LTAT.02.004 Machine Learning II

Multivariate normal distribution

Direct applications

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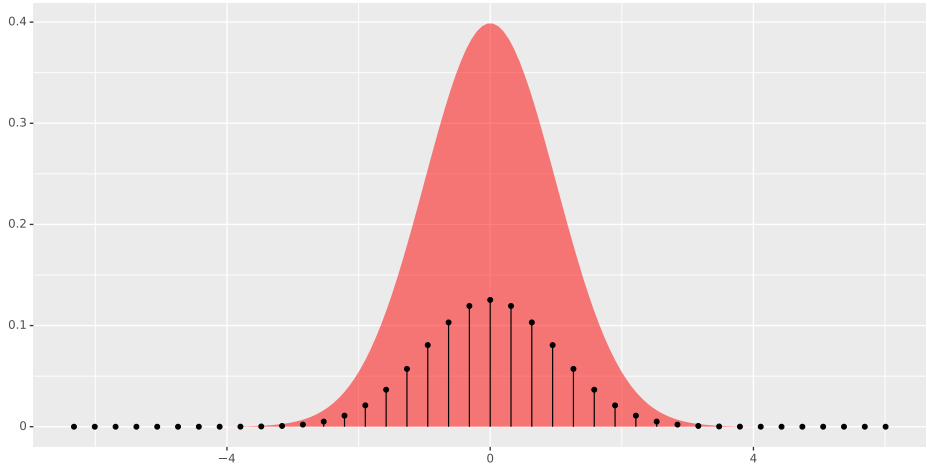
Univariate normal distribution

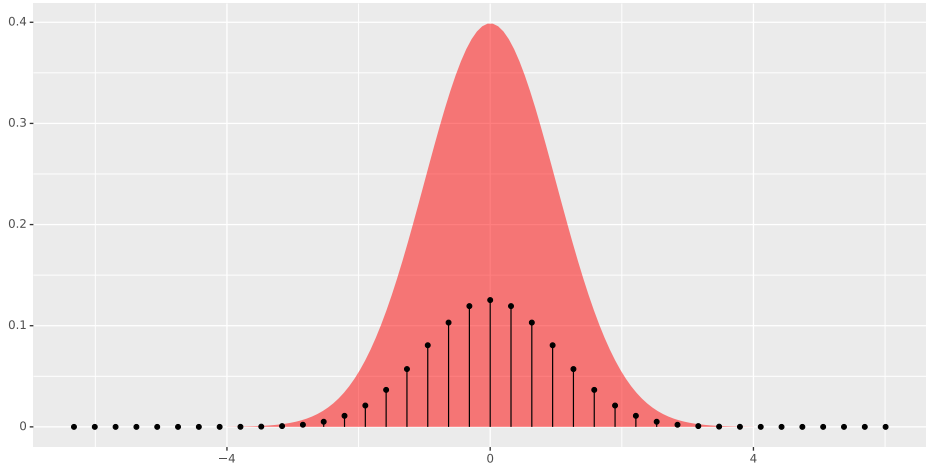
Probability density function



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 $x \in \mathbb{R}$:

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

Probability mass function

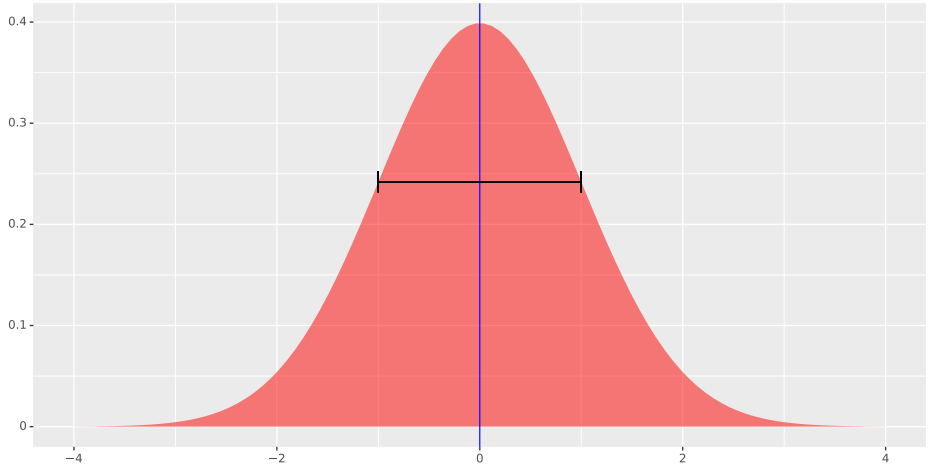


Definition. A real-valued random variable X comes from a discrete distribution with *a probability mass function* $p : \mathbb{R} \to \mathbb{R}^+ \cup \{0\}$ defined as

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

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

$$y = bx + a$$

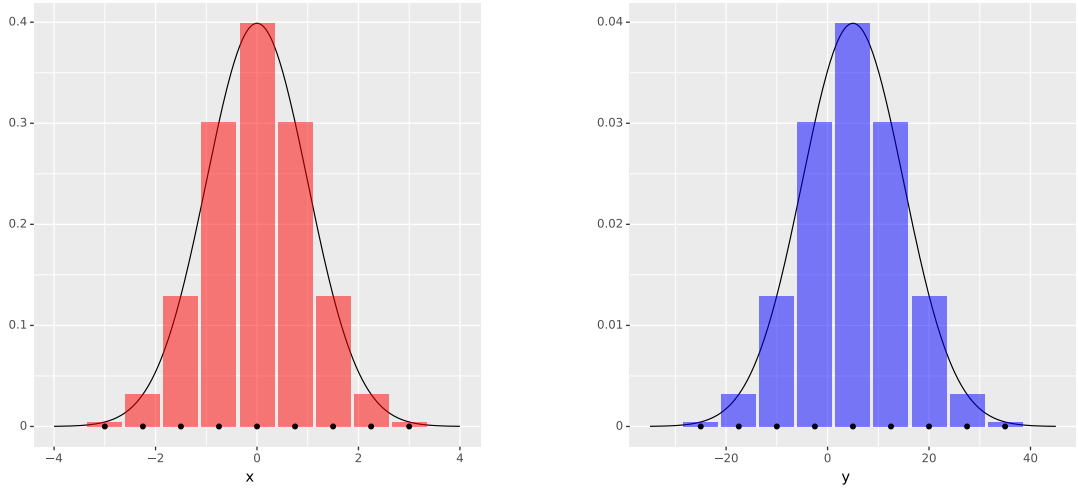
where x is distributed according to standardised normal distribution $\mathcal{N}(0, 1)$.

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 the relation between densities

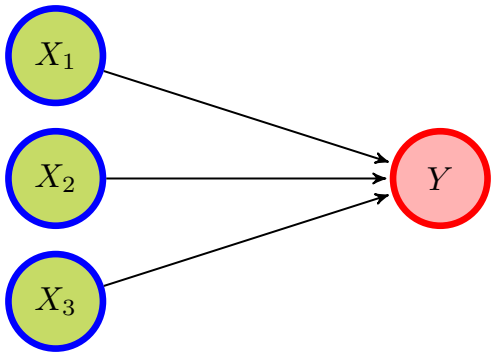
$$p_x(x) = \sigma \cdot p_y(y)$$

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

Motivating examples

Supervised learning

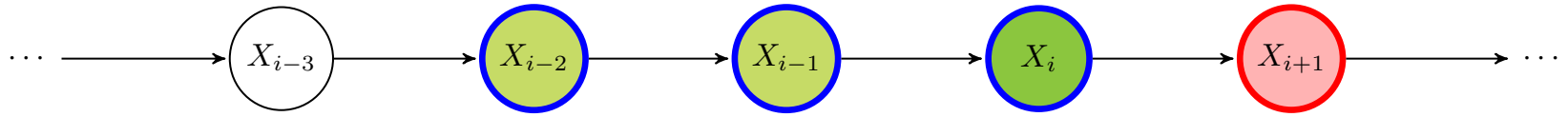
Repeated experiments with external controls



Linear regression models

- ▷ We assume that y_i depends only on the values of $x_{i1}, \ldots, x_{i\ell}$
- ▷ A linear model assumes $y_i = w_1 x_{i1} + \cdots + w_\ell x_{i\ell} + w_0 + \varepsilon_i$.
- ▷ All error terms ε_i are assumed to be independent.
- ▷ All error terms ε_i are drawn from a normal distribution $\mathcal{N}(0, \sigma)$.

Higher-order Markov chains



Time-series models

- ▷ We assume that x_{i+1} depends only on the values of $x_i, \ldots, x_{i-\ell}$
- ▷ A linear model assumes $x_{i+1} = w_0 + w_1 x_i + \cdots + w_{\ell+1} x_{i-\ell} + \varepsilon_i$.
- ▷ All error terms ε_i are assumed to be independent.
- ▷ All error terms ε_i are drawn from a normal distribution $\mathcal{N}(0, \sigma)$.

Univariate linear regression

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

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

- Consequently

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

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

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

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

- Fix a set of initial inputs $x_{-\ell}, \ldots, x_0 \in \mathbb{R}$. Denote them by $\boldsymbol{x}_\circ$.
- 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

$$x_{i+1} = \underbrace{w_0 + w_1 x_i + \ldots w_{\ell+1} x_{i-\ell}}_{\hat{x}_{i+1}} + \varepsilon_i, \qquad \varepsilon_i \sim \mathcal{N}(0, \sigma)$$

- Consequently

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

Maximum likelihood estimate

As usual we can find $\boldsymbol{w} \in \mathbb{R}^{\ell+2}$ and $\sigma \in \mathbb{R}$ that maximise the log-likelihood

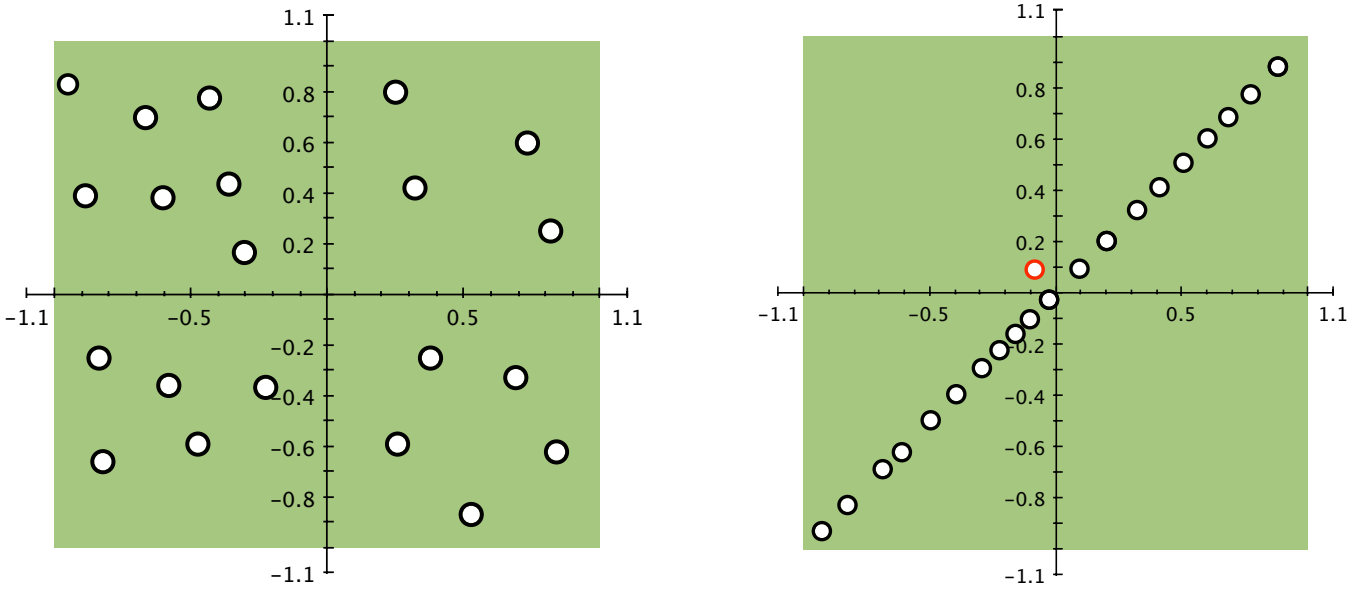
$$\log p[\boldsymbol{x}|\boldsymbol{x}_\circ, \boldsymbol{\beta}, \sigma] = const - n \log \sigma - \sum_{i=1}^{n} \frac{(x_i - \hat{x}_i)^2}{2\sigma^2}$$

and thus we can find $\boldsymbol{w}$ by minimising

$$\mathsf{MSE} = \frac{1}{n} \cdot \sum_{i=1}^{n} (x_i - w_0 - w_1 x_{i-1} - \ldots - w_{\ell+1} x_{i-1-\ell})^2 \ .$$

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.

Input values and numerical stability

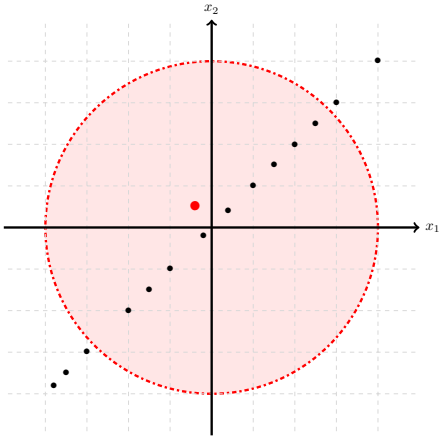


A small error in a point with big leverage can make linear regression function arbitrary large, which can lead to large test errors.

▷ In many case we know that the final output must be in fixed range.

Ridge regression

Let us seek the prediction as a function $f(\boldsymbol{x}) = w_1 x_1 + \cdots + w_k x_k$ with restriction $f(\boldsymbol{x}) \leq c$ inside a unit ball $\|\boldsymbol{x}\|_2^2 = x_1^2 + x_2^2 + \cdots + x_k^2 \leq 1$.



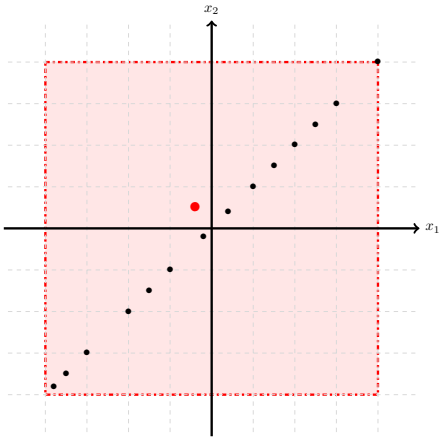
Then we should solve the following task instead:

$$\frac{1}{N} \cdot \sum_{i=1}^{N} \big(y_i - f(\boldsymbol{x}_i)\big)^2 \to \min$$

$$\text{s.t. } w_1^2 + \cdots + w_k^2 \leq c^2$$

LASSO regression

Let us seek the prediction as a function $f(\boldsymbol{x}) = w_1 x_1 + \cdots + w_k x_k$ with restriction $f(\boldsymbol{x}) \leq c$ inside a unit ball $\|\boldsymbol{x}\|_\infty = \max\{|x_1|, \ldots, |x_k|\} \leq 1$.



Then we should solve the following task instead:

$$\frac{1}{N} \cdot \sum_{i=1}^{N} (y_i - f(\boldsymbol{x}_i))^2 \to \min$$

$$\text{s.t.} \quad |w_1| + \cdots + |w_k| \leq c$$

Lagrange' trick

If we want to minimise $f(\boldsymbol{x})$ such that $g(\boldsymbol{x}) \leq c$ for a non-negative function $g(\cdot)$, then there exists $\lambda \geq 0$ such that the solution of the original problem is a minimum for a modified function

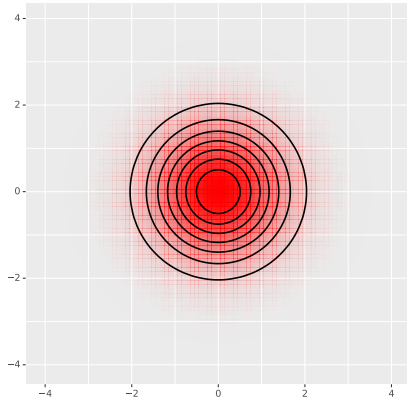
$$f_*(\boldsymbol{x}) = f(\boldsymbol{x}) + \lambda g(\boldsymbol{x})$$

Consequences

- ▷ We can use a penalty term $\lambda \left\|\boldsymbol{w}\right\|_1$ for rectangular area
- ▷ We can use a penalty term $\lambda \left\|\boldsymbol{w}\right\|_2^2$ for circular area

Multivariate normal distribution

White Gaussian noise



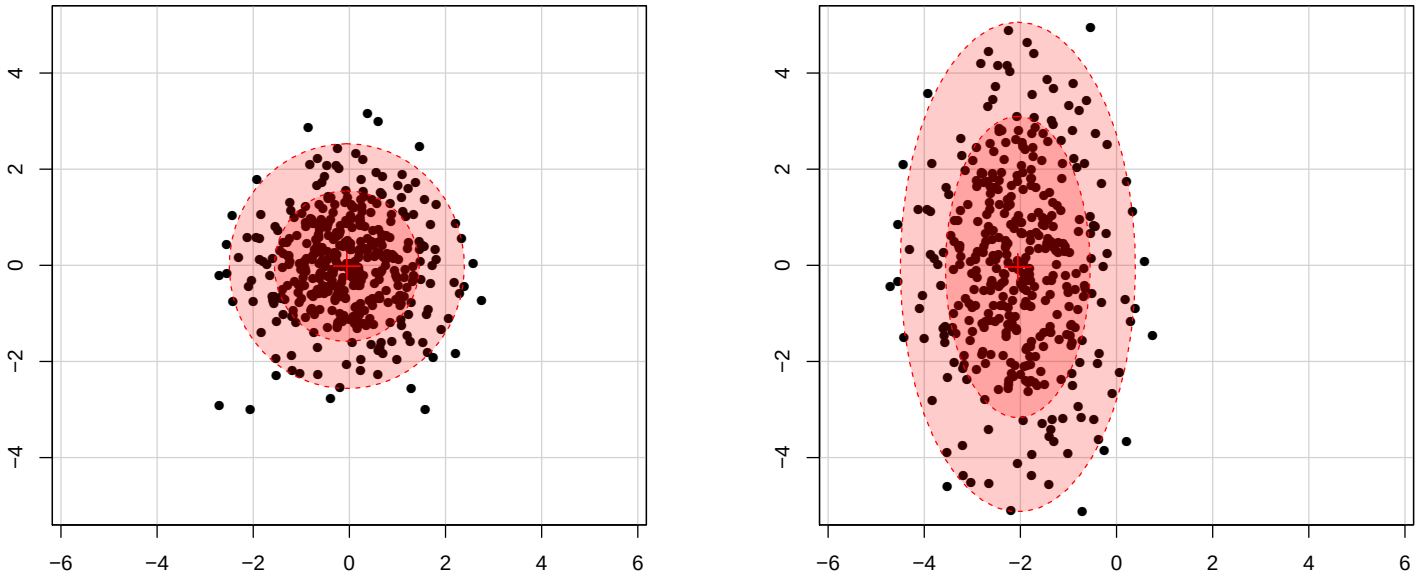
Definition. A random vector $X_1, \ldots, X_n$ is a standard normal random vector if all of its components are independent and and $X_i \sim \mathcal{N}(0, 1)$.

▷ The density can be computed based on independence:

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

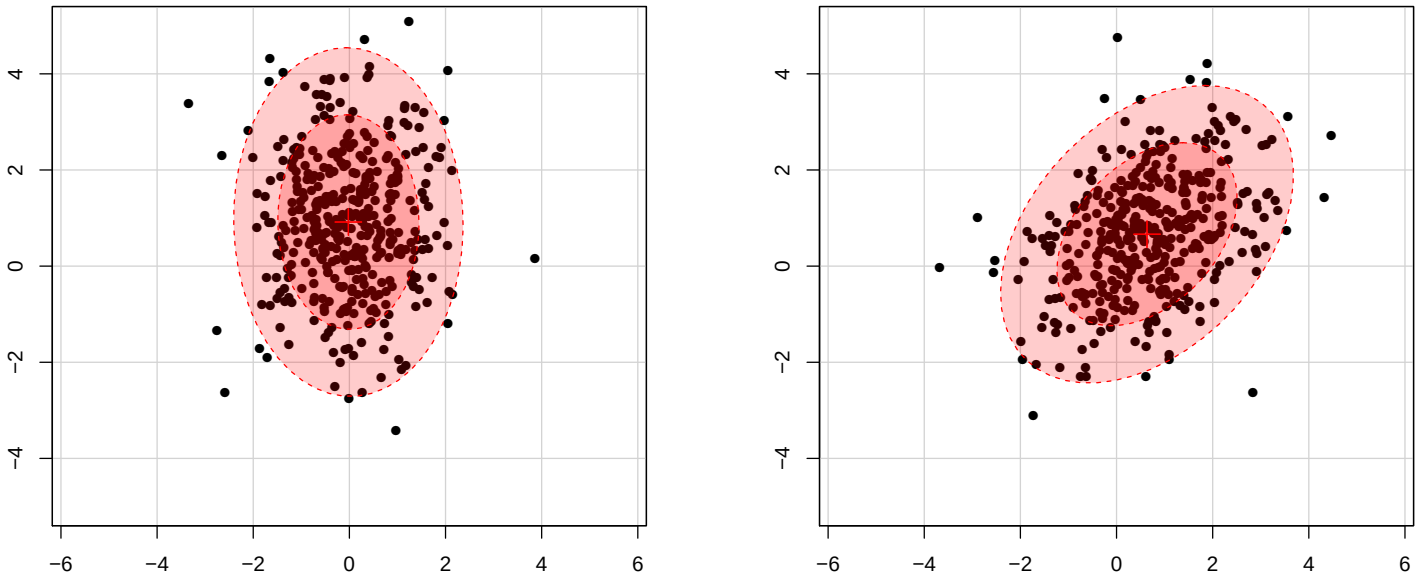
Scaling and shifting

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 $\boldsymbol{x}$ be standard normal random vector and let $\boldsymbol{y}$ be obtained the scaling, translation and rotation of the coordinate plane.

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

$$\begin{aligned} \boldsymbol{y} &= A\boldsymbol{x} + \boldsymbol{\mu} \ , \\ \boldsymbol{x} &= A^{-1}(\boldsymbol{y} - \boldsymbol{\mu}) \ . \end{aligned}$$

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 $\mathcal{R}$:

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

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

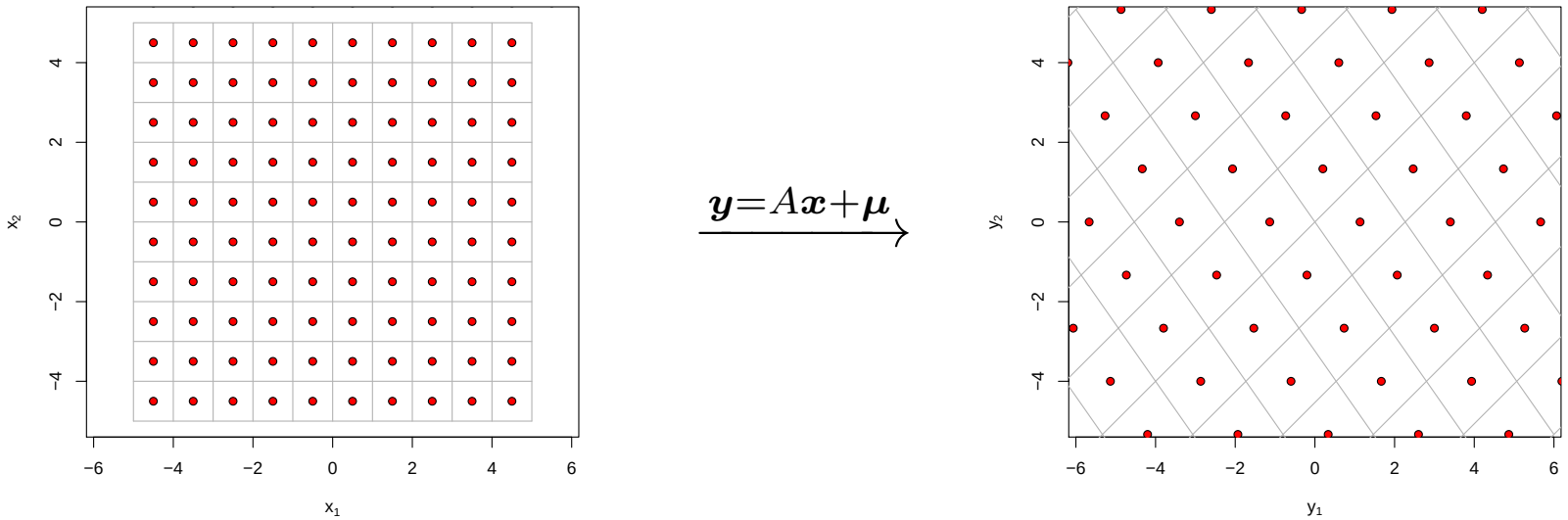
Remark. Regions $\mathcal{R}$ do not have to be rectangular as long as:

- ▷ The area $S(\mathcal{R})$ of a region can be computed.
- ▷ 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:

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

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:

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

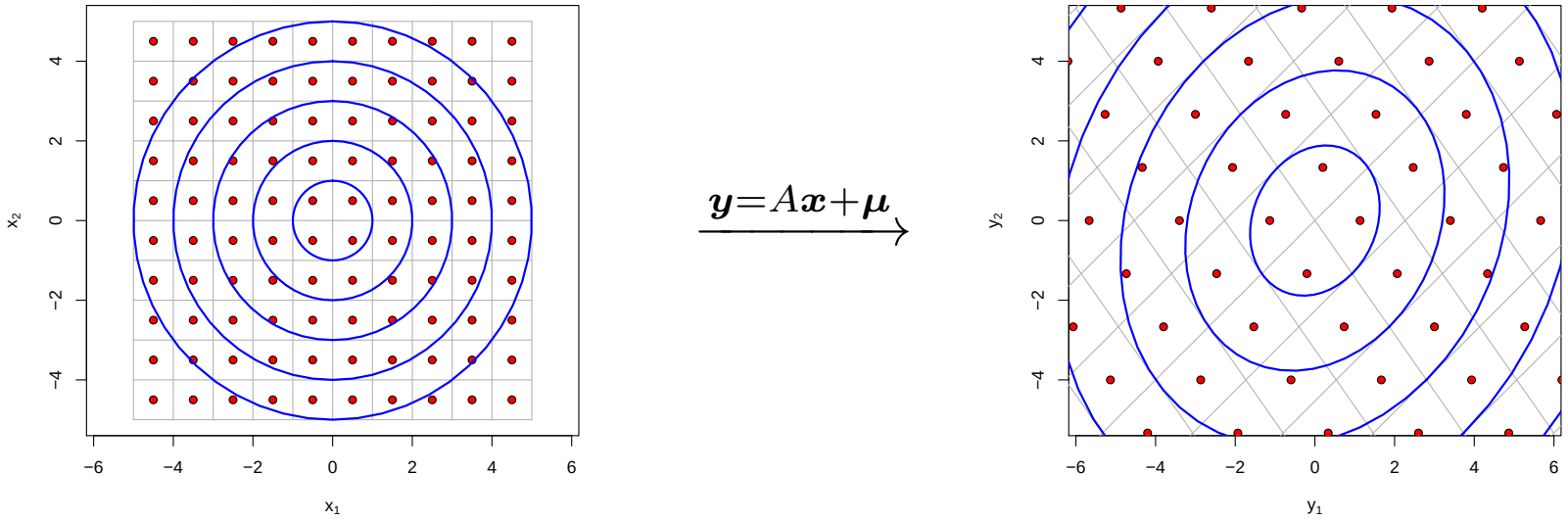
To estimate density $q(y_1, y_2)$, we must find the corresponding (x_1, x_2):

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

Thus we get

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

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 $\boldsymbol{y}$ are generated by applying the affine transformation

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

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:

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

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

Important properties of normal distributions

Closeness under marginalisation

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

▷ Moment matching gives the parameters of the resulting distribution

$$\mathbf{E}(\boldsymbol{x}_{\mathcal{I}}) = \mathbf{E}(\boldsymbol{x})_{\mathcal{I}} = \boldsymbol{\mu}_{\mathcal{I}}$$
$$\mathbf{Cov}(\boldsymbol{x}_{\mathcal{I}}) = \mathbf{Cov}(\boldsymbol{x})_{\mathcal{I} \times \mathcal{I}} = \Sigma[\mathcal{I}, \mathcal{I}]$$

Closeness under linear combinations

Linear combination $y = \boldsymbol{\alpha}_1^T \boldsymbol{x}_1 + \boldsymbol{\alpha}_2^T \boldsymbol{x}_2$ of independent multivariate normal distributions $\boldsymbol{x}_1 \sim \mathcal{N}(\boldsymbol{\mu}_1, \Sigma_1)$ and $\boldsymbol{x}_2 \sim \mathcal{N}(\boldsymbol{\mu}_2, \Sigma_2)$ is also a multivariate normal distribution.

▷ Moment matching gives the parameters of the resulting distribution

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

▷ Closeness under linear combinations holds also for matrix combinations.

Closeness under conditioning

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

▷ Moment matching gives the parameters of the resulting distribution

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

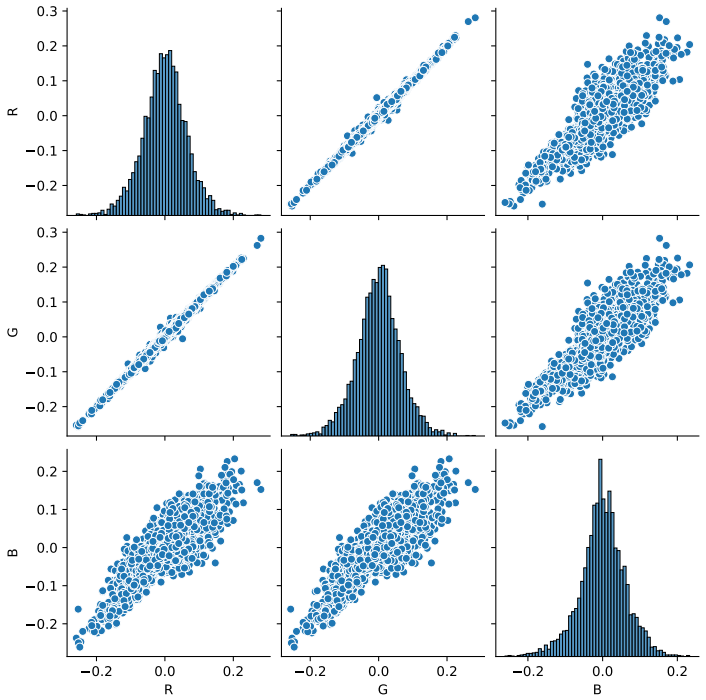
$$\mathbf{Cov}(\boldsymbol{x}|\boldsymbol{y}_*) = \Sigma_{1,1} - \Sigma_{1,2}\Sigma_{2,2}^{-1}\Sigma_{2,1}$$

Motivating examples

Filtering and smoothing

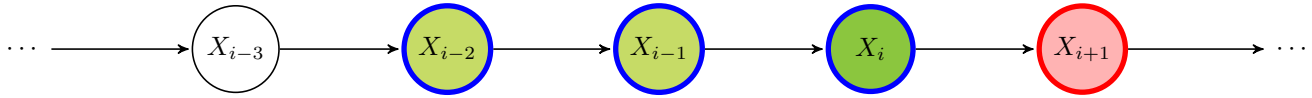
Prediction of vector values

Prediction errors of different vector components can be correlated.



As a result combined model can outperform coordinatewise predictions.

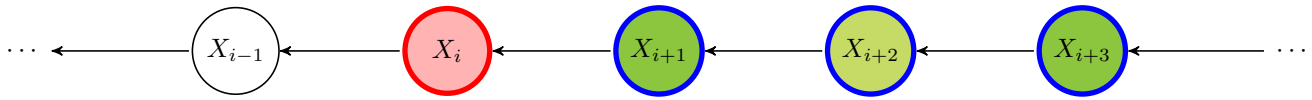
Prediction intervals for time-series



After we have fitted the linear regrssion model to timeseries data we might want to compute prediction intervals for iterative stepwise predictions.

- ▷ Let $\boldsymbol{x}_0$ be the known initial state and $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ iterative predictions.
- ▷ We need priors $\pi[\boldsymbol{x}_i] = p[\boldsymbol{x}_i|\boldsymbol{x}_0]$ to compute confidence intervals.
- ▷ It turns out that all priors $p[\boldsymbol{x}_i]$ are normal distributions.
- ▷ Moment matching allows us to learn the parameters of the distributions.

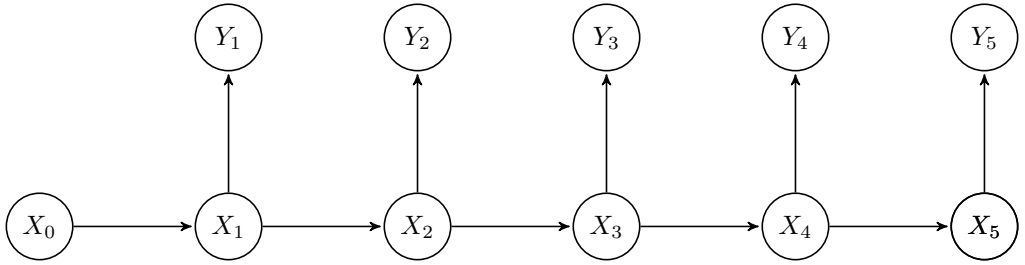
Smoothing and reverse Markov chain



Sometimes we have to interpolate observations in the time series. This can be stated as amoothing task where we know $\boldsymbol{x}_0$ and $\boldsymbol{x}_n$.

- ▷ We need likelihoods $\lambda[\boldsymbol{x}_i] = p[\boldsymbol{x}_n|\boldsymbol{x}_i]$ for the smoothing.
- ▷ Likelihood propagation formula is analogous to the prior propagation.
- ▷ We can define a reverse Markov chain such that the prior $\pi^*[\boldsymbol{x}_i] \propto \lambda[\boldsymbol{x}_i]$.
- ▷ The resulting chain has reversed dynamics.
- ▷ It turns out that all likelihoods $\lambda[\boldsymbol{x}_i]$ are normal distributions.
- ▷ The posterior as product $\pi[\boldsymbol{x}_i] \cdot \lambda[\boldsymbol{x}_i]$ is also a normal distribution.

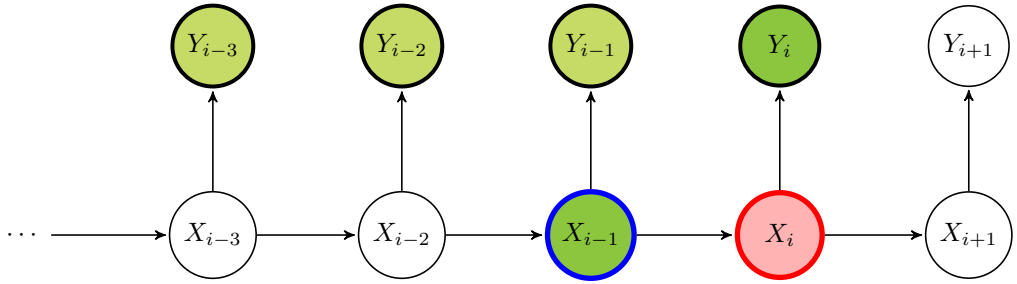
Sensor fusion with Hidden Markov Models



A standard problem in robotics or machine perception is following.

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

Kalman filter

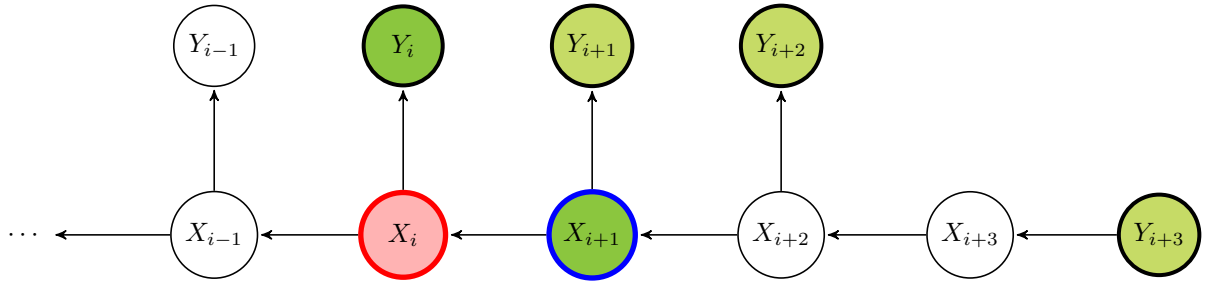


As before we can consider the prior and filter densities

$$\pi[\boldsymbol{x}_i] = p[\boldsymbol{x}_i|\boldsymbol{y}_1, \ldots, \boldsymbol{y}_{i-1}]$$
$$f[\boldsymbol{x}_i] = p[\boldsymbol{x}_i|\boldsymbol{y}_1, \ldots, \boldsymbol{y}_i] \propto \pi[\boldsymbol{x}_i] \cdot p[\boldsymbol{y}_i|\boldsymbol{x}_i]$$

A similar update logic assures that both distributions are normal distributions and that we can only compute the parameters of these normal distributions.

Smoothing and reverse Hidden Markov Model

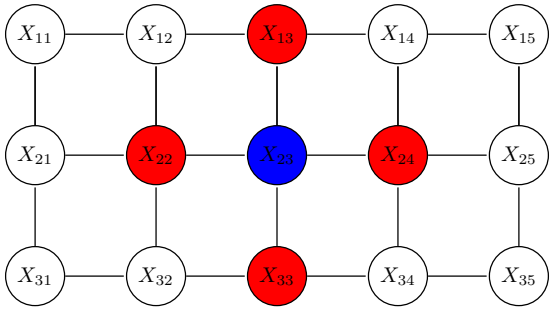


- ▷ We need likelihoods $\lambda[\boldsymbol{x}_i] = p[\boldsymbol{y}_{i+1}, \ldots, \boldsymbol{y}_{\boldsymbol{n}} | \boldsymbol{x}_i]$ for the smoothing.
- ▷ Likelihood propagation formula is analogous to the prior propagation.
- ▷ We can define a reverse HMM such that the prior $\pi^*[\boldsymbol{x}_i] \propto \lambda[\boldsymbol{x}_i]$.
- ▷ The resulting HMM has reversed dynamics.
- ▷ It turns out that all likelihoods $\lambda[\boldsymbol{x}_i]$ are normal distributions.
- ▷ The posterior as product $\pi[\boldsymbol{x}_i] \cdot \lambda[\boldsymbol{x}_i] \cdot p[\boldsymbol{y}_i | \boldsymbol{x}_i]$ is also a normal distribution.

Motivating examples

Markov fields

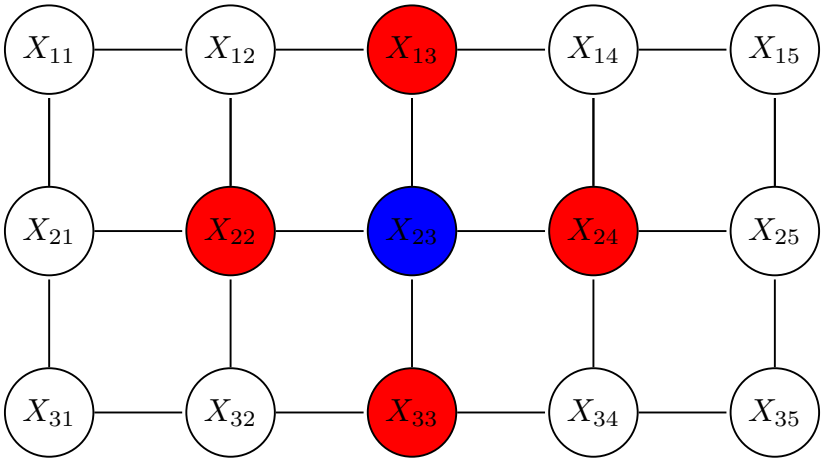
Background model for digital images



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 $\boldsymbol{x} = (x_1, x_2, \ldots)$ generated by a Markov random field can be expressed in the form

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

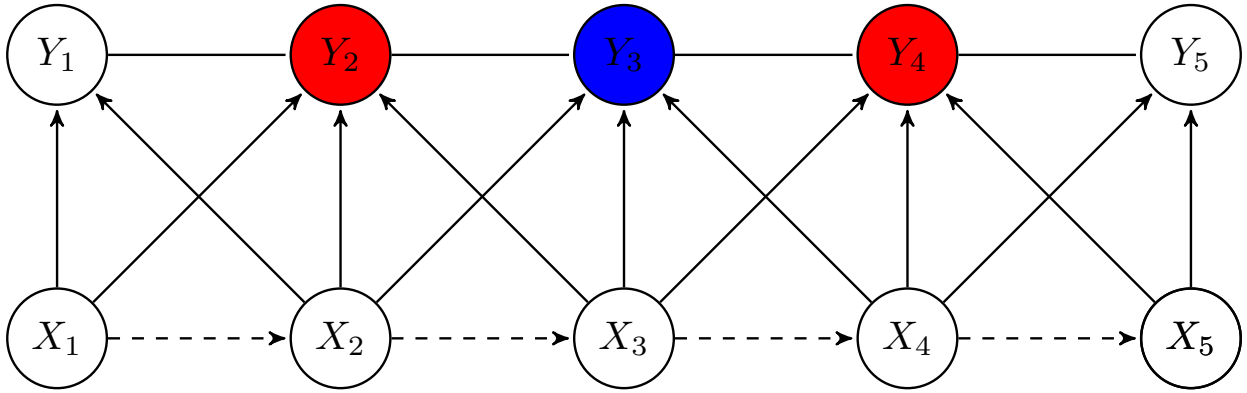
where

- $Z(\omega)$ is a normalising constant
- MaxClique is the set of maximal cliques in the Markov random field
- Ψ_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

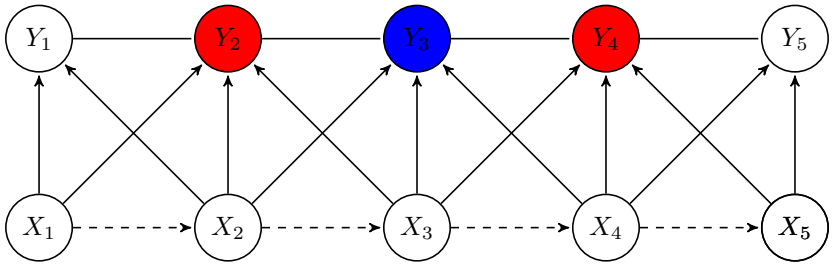


Definition. Let $X_1, X_2, \ldots$ and $Y_1, Y_2, \ldots$ be random variables. The entire process is conditional random field if random variables $Y_1, Y_2, \ldots$ conditioned for any sequence of observations $x_1, x_2, \ldots$ form a Markov random field

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

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

Image segmentation and sequence labelling



- The input $\boldsymbol{x}$ 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

- 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.
- A vertex feature looks only variable y_i associated with the vertex.
- An edge feature looks only variables y_i, y_j associated with the edge.

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:

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

where

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

Multivariate normal distribution as likelihood

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

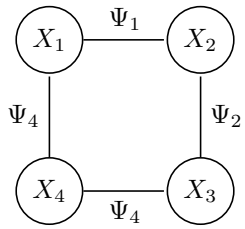
$$\Psi(\boldsymbol{x}) = \sum_{c \in \text{MaxClique}} \Psi_c(\boldsymbol{x}_c, \omega)$$

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

Sub-potentials are often fixed directly based on smoothness constraints

- ▷ Intensities have bounded variance: $\Psi_e = \delta^2 x_{ij}^2$.
- ▷ Intensity changes smoothly vertically: $\Psi_e = \beta(x_{i,j} - x_{i+1,j})^2$.
- ▷ 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 $\boldsymbol{\mu}$ can be computed by matching the shape of the multivariate normal density

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