

Infering Graphical Models from Time Series

Modelling, Simulating, and Inference of Complex Biological Systems

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Sebastian Petry
What are Graphical Models?
Graph Theory
Probability Theory
Infering Grapical Models from Time Series
Summary

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Outline

- 1 What are Graphical Models?
- 2 Graph Theory
 - Graphs and Digraphs
 - Dags
- 3 Probability Theory
 - Association Structures
 - Partial Covariance as a Graphical Model
 - Multivariate Time Series and Stochastic Processes
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Graphical Models

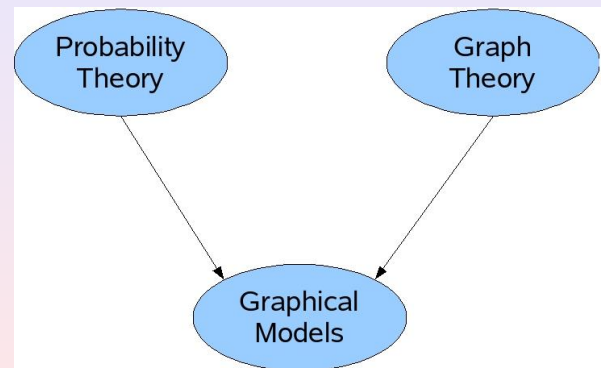
The two parts of the marriage (Quotation from Preface of [1])

Probability theory provides the glue whereby the parts are combined, ensuring that the systems as whole is consistent, and providing ways to interface models to data.

The *graph theoretic* side of graphical models provides both an intuitively appealing interface by which humans can model highly-interacting sets of variables as well as a data structure that lends itself naturally to the design of efficient general-purpose algorithms.

The marriage (Quotation from Preface of [1])

Graphical models are a marriage between probability theory and graph theory. They provide a natural tool for dealing with two problems that occur throughout applied mathematics and engineering — uncertainty and complexity — and in particular they are playing an increasingly important role in design and analysis of machine learning. Fundamental to the idea of graphical model is the notion of modularity — a complex system is built by combining simpler parts.



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Graphs and Digraphs
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Graphs and Digraphs
Dags

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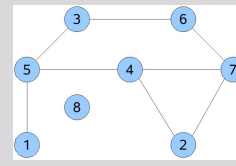
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Definition 1 (graph)

A *graph* G is a tuple $G := (V, E)$ with a finite set $V \neq \emptyset$ and a subset $E \subseteq V \times V$ of two-elementic subsets of V . The elements of V are called *vertices* and the elements of E *edges*. The two vertex $v_i, v_j \in V, v_i \neq v_j$, of a edge $e = \{v_i, v_j\} \in E$ are called *end vertex* of e .

We call v_i and v_j with e incident and v_i and v_j are adjacent.

Example 2



$$G = (V, E)$$

$$V = \{1, 2, 3, 4, 5, 6, 7, 8\}$$

$$E = \{\{1, 5\}, \{5, 4\}, \{5, 3\}, \{4, 7\}, \{3, 6\}, \{2, 4\}, \{2, 7\}, \{6, 7\}\}$$

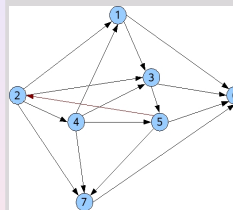
Definition 3 (digraph)

A *directed graph* or *digraph* G is a tuple $G := (V, E)$ with a finite set $V \neq \emptyset$ and a subset $E \subseteq V \times V$ of ordered pairs $(v_i, v_j) \in V \times V, v_i \neq v_j$ and $\exists (v_i, v_j) \Rightarrow \nexists (v_j, v_i)$. The elements of V are also called *vertices* and the elements of E *edges* or *arcs*. For an arc $e = (v_i, v_j) \in E$ v_i is called *tail* and v_j called *head*.

We call v_i and v_j with e incident or v_i and v_j are adjacent.

We call $d_{in}(v)$ the number of arcs with head v *indegree* and $d_{out}(v)$ the number of arcs with tail v *outdegree*.

Example 4



$$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 1 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$

Adjacency matrix: Tails in row and heads in column.

This digraph contains the directed cycle:
 $C := \{(2, 4), (4, 5), (5, 2)\}$.

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Definition 5 (dag)

A digraph $G = (V, E)$ is called *directed acyclic graph (dag)*, iff there exists no sequence in each subset $E' \subseteq E$, with $E' = \{e'_1 = (v'_{1T}, v'_{1H}), \dots, e'_n = (v'_{nT}, v'_{nH})\}, 2 < n \leq |E'|$, for which

- $v'_{iT} = v'_{(i-1)H}$,
- $v'_{iH} = v'_{(i+1)T}, \forall i = 2, \dots, n - 1$,

holds.

Lemma 6

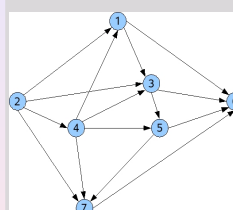
Let $G = (E, V)$ be a dag. Then there exists at least one vertex $v \in V$ for which $d_{in}(v) = 0$ holds.

By Lemma 6 and Definition 5 the following theorem holds.

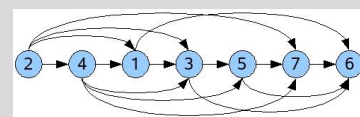
Theorem 7

Every dag has a topological order.

Example 8 (A dag)



$$\begin{pmatrix} 0 & 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 & 1 \\ 0 & 0 & 0 & 0 & 0 & 1 & 1 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & 0 \end{pmatrix}$$



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Lemma 9

Every partial ordered set, i.e. $v_{iT} < v_{iH} \forall i$, can be embedded in a linear ordered set.

In a lot of problems it is necessary to weight the edges. This leads to

Definition 10 (network)

Let $G = (V, E)$ a graph or digraph and $w : E \rightarrow \mathbb{R}$. Then a pair (G, w) is called *network*.

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Basic Situation

Let $\mathbf{Y}^T = (Y_1, \dots, Y_g)$, $\mathbf{X}^T = (X_1, \dots, X_p)$, and $\mathbf{Z}^T = (Z_1, \dots, Z_s)$ be random vectors with metric components. The random vector $(\mathbf{Y}^T, \mathbf{X}^T, \mathbf{Z}^T)^T$ possesses (if they exist) the mean

$$\boldsymbol{\mu} = E((\mathbf{Y}^T, \mathbf{X}^T, \mathbf{Z}^T)^T) = (\boldsymbol{\mu}_Y^T, \boldsymbol{\mu}_X^T, \boldsymbol{\mu}_Z^T)^T$$

and the covariance(matrix)

$$\boldsymbol{\Sigma} = \text{Cov}((\mathbf{Y}^T, \mathbf{X}^T, \mathbf{Z}^T)^T) = \begin{pmatrix} \boldsymbol{\Sigma}_{YY} & \boldsymbol{\Sigma}_{YX} & \boldsymbol{\Sigma}_{YZ} \\ \boldsymbol{\Sigma}_{XY} & \boldsymbol{\Sigma}_{XX} & \boldsymbol{\Sigma}_{XZ} \\ \boldsymbol{\Sigma}_{ZY} & \boldsymbol{\Sigma}_{ZX} & \boldsymbol{\Sigma}_{ZZ} \end{pmatrix}.$$

Three Kinds of Covariance

We can distinguish three kinds of covariance:

- 1 marginal covariance
- 2 conditional covariance
- 3 partial covariance

Marginal Covariance

Definition 11 (marginal covariance)

The *marginal covariance* between two random vectors \mathbf{Y} and \mathbf{X} is given by the submatrix

$$\text{Cov}(\mathbf{Y}, \mathbf{X}) = \boldsymbol{\Sigma}_{YX}$$

of $\boldsymbol{\Sigma}$.

Theorem 12

\mathbf{Y} and \mathbf{X} are marginal uncorrelated, iff $\boldsymbol{\Sigma}_{YX} = \mathbf{0}$.

Conditional Covariance

Definition 13 (conditional covariance)

If the conditional density exists then the *conditional covariance* between \mathbf{Y} and \mathbf{X} given $\mathbf{Z} = \mathbf{z}$, $\text{Cov}(\mathbf{Y}, \mathbf{X} | \mathbf{Z} = \mathbf{z})$, is defined by the covariance of the conditional density of the random vector $\mathbf{Y}, \mathbf{X} | \mathbf{Z} = \mathbf{z}$.

Partial Covariance

Definition 14 (partial covariance)

The *partial covariance* between \mathbf{Y} and \mathbf{X} given \mathbf{Z} , $\text{Cov}(\mathbf{Y}, \mathbf{X} | \mathbf{Z})$, is defined by

$$\text{Cov}(\mathbf{Y}, \mathbf{X} | \mathbf{Z}) = \boldsymbol{\Sigma}_{YX} - \boldsymbol{\Sigma}_{YZ} \boldsymbol{\Sigma}_{ZZ}^{-1} \boldsymbol{\Sigma}_{ZX}^T = \boldsymbol{\Sigma}_{YX} - \boldsymbol{\Sigma}_{YZ} \boldsymbol{\Sigma}_{ZZ}^{-1} \boldsymbol{\Sigma}_{ZX}. \quad (1)$$

Something more about Covariances

Theorem 15

Let $\Sigma^{-1} = \left(\text{Cov} \left(\begin{pmatrix} \mathbf{Y} \\ \mathbf{X} \\ \mathbf{Z} \end{pmatrix} \right) \right)^{-1} = \begin{pmatrix} \mathbf{C}^{\mathbf{Y}\mathbf{Y}} & \mathbf{C}^{\mathbf{Y}\mathbf{X}} & \mathbf{C}^{\mathbf{Y}\mathbf{Z}} \\ \mathbf{C}^{\mathbf{X}\mathbf{Y}} & \mathbf{C}^{\mathbf{X}\mathbf{X}} & \mathbf{C}^{\mathbf{X}\mathbf{Z}} \\ \mathbf{C}^{\mathbf{Z}\mathbf{Y}} & \mathbf{C}^{\mathbf{Z}\mathbf{X}} & \mathbf{C}^{\mathbf{Z}\mathbf{Z}} \end{pmatrix}$ the inverse of Σ . Then $\text{Cov}(\mathbf{Y}, \mathbf{X}|\mathbf{Z}) = \mathbf{0} \Leftrightarrow \mathbf{C}^{\mathbf{Y}\mathbf{X}} = \mathbf{0}$ holds. Or in other words: \mathbf{Y} and \mathbf{X} given \mathbf{Z} are partial uncorrelated, iff $\mathbf{C}^{\mathbf{Y}\mathbf{X}} = \mathbf{0}$.

Theorem 16

In the Gaussian case conditional and partial covariance are equivalent.

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The regression view of partial covariance

Let \mathbf{Y} be a p -dimensional random vector, i and j be two components of \mathbf{Y} , and C the set of the remaining components of \mathbf{Y} being not i or j . Then the two regressions holds

$$\begin{aligned} Y_{i|C} &= Y_i - \Sigma_{i,C} \Sigma_{CC}^{-1} \mathbf{Y}_C, \\ Y_{j|C} &= Y_j - \Sigma_{j,C} \Sigma_{CC}^{-1} \mathbf{Y}_C, \end{aligned} \quad (2)$$

where $\Sigma_{i,C} \Sigma_{CC}^{-1}$ are the submatrices of Σ , because of $\text{Cov}(Y_{i|C}, Y_{j|C}) := \text{Cov}(Y_i, Y_j | \mathbf{Y}_C)$ (see (1)) holds.

Interpretation and Comment

- 1 $\Sigma_{i,C} \Sigma_{CC}^{-1}$ can be interpreted as a regression coefficient vector for i given C .
- 2 Extension to the multivariate case $\mathbf{Y}_{i|C}$ is possible.

Intuitively it makes sense to avoid redundancies what leads to an orthogonal regression system.

In other words we are looking for a regression system of Y_i on $Y_{r(i)}$ for $i = p-1, \dots, 1$ with $r(i) = (i+1, \dots, p)$. This defines a process of successive *orthogonalization*.

Heuristic Illustration I ($p = 4$)

Heuristic Illustration II ($p = 4$)

$$\epsilon = \begin{pmatrix} \epsilon_1 \\ \epsilon_2 \\ \epsilon_3 \\ \epsilon_4 \end{pmatrix} = \begin{pmatrix} 1 & -\beta_{1|2,3,4} & -\beta_{1|3,2,4} & -\beta_{1|4,2,3} \\ 0 & 1 & -\beta_{2|3,4} & -\beta_{2|4,3} \\ 0 & 0 & 1 & -\beta_{3|4} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix} = \mathbf{A}\mathbf{Y}$$

$\beta_{i|k,C}$ denotes the coefficient of Y_k in the regression of Y_i on all variables after the conditioning sign. Computing the covariances matrix $\text{Cov}(\epsilon, \epsilon)$ leads because of independence to

$$\begin{aligned} \text{Cov}(\epsilon, \epsilon) &= E(\epsilon\epsilon^T) \\ &= \text{diag}(\text{Var}(\epsilon_i)) \\ &=: \Delta \\ \Delta &= E((\mathbf{A}\mathbf{Y})(\mathbf{A}\mathbf{Y})^T) \\ &= \mathbf{A}^T E(\mathbf{Y}\mathbf{Y}^T) \mathbf{A} \\ &= \mathbf{A}^T \Sigma \mathbf{A} \\ \Rightarrow \Sigma^{-1} &= \mathbf{A}^T \Delta^{-1} \mathbf{A} \\ \text{and } \Sigma &= \mathbf{A}^{-1} \Delta \mathbf{A}^{-T} \end{aligned}$$

Heuristic Illustration III ($p = 4$)

Heuristic Illustration IV ($p = 4$)

By identifying (2) with the residual ϵ_i it follows

$$\begin{pmatrix} Y_{1|C} \\ Y_{2|C} \\ Y_{3|C} \\ Y_{4|C} \end{pmatrix} = \begin{pmatrix} 1 & -\beta_{1|2,3,4} & -\beta_{1|3,2,4} & -\beta_{1|4,2,3} \\ 0 & 1 & -\beta_{2|3,4} & -\beta_{2|4,3} \\ 0 & 0 & 1 & -\beta_{3|4} \\ 0 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} Y_1 \\ Y_2 \\ Y_3 \\ Y_4 \end{pmatrix}$$

whereas the corresponding set C for each $Y_{i|C}$ is given by the topological order of \mathbf{A} .

The β -elements of \mathbf{A} of each row of \mathbf{A} are consequently given by

$$-a_{i,r(i)} = \Sigma_{i,C} \Sigma_{CC}^{-1}$$

and the diagonal elements of Δ by

$$\Sigma_{i,i} - \Sigma_{i,C} \Sigma_{CC}^{-1} \Sigma_{i,C}^T$$

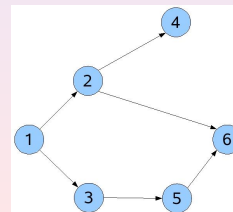
Heuristic Illustration V ($\rho = 4$)

- 1 $\mathbf{A} = \text{diag}(1) - \mathbf{G}$: So \mathbf{G} has the structure of a dag — or can interpreted as a network.
- 2 $\Sigma = \mathbf{A}^{-1} \Delta \mathbf{A}^{-T}$: It is possible to induce the concentration matrices (and by inverting it the covariance matrix) by a network or a dag structure.
- 3 Under conditions you can get a dag network by knowing the concentration and the covariance matrix.

The following theorem holds:

Theorem 17

Let \mathbf{X} be an Gaussian random vector with covariance matrix Σ . The variable \mathbf{X} , or the covariance matrix Σ , is said to factorize in a dag, iff each component X_i of \mathbf{X} is independent from its nondescendant variables, given its parents.



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Definition 18 (multiple time series (MTS))

Let $t \in \mathbb{Z}$ and $\mathbf{X}(t)^T = (X_1(t), \dots, X_m(t))$, with $X_i(t) \in \mathbb{R}$, $\forall i \in \{1, \dots, m\}$, be an m -dimensional random vector. Then the on \mathbb{Z} ordered set $\mathbf{X} := \{\mathbf{X}(t)\}_{t \in \mathbb{Z}}$ is the random process and the realisation \mathbf{x} of \mathbf{X} is called (multiple) time series (MTS).

Definition 19 (autocovariance function (ACF))

For a random process \mathbf{X} the autocovariance function (ACF) is a matrix-valued mapping $\mathbb{Z} \times \mathbb{Z} \rightarrow \mathbb{R}^m \times \mathbb{R}^m$, $(t, s) \mapsto \Gamma(t, s)$,

$$\Gamma(t, s) = E[(\mathbf{X}(t) - E(\mathbf{X}(t)))(\mathbf{X}(s) - E(\mathbf{X}(s)))^T].$$

Definition 20 (stationarity)

A random process \mathbf{X} is called stationary, iff $\mu(t) \equiv \mu^a$ and the ACF only depends on $h = |t - s|$. So the ACF becomes a to matrix-valued mapping $\mathbb{Z} \rightarrow \mathbb{R}^m \times \mathbb{R}^m$, $h \mapsto \Gamma(h)$,

$$\begin{aligned} \Gamma(h) &= E((\mathbf{X}(t+h) - \mu)(\mathbf{X}(t) - \mu)^T) \\ &= E((\mathbf{X}(h) - \mu)(\mathbf{X}(0) - \mu)^T). \end{aligned}$$

^awe only consider $\mu(t) \equiv \mathbf{0}$

Example 21 (ACF, $m = 3$ and $\mu = \mathbf{0}$)

$$\begin{aligned} \Gamma(h) &= E((\mathbf{X}(t+h)(\mathbf{X}(t))^T)) \\ &= E(\mathbf{X}(h)\mathbf{X}(0)^T) \\ &= E \begin{pmatrix} X_1(h)X_1(0) & X_1(h)X_2(0) & X_1(h)X_3(0) \\ X_2(h)X_1(0) & X_2(h)X_2(0) & X_2(h)X_3(0) \\ X_3(h)X_1(0) & X_3(h)X_2(0) & X_3(h)X_3(0) \end{pmatrix} \end{aligned}$$

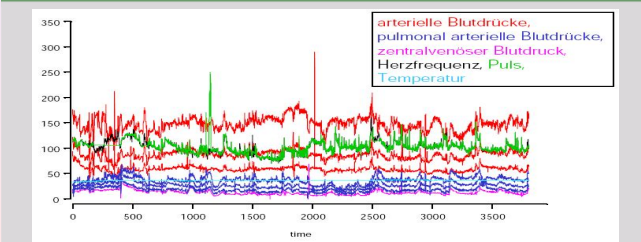
Lemma 22

For a stationary random process the ACF, $\Gamma(h)$, is symmetric and non-negativ.

Definition 23 (Gaussian time series)

A time series is called Gaussian, iff all finite sets of marginals are jointly Gaussian.

Example 24 (MTS)



Definition 25 (spectral density matrix (SDM))

Given an m -dimensional stationary MTS for which $\sum_{h=-\infty}^{+\infty} \|\Gamma(h)\|_2 < +\infty$ holds. Then the spectral density matrix (SDM) is well defined as the matrix-valued mapping $\mathbb{R} \rightarrow \mathbb{R}^m \times \mathbb{R}^m$, $\omega \mapsto \mathbf{f}(\omega)$, with

$$\mathbf{f}(\omega) = \frac{1}{2\pi} \sum_{h=-\infty}^{+\infty} \Gamma(h) \exp(-ih\omega)$$

For SDM the following holds:

- 1 $\mathbf{f}(\omega)$ is Hermitian for each $\omega \in \mathbb{R}$.
- 2 $\omega \mapsto \mathbf{f}(\omega)$ is 2π -periodic.
- 3 for real-valued vectors $\mathbf{f}(\omega) = \mathbf{f}(-\omega)$ holds.
- 4 $\Gamma(h) = \int_0^{2\pi} \mathbf{f}(\omega) \exp(ih\omega) d\omega$.

Definition 26 (sample autocovariance function (SACF))

The sample autocovariance function (SACF) is defined as

$$\hat{\Gamma}(h) = \frac{1}{T} \sum_{t=0}^{T-h-1} (\mathbf{x}(t+h) - \bar{\mathbf{x}})(\mathbf{x}(t) - \bar{\mathbf{x}})^T, \quad h \in [0, T-1]$$

with $\bar{\mathbf{x}} = \frac{1}{T} \sum_{t=0}^{T-1} \mathbf{x}(t)$ as the sample mean of data.

Lemma 27

The SACF is a consistent estimator for the ACF and under weak assumptions normal distributed.

Definition 28 (periodogram)

Let $\mathbf{d}(k) = \frac{1}{\sqrt{T}} \sum_{t=0}^{T-1} \mathbf{x}(t) \exp(-ikt)$ the discrete Fourier transform of data. At each frequencies $\omega_k = \frac{2\pi k}{T}$, $\omega \in [0, 2\pi)$ especially $k \in \{1, \dots, T\}$, the *periodogram* is defined as

$$I(\omega_k) = \frac{1}{2\pi} \mathbf{d}(k) \mathbf{d}(k)^*$$

Lemma 29

The periodogram does not provide a consistent estimator of SDM. Smoothing can solve this problem:

$$\hat{\mathbf{f}}(\omega_k) = \sum_{j=-\infty}^{+\infty} \mathbf{W}_r(j) I(\omega_{j+k}),$$

with the weight-matrix $\mathbf{W}_r(\cdot)$ and r as smoothing parameter.

Comment

A skilled choice of the weight-matrix $\mathbf{W}_r(\cdot)$ makes possible to optimize the periodogram $\hat{\mathbf{f}}(\omega_k)$ by r . For example use $\mathbf{W}_r(j) = \frac{1}{r\sqrt{2\pi}} \exp(-\frac{j^2}{2r^2})$ and minimize AIC with the Whittle approximation of the likelihood by r . (For details see [2])

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Theorem 30

A Gaussian stationary stochastic process with an absolutely summable ACF has the spectral representation

$$\mathbf{X}(t) = \int_0^{2\pi} \exp(it\omega) d\mathbf{Z}(\omega),$$

where $\mathbf{Z}(\omega)$ is a random process with orthogonal increments such that $\omega_1 < \omega_2$, $\text{Cov}(\mathbf{Z}(\omega_2) - \mathbf{Z}(\omega_1)) = \int_{\omega_1}^{\omega_2} \mathbf{f}(\omega) d\omega$. In other words: $\mathbf{X}(t)$ is a superposition of infinite many independent random signals at different frequencies.

The previous theorem 30 in symbiosis with the property that for $X \sim N(\mu, \sigma^2)$

$$E(\exp(itX)) = \exp\left(i\mu t - \frac{1}{2}\sigma^2 t^2\right)$$

holds, makes possible to use the theory of Gaussian random vector on Gaussian stationary MTS by replacing the covariance matrix with the SDM or better periodogram.

Now we apply the theory of Gaussian variables to Gaussian stationary MTS and it follows

Lemma 31

Two time series x_i and x_j are marginally independent iff

$$\forall \omega \in [0, 2\pi), \quad f_{ij}(\omega) = 0.$$

The time series x_i and x_j are partially and therefore conditionally independent given all other times series x_k , $k \neq i, j$ iff

$$\forall \omega \in [0, 2\pi), \quad (f(\omega)^{-1})_{ij} = 0.$$

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- Casting the structure learning as a model selection. The structure is a dag.
- Minimizing the AIC score (3) that is recovered by entropy rates and KL divergence.
- For details see [2].

Comments to AIC

$$J(G) = \sum_{i=1}^m J_i(\pi_i(G)) \quad (3)$$

where the local score is

$$J_i(\pi_i(G)) = \frac{-T}{4\pi} \int_0^{2\pi} \log \frac{\det(\hat{\mathbf{f}}_{\{i\} \cup \pi_i}(\omega))}{\det(\hat{\mathbf{f}}_{\pi_i}(\omega))} d\omega + (2|\pi_i| + 1) \frac{df}{2}. \quad (4)$$

(4) is approximated using the samples of $\hat{f}(\omega)$ as

$$J_i(\pi_i(G)) = \frac{-T}{2H} \sum_{k=0}^{H-1} \log \frac{\det((\mathbf{f}_k^f)_{\{i\} \cup \pi_i})}{\det((\mathbf{f}_k^f)_{\pi_i})} + (2|\pi_i| + 1) \frac{df}{2}. \quad (5)$$

- We learn the structure of G by minimize the AIC $J(G)$. This problem is numerically complex. Using the greedy algorithm and other mathematical tricks can lead to an efficient solving procedures. The problem is NP-complete!
- Often it can be convenient to restrict the number of parents. The dag structure makes this possible.
- One of the major gains from learning a sparse structure for the SDM is that we can perform and optimize the smoothing periodogram locally on cliques of G . The AIC score is given on the next slide.

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$$J(G, r) = \frac{T}{2H} \sum_{k=0}^{H-1} \sum_{i=0}^m \left(\frac{\det((\mathbf{f}_k^f)_{\{i\} \cup \pi_i})}{\det((\mathbf{f}_k^f)_{\pi_i})} + \text{tr} \left\{ (\mathbf{f}_k^f)_{\{i\} \cup \pi_i}^{-1} \mathbf{I}_{\{i\} \cup \pi_i}(\omega_k) \right\} \right) + \sum_{i=1}^m (2|\pi_i| + 1) \frac{df_i}{2}.$$

- Graphical models are special cases of networks.
- Applications are possible in different ways.
- Graphs and Topology
 - A dag is a topological orderable digraphs.
 - Strictly triangular matrices have the structure of a dag
- Multivariate Random Vectors and Times Series
 - The partial covariance has the structure of a dag
 - Using knowledge about random vectors on MTS is in the Gaussian case possible by replacing the covariance matrix by SDM or periodogram
 - Possible to define the independence of MTS
- Searching the structure of independence MTS by using the knowledge of dags and probability theory

Some references

- 📖 Jordan, M.I. (1999). *Learning in Graphical Models*, MIT Press.
- 📖 Francis R., Bach and Jordan, M.I. (2004). *Learning in Graphical Models for Stationary Time Series*, IEEE Transactions on Signal Processing, Vol52, No.8, August 2004.
- 📖 Jungnickel, D. (1987). *Graphen, Netzwerke und Algorithmen*, B.I.-Wissenschaftsverlag.
- 📖 Wermuth, N., Cox, D.R., Marchetti, G.M.. *Covariance chains*.
- 📖 Murphy, K.P. (2001). *An introduction to graphical models*.