Probability Based Learning

Lecture 7, DD2431 Machine Learning

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Advantages of Probability Based Methods

- Work with sparse training data. More powerful than deterministic methods decision trees when training data is sparse.
- **Results are interpretable.** More transparent and mathematically rigorous than methods such as *ANN*, *Evolutionary methods*.
- Tool for interpreting other methods. Framework for formalizing other methods *concept learning, least squares.*

- Probability Theory Basics
 - $\checkmark~$ Bayes' rule
 - $\checkmark~$ MAP and ML estimation
 - $\checkmark~$ Minimum Description Length principle
- Naïve Bayes Classifier
- EM Algorithm

Probability Theory Basics

- A random variable x denotes a quantity that is uncertain
 - $\checkmark~$ the result of flipping a coin,
 - $\checkmark~$ the result of measuring the temperature
- The probability distribution P(x) of a random variable (r.v.) captures the fact that
 - $\checkmark~$ the r.v. will have different values when observed ${\bf and}$
 - $\checkmark\,$ Some values occur more than others.

Random Variables

- A discrete random variable takes values from a predefined set.
- For a **Boolean discrete random variable** this predefined set has two members {0,1}, {yes, no} etc.
- A continuous random variable takes values that are real numbers.



Figures taken from Computer Vision: models, learning and inference by Simon Prince.

Joint Probabilities

- Consider two random variables x and y.
- Observe multiple paired instances of x and y. Some paired outcomes will occur more frequently.
- This information is encoded in the joint probability distribution P(x, y).
- $P(\mathbf{x})$ denotes the joint probability of $\mathbf{x} = (x_1, \dots, x_K)$.



Figure from Computer Vision: models, learning and inference by Simon Prince.

Joint Probabilities (cont.)



Figure from Computer Vision: models, learning and inference by Simon Prince.

The probability distribution of any single variable can be recovered from a joint distribution by summing for the discrete case

$$P(x) = \sum_{y} P(x, y)$$

and integrating for the continuous case

$$P(x) = \int_{\mathcal{Y}} P(x, y) \, dy$$

Marginalization (cont.)



Figure from Computer Vision: models, learning and inference by Simon Prince.

Conditional Probability

- The conditional probability of x given that y takes value y^* indicates the different values of r.v. x which we'll observe given that y is fixed to value y^* .
- The conditional probability can be recovered from the joint distribution P(x, y):

$$P(x \mid y = y^*) = \frac{P(x, y = y^*)}{P(y = y^*)} = \frac{P(x, y = y^*)}{\int_x P(x, y = y^*) \, dx}$$

• Extract an appropriate slice, and then normalize it.



Figure from Computer Vision: models, learning and inference by Simon Prince.

Bayes' Rule

$$P(y \,|\, x) = \frac{P(x \,|\, y) P(y)}{P(x)} = \frac{P(x \,|\, y) P(y)}{\sum_y P(x \,|\, y) P(y)}$$

Each term in Bayes' rule has a name:

- $P(y | x) \leftarrow Posterior$ (what we know about y given x.)
- $P(y) \leftarrow Prior$ (what we know about y before we consider x.)
- P(x | y) ← Likelihood (propensity for observing a certain value of x given a certain value of y)
- $P(x) \leftarrow Evidence$ (a constant to ensure that the l.h.s. is a valid distribution)

In many of our applications y is a discrete variable and \mathbf{x} is a multi-dimensional data vector extracted from the world.

$$P(y \mid \mathbf{x}) = \frac{P(\mathbf{x} \mid y)P(y)}{P(\mathbf{x})}$$

Then

- P(x | y) ← Likelihood represents the probability of observing data x given the hypothesis y.
- $P(y) \leftarrow Prior \text{ of } y$ represents the background knowledge of hypothesis y being correct.
- P(y | x) ← Posterior represents the probability that hypothesis y is true after data x has been observed.

- Bayesian Inference: The process of calculating the posterior probability distribution $P(y | \mathbf{x})$ for certain data \mathbf{x} .
- Bayesian Learning: The process of learning the likelihood distribution $P(\mathbf{x} | y)$ and prior probability distribution P(y) from a set of training points

$$\{(\mathbf{x}_1, y_1), (\mathbf{x}_2, y_2), \dots, (\mathbf{x}_n, y_n)\}$$

Example: Which Gender?

Task: Determine the gender of a person given their measured hair length.

Notation:

- Let $g \in \{$ 'f', 'm' $\}$ be a r.v. denoting the gender of a person.
- Let x be the measured length of the hair.

Information given:

• The hair length observation was made at a boy's school thus

$$P(g = \text{'m'}) = .95, \quad P(g = \text{'f'}) = .05$$

• Knowledge of the likelihood distributions $P(x | g = {}^{\circ}f)$ and $P(x | g = {}^{\circ}m')$

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Task: Determine the gender of a person given their measured hair length \implies calculate $P(g \mid x)$.

Solution:

Apply Bayes' Rule to get

$$\begin{split} P(g = \text{'m'} | x) &= \frac{P(x | g = \text{'m'})P(g = \text{'m'})}{P(x)} \\ &= \frac{P(x | g = \text{'m'})P(g = \text{'m'})}{P(x | g = \text{'f'})P(g = \text{'m'}) + P(x | g = \text{'m'})P(g = \text{'m'})} \end{split}$$

Can calculate $P(g = \mathbf{\dot{f}} | x) = 1 - P(g = \mathbf{\dot{m}} | x)$

Selecting the most probably hypothesis

• Maximum A Posteriori (MAP) Estimate:

Hypothesis with highest probability given observed data

$$y_{\text{MAP}} = \arg \max_{y \in \mathcal{Y}} P(y \mid \mathbf{x})$$
$$= \arg \max_{y \in \mathcal{Y}} \frac{P(\mathbf{x} \mid y) P(y)}{P(\mathbf{x})}$$
$$= \arg \max_{y \in \mathcal{Y}} P(\mathbf{x} \mid y) P(y)$$

• Maximum Likelihood Estimate (*MLE*): Hypothesis with highest likelihood of generating observed data

$$y_{\text{MLE}} = \arg \max_{y \in \mathcal{Y}} P(\mathbf{x} \mid y)$$

Useful if we do not know prior distribution or if it is uniform.

Selecting the most probably hypothesis

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Scenario:

A patient takes a lab test and the result comes back positive. The test returns a correct positive result in only 98% of the cases in which the disease is actually present, and a correct negative result in only 97% of the cases in which the disease is not present. Furthermore, 0.8% of the entire population have cancer.

Scenario in probabilities:

- Priors:
- $P(\text{disease}) = .008 \qquad P(\text{not disease}) = .992$

• Likelihoods:

 $\begin{aligned} P(+ | \text{disease}) &= .98 \\ P(- | \text{disease}) &= .03 \\ P(- | \text{disease}) &= .02 \end{aligned} \qquad P(+ | \text{not disease}) &= .97 \end{aligned}$

Example: Cancer or Not?

Find MAP estimate:

When test returned a positive result,

 $y_{\text{MAP}} = \arg \max_{\substack{y \in \{\text{disease, not disease}\}}} P(y \mid +)$ $= \arg \max_{\substack{y \in \{\text{disease, not disease}\}}} P(+ \mid y) P(y)$

Substituting in the correct values get

 $P(+ | \text{disease}) P(\text{disease}) = .98 \times .008 = .0078$ $P(+ | \text{not disease}) P(\text{not disease}) = .03 \times .992 = .0298$

Therefore $y_{\text{MAP}} =$ "not disease".

The Posterior probabilities:

$$P(\text{disease} | +) = \frac{.0078}{(.0078 + .0298)} = .21$$
$$P(\text{not disease} | +) = \frac{.0298}{(.0078 + .0298)} = .79$$

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Relation to Occams's Razor

Occam's Razor:

Choose the simplest explanation for the observed data

- Information theoretic perspective Occam's razor corresponds to choosing the explanation requiring the fewest bits to represent.
- The optimal representation requires $-\log_2 p(y | \mathbf{x})$ bits to store. (Remember: the Shannon information content)
- Minimum description length principle: Choose hypothesis

$$y_{\text{MDL}} = \arg\min_{y \in \mathcal{Y}} -\log_2 P(y \mid \mathbf{x})$$
$$= \arg\min_{y \in \mathcal{Y}} -\log_2 P(\mathbf{x} \mid y) - \log_2 P(y)$$

• The MDL estimate is equal to the MAP estimate $y_{\text{MAP}} = \arg \max \log_2 P(\mathbf{x} \mid y) + \log_2 P(\mathbf{x} \mid y)$

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$$y_{\text{MAP}} = \arg \max_{y \in \mathcal{Y}} \ \log_2 P(\mathbf{x} \,|\, y) + \log_2 P(y)$$

- Sensors give *measurements* which can be converted to *features*.
- Ideally a feature value is identical for all *samples* in one *class*.





Samples

Feature space

Feature Space

• Sensors give *measurements* which can be converted to *features*.

Feature space

• However in the real world



Samples

because of

- $\checkmark~$ Measurement noise
- $\checkmark~$ Intra-class variation
- $\checkmark~$ Poor choice of features

End result: a *K*-dimensional space

- in which each dimension is a **feature**
- containing *n* labelled **samples** (objects)



Problem: Large Feature Space

- Size of feature space exponential in number of features.
- More features ⇒ potential for better description of the objects but...

More features \implies more difficult to model $P(\mathbf{x} | y)$.

- Extreme Solution: Naïve Bayes classifier
 - $\checkmark\,$ All features (dimensions) regarded as independent.
 - $\checkmark~$ Model k one-dimensional distributions instead of one k-dimensional distribution.

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 - $\checkmark~$ Model k one-dimensional distributions instead of one k-dimensional distribution.

- One of the most common learning methods.
- When to use:
 - $\checkmark\,$ Moderate or large training set available.
 - ✓ Features x_i of a data instance **x** are conditionally independent given classification (or at least reasonably independent, still works with a little dependence).
- Successful applications:
 - \checkmark Medical diagnoses (symptoms independent)
 - $\checkmark\,$ Classification of text documents (words independent)

- **x** is a vector (x_1, \ldots, x_K) of attribute or feature values.
- Let $\mathcal{Y} = \{1, 2, \dots, Y\}$ be the set of possible classes.
- The MAP estimate of y is

$$y_{\text{MAP}} = \arg \max_{y \in \mathcal{Y}} P(y \mid x_1, \dots, x_K)$$

=
$$\arg \max_{y \in \mathcal{Y}} \frac{P(x_1, \dots, x_K \mid y) P(y)}{P(x_1, \dots, x_K)}$$

=
$$\arg \max_{y \in \mathcal{Y}} P(x_1, \dots, x_K \mid y) P(y)$$

- Naïve Bayes assumption: $P(x_1, ..., x_K | y) = \prod_{k=1}^K P(x_k | y)$
- This give the *Naïve Bayes classifier*:

$$y_{\text{MAP}} = \arg \max_{y \in \mathcal{Y}} P(y) \prod_{k=1}^{K} P(x_k \mid y)$$

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Question: Will I go and play tennis given the forecast?

My measurements:

• forecast \in {sunny, overcast, rainy},

2 temperature \in {hot, mild, cool},

3 humidity \in {high, normal},

windy $\in \{ false, true \}.$

Possible decisions: $y \in \{\text{yes, no}\}$

What I did in the past:

| outlook | temp. | humidity | windy | play | outlook | temp. | humidity | windy | play |
|----------|-------|----------|-------|------|----------|-------|----------|-------|------|
| sunny | hot | high | false | no | sunny | mild | high | false | no |
| sunny | hot | high | true | no | sunny | cool | normal | false | yes |
| overcast | hot | high | false | yes | rainy | mild | normal | false | yes |
| rainy | mild | high | false | yes | sunny | mild | normal | true | yes |
| rainy | cool | normal | false | yes | overcast | mild | high | true | yes |
| rainy | cool | normal | true | no | overcast | hot | normal | false | yes |
| overcast | cool | normal | true | yes | rainy | mild | high | true | no |

Counts of when I played tennis (did not play)

| Outlook | | | Temperature | | | Hur | nidity | Windy | |
|---------|----------|------|-------------|-------|------|------|--------|-------|------|
| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| 2 (3) | 4 (0) | 3(2) | 2(2) | 4 (2) | 3(1) | 3(4) | 6 (1) | 6 (2) | 3(3) |

Prior of whether I played tennis or not

| | Pl | | Play | | |
|---------|----|----------------------|----------------|--|--|
| Counts: | | Prior Probabilities: | | | |
| | | | $\frac{9}{14}$ | | |

Likelihood of attribute when tennis played $P(x_i | y=yes)(P(x_i | y=no))$

| Outlook | | | Temperature | | | Hun | nidity | Windy | |
|---------|--|--|-------------|--|--|-----|--------|-------|--|
| | | | | | | | | | |
| | | | | | | | | | |

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Prior of whether I played tennis or not

| | Pl | ay | | Play | |
|---------|-----|----|----------------------|----------------|----------------|
| Counts: | yes | no | Prior Probabilities: | yes | no |
| | 9 | 5 | | $\frac{9}{14}$ | $\frac{5}{14}$ |

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| | | | | | | | | | |

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| sunny | overcast | rain | hot | mild | cool | high | normal | false | true |
| $\frac{2}{9}(\frac{3}{5})$ | $\frac{4}{9}(\frac{0}{5})$ | $\frac{3}{9}(\frac{2}{5})$ | $\frac{2}{9}(\frac{2}{5})$ | $\frac{4}{9}(\frac{2}{5})$ | $\frac{3}{9}(\frac{1}{5})$ | $\frac{3}{9}(\frac{4}{5})$ | $\frac{6}{9}(\frac{1}{5})$ | $\frac{6}{9}(\frac{2}{5})$ | $\frac{3}{9}(\frac{3}{5})$ |

Inference: Use the learnt model to classify a new instance. **New instance:**

$$\mathbf{x} = (\text{sunny, cool, high, true})$$

Apply Naïve Bayes Classifier:

$$y_{\text{MAP}} = \arg \max_{y \in \{\text{yes, no}\}} P(y) \prod_{i=1}^{4} P(x_i | y)$$

 $P(\text{yes}) P(\text{sunny} | \text{yes}) P(\text{cool} | \text{yes}) P(\text{high} | \text{yes}) P(\text{true} | \text{yes}) = \frac{9}{14} \times \frac{2}{9} \times \frac{3}{9} \times \frac{3}{9} \times \frac{3}{9} = .005$ $P(\text{no}) P(\text{sunny} | \text{no}) P(\text{cool} | \text{no}) P(\text{high} | \text{no}) P(\text{true} | \text{no}) = \frac{5}{14} \times \frac{3}{5} \times \frac{1}{5} \times \frac{4}{5} \times \frac{3}{5} = .021$

 $\implies y_{MAP} = no$

Naïve Bayes: Independence Violation

• Conditional independence assumption:

$$P(x_1, x_2, \dots, x_K | y) = \prod_{k=1}^K P(x_k | y)$$

often violated - but it works surprisingly well anyway!

- Note: Do not need the posterior probabilities $P(y | \mathbf{x})$ to be correct. Only need y_{MAP} to be correct.
- Since dependencies ignored, naïve Bayes posteriors often unrealistically close to 0 or 1. Different attributes say the same thing to a higher degree than we expect as they are correlated in reality.

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Naïve Bayes: Estimating Probabilities

• **Problem:** What if none of the training instances with target value y have attribute x_i ? Then

$$P(x_i \mid y) = 0 \quad \Longrightarrow \quad P(y) \prod_{i=1}^{K} P(x_i \mid y) = 0$$

• Solution: Add as prior knowledge that $P(x_i | y)$ must be larger than 0:

$$P(x_i \mid y) = \frac{n_y + mp}{n+m}$$

where

n = number of training samples with label y $n_y =$ number of training samples with label y and value x_i p = prior estimate of $P(x_i | y)$ m = weight given to prior estimate (in relation to data)

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• Aim: Build a classifier to identify spam e-mails.

• How:

Training

- ✓ Create dictionary of words and tokens $W = \{w_1, ..., w_L\}$. These words should be those which are specific to spam or non-spam e-mails.
- ✓ E-mail is a concatenation, in order, of its words and tokens: $\mathbf{e} = (e_1, e_2, \dots, e_K)$ with $e_i \in \mathcal{W}$.
- ✓ Must model and learn $P(e_1, e_2, ..., e_K | _{spam})$ and $P(e_1, e_2, ..., e_K | _{not spam})$

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Email: E



Vector: e

('dear', 'customer', ',', 'a', 'fully', 'licensed',, '/')



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- ✓ Must model and learn $P(e_1, e_2, ..., e_K | _{spam})$ and $P(e_1, e_2, ..., e_K | _{not spam})$ Inference
 - ✓ Given an e-mail, E, compute $\mathbf{e} = (e_1, \ldots, e_K)$.
 - $\checkmark~$ Use Bayes' rule to compute

 $P(\text{spam} | e_1, \dots, e_K) \propto P(e_1, \dots, e_K | \text{spam}) P(\text{spam})$

• How is the joint probability distribution modelled?

$$P(e_1,\ldots,e_K \,|_{\mathrm{spam}})$$

Remember K will be very large and vary from e-mail to e-mail.

• Make conditional independence assumption:

$$P(e_1, \dots, e_K \,|_{\operatorname{spam}}) = \prod_{k=1}^K P(e_k \,|_{\operatorname{spam}})$$

Similarly

$$P(e_1,\ldots,e_K \mid ext{not spam}) = \prod_{k=1}^K P(e_k \mid ext{not spam})$$

• Have assumed the position of word is not important.

• How is the joint probability distribution modelled?

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Remember K will be very large and vary from e-mail to e-mail.

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Learning:

Assume one has n training e-mails and their labels - spam /non-spam

$$\mathcal{S} = \{(\mathbf{e}_1, y_1), \dots, (\mathbf{e}_n, y_n)\}$$

Note: $\mathbf{e}_i = (e_{i1}, \dots, e_{iK_i}).$

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Create dictionary



Make a union of all the distinctive words and tokens in $\mathbf{e}_1, \ldots, \mathbf{e}_n$ to create $\mathcal{W} = \{w_1, \ldots, w_L\}$. (Note: words such as and, the, ... omitted)

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Learn probabilities

For $y \in \{\text{spam}, \text{not spam}\}$

• Set $P(y) = \frac{\sum_{i=1}^{n} \operatorname{Ind}(y_i=y)}{n} \leftarrow \text{proportion of e-mails from class } y.$

2 $n_y = \sum_{i=1}^n K_i imes \mathrm{Ind}\,(y_i = y) \leftarrow \mathrm{total} \ \# \ \mathrm{of} \ \mathrm{words} \ \mathrm{in} \ \mathrm{the} \ \mathrm{class} \ y \ \mathrm{e} ext{-mails}.$

3 For each word w_l compute $n_{yl} = \sum_{i=1}^{n} \operatorname{Ind} (y_i = y) \times \left(\sum_{k=1}^{K_i} \operatorname{Ind} (e_{ik} = w_l) \right) \leftarrow \# \text{ of}$

occurrences of word w_l in the class y e-mails.

3
$$P(w_l \mid y) = rac{n_{yl}+1}{n_y+|\mathcal{W}|} \leftarrow$$
 assume prior value of $P(w_l \mid y)$ is $1/|\mathcal{W}|$.

Inference: Classify a new e-mail $\mathbf{e}^* = (e_1^*, \dots, e_{K^*}^*)$

$$y^* = \arg \max_{y \in \{-1,1\}} P(y) \prod_{k=1}^{K^*} P(e_k^*|y)$$

- **Bayesian theory**: Combines prior knowledge and observed data to find the most probable hypothesis.
- Naïve Bayes Classifier: All variables considered independent.

Expectation-Maximization (EM) Algorithm

Mixture of Gaussians

This distribution is a weight sum of K Gaussian distributions



This model can describe **complex multi-modal** probability distributions by combining simpler distributions.

$$P(x) = \sum_{k=1}^{K} \pi_k \mathcal{N}(x; \mu_k, \sigma_k^2)$$

- Learning the parameters of this model from training data x_1, \ldots, x_n is not trivial using the usual straightforward maximum likelihood approach.
- Instead learn parameters using the **Expectation-Maximization** (EM) algorithm.

Mixture of Gaussians as a marginalization

We can interpret the Mixture of Gaussians model with the introduction of a discrete hidden/latent variable h and P(x, h):



Figures taken from Computer Vision: models, learning and inference by Simon Prince.

Assume: We know the pdf of x has this form:

$$P(x) = \pi_1 \mathcal{N}(x; \mu_1, \sigma_1^2) + \pi_2 \mathcal{N}(x; \mu_2, \sigma_2^2)$$

where $\pi_1 + \pi_2 = 1$ and $\pi_k > 0$ for components k = 1, 2.

Unknown: Values of the parameters (Many!)

$$\Theta = (\pi_1, \mu_1, \sigma_1, \mu_2, \sigma_2).$$

Have: Observed *n* samples x_1, \ldots, x_n drawn from p(x). **Want to:** Estimate Θ from x_1, \ldots, x_n .

How would it be possible to get them all???

For each sample x_i introduce a *hidden variable* h_i

$$h_i = \begin{cases} 1 & \text{if sample } x_i \text{ was drawn from } \mathcal{N}(x;\mu_1,\sigma_1^2) \\ 2 & \text{if sample } x_i \text{ was drawn from } \mathcal{N}(x;\mu_2,\sigma_2^2) \end{cases}$$

and come up with initial values

$$\Theta^{(0)} = (\pi_1^{(0)}, \mu_1^{(0)}, \sigma_1^{(0)}, \mu_2^{(0)}, \sigma_2^{(0)})$$

for each of the parameters.

EM is an *iterative algorithm* which updates $\Theta^{(t)}$ using the following two steps...

EM for two Gaussians: E-step

The responsibility of k-th Gaussian for each sample x (indicated by the size of the projected data point)



Look at each sample x along hidden variable h in the E-step

Figure from Computer Vision: models, learning and inference by Simon Prince.

E-step: Compute the "posterior probability" that x_i was generated by component k given the current estimate of the parameters $\Theta^{(t)}$. (responsibilities)

for i = 1, ... nfor k = 1, 2 $\gamma_{ik}^{(t)} = P(h_i = k | x_i, \Theta^{(t)})$ $= \frac{\pi_k^{(t)} \mathcal{N}(x_i; \mu_k^{(t)}, \sigma_k^{(t)})}{\pi_1^{(t)} \mathcal{N}(x_i; \mu_1^{(t)}, \sigma_1^{(t)}) + \pi_2^{(t)} \mathcal{N}(x_i; \mu_2^{(t)}, \sigma_2^{(t)})}$

Note: $\gamma_{i1}^{(t)} + \gamma_{i2}^{(t)} = 1$ and $\pi_1 + \pi_2 = 1$

EM for two Gaussians: M-step

Fitting the Gaussian model for each of k-th constinuent. Sample x_i contributes according to the responsibility γ_{ik} .



(dashed and solid lines for fit before and after update) Look along samples x for each h in the M-step

Figure from Computer Vision: models, learning and inference by Simon Prince.

EM for two Gaussians: M-step (cont.)

M-step: Compute the Maximum Likelihood of the parameters of the mixture model given out data's membership distribution, the $\gamma_i^{(t)}$'s:

for k = 1, 2

$$\mu_k^{(t+1)} = \frac{\sum_{i=1}^n \gamma_{ik}^{(t)} x_i}{\sum_{i=1}^n \gamma_{ik}^{(t)}},$$

$$\sigma_k^{(t+1)} = \sqrt{\frac{\sum_{i=1}^n \gamma_{ik}^{(t)} (x_i - \mu_k^{(t+1)})^2}{\sum_{i=1}^n \gamma_{ik}^{(t)}}},$$

$$\pi_k^{(t+1)} = \frac{\sum_{i=1}^n \gamma_{ik}^{(t)}}{n}.$$

EM in practice



- **Bayesian theory**: Combines prior knowledge and observed data to find the most probable hypothesis.
- Naïve Bayes Classifier: All variables considered independent.
- **EM algorithm**: Learn probability destribution (model parameters) in presence of hidden variables.

If you are interested in learning more take a look at: C. M. Bishop, *Pattern Recognition and Machine Learning*, Springer Verlag 2006.