LTAT.02.004 MACHINE LEARNING II

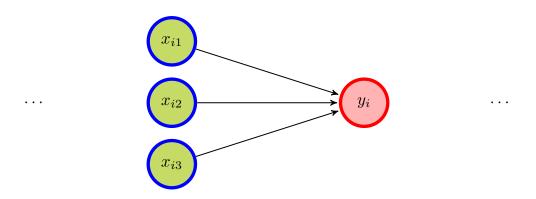
Multivariate normal distribution Direct applications

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Motivating examples

Supervised learning

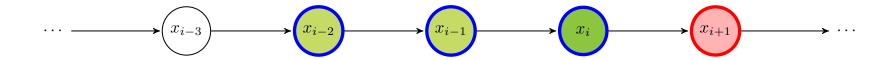
Repeated controlled coin tosses



Linear regression models

- \triangleright We assume that y_i depends only on the values of $x_{i1},\ldots,x_{i\ell}$
- \triangleright A linear model assumes $y_i = \beta_1 x_{i1} + \cdots + \beta_\ell x_{i\ell} + \beta_0 + \varepsilon_i$.
- \triangleright All error terms ε_i are assumed to be independent.
- \triangleright All error terms ε_i are drawn from a normal distribution $\mathcal{N}(0,\sigma)$.

Higher-order Markov chains

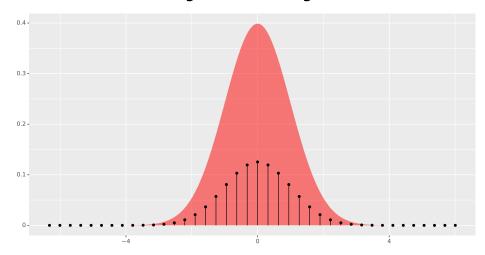


Time-series models

- \triangleright We assume that x_{i+1} depends only on the values of $x_i, \ldots, x_{i-\ell}$
- \triangleright A linear model assumes $x_{i+1} = \alpha_0 x_i + \cdots + \alpha_\ell x_{i-\ell} + \alpha_{\ell+1} + \varepsilon_i$.
- \triangleright All error terms ε_i are assumed to be independent.
- \triangleright All error terms ε_i are drawn from a normal distribution $\mathcal{N}(0,\sigma)$.

Univariate normal distribution

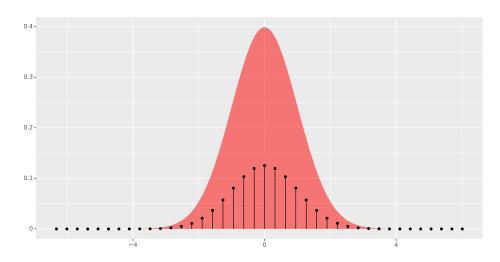
Probability density function



Definition. A real-valued random variable X comes from a continuous distribution with a probability density function $p: \mathbb{R} \to \mathbb{R}^+ \cup \{0\}$ if the following limit exists for any $x \in \mathbb{R}$:

$$p(x) = \lim_{\Delta x \to 0^+} \frac{\Pr\left[x - \Delta x \le X \le x + \Delta x\right]}{2 \cdot \Delta x} .$$

Probability mass function

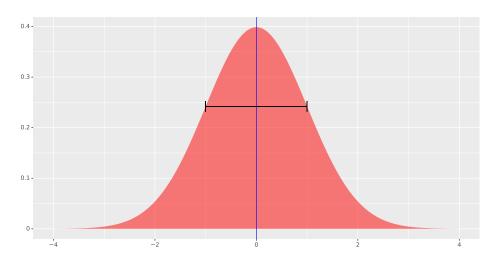


Definition. A real-valued random variable X comes from a discrete distribution with a probability mass function $p: \mathbb{R} \to \mathbb{R}^+ \cup \{0\}$ defined as

$$p(x) = \Pr\left[X = x\right] = \lim_{\Delta x \to 0^+} \Pr\left[x - \Delta x \le X \le x + \Delta x\right]$$

if there exist a sequence $(x_i)_{i=1}^{\infty}$ such that $p(x_1) + \ldots + p(x_i) + \ldots = 1$.

Standard normal distribution



Standard normal distribution $\mathcal{N}(\mu=0,\sigma=1)$ is a continuous distribution with a probability density function

$$p(x) = \frac{1}{\sqrt{2\pi}} \cdot \exp\left(-\frac{x^2}{2}\right)$$

The mean value $\mu=0$ and variance $\sigma^2=1$ for this distribution.

Univariate normal distribution

Definition. A random variable y is distributed according to a normal distribution $\mathcal{N}(\mu=a,\sigma=b)$ if it can be expressed

$$y = bx + a$$

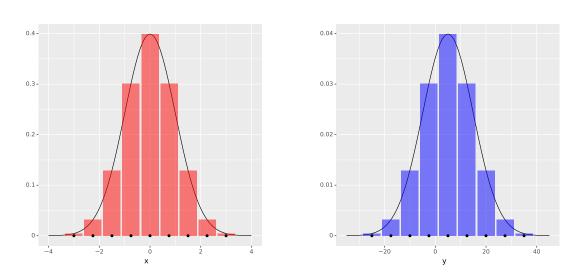
where x is distributed according to standardised normal distribution $\mathcal{N}(0,1)$.

The corresponding probability density functions is

$$p[y|\mu,\sigma] = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(\frac{(x-\mu)^2}{2\sigma^2}\right)$$

and the mean value μ and variance σ^2 for this distribution.

Density derivation



Let y = ax + b the relation between densities

$$p_x(x) = \sigma \cdot p_y(y)$$

follows form the fact that areas of red and blue columns must be the same.

Univariate linear regression

- \triangleright Fix a set of inputs $x_1, \ldots, x_n \in \mathbb{R}$.
- \triangleright A probabilistic model is defined by three coefficients $a, b, \in \mathbb{R}$.
- \triangleright The model assigns a probability to outcomes y_1, \ldots, y_n through the following observation generation mechanism

$$y_i = ax_i + b + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma)$$

$$p[\boldsymbol{y}|\boldsymbol{x},a,b] = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(y_i - ax_i - b)^2}{2\sigma^2}\right)$$

Maximum likelihood estimate

As usual we can find $a,b,\sigma\in\mathbb{R}$ that maximise the log-likelihood

$$\log p[\boldsymbol{y}|\boldsymbol{x}, a, b, \sigma] = const - n\log\sigma - \sum_{i=1}^{n} \frac{(y_i - ax_i - b)^2}{2\sigma^2}$$

and thus we can find a and b by minimising

MSE =
$$\frac{1}{n} \cdot \sum_{i=1}^{n} (y_i - ax_i - b)^2$$
.

Residuals and the variance parameter

For fixed $a,b \in \mathbb{R}$ we can define predictions and residuals

$$\hat{y}_i = ax_i - b$$

$$r_i = y_i - \hat{y}_i$$

To find the optimal variance σ^2 we need to maximise

$$\log p[\boldsymbol{y}|\boldsymbol{x}, a, b, \sigma] = const - n\log \sigma - \sum_{i=1}^{n} \frac{r_i^2}{2\sigma^2}$$

The resulting solution is

$$\sigma^2 = \frac{1}{n} \cdot \sum_{i=1}^{n} (y_i - \hat{y}_i)^2$$

Linear time-series model

- \triangleright Fix a set of initial inputs $x_{-\ell}, \ldots, x_0 \in \mathbb{R}$. Denote them by \boldsymbol{x}_{\circ} .
- \triangleright Think of x_1, x_2, \ldots, x_n as observations. Denote them by \boldsymbol{x} .
- > A probabilistic model for state transitions is defined as follows

$$x_{i+1} = \underbrace{\alpha_0 x_i + \dots \alpha_\ell x_{i-\ell} + \alpha_{\ell+1}}_{\hat{x}_{i+1}} + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma)$$

$$p[\boldsymbol{x}|\boldsymbol{x}_{\circ},\boldsymbol{\beta},\sigma] = \prod_{i=1}^{n} \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x_{i} - \hat{x}_{i})^{2}}{2\sigma^{2}}\right)$$

Maximum likelihood estimate

As usual we can find $\pmb{\alpha} \in \mathbb{R}^{\ell+1}$ and $\sigma \in \mathbb{R}$ that maximise the log-likelihood

$$\log p[\boldsymbol{x}|\boldsymbol{x}_{\circ},\boldsymbol{\beta},\sigma] = const - n\log\sigma - \sum_{i=1}^{n} \frac{(x_{i} - \hat{x}_{i})^{2}}{2\sigma^{2}}$$

and thus we can find β by minimising

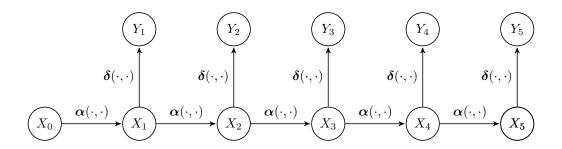
$$MSE = \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - \alpha_0 x_{i-1} + \dots \alpha_{\ell} x_{i-1-\ell} + \alpha_{\ell+1})^2.$$

The latter is the standard multivariate linear regression setup. The variance of the model σ^2 can be found by the same formula as for linear regression.

Motivating examples

Unsupervised learning

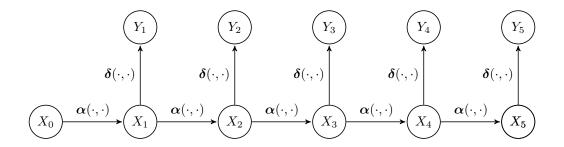
Hidden Markov Model



Sensor fusion problem

- ▷ Several sensors measure a physical system
- hd Measurements are observable as $oldsymbol{y} \in \mathbb{R}^p$.
- hd Physical system has an hidden state $oldsymbol{x} \in \mathbb{R}^n$.
- riangleright Physical system evolves linearly $oldsymbol{x}_{i+1} = Aoldsymbol{x}_i + oldsymbol{w}_i$.
- \triangleright Measurements are linear from the state $oldsymbol{y}_i = Coldsymbol{x}_i + oldsymbol{v}_i$.
- \triangleright Distribution of error terms $oldsymbol{v}_i$ and $oldsymbol{w}_i$ is known.
- \triangleright Error terms $oldsymbol{v}_i$ and $oldsymbol{w}_i$ are independently drawn.

Belief propagation for continous distibutions

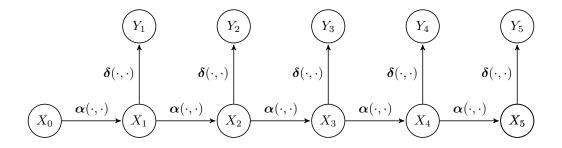


Continuous distributions are rarely compatible with belief propagation

$$\pi_{X_i}(\boldsymbol{x}_i) \propto \int_{\boldsymbol{x}_{i-1}} \alpha[\boldsymbol{x}_{i-1}, \boldsymbol{x}_i] \cdot \lambda_{i-1}^*(\boldsymbol{x}_{i-1}) \cdot \pi_{X_{i-1}}(\boldsymbol{x}_{i-1}) d\boldsymbol{x}_{i-1}$$
$$\lambda_{X_i}(\boldsymbol{x}_i) \propto \int_{\boldsymbol{x}_{i+1}} \alpha[\boldsymbol{x}_i, \boldsymbol{x}_{i+1}] \cdot \lambda_i^*(\boldsymbol{x}_i) \cdot \lambda_{X_{i+1}}(\boldsymbol{x}_{i+1}) d\boldsymbol{x}_{i+1}$$

but normal distributions form a rare exception.

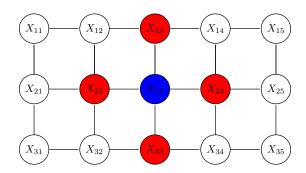
Kalman filter



Belief propagation becomes tractable under following assumptions:

- \triangleright Measurement noise v_t is modelled with a normal distribution.
- hd Unknown control signal $oldsymbol{w}_i$ is modelled with a normal distribution.
- \triangleright Unknown initial state x_0 is modelled with a normal distribution.
- \triangleright Quantities $oldsymbol{x}_0, oldsymbol{v}_i, oldsymbol{w}_i$ are assumed to be independent.
- > All normal distributions can have complex correlation structure.

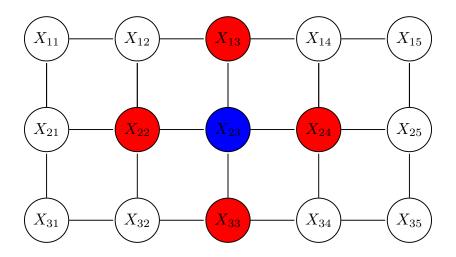
Background model for digital images



In most images intensity of pixel is influenced only by its neighbours:

- > For simple textures the neighbourhood consist of four adjacent pixels.
- > For complex textures the the neighbourhood contains much more pixels.
- ▶ For homogenous textures the conditional probabilities are universal.
 - Generative repetitive patterns for textile and grass
- > For complex patterns conditional probabilities can be location dependent.
 - Generative patterns for human faces and fashion accessories

Random Markov Fields



Definition. Markov random field is specified by undirected graph connecting random variables X_1, X_2, \ldots such that for any node X_i

$$\Pr\left[x_i|(x_j)_{j\neq i}\right] = \Pr\left[x_i|(x_j)_{j\in\mathcal{N}(X_i)}\right]$$

where the set of neighbours $\mathcal{N}(X_i)$ is also known as *Markov blanket* for X_i .

Hammersley-Clifford theorem

The probability of an observation $x = (x_1, x_2, ...)$ generated by a Markov random field can be expressed in the form

$$\Pr\left[\boldsymbol{x}\right] = \frac{1}{Z(\omega)} \cdot \exp\left(-\sum_{c \in \mathsf{MaxClique}} \Psi_c(\boldsymbol{x}_c, \omega)\right)$$

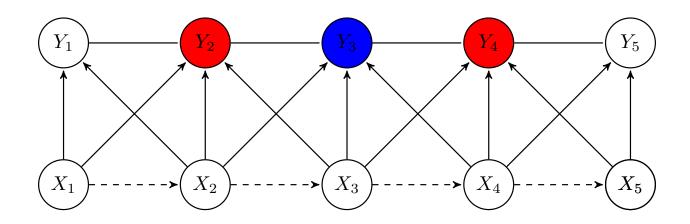
where

- $\triangleright Z(\omega)$ is a normalising constant
- MaxClique is the set of maximal cliques in the Markov random field
- $hd \Psi_c$ is defined on the variables in the clique c

The formula implies that the distribution belongs to the exponential family.

▶ Multivariate normal distribution belongs to the exponential family

Conditional Random Fields

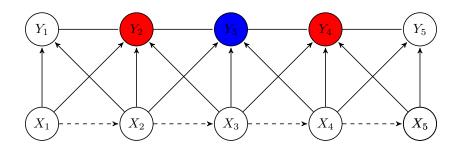


Definition. Let X_1, X_2, \ldots and Y_1, Y_2, \ldots be random variables. The entire process is conditional random field if random variables Y_1, Y_2, \ldots conditioned for any sequence of observations x_1, x_2, \ldots form a Markov random field

$$\Pr[y_i|(x_k)_{k=1}^{\infty}, (y_j)_{j\neq i}] = \Pr[y_i|(x_k)_{k=1}^{\infty}, (y_j)_{j\in\mathcal{N}(Y_i)}]$$

where the set of neighbours $\mathcal{N}(Y_i)$ is a *conditional Markov blanket* for Y_i .

Image segmentation and sequence labelling



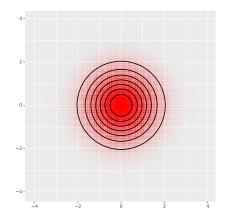
- \triangleright The input $m{x}$ is used to predict labels y_1, y_2, \ldots
- > A correct label sequence must satisfy possibly unknown restrictions.
- > These restrictions are captured by conditional random random field.

Consequences of Hammersley-Clifford theorem

- \triangleright Clique features Ψ_c can depend on $(y_i)_{i \in c}$, $(x_i)_{i=1}^{\infty}$
- ▷ Features can be defined as linear combination of vertex and edge features.
- \triangleright A vertex feature looks only variable y_i associated with the vertex.
- \triangleright An edge feature looks only variables y_i, y_j associated with the edge.

Multivariate normal distribution

White Gaussian noise



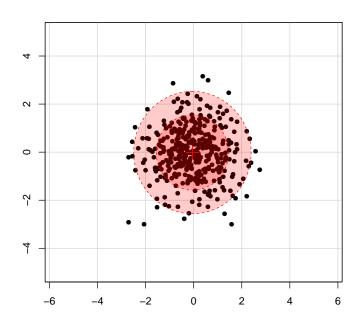
Definition. A random vector X_1, \ldots, X_n is a standard normal random vector if all of its components are independent and and $X_i \sim \mathcal{N}(0, 1)$.

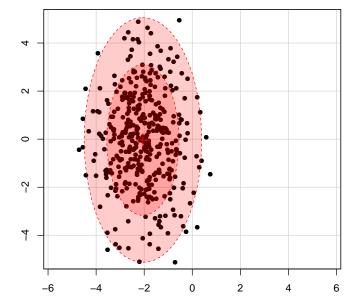
▶ The density can be computed based on independence:

$$p(x_1, \dots, x_n) = p(x_1) \cdots p(x_n) = \frac{1}{(2\pi)^{n/2}} \cdot \exp\left(-\frac{x_1^2 + \dots + x_n^2}{2}\right)$$
.

Scaling and shifting

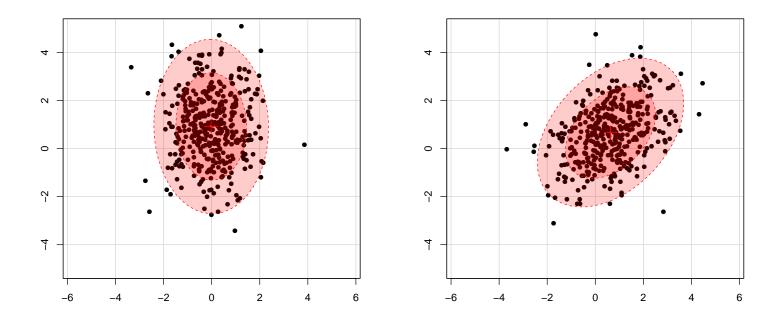
By shifting and scaling the source distribution $\mathcal{N}(\mathbf{0}, I)$ we can obtain some other instances of multivariate normal distribution.





Necessity of rotations

As the choice of coordinate axis is sometimes arbitrary, there must be other ways to form a normal distribution – rotations of coordinate axis.



Any affine transformation can be expressed as scaling, rotating and shifting.

Affine transformations

Let x be standard normal random vector and let y be obtained the scaling, translation and rotation of the coordinate plane.

Then we can express $oldsymbol{x}$ and $oldsymbol{y}$ in terms of an affine transformation

$$\mathbf{y} = A\mathbf{x} + \boldsymbol{\mu}$$
,
 $\mathbf{x} = A^{-1}(\mathbf{y} - \boldsymbol{\mu})$.

Observation. Affine transformations are closed with respect to composition, i.e., applying two affine transformations yields a new affine transformation.

Remark. Not all affine transformations are invertible.

What is density in 2D?

Recall that density assigns probability to small enough regions \mathcal{R} :

$$\Pr_{x_1^*, x_2^*} \begin{bmatrix} x_1 \le x_1^* \le x_1 + \Delta x_1 \\ x_2 \le x_2^* \le x_2 + \Delta x_2 \end{bmatrix} = p(x_1, x_2) \cdot \underbrace{\Delta x_1 \Delta x_2}_{S} + \varepsilon$$

where $\varepsilon = o(\Delta x_1 \cdot \Delta x_2)$ in the process $\Delta x_1 \to 0$ and $\Delta x_2 \to 0$.

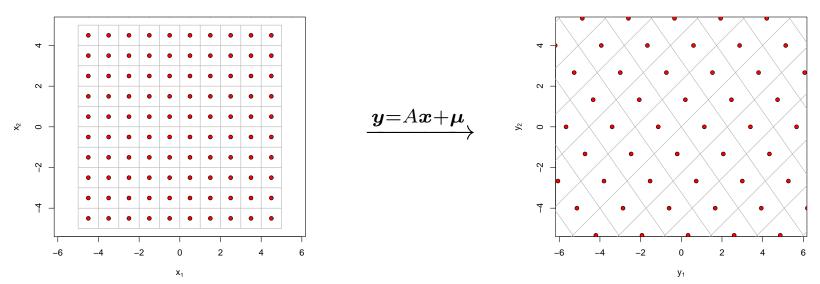
Remark. Regions \mathcal{R} do not have to be rectangular as long as:

- \triangleright The area $S(\mathcal{R})$ of a region can be computed.
- \triangleright Probability can be assigned to the region $\mathcal R$ and its scalings.

Then $\varepsilon = o(S)$ when we rescale the region \mathcal{R} around the point (x_1, x_2) .

Density recalibration

Any affine transformation changes a square grid into parallelograms.



As a result, the area of the regions is different on the left and on the right:

$$p(x_1, x_2) \cdot S_1 \approx q(y_1, y_2) \cdot S_2 \implies q(y_1, y_2) = \frac{S_1}{S_2} \cdot p(x_1, x_2)$$

Fortunately, the ratio between areas are constant over the entire plane!

Density of two-variate normal distribution

The density of (x_1, x_2) pairs can be computed based on independence:

$$p(x_1, x_2) = p(x_1) \cdot p(x_2) = \frac{1}{2\pi} \cdot \exp\left(-\frac{x_1^2 + x_2^2}{2}\right)$$
.

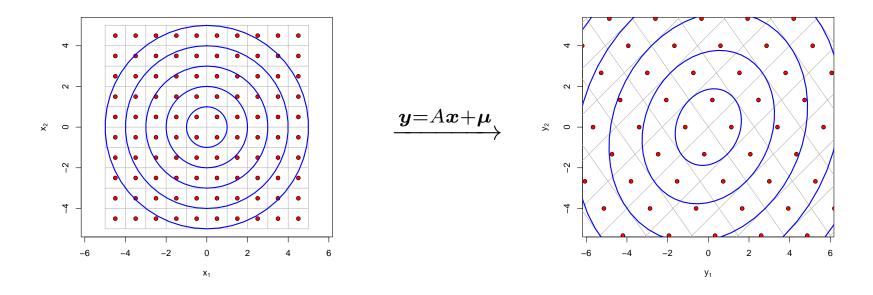
To estimate density $q(y_1, y_2)$, we must find the corresponding (x_1, x_2) :

$$y = Ax + \mu \Leftrightarrow x = A^{-1}(y - \mu)$$
.

Thus we get

$$q(y_1, y_2) = \frac{S_1}{S_2} \cdot \frac{1}{2\pi} \cdot \exp\left(-\frac{(\mathbf{y} - \boldsymbol{\mu})^T A^{-T} A^{-1} (\mathbf{y} - \boldsymbol{\mu})}{2}\right)$$
$$= \frac{1}{\sqrt{\det(\Sigma)}} \cdot \frac{1}{2\pi} \cdot \exp\left(-\frac{(\mathbf{y} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu})}{2}\right) .$$

Illustrative example



- > Affine transformation changes the square grid into parallelograms.
- > Affine transformation changes circular equiprobability lines into ellipses.
- > The axes of the ellipses may intersect with the sides of parallelograms.

Generalisation to multivariate case

If observed quantities $oldsymbol{y}$ are generated by applying the affine transformation

$$y = Ax + \mu \quad \Leftrightarrow \quad x = A^{-1}(y - \mu)$$

to the *independent source signals* $x_1, \ldots, x_n \sim \mathcal{N}(0, 1)$, then the resulting distribution is a multivariate normal distribution with the density:

$$p(\mathbf{y}) = \frac{1}{(2\pi)^{n/2}} \cdot \frac{1}{\sqrt{\det(\Sigma)}} \cdot \exp\left(-\frac{(\mathbf{y} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{y} - \boldsymbol{\mu})}{2}\right)$$

where $\Sigma^{-1} = A^{-T}A^{-1}$ is a positively definite symmetric matrix.

Markov fields with multivariate normal distributions

General form of the likelihood function

The celebrated Hammersley-Clifford theorem fixes the format in which the corresponding probability distribution must be sought:

$$p[\boldsymbol{x}|\omega] = \frac{1}{Z(\omega)} \cdot \exp\left(-\sum_{c \in \mathsf{MaxClique}} \Psi_c(\boldsymbol{x}_c, \omega)\right)$$

where

- $\triangleright \omega$ is a set of model parameters
- $\triangleright Z(\omega)$ is a normalising constant
- ▷ MaxClique is the set of maximal cliques in the Markov random field
- $\triangleright \Psi_c$ is defined on the variables x_i in the clique c.

Multivariate normal distribution as likelihood

If individual sub-potentials $\Psi_c({m x}_c,\omega)$ are quadratic forms then the energy

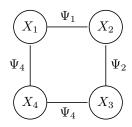
$$\Psi(oldsymbol{x}) = \sum_{c \in \mathsf{MaxClique}} \Psi_c(oldsymbol{x}_c, \omega)$$

is also a quadratic form and thus $p[x|\omega]$ is a multivariate normal distribution.

Sub-potentials are often fixed directly based on smoothness constraints

- \triangleright Intensities have bounded variance: $\Psi_e = \delta^2 x_{ij}^2$.
- \triangleright Intensity changes smoothly vertically: $\Psi_e = \beta(x_{i,j} x_{i+1,j})^2$.
- \triangleright Intensity changes smoothly horizontally: $\Psi_e = \alpha (x_{i,j} x_{i,j+1})^2$.

Toy example



Sub-potentials corresponding four edges are:

$$\Psi_1(x_1, x_2) = \alpha_1(x_1 - x_2)^2 = \alpha_1 x_1^2 - 2\alpha_1 x_1 x_2 + \alpha_1 x_2^2$$

$$\Psi_2(x_2, x_3) = \alpha_2(x_2 - x_3)^2 = \alpha_2 x_2^2 - 2\alpha_2 x_2 x_3 + \alpha_2 x_3^2$$

$$\Psi_3(x_3, x_4) = \alpha_3(x_3 - x_4)^2 = \alpha_3 x_3^2 - 2\alpha_3 x_3 x_4 + \alpha_3 x_4^2$$

$$\Psi_4(x_4, x_1) = \alpha_4(x_4 - x_1)^2 = \alpha_4 x_4^2 - 2\alpha_4 x_4 x_1 + \alpha_4 x_1^2$$

Sub-potentials corresponding to four vertices are $\Psi_i^*(x_i) = \delta_i^2 x_i^2$

Resulting potential function

$$\Psi(\boldsymbol{x}) = \boldsymbol{x}^T \begin{pmatrix} \alpha_1 + \alpha_4 + \delta_1^2 & -\alpha_1 & 0 & -\alpha_4 \\ -\alpha_1 & \alpha_1 + \alpha_2 + \delta_2^2 & -\alpha_2 & 0 \\ 0 & -\alpha_2 & \alpha_2 + \alpha_3 + \delta_3^2 & -\alpha_3 \\ -\alpha_4 & 0 & -\alpha_3 & \alpha_3 + \alpha_4 + \delta_4^2 \end{pmatrix} \boldsymbol{x}$$

and thus the covariance matrix Σ and mean μ can be computed by matching the shape of the multivariate normal density

$$p[\boldsymbol{x}|\boldsymbol{\mu}, \Sigma] \propto \frac{1}{\sqrt{\det \Sigma}} \cdot \exp\left(-\frac{1}{2} \cdot (\boldsymbol{x} - \boldsymbol{\mu})^T \Sigma^{-1} (\boldsymbol{x} - \boldsymbol{\mu})\right)$$

Important properties of normal distributions

Closeness under marginalisation

Let $x_{\mathcal{I}} = (x_i)_{i \in \mathcal{I}}$ be a subvector determined by the coordinate set \mathcal{I} . Then $x_{\mathcal{I}}$ is distributed according to a multivariate normal distribution as long as the vector x comes form a multivariate normal distribution $\mathcal{N}(\mu, \Sigma)$.

▶ Moment matching gives the parameters of the resulting distribution

$$egin{aligned} \mathbf{E}(oldsymbol{x}_{\mathcal{I}}) &= \mathbf{E}(oldsymbol{x})_{\mathcal{I}} = oldsymbol{\mu}_{\mathcal{I}} \ \mathbf{Cov}(oldsymbol{x}_{\mathcal{I}}) &= \mathbf{Cov}(oldsymbol{x})_{\mathcal{I} imes\mathcal{I}} = \Sigma[\mathcal{I},\mathcal{I}] \end{aligned}$$

Closeness under linear combinations

Linear combination $y = \alpha_1^T x_1 + \alpha_2^T x_2$ of independent multivariate normal distributions $x_1 \sim \mathcal{N}(\mu_1, \Sigma_1)$ and $x_2 \sim \mathcal{N}(\mu_2, \Sigma_2)$ is also a multivariate normal distribution.

▶ Moment matching gives the parameters of the resulting distribution

$$\begin{split} \mathbf{E}(y) &= \boldsymbol{\alpha}_1^T \, \mathbf{E}(\boldsymbol{x}_1) + \boldsymbol{\alpha}_2^T \, \mathbf{E}(\boldsymbol{x}_2) = \boldsymbol{\alpha}_1^T \boldsymbol{\mu}_1 + \boldsymbol{\alpha}_2^T \boldsymbol{\mu}_2 \\ \mathbf{Var}(y) &= \mathbf{Cov}(\boldsymbol{\alpha}_1^T \boldsymbol{x}_1) + \mathbf{Cov}(\boldsymbol{\alpha}_2^T \boldsymbol{x}_2) \\ &= \boldsymbol{\alpha}_1^T \mathbf{Cov}(\boldsymbol{x}_1) \boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2^T \mathbf{Cov}(\boldsymbol{x}_2) \boldsymbol{\alpha}_2 \\ &= \boldsymbol{\alpha}_1^T \Sigma_1 \boldsymbol{\alpha}_1 + \boldsymbol{\alpha}_2^T \Sigma_2 \boldsymbol{\alpha}_2 \end{split}$$

▷ Closeness under linear combinations holds also for matrix combinations.

Closeness under conditioning

Let x and y be related random variables. Let $x|y_*$ denote the conditional distribution of x given that a random variable y has a fixed value y_* . Then $x|y_*$ is distributed according to a multivariate normal distribution provided that (x,y) comes form a multivariate normal distribution $\mathcal{N}((\mu_i),(\Sigma_{ij}))$

▶ Moment matching gives the parameters of the resulting distribution

$$\mathbf{E}(m{x}|m{y}_*) = m{\mu}_1 + \Sigma_{1,2}\Sigma_{2,2}^{-1}(m{y} - m{\mu}_2)$$
 $\mathbf{Cov}(m{x}|m{y}_*) = \Sigma_{1,1} - \Sigma_{1,2}\Sigma_{2,2}^{-1}\Sigma_{2,1}$

Kalman filter

To be completed next year