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#### Definition 1.1:

1. Let [0,T] be an observation intervall, then we call

$$x(t): [0,T] \to \Psi \subset \mathbb{R}^n \tag{1.1}$$

a time series.

2. Let  $\mathcal{F}([0,T],\Psi)$  be the space of all functions from [0,T] to  $\Psi$ , then we call

$$g(x,\Theta): \mathcal{F}([0,T],\Psi) \times \Omega \to [0,\infty)$$
(1.2)

the model functional.  $\Theta \in \Omega$ ,  $(\Omega \subset \mathbb{R}^d)$  are the modell parameters.

3. We denote by "problem of time series analysis" the solution of:

$$\Theta^* = \arg\min_{\Theta \in \Omega} g(x, \Theta) \tag{1.3}$$

for given  $x(t), t \in [0, T]$  and formaly given  $g(x, \Theta)$ .

These general definitions will give us the possibility to solve a lot of problems

**Example 1.1: (analysis of a time series using a gaussian model)** Let  $t \in \{0, 1, ..., T\}$  and  $x(t) = x_t$  be normaly distributed with mean  $\bar{\mu}$  and variance  $\bar{\sigma}^2$ . Moreover, let  $x_0, x_1, ..., x_T$  be independend. Our model parameters are choosen to be  $\Theta = (\mu, \sigma^2)$ . We look for the best parameters  $\bar{\mu}$  and  $\bar{\sigma}^2$  for the given dataset. Since  $x_t$  are normaly distributed, the density of the  $x_t$  is

$$f_t = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(x_t - \mu)^2}{2\sigma^2}\right).$$
 (1.4)

Given the independence of the  $x_t$  we can calculate the joint distribution of  $(x_t), t \in \{0, \ldots, T\}$ :

$$f_x = \prod_{t=0}^T f_t = \left(\frac{1}{\sqrt{2\pi\sigma^2}}\right)^{T+1} \exp\left[-\frac{\sum_{t=0}^T (x_t - \bar{x})^2 + (T+1)(\bar{x} - \mu)^2}{2\sigma^2}\right],$$
(1.5)

where  $\bar{x} = E[x_t] = \frac{1}{T+1} \sum_{t=0}^{T} x_t$ . If we define the Gaussian model functional as

$$g := -\ln f_x = \frac{T+1}{2}\ln(2\pi\sigma^2) + \frac{\sum_{t=0}^T (x_t - \bar{x})^2 + (T+1)(\bar{x} - \mu)^2}{2\sigma^2}$$
(1.6)

we can solve the problem of the time series analysis analytically by solving the system of equations:

$$\left(\frac{\partial g}{\partial \mu}, \frac{\partial g}{\partial \sigma^2}\right) = 0 \tag{1.7}$$

thus

$$\frac{\partial g}{\partial \mu} = -\frac{2(T+1)(\bar{x}-\mu)}{2\sigma^2} = 0,$$
(1.8)

$$\frac{\partial g}{\partial \sigma^2} = \frac{T+1}{2\sigma^2} - \frac{\sum_{t=0}^T (x_t - \bar{x})^2 + (T+1)(\bar{x} - \mu)^2}{2\sigma^4} = 0.$$
(1.9)

The solution is:

$$\mu = \bar{x},\tag{1.10}$$

$$\sigma^2 = \frac{1}{T+1} \sum_{t=0}^{T} (x_t - \bar{x})^2.$$
(1.11)

These are the known formulars for mean and variance from statistics.

 $\diamond$ 

 $\diamond$ 

**Example 1.2: (K-Means clustering)** Given a set of points x(t) for  $t \in \mathcal{T} \subset [0, T]$ , we look for K clusters  $C_1, \ldots, C_K$ . Therefore let  $\gamma_i(t)$  for  $i = 1, \ldots, K$  and  $t \in \mathcal{T}$  be the probabilities for point x(t) to belong to cluster  $C_i$ . Moreover let

$$\sum_{i=1}^{K} \gamma_i(t) = 1, \forall t \in \mathcal{T}$$
(1.12)

$$\gamma_i(t) \ge 0, \forall t \in \mathcal{T}, i = 1, \dots, K.$$
(1.13)

Now let  $C_i$  be the central point of the *i*th cluster and a point should belong to this cluster, if the function of distance  $d(x(t), C_i) \leq d(x(t), C_j)$  for all j = 1, ..., K. Then we can choose the model parameters according to

$$\Theta(t) = (C_1, \dots, C_K, \gamma_1(t), \dots, \gamma_K(t)).$$
(1.14)

The model function should be

$$g = \sum_{i=1}^{K} \sum_{t \in \mathcal{T}} \gamma_i(t) ||x(t) - C_i||_2.$$
(1.15)

For given  $C_1, \ldots, C_K$  the  $\gamma_i^*(t)$  can be calculated easily: Choose  $\gamma_i(t) = 1$  if x(t) belongs to cluster  $C_i$  and else  $\gamma_i(t) = 0$ . On the other hand, for given  $\gamma_i$ , the  $C_i^*$  can be choosen optimally by setting  $C_i^*$  to be the mean of all points belonging to the *i*th cluster. This leads to the following algorithm:

- 1. Choose the initial  $C_1^0, \ldots, C_K^0$  randomly.
- 2. Repeat for j = 1, 2, ... unitle some stopping criteria is satisfied:
  - (a) Choose  $\gamma_i^j(t) = 1$  if x(t) belongs to cluster  $C_i$ , else  $\gamma_i^j(t) = 0$ .
  - (b) Choose  $C_i^j$  by calculation the mean of all points belonging to the *i*th cluster.

One can prove: Every step of this algorithm improves the result (in sense of making g smaller).

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of June 24, 2008

**Example 2.1: (Markov chain)** In this example we will have a closer look at the discrete time series that satisfy certain independency conditions. Let

 $x = x(t), t \in \{t_0, t_1, \ldots, t_N\} \subset [0, T]$  with equidistant timesteps  $t_i = t_0 + i\Delta_t$  a time series. Moreover, the set of states shall be  $\Psi^N \in \mathbb{R}^N$  with  $x(t) \in \Psi = \{1, \ldots, K\}$ . We abreviate  $x_k = x(t_k)$ .

**Definition 2.1:** A process x is called Markovian or a Markov process, if x satisfies

$$\mathbb{P}[x_{k+1} = j | x_k = i_k, \dots, x_0 = i_0] = \mathbb{P}[x_{k+1} = j | x_k = i_k].$$
(2.1)

If the term above does not depend on the time  $t_k$ , the Markov process is called **homogeneous**. For a homogeneous Markov processes is the **transition matrix** P with  $P = [p_{ij}], p_{ij} = \mathbb{P}[x_{k+1} = j | x_k = i]$  time-invariant. The transition matrix satisfies the following conditions:

- 1.  $0 \le p_{ij} \le 1$
- 2.  $\sum_{j} p_{ij} = 1, \forall i$
- 3.  $P \mathbb{1}^K = \mathbb{1}^K$ , where  $\mathbb{1}^K = (1, 1, \dots, 1)^T$
- 4.  $|\lambda| \leq 1$  where  $\lambda$  is any eigenvalue of P.
- 5. If the process is reversible, thus  $\pi_i p_{ij} = \pi_j p_{ji}$  for some  $\pi$  we get:  $\lambda \in \mathbb{R}$ .

Now we want to solve the minimization problem:

$$\Theta^* = \arg\min_{\Theta} g(x, \Theta). \tag{2.2}$$

Using the homogeneous Markovian property of x we can state:

$$\mathbb{P}[x = (x_0, x_1, \dots, x_T) | P] = \mathbb{P}[x(0) = x_0] \prod_{t=1}^T p_{x_{t-1}, x_t}.$$
(2.3)

**Remark:** We start by expressing this probabilities depending on the whole series to time t. Then we use the Markov property to truncate all but the last dependency and in the end we use the homogeneous property to express the probabilities by the components of P.

Now we denote by  $N_{ij}$  the number of jumps from i to j during the lifetime of x. Then we

can write:

$$\mathbb{P}[x = (x_0, x_1, \dots, x_T)|P] = \mathbb{P}[x(0) = x_0] \prod_{i=1}^K \prod_{j=1}^K p_{ij}^{N_{ij}}.$$
(2.4)

Using  $\tilde{g}(\cdot) = -\ln(\cdot)$  we get

$$\tilde{g}(P) = -\ln(\mathbb{P}[x = (x_0, \dots, x_T)|P]) = -\ln(\mathbb{P}[x(0) = x_0]) - \sum_{i=1}^K \sum_{j=1}^K N_{ij} \ln p_{ij}.$$
(2.5)

We use only the condition  $\forall i : \sum_{j} p_{ij} = 1$ , the other ones will be satisfied automaticaly (has to checked afterwards). Using the Lagrange technic we get the extended problem:

$$g(P,\mu) = -\log \mathbb{P}[x(0) = x_0] - \sum_{i=1}^K \sum_{j=1}^K N_{ij} \ln p_{ij} + \sum_{i=1}^K \mu_i \left(\sum_{j=1}^K p_{ij} - 1\right).$$
(2.6)

Now we can write the derivatives:

$$\frac{\partial g}{\partial p_{ij}} = -\frac{N_{ij}}{p_{ij}} + \mu_i. \tag{2.7}$$

Setting this equal to zero we get:

$$p_{ij}^* = \frac{N_{ij}}{\mu_i}.$$
(2.8)

Now we put this into the condition to get:

$$1 = \sum_{j} p_{ij}^* = \frac{1}{\mu_i^*} \sum_{j} N_{ij}, \mu_i^* = \sum_{j} N_{ij} \,\forall i.$$
(2.9)

Using this for  $p_{ij}^*$  we get:

$$p_{ij}^* = \frac{N_{ij}}{\sum_l N_{il}}.$$
 (2.10)

This is a good point to introduce the robustness:

**Definition 2.2: Robustness** is a measure of the influence of small perturbations on the optimal solution.

Since  $\tilde{g}$  as a function of  $\Theta$  is convex, we have a closer look at the second derivative:

$$\frac{\partial^2 g}{\partial p_{ij}^2}(p_{ij}^*) = \frac{N_{ij}}{p_{ij}^2}(p_{ij}^*) = \frac{(\sum_l N_{il})^2}{N_{ij}}.$$
(2.11)

Thus we can state: The more information we have (thus  $N_{ij}$  is large) the more stability we have in the solution.

We will need some convergence for stochastic objects, so we define:

#### Definition 2.3:

- 1.  $X_n$  converges almost surely (a.s.) to X if  $\mathbb{P}[X_n \to X] = 1$ .
- 2.  $X_n$  converges in probability to X if  $\mathbb{P}[|X_n X| > \varepsilon] \to 0$ .
- 3.  $X_n$  converges in distribution to X if  $\mathbb{E}[X_n] \to \mathbb{E}[X]$ .

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 1, 2008

We start by bringing some definitions back in mind:

**Definition 3.1:** The expectation  $\mathbb{E}_{\omega}[X(\omega)]$  can be calculated by

$$\mathbb{E}_{\omega}[X(\omega)] = \int_{\Omega} X(\omega) P(d\omega).$$
(3.1)

The variance of a random variable is defined by

$$Var_{\omega}[X(\omega)] = \mathbb{E}[(X - \mathbb{E}[X])(X - \mathbb{E}[X])^T].$$
(3.2)

This is a good point, to repeat the Central Limit Theorem:

**Theorem 3.1** Let  $X_n, X_n : \Omega \to \mathbb{R}$  be a sequence of iid random variables with  $\mathbb{E}[X_n] = \mu$ ,  $Var[X_n] = \sigma^2$  for all n. Moreover, let

$$S_{N} = \frac{\frac{1}{N} \sum_{i=1}^{N} X_{i} - \mu}{\frac{1}{\sqrt{N}} \sigma}.$$
(3.3)

Then  $S_n \xrightarrow{n \to \infty} \mathcal{N}(0,1)$  in distribution. Moreover, the probability for  $S_{\infty}$  to be in an intervall [a,b) is given by

$$\mathbb{P}[a \le S_{\infty} < b] = \frac{1}{\sqrt{2\pi}} \int_{a}^{b} \exp\left(-\frac{x^{2}}{2}\right) dx.$$
(3.4)

The second important theorem is the Law of Large Numbers:

**Theorem 3.2** Let  $X_n$  iid with  $\mathbb{E}[X_n] = \mu < \infty$  and  $Var[X] = \sigma^2 < \infty$ . Then

$$\mathbb{P}\left[\left|\frac{1}{N}\sum_{l=1}^{N}X_{l}-\mu\right| \geq \varepsilon\right] \leq \frac{\sigma^{2}}{N\varepsilon^{2}}.$$
(3.5)

Now let  $\Psi = \{1, 2, 3, ..., K\}$  be the **state space** and P the transition matrix for a Markovian process. Moreover  $v \in \mathbb{R}^K$  with  $0 \le v_i \le 1$  and  $\sum_i v_i = 1$  should be a vector of state probabilities, i.e. this is a distribution. Then we have the sequence of distributions starting by some  $v^0$  given by

$$v^{t+1} = P^T v^t. aga{3.6}$$

Translating the fixed point theorem of Banach to our setting, we get:

**Theorem 3.3** If the eigenvalue  $\lambda = 1$  has a geometric size of 1, thus the sub space of the eigenvectors has dimension 1, then  $v^t \xrightarrow{t \to \infty} \pi$ . Where  $\pi$  is the stationary distribution.

This leads us to the Law of Large Numbers for Markovian processes

**Theorem 3.4** Let  $\pi$  be unique and  $f: \Psi \to \mathbb{R}$ . Then

$$\mathbb{E}_{\pi}[f] = \sum_{j \in \Psi} \pi_j f(j).$$
(3.7)

If  $\mathbb{E}_{\pi}[|f|] < \infty$ , then

$$\frac{1}{N} \sum_{j=1}^{N} f(x_j) \xrightarrow{N \to \infty} \mathbb{E}_{\pi}[f]$$
(3.8)

almost surely.

We might be interested in the leaving time, this is the average time we stay in a specific state:

$$\tau(i) = \min\{t \ge 0 : X_{t_0} = i, X_{t_0+t} \ne i\}$$
(3.9)

The average leaving time would be:

$$\mathbb{E}[\tau(i)] = \Delta t \sum_{k=1}^{\infty} k(1 - p_{ii}) p_{ii}^{k-1}$$
(3.10)

where  $\Delta t$  is the step size we use during the time. We can calculate this by using:

$$\mathbb{E}[\tau(i)] = \Delta t \sum_{k=0}^{\infty} p_{ii}^k = \frac{\Delta t}{1 - p_{ii}}$$
(3.11)

if and only if  $p_{ii} < 1$ . This is a measure for the metastability of the time series.

**Definition 3.2:** For  $x \in \Psi$ ,  $y \in \Psi$  we write  $x \mapsto y$  if  $P[X_t = y | X_0 = x] > 0$  for some t. Then y is called **attainable from** x. We write  $x \mapsto y \mapsto x$  as  $x \leftrightarrow y$ .

We can use this to define communication classes:

**Theorem 3.5** Let  $\mathbb{K}$  be the set of close disjunct communication classes (thus  $x, y \in K \in \mathbb{K} \Leftrightarrow x \leftrightarrow y$ ), then  $\lambda = 1$  is  $\#\mathbb{K}$  times an eigenvalue.

**Theorem 3.6** Let C be a close, disjunct communication class and  $P_C$  with  $p_{C,kl} = p_{kl}$  for  $k, l \in C$ . Then there exists an irreducible Markovian process with transition matrix  $P_C$ .

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 1, 2008

**Definition 4.1:**  $E_1, \ldots, E_d$  are called cyclic or periodic classes, if

$$\mathbb{P}[x_1 \in E_{k+1} | x_0 \in E_k] = 1 \tag{4.1}$$

and  $E_{d+1} = E_1$ .

Example 4.1: (deterministic chain) We have a markov chain with transistion matrix

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$
 (4.2)

Then this chain has two communication classes  $C_1 = \{1,2\}$  and  $C_2 = \{3\}$ .  $C_1$  can be split in two periodic classes.

**Definition 4.2:** If for all cyclic classes  $E_1, \ldots, E_d$  of a Markov chain d = 1 then the chain is called aperiodic.

**Theorem 4.1** The following statements are equivalent:

- P has K eigenvalues with  $|\lambda| = 1$
- d = K

**Theorem 4.2 Frobenius-Perron** Let a Markov chain be irreducible and aperiodic, then  $\lambda_1 = 1$  is a unique eigenvalue and  $|\lambda_i| < 1$  for i > 1 and there exists a unique stationary distribution  $\pi^T = \pi^T P$ .

If  $A, B \subset S$  where S is the state space of a Markov chain, then

$$\mathbb{P}[x_1 \in B | x_0 \in A] = \sum_{l \in A} \mathbb{P}[x_1 \in B | x_0 = l] \mathbb{P}[x_0 = l | x_0 \in A]$$
(4.3)

$$=\sum_{\substack{l\in A\\m\in B}} \underbrace{\mathbb{P}[x_1=m|x_0=l]}_{p_{lm}} \mathbb{P}[x_0=l|x_0\in A]$$
(4.4)

**Example 4.2:** (stochastic periodic markov chain) Let P be the transition matrix for a Markov chain with

$$P = \begin{pmatrix} \frac{1}{2} & 0 & \frac{1}{2} \\ 0 & 1 & 0 \\ \frac{1}{2} & 0 & \frac{1}{2} \end{pmatrix}.$$
 (4.5)

 $\lambda = 1$  is two times an eigenvalue of this matrix, we have  $C_1 = \{2\}$  and  $C_2 = \{1,3\}$ , thus by exchanging the states 2 and 3 we get the block structure. For this blocks the assumptions of Frobenius-Perron are satisfied and indeed:  $\lambda_1 = 1$  is unique and  $\pi^1 = 1$  respectively  $\pi^2 = \left(\frac{1}{2}, \frac{1}{2}\right)^T$  are the unique stationary distributions.

**Definition 4.3:** Let  $(X_n)_n$  be a sequence of outputs of a Markov chain, with  $X_n \in \{1, 2\}$ and  $(\mu_1, \sigma_1)$  and  $(\mu_2, \sigma_2)$  two parameter sets. Now let  $O_i \sim \mathcal{N}(\mu_{X_i}, \sigma_{X_i}^2)$ . This is called a (Gaussian) Hidden Markov Modell (HMM).

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 7, 2008

This time, we will have a closer look to so called **Gaussian Mixture Models** (GMMs) and **Finite Mixture Models** (FMMs). Let  $\mu_i, \theta_i$  be sequences of mean and variance for some gaussian processes. Let  $f_i$  be the density of  $\mathcal{N}(\mu_i, \theta_i)$ . Now we construct the density function

$$f = \sum_{y} \alpha_{y} f_{y} \tag{5.1}$$

with  $\sum_{y} \alpha_{y} = 1$  and  $0 \le \alpha_{y} \le 1$ . Where  $f_{y}$  and  $\alpha_{y}$  depend on the random variable Y. For the Likelyhood operator  $\mathbb{L}$  we can define the problem as

$$\tilde{\Theta} = \arg\max_{\Theta} \mathbb{L}[\Theta|x_0, \dots, x_T] = \arg\max_{\Theta} \prod_{t=0}^T \mathbb{P}[X_t = x_t|\Theta]$$
(5.2)

Given this we could use the Loglikelihood  $\mathcal{L}$ , thus:

$$\tilde{\Theta} = \arg\max_{\Theta} \sum_{t=0}^{T} \log\left(\sum_{y} \mathbb{P}[X_t = x_t | Y_t = y, \Theta] \mathbb{P}[Y_t = y]\right)$$
(5.3)

Now we reduce this to the problem with marginal distribution:

$$\hat{\Theta} = \arg\max_{\Theta} \log \mathbb{L}[\Theta|X] = \arg\max_{\Theta} \log \left( \int_{\mathcal{Y}} \mathbb{P}[x_0, \dots, x_T, y|\Theta] dy \right)$$
(5.4)

where  $Y: \Omega \to \mathcal{Y}$ . Defining a family of lower bounds  $B(\Theta)$  with

$$B(\Theta) \le \log \mathbb{L}[\Theta, x], \, \forall \Theta \tag{5.5}$$

we let  $\Theta^i$  be the first *i* elements of this family with

$$\log \mathbb{L}[\Theta|x] = \log \mathbb{P}[x_0, \dots, x_T|\Theta] = \log \int_{\mathcal{Y}} \mathbb{P}[x, y|\Theta] \, dy \tag{5.6}$$

$$= \log \int_{\mathcal{Y}} \frac{\mathbb{P}[X,Y]}{f(y)} f(y) \, dy \tag{5.7}$$

$$= \log \mathbb{E}_{f(Y)} \left[ \frac{\mathbb{P}[X, Y]}{f(Y)} \right].$$
(5.8)

Now we use the Jensen inequation to get

$$\log \mathbb{L}[\Theta|x] \ge \mathbb{E}_{f(Y)} \left[ \log \frac{\mathbb{P}[X,Y]}{f(y)} \right]$$
(5.9)

**Theorem 5.1 Jensen inequation** Let  $u: D \subset \mathbb{R} \to \mathbb{R}$  be a convex function then:

$$\mathbb{E}[u(X)] \ge u(\mathbb{E}[X]) \tag{5.10}$$

This leads us to the formal equation:

$$LB = \left\{ B_f(\Theta) = \mathbb{E}_{f(Y)} \left[ \log \frac{\mathbb{P}[x, Y|\Theta]}{f(Y)} \right] \right\}$$
(5.11)

where f is a density function with  $f : \mathcal{Y} \to \mathbb{R}$ . This leads to the Expectation-Maximization (EM) algoritm. This algorithm consists of two steps: Expectation and Maximization. We have a look at the first step. Here we try to solve the following problem:

$$B_{\max} = \arg \max_{B_f \in LB} B_f(\Theta^i)$$
(5.12)

With  $\int_{\mathcal{Y}} f(y) \, dy = 1$ , therefore we define the Lagrangian

$$J(f,\Theta^{i}) = B_{f}(\Theta^{i}) + \lambda \left(1 - \int_{\mathcal{Y}} f(y) \, dy\right).$$
(5.13)

with

$$\frac{dJ}{df} = \lim_{\varepsilon \to 0} \frac{J(f + \varepsilon g) - J(f)}{\varepsilon}$$
(5.14)

For some test function g. We will have a look at the result during the next lecture.

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 7, 2008

Last time we defined a family of lower bounds to use the EM-Algorithm. In step one (the expectation step) we need to solve the following problem:

$$\max_{f} B_{f}(\Theta) \text{ with } \int_{\mathcal{Y}} f(y) \, dy = 1 \tag{6.1}$$

Thus we use the Lagrangian J to get

$$J(f,\Theta) = B_f(\Theta) + \lambda \left( \int_{\mathcal{Y}} f(y) \, dy - 1 \right)$$
(6.2)

$$\frac{\partial J}{\partial f} = 0$$
(How do we solve this?) (6.3)

$$\frac{\partial J}{\partial \lambda} = 0 \tag{6.4}$$

Equation (6.3) is not a typical problem, here we have to use a variational differential:

$$\frac{\partial J}{\partial f} = \lim_{\varepsilon \to 0} \frac{J(f + \varepsilon g) - J(f)}{\varepsilon} = 0$$
(6.5)

$$\Rightarrow 0 = \lambda + \log \mathbb{P}(x, y | \Theta^{(i)}) - (1 + \log f(Y))$$
(6.6)

To get the following solution

$$f^*(y) = \frac{\mathbb{P}(x, y|\Theta(i))}{\mathbb{P}(x|\Theta^{(i)})} = \mathbb{P}(y|x, \Theta^{(i)})$$
(6.7)

Now we use this within our family to get

$$B_{f^*}(\Theta) = \int_{\mathcal{Y}} \mathbb{P}(y|x,\Theta^{(i)}) \log \frac{\mathbb{P}(x,y|\Theta)}{\mathbb{P}(y|x,\Theta^{(i)})} \, dy$$
(6.8)

And thus

$$B_{f^*}(\Theta^{(i)}) = \int_{\mathcal{Y}} \mathbb{P}(y|x,\Theta^{(i)}) \log \frac{\mathbb{P}(x,y|\Theta^{(i)})}{\mathbb{P}(y|x,\Theta^{(i)})} dy$$
(6.9)

$$= \int_{\mathcal{Y}} \mathbb{P}(y|x,\Theta^{(i)}) \log \mathbb{P}(x|\Theta^{(i)}) \, dy \tag{6.10}$$

$$= \int_{\mathcal{Y}} \mathbb{P}(y|x,\Theta^{(i)}) \, dy \log \mathbb{P}(x|\Theta^{(i)}) \tag{6.11}$$

$$= \log \mathbb{P}(x|\Theta^{(i)}) = \log \mathbb{L}(\Theta^{(i)}|x)$$
(6.12)

Thus, since  $B_f \leq \log \mathbb{L}$  we have the maximum property. Now we can proceed to the second step: Our new problem is

$$\arg\max_{\Theta} B_{f^*}(\Theta) = \arg\max_{\Theta} \int_y \mathbb{P}(y|x,\Theta^{(i)}) \log \frac{\mathbb{P}(x,y|\Theta)}{\mathbb{P}(y|x,\Theta^{(i)})} dy$$

$$= \arg\max_{\Theta} \int_y \mathbb{P}(y|x,\Theta^{(i)}) \log \mathbb{P}(x,y|\Theta) dy =: \arg\max_{\Theta} Q^{(i)}(\Theta) = \Theta^{(i+1)}$$

$$(6.14)$$

**Theorem 6.1** Let  $\Theta^{(i)}$  be output of the algorithm above. Then  $\mathbb{L}(\Theta^{(i+1)}|x) \ge \mathbb{L}(\Theta^{(i)}|x)$ .

**Proof:** 

$$\log \mathbb{L}(\Theta^{i+1}|x) \ge B_f(\Theta^{(i+1)}) = \max_{\Theta} B_f(\Theta) \ge B_f(\Theta^{(i)}) = \log \mathbb{L}(\Theta^{(i)}|x)$$
(6.15)

Nevertheless, solving these problems is no trivial task. Let's have a closer look to the solutions: If the timesteps are statistical independend we get

$$f^* = \mathbb{P}(y|x, \Theta^{(i)}) = \prod_{t=1}^T \mathbb{P}(y_t|x, \Theta^{(i)}) = \prod_{t=1}^T \gamma_t(y_t)$$
(6.16)

with

$$\mathbb{P}(y|x_t, \Theta^{(i)}) = \frac{P(x_t, y|\Theta^{(i)})}{\sum_{y=1}^{K} P(x_t, y|\Theta^{(i)})} = \gamma_t(y)$$
(6.17)

then

$$f^* = \gamma_t(y). \tag{6.18}$$

Now we might use this for  $Q^{(i)}$ :

$$Q^{(i)}(\Theta) = \sum_{y=1}^{K} \gamma_t(y) \log \mathbb{P}(x_t, Y_t = y | \Theta)$$
(6.19)

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 7, 2008

While the theory of the last lectures was for general Mixture Models, we will now have a special look at Gaussian Mixture Models. Let  $G(\cdot, \mu_y, \Sigma_y)$  be the density function of  $\mathcal{N}(\mu_y, \Sigma_y)$ , thus

$$G(x, \mu_y, \Sigma_y) = \frac{1}{z} \exp\left(-(x - \mu_y)^T \Sigma_y^{-1} (x - \mu_y)\right)$$
(7.1)

where z is used to normalize the measure. Additionally let

$$\alpha_y = P(Y = y|\Theta) \tag{7.2}$$

with  $\Theta = (\mu_1, \ldots, \mu_K, \Sigma_1, \ldots, \Sigma_K, \alpha_1, \ldots, \alpha_K)$ . Then we write a Lagrangian:

$$J(\Theta) = Q^{(i)}(\Theta) + \lambda \left(\sum_{y=1}^{K} \alpha_y - 1\right)$$
(7.3)

and differentiate with respect to  $\Theta$  and set those to zero.

$$\partial_{\Sigma_y^{-1}} J(\Theta) = \sum_{t=0}^T \gamma_t(y) (-(x_t - \mu_y)(x_t - \mu_y)^T + \partial_{\Sigma_y^{-1}} \log(z(\Sigma_y))) = 0$$
(7.4)

$$\partial_{\mu_y} J(\Theta) = -2 \sum_{t=0}^T \gamma_t(y) (-(x_t - \mu_y)) = 0$$
(7.5)

$$\partial_{\lambda}J(\Theta) = \sum_{y=1}^{K} \alpha_y - 1 = 0 \tag{7.6}$$

$$\partial_{\alpha_y} J(\Theta) = \sum_{t=0}^T \frac{\gamma_t(y)}{\alpha_y} - \lambda = 0$$
(7.7)

Now we start to solve these equations

$$\mu_y^* = \frac{\sum_t \gamma_t x_t}{\sum_t \gamma_t} \tag{7.8}$$

$$\Sigma_y^* = \frac{1}{\sum_t \gamma_t} \sum_t \gamma_t (x_t - \mu_y^*) (x_t - \mu_y^*)^T$$
(7.9)

$$\alpha_y^* = \frac{1}{\sum_y \gamma(y)} \sum_t \gamma_t, \gamma_y = \sum_{t=0}^T \gamma_t(y).$$
(7.10)

At this point, the lecture was continued by a computational and graphical example, this will not be included in this file.

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

version of July 7, 2008

During this lecture, we will have a look at high-dimensional problems. Therefore we assume there are some correlations between the different dimensions. Now we want to keep as much information as possible while reducing the dimensions. Thus let T be a matrix where the columns define a basis of some submanifold. Moreover, the columns should be orthonormal. Then we have a look at

$$\sum_{t} \|(x_t - \mu) - TT^T(x_t - \mu)\|_2^2 \to \min_{T}, T^TT = \mathbb{1}^{m \times m}$$
(8.1)

for some  $\mu$ . To solve this, we use once more the Lagrangian principle:

$$L := \sum_{t} \|(x_t - \mu) - TT^T(x_t - \mu)\|_2^2 + \sum_{i,j=1}^m \lambda_{ij} (T^T T - \mathbb{1}^{m \times m})$$
(8.2)

$$= \sum_{t} \|(x_t - \mu) - TT^T(x_t - \mu)\|_2^2 + e^T \lambda \odot (T^T T - 1)e$$
(8.3)

Where e is a vector full of ones. Let's have a look at the first part of the L:

$$\|(x_t - \mu) - TT^T(x_t - \mu)\|_2^2$$
(8.4)

$$=((x_t - \mu) - TT^T(x_t - \mu))^T((x_t - \mu) - TT^T(x_t - \mu))$$
(8.5)

$$=((x_t - \mu)^T (x_t - \mu) - (x_t - \mu)^T T T^T (x_t - \mu) - (x_t - \mu)^T T T^T (x_t - \mu)$$
(8.6)

$$+ (x_t - \mu)^T T T^T T T^T (x_t - \mu))$$
(8.7)

$$=((x_t - \mu)^T (x_t - \mu) - (x_t - \mu)^T T T^T (x_t - \mu)$$

$$=(x_t - \mu)^T (\mathbb{1} - T T^T) (x_t - \mu)$$
(8.8)
(8.9)

$$= (x_t - \mu)^T \underbrace{(\mathbb{1} - TT^T)}_{=:Q} (x_t - \mu)$$
(8.9)

Thus

$$\frac{\partial L}{\partial \mu} = -2Q \sum_{t} (x_t - \mu) \tag{8.10}$$

By setting this to zero, we get

$$\sum_{t} (x_t - \mu) \in \operatorname{Kern}(Q) \ni \xi, \bar{x} = \frac{1}{N} \sum_{t} x_t, \mu = \bar{x} + \xi.$$
(8.11)

We need one more derivative:

$$\frac{\partial L}{\partial T} = -2\sum_{t} (x_t - \mu)(x_t - \mu)^T T - 2T\lambda$$
(8.12)

Now we set this to zero, too:

$$\sum_{t} (x_t - \mu)(x_t - \mu)^T T = -T\lambda$$
(8.13)

For m = 1 this is an eigenvalue problem. Thus we can solve this problem step by step by solving *m* eigenvalue problems. Therefore, this approach is called "principle components analysis". Let us have a closer look at this stuff:

$$\sum_{t} ((x_t - \mu) - TT^T (x_t - \mu))^T ((x_t - \mu) - TT^T (x_t - \mu))$$
(8.14)

$$= \sum_{t} (x_t - \mu)^T (x_t - \mu) - \sum_{t} \operatorname{trace}(T^T (x_t - \mu) (x_t - \mu)^T T)$$
(8.15)

$$= \sum_{t} (x_t - \mu)^T (x_t - \mu) - \operatorname{trace}(T^T \underbrace{\sum_{t} (x_t - \mu) (x_t - \mu)^T T}_{=\operatorname{Cov}} T)$$
(8.16)

$$=\sum_{t} (x_t - \mu)^T (x_t - \mu) - \operatorname{trace}(T^T \Lambda T)$$
(8.17)

$$=\sum_{t}^{T} (x_t - \mu)^T (x_t - \mu) - \operatorname{trace}(\Lambda)$$
(8.18)

$$=\sum_{i=m+1}^{n}\lambda_{i} \tag{8.19}$$

Lecture by: Prof. Illia Horenko deputized by: Eike Meerbach Notes by: Lars Putzig

version of July 8, 2008

This time we have a look at autoregressive processes. Therefore let  $Z = \{z_1, \ldots, z_t\}$  with  $z_i \in \mathbb{R}^d$  be a time series. Normally, we are looking for some  $f : \mathbb{R}^d \to \mathbb{R}^d$  such that  $\hat{Z}_{k+1} = f(Z_k)$  and  $||\hat{Z}_{k+1} - Z_{k+1}||$  should be as small as possible. Now we add additional information to this function, thus  $\hat{Z}_{k+1} = f(Z_k, Z_{k-1}, \ldots, Z_{k-p})$ . We will use some general assumptions throughout this lecture:

- 1. f should be affin multilinear, thus  $\hat{Z}_t = \nu + A_1 z_{t-1} + A_2 z_{t-2} + \dots + A_p z_{t-p}$  with  $\nu \in \mathbb{R}^d$ and  $A_i \in \mathbb{R}^{d \times d}$ .
- 2. The error  $\varepsilon_t = z_t \hat{Z}_t \in \mathbb{R}^d$  should be white noise, thus  $\varepsilon_t$  is a stochastic process with  $E[\varepsilon_t] = 0 \forall t$  and  $E[\varepsilon_t \varepsilon_t^T] = R \forall t$  and  $E[\varepsilon_t \varepsilon_s^T] = 0 \forall, s \neq t$ .

**Definition 9.1:** A stochastic process  $Z = \{z_t\}$  is called a **VAR(p)-process** (Vector AutoRegressive), if a process  $\varepsilon = \{\varepsilon_t\}$  exists such that

$$z_{t+1} = \nu + A_1 z_t + A_2 z_{t-1} + \dots + A_p z_{t-p+1} + \varepsilon_{t+1}$$
(9.1)

with  $\varepsilon_t, \nu \in \mathbb{R}^d$  and  $A_i \in \mathbb{R}^{d \times d}$ .

There are two different ways to initialize VAR(p)-processes:

- 1. We assume Z to be stationary (e.g. we started the process at  $t = -\infty$ ).
- 2. We initialize Z with arbitrary values  $(z_1, \ldots, z_p)$ .

For now, let p = 1, thus

$$Z_t = \nu + A_1 z_{t-1} + \varepsilon_t \tag{9.2}$$

For some given  $z_0$  we get

$$z_1 = \nu + A_1 z_0 + \varepsilon_1 \tag{9.3}$$

$$z_{2} = \nu + A_{1}(\nu + A_{1} + z_{0} + \varepsilon_{1}) + \varepsilon_{2} = (I + A_{1})\nu + A_{1}^{2}z_{0} + A_{1}\varepsilon_{1} + \varepsilon_{2}$$
(9.4)

$$z_t = (I + A_1 + \dots + A_1^{t-1})\nu + A_1^t z_0 + \sum_{k=0}^{t-1} A_1^k \varepsilon_{t-k}$$
(9.5)

$$z_{\infty} = \lim_{t \to \infty} z_t = (I - A_1)^{-1} \nu + \sum_{k=0}^{\infty} A_1^k \varepsilon_{t-k}$$
(9.6)

if and only if  $\sigma(A_1) < 1$ , where  $\sigma(A_1)$  is the spectral radius of  $A_1$ .

**Definition 9.2:** A VAR(1)-process is called stable, if  $\sigma(A_1) < 1$ . This is equivalent to  $\det(I - sA) \neq 0$  for  $s \leq 1$ .

Now we expand this theory to VAR(p)-processes by splitting these into VAR(1)-processes:

$$\bar{Z}_t = [z_t, z_{t-1}, \dots, z_{t-p+1}]^T, \bar{\nu} = [\nu, 0, \dots, 0]^T$$

$$(9.7)$$

$$(4_1 \dots A_p)$$

$$\bar{A} = \begin{pmatrix} I & & & \\ I & & & \\ & \ddots & & \vdots \\ 0 & & I & 0 \\ & & & & 0 \end{pmatrix}, \bar{\varepsilon}_t = [\varepsilon_t, 0, \dots, ]^T$$
(9.8)

$$\bar{Z}_t = \bar{\nu} + \bar{A}\bar{z}_{t-1} + \bar{\varepsilon}_t \tag{9.9}$$

Thus a VAR(p)-process could be called stable, if  $\sigma(\bar{A}) < 1$  or det $(I - A_1 s - A_2 s^2 - \cdots - A_p s^p) \neq 0$  for all  $s \leq 1$ . A stable VAR(p)-process started by  $t = -\infty$  will be stationary. How about prediction?

$$\bar{z}_{t+1} = \mathbb{E}[z_{t+1}|z_t, \dots, z_{t-p+1}] = \nu + A_1 z_t + \dots + A_p z_{t-p+1}$$
(9.10)

Multi-step prediction works the same way, we simply use the predicted values to calculate the missing ones recursively. The error is  $\varepsilon_{t+1}$ . For multi-step predictions the errors sum up, thus:

$$z_{t+j} - \bar{z}_{t+j} = \sum_{i=1}^{j} A_i^{j-1} \varepsilon_{t+i}$$
(9.11)

The expectation of the error is always zero, thus the guess is unbiased. Moreover, this is a minimal MSE-estimator. As a last point, we try to estimate the parameters of the VAR(p) model. Let  $Z = \{z_1, \ldots, z_T\}$  where the first p elements are used as initial values. We define

$$\Phi := (\nu, A_1, A_2, \dots, A_p) \in \mathbb{R}^{d \times (dp+1)}$$

$$(9.12)$$

$$Y := (z_{p+1}, z_{p+2}, \dots, z_T) \in \mathbb{R}^{d \times (T-p)}$$
(9.13)

$$X_t := \begin{pmatrix} 1 \\ z_t \\ \vdots \\ z_{t-p+1} \end{pmatrix} \in \mathbb{R}^{dp+1}$$

$$(9.14)$$

$$X := (X_p, X_{p+1}, \dots, X_T) \in \mathbb{R}^{(dp+1) \times (T-p+1)}$$
(9.15)

Thus  $z_t = \Phi X_{t-1} + \varepsilon_t$  for t > p. Then we get

$$z_t X_{t-1}^T = \Phi X_{t-1} X_{t-1}^T + \varepsilon_t X_{t-1}$$
(9.16)

$$\mathbb{E}[z_t X_{t-1}^T] = \mathbb{E}[\Phi X_{t-1} X_{t-1}^T]$$
(9.17)

The lefthand side of this equations could be estimated by

$$\mathbb{E}[z_t X_{t-1}^T] \approx \frac{1}{T-p} \sum_{i=p+1}^T z_i X_{i-1}^T = \frac{1}{T-p} Y X^T,$$
(9.18)

while the righthand side is approximatly

$$\mathbb{E}[\Phi X_{t-1} X_{t-1}^T] \approx \frac{1}{T-p} \sum_{i=p+1}^T X_{i-1} X_{i-1}^T = \frac{1}{T-p} X X^T.$$
(9.19)

Putting these estimators together, we get:

$$YX^T = \Phi XX^T \Rightarrow \hat{\Phi} = YX^T (XX^T)^{-1}$$
(9.20)

Lecture by: Prof. Illia Horenko Notes by: Lars Putzig

July 8, 2008

Let  $Z_t \in \mathbb{R}^n$  with

$$Z_{t+\tau} = \sum_{i=0}^{p} A_i(\tau) Z_{t-i\tau} + B(\tau) \varepsilon_{t+\tau}$$
(10.1)

with  $A_i(\tau), B(\tau) \in \mathbb{R}^{n \times n}, \mathbb{E}[\varepsilon_t] = 0$  and  $\mathbb{E}[\varepsilon_{t_1}^T \varepsilon_{t_2}] = \delta(t_1 - t_2)$ . Then we get

$$\mathbb{E}[Z_{t+\tau}] = \sum_{i=0}^{p} A_i(\tau) \mathbb{E}[Z_{t-i\tau}]$$
(10.2)

Now we multiply the  $Z_{t+\tau}$  by  $Z_{t-j\tau}^T$  for j = 0, 1, ... to see

$$\mathbb{E}[Z_{t+\tau}Z_{t-j\tau}^T] = \sum_{i=0}^p A_i(\tau)\mathbb{E}[Z_{t-i\tau}Z_{t-j\tau}^T].$$
(10.3)

**Definition 10.1:** We denote by  $\rho(t-\tau)$  the **auto-covariance**. We define

$$\rho(t-\tau) = \mathbb{E}[(Z_t - \mathbb{E}[Z_t])(Z_\tau - \mathbb{E}[Z_\tau])^T].$$
(10.4)

A special property of the auto-covariance is  $\rho(t-\tau) = \rho(\tau-t)$ .

This allows us to write the equation (10.3) as

$$\rho((1-j)\tau) = \sum_{i=0}^{p} A_i(\tau)\rho((j-i)\tau).$$
(10.5)

This is the Jule-Walker-equation. Now let  $Z_t$  be an auto-regressive process of order p. Therefore let

$$\alpha = [A_0, A_1, \dots, A_p] \in \mathbb{R}^{n \times (p+1)n}$$
(10.6)

and

$$Y^{T} = [Z_{p+1}, \dots, Z_{T}],$$

$$\begin{bmatrix} Z_{p} & Z_{p+1} & \dots & Z_{T} \end{bmatrix}$$
(10.7)

$$X^{T} = \begin{bmatrix} Z_{p} & Z_{p+1} & \dots & Z_{T} \\ \vdots & \vdots & \ddots & \vdots \\ Z_{0} & Z_{1} & \dots & Z_{T-p} \end{bmatrix},$$
 (10.8)

$$\epsilon^T = (\varepsilon_{p+1} \dots \varepsilon_T) \tag{10.9}$$

Then we can write

$$Y = X\alpha + \epsilon B^T \tag{10.10}$$

and thus

$$\mathbb{E}[Y - X\alpha] = \mathbb{E}[\epsilon B^T] = 0 \tag{10.11}$$

so we try to solve

$$||Y - X\alpha|| \to \min.$$
 (10.12)

We denote by  $\hat{\alpha}$  so solution of this problem, therefore we get

$$\hat{\alpha} = (X^T X)^{-1} X^T Y \tag{10.13}$$

For ergodic  $Z_t$  the  $(X^T X)$  is just the empiric auto-covariance matrix. If Z is periodic, then we might get an eigenvalue of zero, thus the problem is no longer solveable. By changing the problem to

$$||Y - X\alpha|| + \Gamma||\alpha|| \to \min, \qquad (10.14)$$

we might get better results. Thus we define:

$$\tilde{Y} = [Y\,0] \tag{10.15}$$

$$\tilde{Y} = [Y \ 0]$$
(10.15)
  
 $\tilde{X} = [X \ \Gamma]$ 
(10.16)

Then we can solve the problem  $||\tilde{Y} - \tilde{X}\alpha||$  by using

$$\widehat{\hat{\alpha}}(\tilde{X}^T \tilde{X})^{-1} \tilde{X}^T \tilde{Y} = (X^T X + \Gamma^T \Gamma)^{-1} X^T Y$$
(10.17)