterior
will lead to two difference approaches we can do parameter estimation

A simple decision rule

- If we can know either p(x|w) or p(w|x) we can make a classification guess

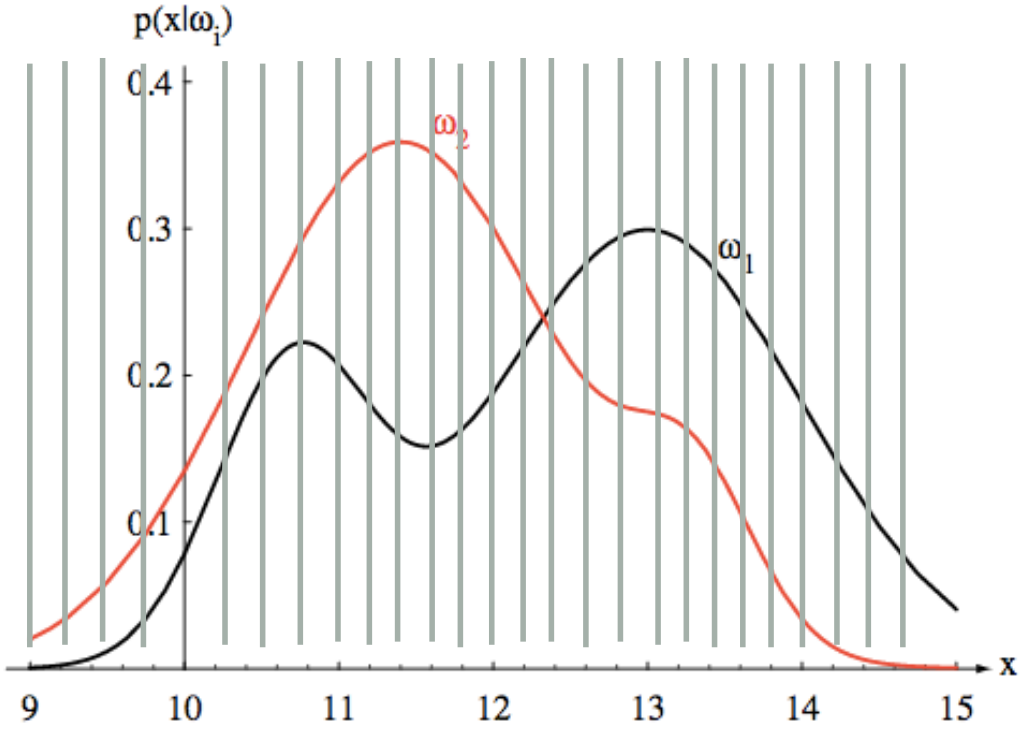




Goal: Find p(x|w) or p(w|x)

Duda et al. Pattern Classification

A simple way to estimate p(x|w)



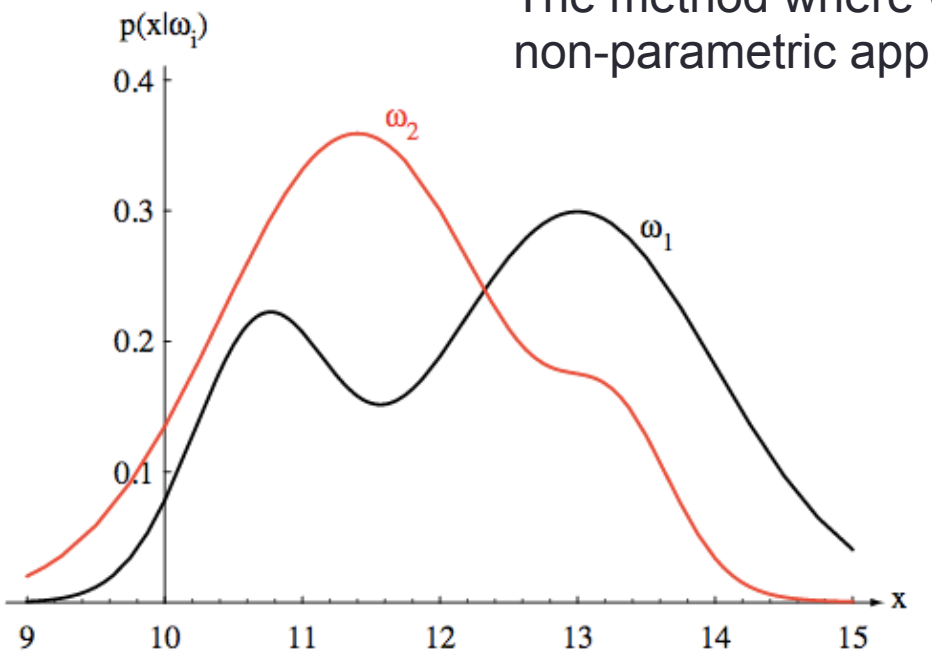
Make a histogram!

What happens if there is no data in a bin?

The parametric approach

- We assume p(x|w) or p(w|x) follow some distributions with parameter θ

The method where we find the histogram is the non-parametric approach



$$p(x) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-(x-\mu)^2/2\sigma^2}$$

Goal: Find θ so that we can estimate p(x|w) or p(w|x)

Maximum Likelihood Estimate (MLE)

$$p(w_i|x) = \frac{p(x|w_i)p(w_i)}{p(x)}$$

$$\text{Posterior} = \frac{\text{likelihood} * \text{prior}}{\text{evidence}}$$

- Maximizing the likelihood (probability of data given model parameters)

$p(\mathbf{x}|\theta) = L(\theta)$ <- This assumes the data is fixed

- Usually done on log likelihood

- Take the partial derivative wrt to θ and solve for the θ that maximizes the likelihood

MLE of binomial trials

- A coin with bias is tossed N times. k times are heads. Find θ, the probability of the coin landing head.

MLE of Gaussian

Maximum Likelihood Estimate (MLE)

$$p(w_i|x) = \frac{p(x|w_i)p(w_i)}{p(x)}$$

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$p(\mathbf{x}|\theta) = L(\theta)$ <- This assumes the data is fixed

- Usually done on log likelihood

- Take the partial derivative wrt to θ and solve for the θ that maximizes the likelihood

Maximum A Posteriori (MAP) Estimate

MLE

- Maximizing the likelihood (probability of data given model parameters)

$$\underset{\theta}{\operatorname{argmax}}\ p(\mathbf{x}|\theta)$$

$$p(\mathbf{x}|\theta) = L(\theta)$$

- Usually done on log likelihood

- Take the partial derivative wrt to θ and solve for the θ that maximizes the likelihood

MAP

- Maximizing the posterior (model parameters given data)

$$\underset{\theta}{\operatorname{argmax}}\ p(\theta|\mathbf{x})$$

- But we don't know $p(\theta|\mathbf{x})$

- Use Bayes rule

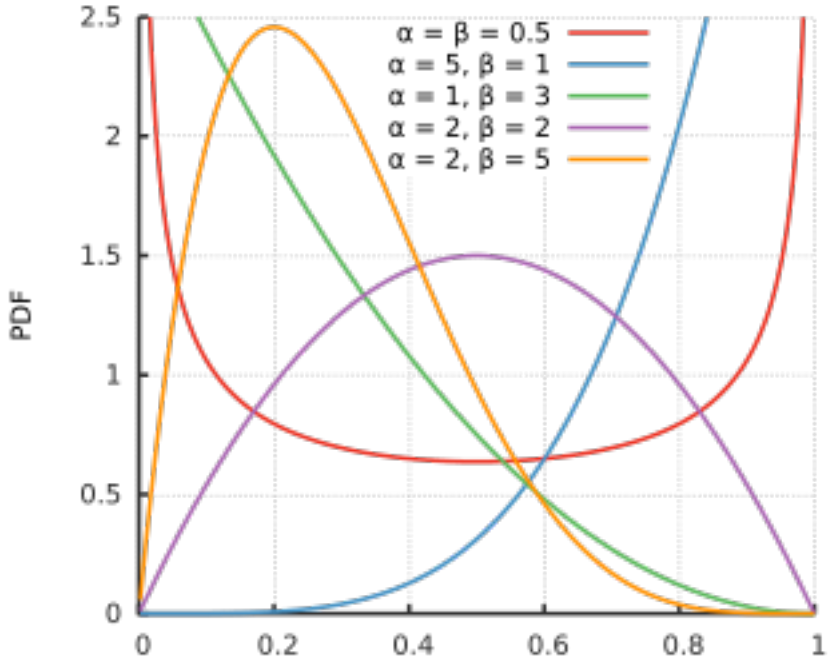
$$p(\theta|\mathbf{x}) = \frac{p(\mathbf{x}|\theta)p(\theta)}{p(\mathbf{x})}$$

- Taking the argmax for θ we can ignore $p(\mathbf{x})$

- $\underset{\theta}{\operatorname{argmax}}\ p(\mathbf{x}|\theta)\ p(\theta)$

MAP on binomial trials

- A coin with bias is tossed N times. k times are heads. Find θ, the probability of the coin landing head.
- We assume θ comes from a Beta distribution



$$p(x) = \frac{1}{\mathrm{B}(\alpha,\beta)} x^{\alpha-1}(1-x)^{\beta-1}$$

The parameters α, β are assume given and constant throughout the derivation (Called hyperparameters)
α, β represents our knowledge of the world

MAP on Gaussian

- We know x is Gaussian with unknown mean μ that we need to estimate and known variance σ^2
- Assume the prior of μ is $N(\mu_0, \sigma_0^2)$

- MAP estimate of μ is

$$\mu_n = \left(\frac{n\sigma_0^2}{n\sigma_0^2 + \sigma^2}\right)\left[\frac{1}{n}\Sigma_{i=1}^{n} x_i\right] + \frac{\sigma^2}{n\sigma_0^2 + \sigma^2}\mu_0$$

Notes of MAP estimate

- Usually harder to estimate that MLE
- If we use a uniform prior distribution for θ
  - MAP estimate = MLE
- Given infinite data
  - MAP estimate converges to MLE
- MAP is useful when you have less data, so you need additional knowledge about the domain
  - MAP estimate tends to converges to faster than MLE even with an arbitrary distribution
  - Can help prevent overfitting
- Useful for model adaptation (MAP adaptation)
  - Learn MLE on larger dataset, use this as your prior distribution
  - Learn MAP estimate on your dataset

Notes on MAP estimate

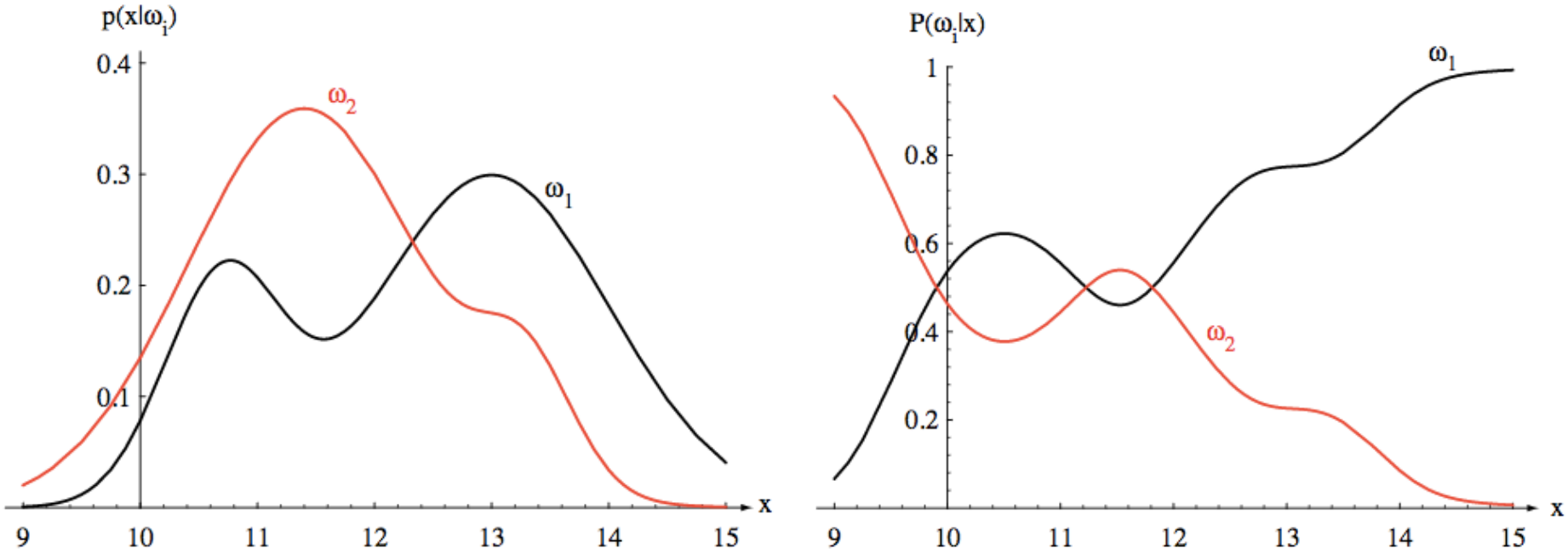
- What is the choice of distribution for the prior?
  - Pick the conjugate priors
  - Makes the math simple without loss of generalizability

https://en.wikipedia.org/wiki/Conjugate_prior

Likelihood	Model parameters	Conjugate prior distribution	Prior hyperparameters	Posterior hyperparameters	h
Bernoulli	p (probability)	Beta	$\alpha,\ \beta$	$\alpha+\sum_{i=1}^{n}x_i,\ \beta+n-\sum_{i=1}^{n}x_i$	α β
Binomial	p (probability)	Beta	$\alpha,\ \beta$	$\alpha+\sum_{i=1}^{n}x_i,\ \beta+\sum_{i=1}^{n}N_i-\sum_{i=1}^{n}x_i$	α β
Negative binomial with known failure number, r	p (probability)	Beta	$\alpha,\ \beta$	$\alpha+\sum_{i=1}^{n}x_i,\ \beta+rn$	α β (i e r
Poisson	λ (rate)	Gamma	$k,\ \theta$	$k+\sum_{i=1}^{n}x_i,\ \frac{\theta}{n\theta+1}$	k $\frac{1}{\theta}$
			$\alpha,\ \beta$[note 3]	$\alpha+\sum_{i=1}^{n}x_i,\ \beta+n$	α in
	p				

A simple decision rule

- If we can know either p(x|w) or p(w|x) we can make a classification guess



Goal: Find p(x|w) or p(w|x) by finding the parameter of the distribution

Likelihood ratio test

- If $P(w_1|x) > P(w_2|x)$, that x is more likely to be class w_1
- Again we know $P(x|w_1)$ is more intuitive and easier to calculate than $P(w_1|x)$

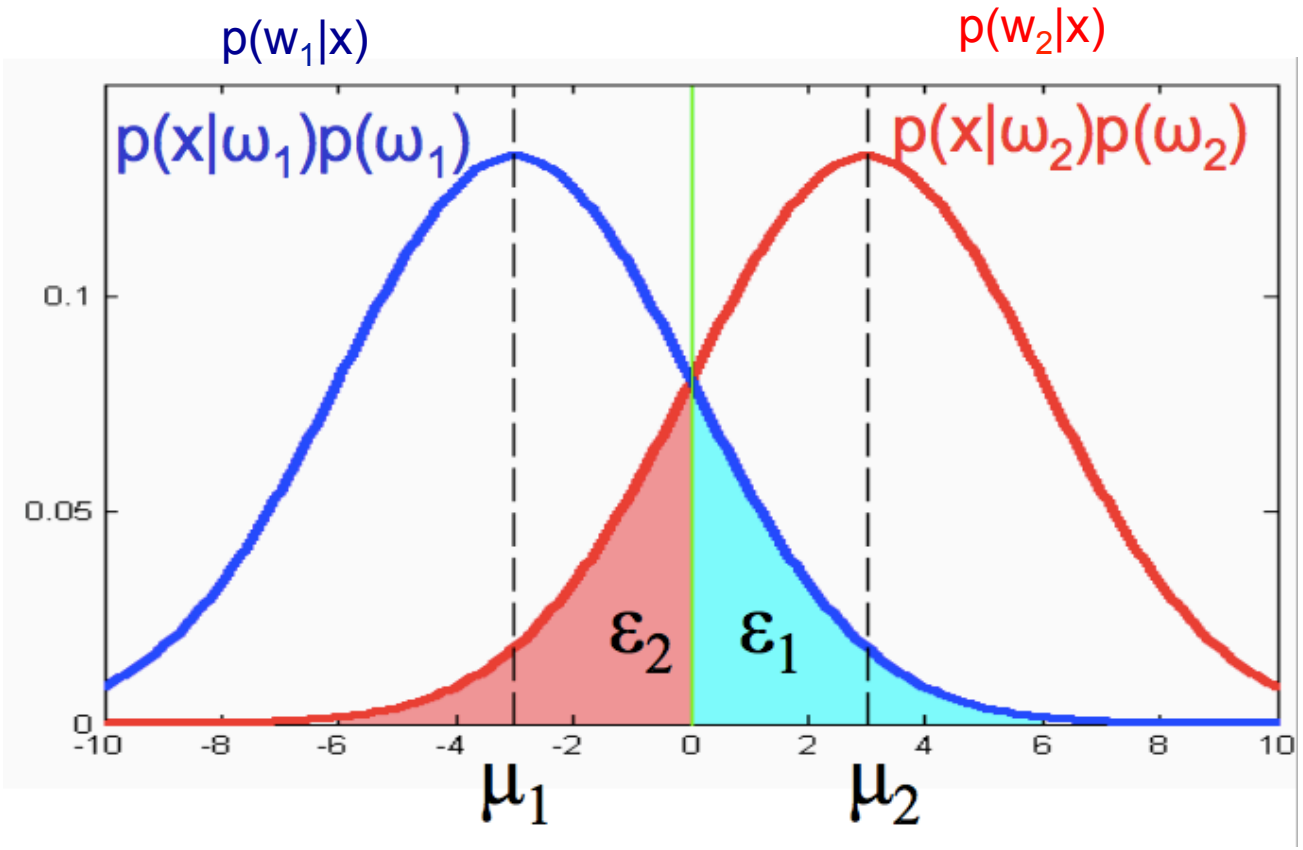
- Our classifier becomes
- $$P(x|w_1)P(w_1) \quad ? \quad P(x|w_2)P(w_2)$$
- $$\frac{P(x|w_1)}{P(x|w_2)} \quad ? \quad \frac{P(w_2)}{P(w_1)}$$

Likelihood ratio

Ratio of priors

Notes on likelihood ratio test (LRT)

- LRT minimizes the classification error (all errors are equally bad)



Notes on LRT

- If $P(w_1|x) > P(w_2|x)$, that x is more likely to be class w_1
  - Also known as MAP decision rule
  - The classifier is sometimes called the Bayes classifier
- If we do not want to treat all error equally, we can assign different loss to each error, and minimize the expected loss. This is called Bayes loss/risk classifier
- $$\frac{P(x|w_1)}{P(x|w_2)} \quad ? \quad \frac{P(w_2)(L_{1|2} - L_{2|2})}{P(w_1)(L_{2|1} - L_{1|1})}$$
- When we treat errors equally we refer to the zero-one loss

Notes on LRT

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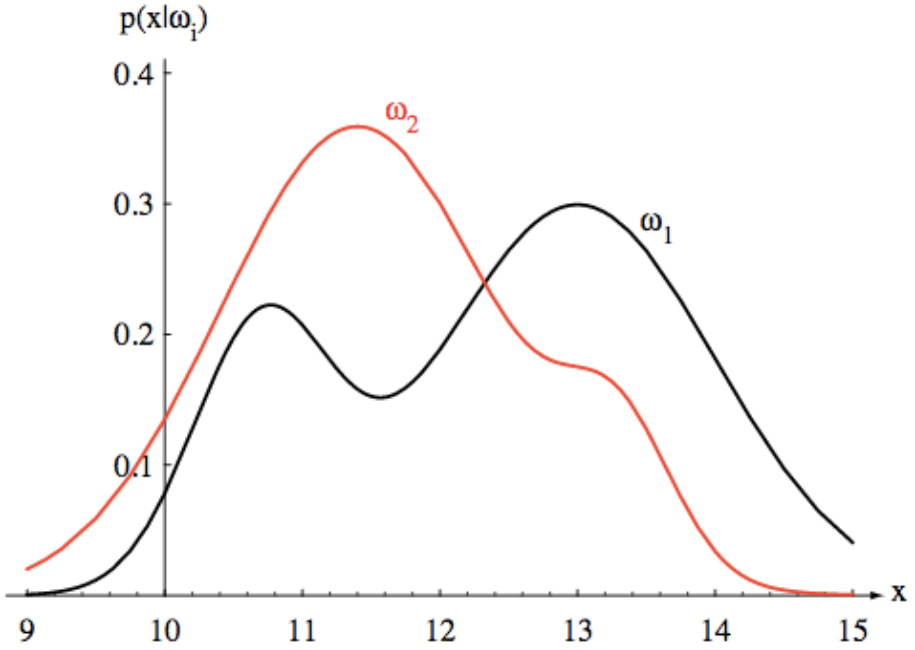
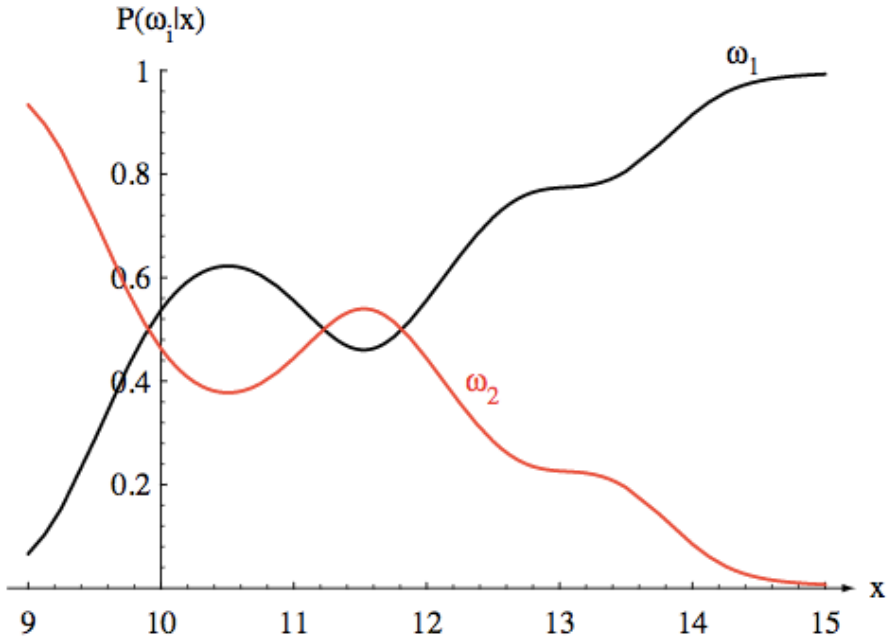
- When we treat errors equally we refer to the zero-one loss
- $L_{1|2} = 1, L_{2|2} = 0, L_{2|1} = 1, L_{1|1} = 0$

Notes on LRT

- If we treat the priors as equal, we get the maximum likelihood criterion
- $$\frac{P(x|w_1)}{P(x|w_2)} \quad ? \quad 1$$





Naïve Bayes

- Below is the LRT or the Bayes classifier

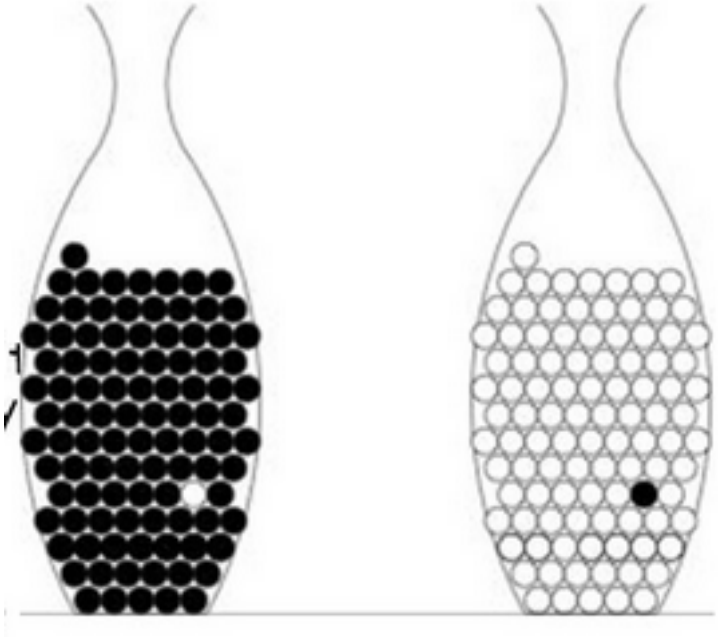
$$P(x|w_1)P(w_1) \quad ? \quad P(x|w_2)P(w_2)$$

- What about Naïve Bayes?

- Here x is a vector with m features $[x_1,x_2,\ldots x_m]$
- $P(x|w_i)$ is m+1 dimensional
  - Sometimes to hard to model, not enough data, overfit, *curse of dimensionality*, etc.
- Assumes $x_1,x_2,\ldots x_m$ independent given w_i (conditional independence)
  - What does this mean?

Conditional independence

- x1 x2 are two drawns from the same urn
- w represents the urn being drawn



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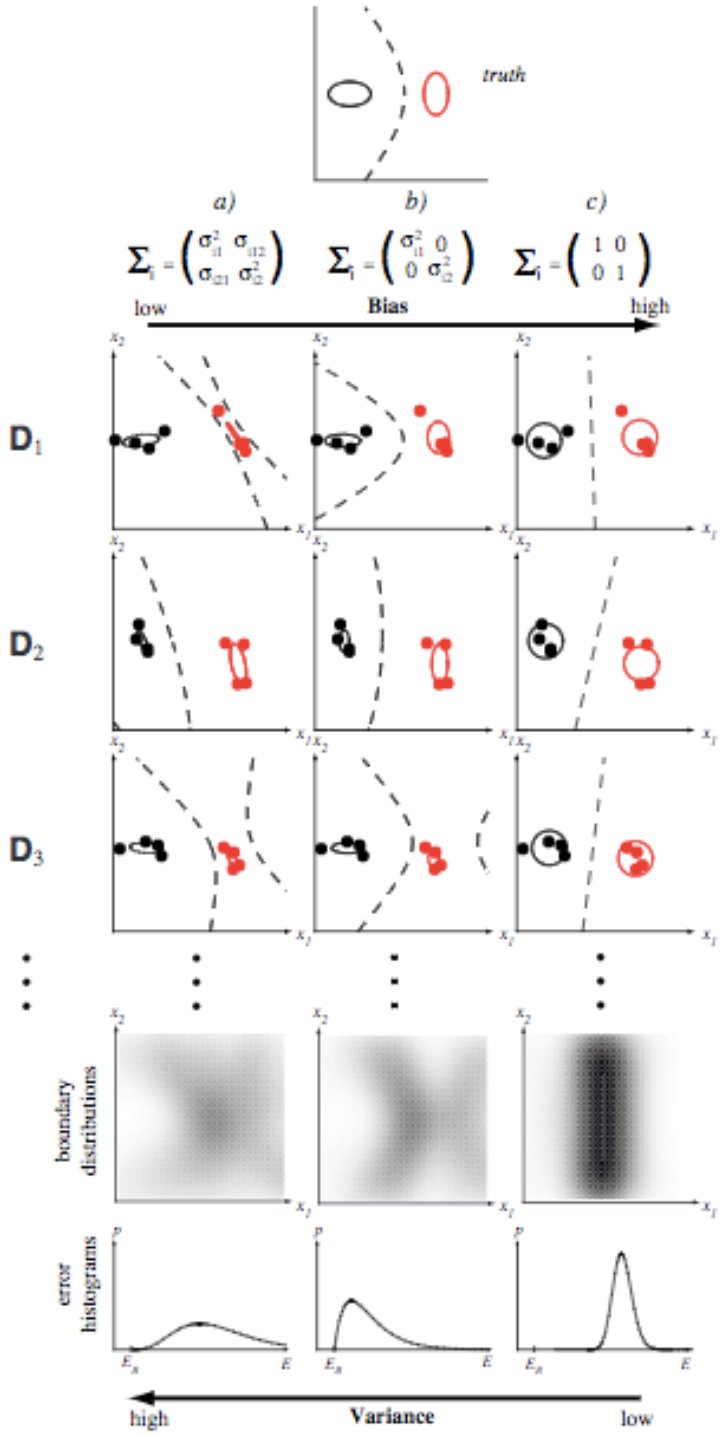
Naïve Bayes

- $P(\mathbf{x}|w_i)P(w_i) = P(w_i) \prod_j P(x_j|w_i)$

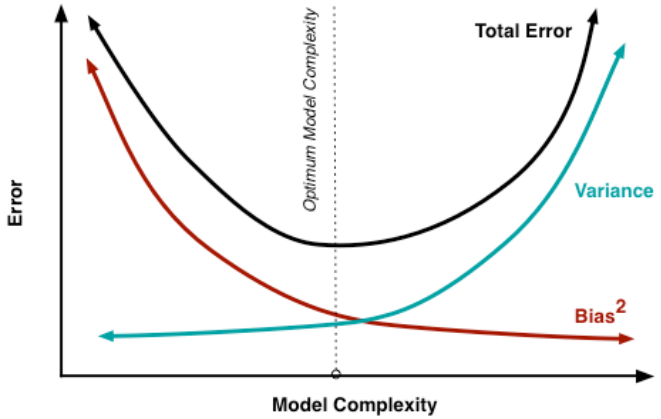
- This assumption simplifies the calculation
- Note that we do not say anything about what kind of distribution $P(x_j|w_i)$ is.
  - In the homework you will play with this
    - Clean data
    - Estimate $P(x_j|w_i)$ using MLE
    - Do prediction



Duda et al. Pattern Classification

Summary

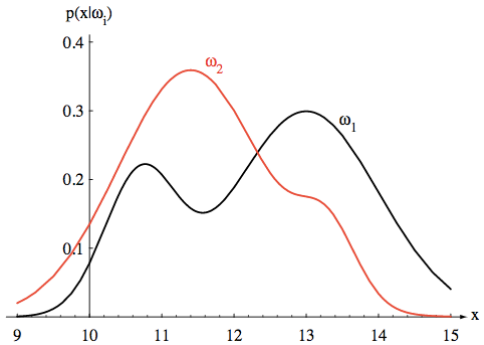
- Normalization
- Bias-Variance trade-off
  - Overfitting and underfitting
- MLE vs MAP estimate
  - How to use the prior
- LRT (Bayes Classifier)
  - Naïve Bayes

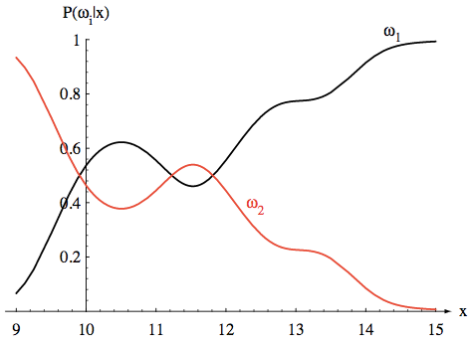


$$\frac{P(x|w_1)}{P(x|w_2)} \quad ? \quad \frac{P(w_2)}{P(w_1)}$$

Likelihood ratio

Ratio of priors





Next homework