02457 Signal Processing in Non-linear Systems: Lecture 7

The EM algorithm and K-means

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- Hour 1
  - Neural networks for classification (signal detection)
  - Your turn! Construct neural network for AND and XOR
  - Exercise 6 walk through
- Hour 2
  - Your turn! Exercise 6 quiz
  - Unsupervised learning
  - Estimating a Gaussian distribution from data revisited
  - Mixture of Gaussians (MoG)
- Hour 3
  - Learning with expectation-maximization (EM)
  - Your turn! Derive EM updates for MoG

Next lecture - lecture 8

- Clustering
  - K-means and family
  - Hierarchical clustering (not part of curriculum but still useful)
- Summary likelihoods
  - What is a likelihood function?
  - Which one to use in a given problem?
- Radial basis networks - from $p(\mathbf{x}, t)$ to $p(t|\mathbf{x})$

- Training data $\mathcal{D} = \{(\mathbf{x}_n, t_n) | n = 1, \ldots, N\}$
- Likelihood function for independent identically distributed (iid) examples, factorizes

$$p(\mathcal{D}|\mathbf{w}) = \prod_{n=1}^{N} [p(t_n|\mathbf{x}_n, \mathbf{w}) p(\mathbf{x}_n|\mathbf{w})] = \underbrace{p(\mathbf{t}|\mathbf{X}, \mathbf{w})}_{\text{supervised}} \quad \overbrace{p(\mathbf{X}|\mathbf{w})}^{\text{unsupervised}}$$

- For regression, we can use least squares learning

$$E(\mathbf{w}) = \sum_{n=1}^{N} (t_n - y(\mathbf{x}_n, \mathbf{w}))^2$$

- More general learning principle maximum likelihood

- Maximum likelihood, that is maximize

$$\log p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \sum_{n=1}^{N} \log p(t_n|\mathbf{x}_n, \mathbf{w})$$

- New convenient definition of cost function

$$E(\mathbf{w}) = -\log p(\mathbf{t}|\mathbf{X}, \mathbf{w})$$

- The *training error per example*

$$e_{\mathrm{tr}}(\mathbf{w}) = \frac{1}{N}\sum_{n=1}^{N} -\log p(t_n|\mathbf{x}_n, \mathbf{w})$$

- A *good generalizer* assigns high probability to the true output for a given *new input*:
- We define *the generalization error*:

$$\begin{aligned} e_{\mathrm{gen}} &= \lim_{M\to\infty} \frac{1}{M}\sum_{m=1}^{M} -\log p(t_m|\mathbf{x}_m, \mathbf{w}) \\ &= \int\int -\log p(t|\mathbf{x}, \mathbf{w})\, p(t|\mathbf{x})\, dt\, p(\mathbf{x})\, d\mathbf{x} \end{aligned}$$

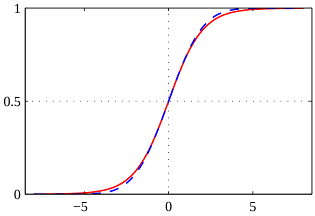
This is the average (expected) error on a test datum $(\mathbf{x}, t)$.

- Labels two class problem: $t_n = 1$ for class one and $t_n = 0$ for class two
- Logistic regression recap – start with real valued function of inputs:

$$a(\mathbf{x}; \mathbf{w}) = \mathbf{w} \cdot \mathbf{x} + w_0$$

- and apply logistic transformation

$$P(t = 1|\mathbf{x}) = y(\mathbf{x}, \mathbf{w}) = \sigma(\, a(\mathbf{x}; \mathbf{w})\,) \quad \text{with} \quad \sigma(a) \equiv \frac{1}{1 + \exp(-a)}$$



Two class problem - cost function

- Labels: $t_n = 1$ for class one and $t_n = 0$ for class two
- Let the network output $y \in [0, 1]$ be the probability of $t = 1$,
- then we can write the likelihood as

$$p(\mathbf{t}|\mathbf{X}, \mathbf{w}) = \prod_{n=1}^{N} p(t_n|\mathbf{x}_n, \mathbf{w}) = \prod_{n=1}^{N} \left\{ y(\mathbf{x}_n|\mathbf{w})^{t_n} [1 - y(\mathbf{x}_n|\mathbf{w})]^{(1-t_n)} \right\}$$

- and the cost function becomes

$$E(\mathbf{w}) = -\sum_{n=1} \{ t_n \log y(\mathbf{x}_n|\mathbf{w}) + (1 - t_n) \log[1 - y(\mathbf{x}_n|\mathbf{w})] \}$$

- This is called the *entropic cost function*

- MLP w linear output: $a(\mathbf{x}; \mathbf{w}) = \mathbf{w}^{(2)} \cdot \mathbf{z}$:

$$y(\mathbf{x}|\mathbf{w}) = \frac{1}{1 + \exp(-a(\mathbf{x}; \mathbf{w}))}$$

- Backprop rule: $\frac{\partial E_n}{\partial w_{jk}} = \delta_{nj} z_{nk}$
- Output unit δ-rule

$$\delta_n = \frac{\partial E_n}{\partial a_n} = \frac{\partial E_n}{\partial y_n} \frac{\partial y_n}{\partial a_n} = \frac{y_n - t_n}{y_n(1 - y_n)} y_n(1 - y_n) = y_n - t_n$$

- Derivative of logistic function:

$$\frac{\partial y_n}{\partial a_n} = \frac{\partial}{\partial a_n} \frac{1}{1 + \exp(-a_n)} = y_n(1 - y_n)$$

- Derivative wrt y:

$$\frac{\partial E}{\partial y_n} = -\left[\frac{t_n}{y_n} - \frac{1 - t_n}{1 - y_n}\right] = \ldots = \frac{y_n - t_n}{y_n(1 - y_n)}$$

Multiple classes

- We use $0 \leq y \leq 1$ coding for C classes and we want the outputs to be the posterior probabilities $P(C|\mathbf{x})$, hence they "should sum to one"

$$y_k(\mathbf{x}) = \frac{\exp a_k(\mathbf{x})}{\sum_{k'} \exp a_{k'}(\mathbf{x})}$$

- Targets are represented by '1 of K'-vectors. If class k:

$$\mathbf{t} = [0, 0, 0, ..., \underbrace{1}_{k}, 0, \ldots, 0]$$

- The likelihood function is given by

$$p(\mathbf{t}|\mathbf{x}) = \prod_{k=1}^{C} y_k(\mathbf{x})^{t_k}$$

- The likelihood and cost function are given by

$$p(\mathbf{t}|\mathbf{x},\mathbf{w}) \quad = \quad \prod_{k=1}^{C} y_k(\mathbf{x})^{t_k} \qquad E = -\sum_n \sum_k t_{nk} \log y_{nk}$$

- The derivatives are relatively simple again

$$\begin{aligned}
\frac{\partial E_n}{\partial a_k} &= \sum_{k'} \frac{\partial E_n}{\partial y_{k'}} \frac{\partial y_{k'}}{\partial a_k} \\
\frac{\partial y_{k'}}{\partial a_k} &= \delta_{kk'} y_k - y_{k'} y_k \\
\frac{\partial E_n}{\partial y_{k'}} &= -\frac{t_{k'}}{y_{k'}}
\end{aligned}$$

$$\frac{\partial E_n}{\partial a_k} \quad = \quad \sum_{k'} -\frac{t_{k'}}{y_{k'}}(\delta_{kk'} y_k - y_k y_{k'}) = -(t_k - y_k \sum_{k'} t_{k'}) = y_k - t_k$$

Your turn! Neural networks for AND and XOR

- Consider 2d inputs $\mathbf{x} = (x_1, x_2)$.
- Represent AND and XOR in truth table & graphically (2d)
- The decision boundary is defined as those points in input space with $p(t = 1|\mathbf{x}, \mathbf{w}) = \frac{1}{2}$
- What is the shape of the decision boundary for logistic regression

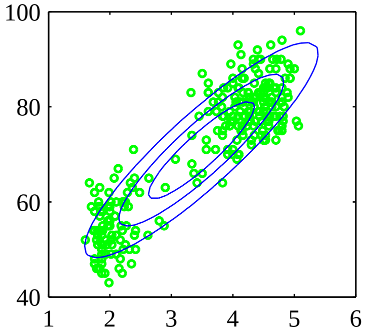
$$P(t = 1|\mathbf{x}) = y(\mathbf{x}, \mathbf{w}) = \sigma(\ \mathbf{w} \cdot \mathbf{x} + w_0\ )$$

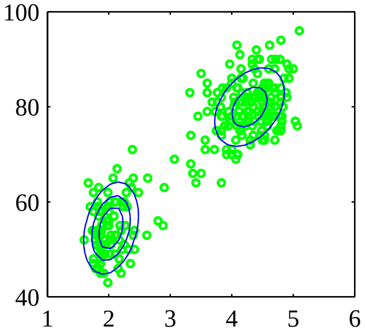
- Try to find **w**-values to solve the AND and XOR problems.
- XOR – use hidden layer and two hidden units
- Hint: each hidden unit acts logistic regressor.

- Exercise 6 walk through
- Your turn! Exercise 6 quiz

Unsupervised learning

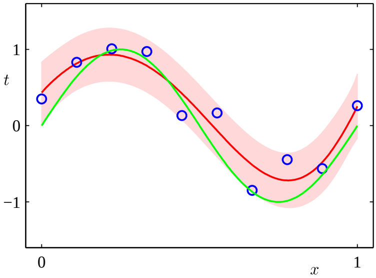
- Learning the distribution of a set of variables $p(\text{input})$.
- Or perhaps just some important characteristics of the distribution

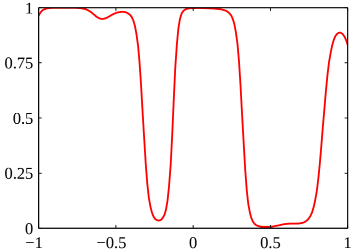




Supervised learning

- Learning the conditional distribution $p(\text{output}|\text{input})$.
- Regression – output continuous
- Classification – output discrete (e.g. positive diagnosis)



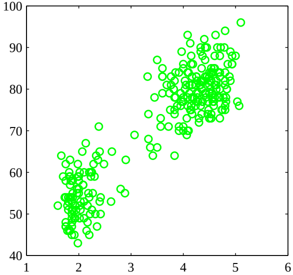


Unsupervised learning task

- Density estimation
  - Compression, creating compact representation of data
  - Generative modeling $P(\mathcal{C}_k|\mathbf{x}) \propto p(\mathbf{x}|\mathcal{C}_k)p(\mathcal{C}_k)$
  - Outlier detection, identification
  - In this course only continuous densities: Gaussian, mixture of Gaussians and non-parametric (histogram and kernel densities)
- Clustering
  - unsupervised classification
  - prototypical summary
- Feature extraction/visualization –
  - finding sub-space with most variance (PCA)
  - finding regions with high density (K-means).

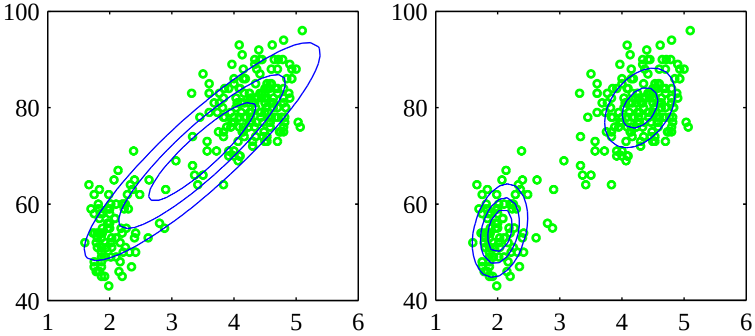
Old Faithful

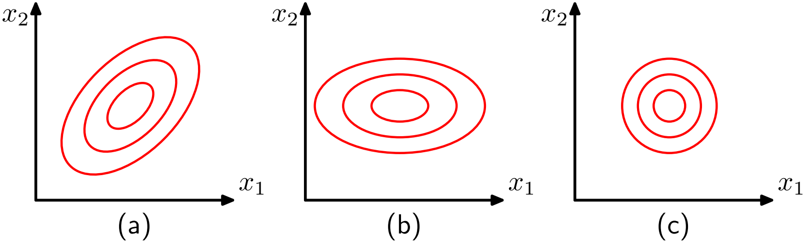
- Hydrothermal geyser in Yellowstone National Park, Wyoming, USA.



- x-axis duration of eruption in minutes
- y-axis time to next eruption in minutes

Density estimation





$$\Sigma = \begin{pmatrix} \alpha & \gamma \\ \gamma & \beta \end{pmatrix}$$

Maximum likelihood

- Bishop 2.3.4 - show on black board
- Training set: $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, ..., \mathbf{x}_N\}$
- Mean value

$$\mu_{\mathrm{ML}} = \frac{1}{N} \sum_n \mathbf{x}_n$$

- Covariance

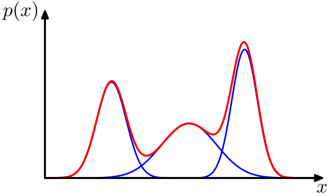
$$\Sigma_{\mathrm{ML}} = \frac{1}{N} \sum_n (\mathbf{x}_n - \mu_{\mathrm{ML}})(\mathbf{x}_n - \mu_{\mathrm{ML}})^T$$

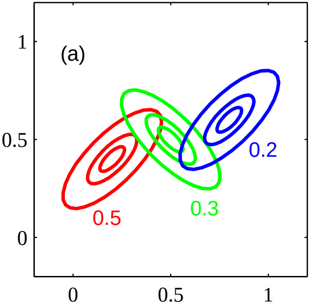
- Overfitting (underestimates covariance):

$$\mathbb{E}_{\mathcal{D}}\left[\Sigma_{\mathrm{ML}}\right] = \frac{N-1}{N} \Sigma_{\mathrm{true}}$$

- Mixture modeling – convex combinations of simpler models

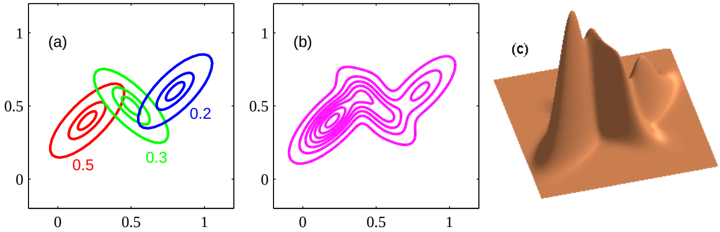
$$p(\mathbf{x}) = \sum_{k=1}^{K} p(k)p(\mathbf{x}|k) \,, \qquad \sum_k p(k) = 1$$





Mixture of Gaussians (MoG)

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \; , \qquad \sum_k \pi_k = 1$$



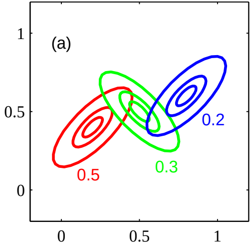
Generative process

- MoG density

$$p(\mathbf{x}) = \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \,, \qquad \sum_k \pi_k = 1$$

- Take a generative view of model:

1. first draw a component number k with relative probabilities π_k,
2. then draw a random vector $\mathbf{x}$ from the given component with density $\mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)$.



- The training set is $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \mathbf{x}_3, ..., \mathbf{x}_N\}$
- the likelihood function is given by

$$p(\mathbf{X}|\mathbf{w}) = \prod_{n=1}^{N} p(\mathbf{x}_n|\mathbf{w})$$

- Parameters $\mathbf{w} = \{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$
- The cost function is then (notice sum inside log)

$$\begin{aligned} E(\mathbf{w}) &= -\sum_{n=1}^{N} \log p(\mathbf{x}_n|\mathbf{w}) = -\sum_{n=1}^{N} \log \sum_{k=1}^{K} p(\mathbf{x}_n|\mathbf{w}_k)\pi_k \\ &= -\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \end{aligned}$$

- We will try to maximize the log likelihood by setting the gradient to zero wrt to the parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \, .$$

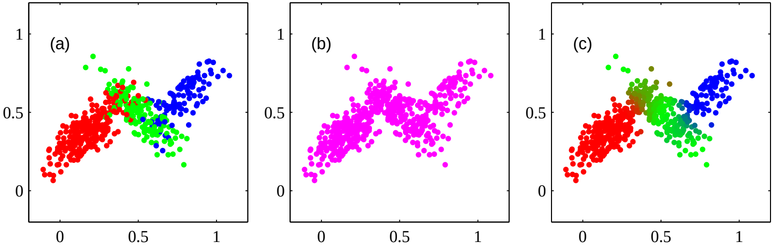
- Introduce the so-called responsibility

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'}, \Sigma_{k'})} \in [0, 1] \, .$$

Responsibility – soft assignments

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'}, \Sigma_{k'})}$$

$$= \frac{p(k)p(\mathbf{x}_n|k)}{\sum_{k'} p(k')p(\mathbf{x}_n|k')} = p(k|\mathbf{x}_n) \in [0, 1] \,.$$



MoG maximum likelihood - π_k

Derivative wrt π_k of

$$\mathcal{L}(\mathbf{w}, \lambda) = E(\mathbf{w}) + \lambda \left[\sum_{k'=1}^{K} \pi_{k'} - 1 \right] .$$

Cost function and responsibility

$$\begin{aligned} E(\mathbf{w}) &= -\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) \\ \gamma_{nk} &= \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'}, \Sigma_{k'})} . \end{aligned}$$

MoG maximum likelihood - $\boldsymbol{\mu}_k$

Use (see appendix C)

$$\frac{\partial}{\partial \boldsymbol{\mu}_k} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \Sigma_k) = \Sigma_k^{-1}(\mathbf{x}_n - \boldsymbol{\mu}_k) \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \Sigma_k)$$

Cost function and responsibility

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MoG maximum likelihood - Σ_k

Use (see appendix C)

$$\frac{\partial}{\partial \Sigma_k} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \Sigma_k) = -\frac{1}{2} \left[\Sigma_k^{-1} - \Sigma_k^{-1} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T \Sigma_k^{-1} \right] \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}$$

Cost function and responsibility

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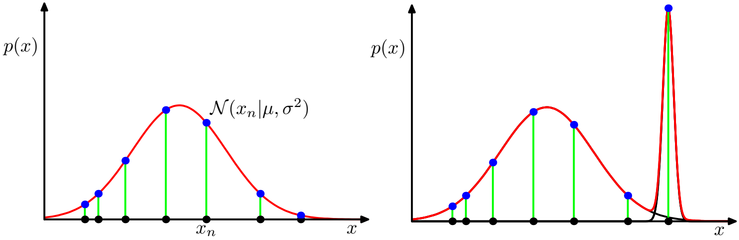
E-step - for $n = 1, \ldots, N$ and $k = 1, \ldots, K$:

$$\gamma_{nk} \leftarrow \frac{\pi_k \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n | \boldsymbol{\mu}_{k'}, \Sigma_{k'})}.$$

M-step - for $k = 1, \ldots, K$:

$$\begin{aligned}
N_k &\leftarrow \sum_{n=1}^{N} \gamma_{nk} \\
\pi_k &\leftarrow \frac{N_k}{N} \\
\boldsymbol{\mu}_k &\leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} \mathbf{x}_n \\
\Sigma_k &\leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T
\end{aligned}$$

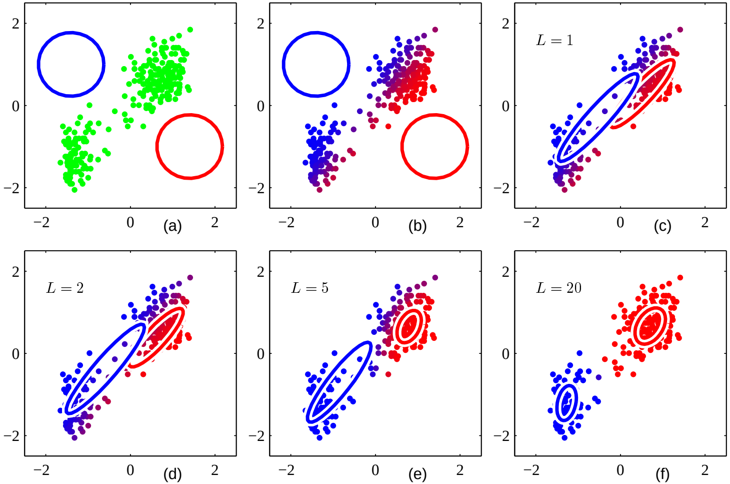
Nature of the maximum likelihood solution



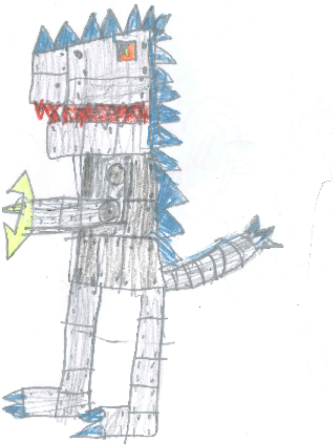
$$E(\mathbf{w}) \quad = \quad -\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k)$$

Consider cost when $\mu_k = \mathbf{x}_n$, $\pi_k > 0$ and $\Sigma_k \to 0$.

MoG for Old Faithful



- Unsupervised learning task
- Mixture models
- Learning with expectation maximization (EM)



- Gaussian – Bishop 2.3 especially 2.3.4
- Mixture of Gaussians – Bishop 2.3.9
- Mixture models – Bishop 9, 9.2-9.3.1
- Alternative free pdf books:
- Hastie, Tibshirani and Friedman, The Elements of Statistical Learning, Springer and
- MacKay, Information Theory, Inference, and Learning Algorithms, Cambridge

Your turn! Derive EM update for MoG

- We will try to maximize the log likelihood by setting the gradient to zero wrt to the parameters $\{\pi_k, \boldsymbol{\mu}_k, \Sigma_k\}$

$$E(\mathbf{w}) = -\sum_{n=1}^{N} \log \sum_{k=1}^{K} \pi_k \mathcal{N}(\mathbf{x}|\boldsymbol{\mu}_k, \Sigma_k) .$$

- Introduce the so-called responsibility

$$\gamma_{nk} = \frac{\pi_k \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_k, \Sigma_k)}{\sum_{k'} \pi_{k'} \mathcal{N}(\mathbf{x}_n|\boldsymbol{\mu}_{k'}, \Sigma_{k'})} \in [0, 1] .$$

Responsibility – soft assignments

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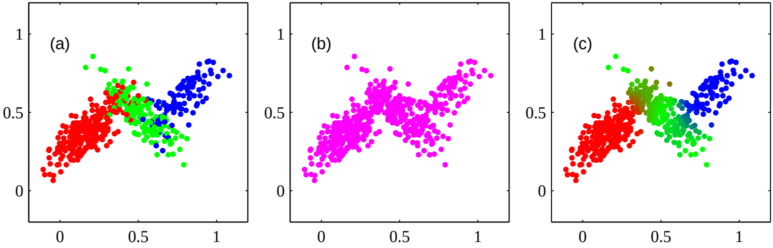

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Derivative wrt π_k of

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Cost function and responsibility

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MoG maximum likelihood - $\boldsymbol{\mu}_k$

Use (see appendix C)

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Cost function and responsibility

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E-step - for $n = 1, \ldots, N$ and $k = 1, \ldots, K$:

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M-step - for $k = 1, \ldots, K$:

$$\begin{aligned} N_k &\leftarrow \sum_{n=1}^{N} \gamma_{nk} \\ \pi_k &\leftarrow \frac{N_k}{N} \\ \boldsymbol{\mu}_k &\leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} \mathbf{x}_n \\ \Sigma_k &\leftarrow \frac{1}{N_k} \sum_{n=1}^{N} \gamma_{nk} (\mathbf{x}_n - \boldsymbol{\mu}_k)(\mathbf{x}_n - \boldsymbol{\mu}_k)^T \end{aligned}$$