## Intelligent Systems for Pattern Recognition

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# Index

0.1	Introd	uction
0.2	Pattern Recognition	
	0.2.1	Signals
	0.2.2	Image Processing
	0.2.3	Wavelets
0.3	Generative and Graphical Models	
	0.3.1	Probability Refresher
	0.3.2	Graphical Models
	0.3.3	Conditional Independence and Causality
	0.3.4	Fundamental Bayesian Network Structures
	0.3.5	Markov Random Fields
	0.3.6	Learning Causation from Data

## 0.1 Introduction

Prof.s: Davide Bacciu and Antonio Carta

**Objectives** Train ML specialists capable of: designing novel learning models, developing pattern recognition applications using ML, developing intelligent agents using **Reinforcement Learning**.

We're referring to images and signals, but not limited to that: practical applications.

Focusing on challenging and complex data: **machine vision** (noisy, hard to interpret, semantically rich...) and **structured data** (relational information: sequences, trees, graphs...)

Natural Language Processing will be used as an example, but will not be the focus of this course.

**Methodology-Oriented Outcomes** Gain in-depth knowledge of advanced machine learning models, understanding the underlying theory. This gives the ability to read and understand and discuss research works in the field.

**Application-Oriented Outcomes** Learn to address modern pattern recognition applications, gain knowledge of ML, PR and RL libraries and be able to develop an application using ML and RL models.

**Prerequisites** Knowledge of ML fundamentals, mathematical tools for ML and Python.

## 0.2 Pattern Recognition

Automated recognition of meaningful patterns in noisy data.

#### **Origins**

**Viola-Jones Algorithm** Framework for face recognition. Sum pixel in white area and subtract those in the black portion. The VJ algorithm positions the masks on the image and combines the responses (training set of  $\simeq$ 5k images with hand-aligned filters)

#### An historical view

- 1. Identification of distinguishing features of the object/entity (**feature detection**)
- 2. Extraction of features for the defining attributes (feature extraction)
- 3. Comparison with known patterns (matching)

Basically, lots of time spent hand-engineering the best data features.

**A modern view** Data is thrown into a neural network. A single stage process with a data crushing-and-munching neural network spitting out prediction, which encapsulates the three historical steps. But the time is now spent in fine-tuning the neural network.

The deep learning Lego Creating applications by putting together various combinations of CNN and LSTM modules.

## 0.2.1 Signals

Signals are time series: a sequence of measurements in time. Examples of sources are: medicine, finance, geology, IoT, biometrics...

**Formalization** A time series x is a sequence of measurements in time t

$$\mathbf{x} = x_0, \dots, x_N$$

where  $x_t$  or x(t) is the measurement at time t.

Observation can be at **irregular** time intervals.

We assume weakly stationary (or second-order stationary) data

$$\forall t \ E[x_t] = \mu$$
  
  $\forall t \ \text{Cov}(x_{t+\tau}, x_t) = \gamma_{\tau} \text{ with } \gamma \text{ depending only on the lag } \tau$ 

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#### Goals

Description

Analysis: identify and describe dependencies in data

**Prediction**: forecast next values given information up to t

Control: adjust parameters of the generative process to make the time series fit a target

## **Key Methods**

Time domain analysis: assesses how a signal changes over time (correlation, convolution, auto-regressive models)

**Spectral domain analysis**: assesses the distribution of the signal over a range of frequencies (Fourier analysis, wavelets)

#### Time Domain Analysis

Mean

$$\hat{\mu} = \frac{1}{N} \sum_{t=1}^{N} x_t$$

Can be used to subtract mean from values and "standardize" the two series.

**Autocovariance** For lag  $-N \le \tau \le N$ 

$$\hat{\gamma}_x(\tau) = \frac{1}{N} \sum_{t=1}^{N-|\tau|} (x_{t+|\tau|} - \hat{\mu})(x_t - \hat{\mu})$$

Autocorrelation The correlation of a signal with itself.

$$\hat{\rho}_x(\tau) = \frac{\hat{\gamma}_x(\tau)}{\hat{\gamma}_x(0)}$$

We can compute this with every possible  $\tau$ , finding the max/min which gives the  $\tau$  where the autocorrelation is max/min, which means the lag where the signal starts repeating itself. The lags near zero typically dominates, so we want the maximum lag reasonably far from 0.

Autocorrelation plot It's a revealing view on time series statistics.

Cross-Correlation A measure of similarity of  $x_1$  and  $x_2$  as a function of a time lag  $\tau$ 

$$\phi_{\mathbf{X}_1 \mathbf{X}_2}(\tau) = \sum_{t = \max\{0, \tau\}}^{\min\{(T_1 - 1 + \tau), (T_2 - 1)\}} \mathbf{x}_1(t - \tau) \cdot \mathbf{x}_2(t)$$

Normalized cross-correlation Returns an amplitude independent value

$$\overline{\phi}_{\mathbf{X}_1 \, \mathbf{X}_2}(\tau) = \frac{\phi_{\mathbf{X}_1 \, \mathbf{X}_2}}{\sqrt{\sum_{t=0}^{T_1-1} (x_1(t))^2 \cdot \sum_{t=0}^{T_2-1} (x_2(t))^2}} \in [-1, +1]$$

With  $\overline{\phi}_{X_1 X_2}(\tau) = +1$  mean that the two time series have the exact same shape if aligned at time  $\tau$ . Nearing -1 we get the maximum anticorrelation, same shape but opposite sign. Near 0 we get that the two signals are completely linearly uncorrelated.

Note that we measure linear correlation.

Cross correlation looks like the convolution

$$(f * g)[n] = \sum_{t=-M}^{M} f(n-t)g(t)$$

but we have a flipped sign (n-t) instead of  $t-\tau$ ).

Cross-correlation is not symmetric, whereas convolution is (f \* g = g \* f).

Autoregressive Process A timeseries autoregressive process (AR) of order K is the linear system

$$x_t = \sum_{k=1}^{K} \alpha_k x_{t-k} + \epsilon_t$$

Autoregressive means  $x_t$  regresses on itself

 $\alpha_k \Rightarrow \text{linear coefficients} | |\alpha| < 1$ 

 $\epsilon_t \Rightarrow$  sequence of independent and identically distributed values with mean 0 and fixed variance.

We look backward K steps, so limited memory.

### ARMA Autoregressive with Moving Average process

$$x_t = \sum_{k=1}^{K} \alpha_k x_{t-k} + \sum_{q=1}^{Q} \beta_q \epsilon_{t-1} + \epsilon_t$$

With  $\epsilon_t$  Random white noise (again)

The current time series values is the result of a regression on its past values plus a term that depends on a combination of stochastically uncorrelated information

Estimating Autoregressive Models Need to estimate: the values of the linear coefficients  $\alpha_t$  and  $\beta_t$  and the order of the autoregressor K and Q

Estimation of the  $\alpha$ ,  $\beta$  is performed with the Levinson-Durbin Recursion (levinson(x, K) in matlab, and included in several Python modules).

The order is often estimated with a Bayesian model selection criterion, choosing the largest K and Q possible. E.g.: BIC, AIC...

The set of autoregressive parameters  $\alpha_{i,1}, \ldots, \alpha_{i,K}$  fitted to a specific time series  $x_i$  is used to confront it with other time series. Same thing for  $\beta$  so we can use  $\alpha$  for both sets.

## Comparing time series by AR

timeseries clustering:  $d(\mathbf{x}_1, \mathbf{x}_2) = \|\alpha_1 - \alpha_2\|_M^2$ 

novelty/anomaly detection: TestErr $(x_t, \hat{x}_t) < \xi$  with  $\hat{x}_t$  being the AR predicted value.

#### Spectral Domain Analysis

Analyze the time series in the frequency domain. Key idea: decomposing the time series into a linear combination of sines and cosines with random and uncorrelated coefficients. So a **regression on sinusoids** with Fourier analysis.

**Fourier Transform** Discrete Fourier Transform (DFT): transform a time series from the time domain to the frequency domain. Can be easily inverted back to the time domain.

Useful to handle periodicity in the time series: seasonal trends, cyclic processes...

**Representing functions** We know that, given an orthonormal system for E we can use linear combinations of the basis  $\{e_1, \ldots, e_k\}$  to represent any function  $f \in E$ 

$$\sum_{k=1}^{\infty} \langle f, e_k \rangle e_k$$

Given the orthonormal system

$$\left\{\frac{1}{\sqrt{2}}, \sin(x), \cos(x), \sin(2x), \cos(2x), \ldots\right\}$$

then the linear combination above becomes the Fourier series

$$\frac{a_0}{2} + \sum_{k=1}^{\infty} \left( a_k \cos(kx) + b_k \sin(kx) \right)$$

Representing function in Complex space Using  $\cos(kx) - i \sin(kx) = e^{-ikx}$  with  $i = \sqrt{-1}$  we can rewrite the Fourier series as

$$\sum_{k=-\infty}^{\infty} c_k e^{ikx}$$

on the orthonormal system

$$\{1, e^{ix}, e^{-ix}, e^{2ix}, e^{-2ix}, \ldots\}$$

Representing Discrete Time Series Consider x of length N and  $x_n \in R$ . Using the exponential formulation, the orthonormal system is finite, from  $e_0$  to  $e_{N-1}$  each  $\in C^N$ 

The n-th component of the k-th vector is

$$[e_k]n = e^{\frac{-2\pi i n k}{2}}$$

**Discrete Fourier Transform** Given a time series  $\mathbf{x} = x_0, \dots, x_{N-1}$  its DFT is the sequence

Spectral domain 
$$X_k = \sum_{n=1}^{N-1} x_n e^{\frac{-2\pi i n k}{N}}$$
 Time domain

And can be inverted

$$x_k = \frac{1}{N} \sum_{k=1}^{N-1} X_k e^{\frac{2\pi i n k}{N}}$$

#### Basic Spectral Quantities in SFT

Amplitude 
$$A_k = |X_k| = \sqrt{Re^2(X_k) + Im^2(X_k)}$$

Power  $P_k = \frac{|X_k|^2}{N}$ , more used in reality and under some conditions this is a reasonable estimate of the power spectral density

**DFT in Action** We use the DFT elements  $X_1, \ldots, X_K$  as representation of the signal to train the predictor/classifier. This representation can reveal patterns that are not clear in the time domain.

## 0.2.2 Image Processing

Bidimentional series. Basically same approach to signals.

#### Descriptors

An image is a matrix of pixel intensities or color values (RGB). There are other representations, not interesting for this course. CIE-LUV often used in image processing due to perceptual linearity (image difference is more coherent)

Machine Vision Applications For example region of interest, or object classification.

Even pixel-level tasks, for example image segmentation (regions of the image) or semantic segmentation (classifying regions of the image).

Up one level of abstraction: automated image captioning, requiring identifying objects, generating sentences and ranking those sentences.

#### **Key Questions**

How to represent visual information? It has to be:

Informative, carrying all the information

Invariant to photometric (different illuminations) and geometric transformation (position in the picture, rotation...)

Efficient for indexing and querying

How to identify informative parts?

Whole image is generally not a good idea

Must lead to good representations

**Image Histograms** One of the first answer. Describes the distribution of some visual information on the whole image: colors, edges, corners...depending on the goals.

Color Histograms, one of the earliest image descriptors.

Count the number of pixels of a given color (normalize!). We need to discretize and group the RGB colors.

Any information concerning shapes and position is lost. Two image with a random permutation of the same pixels produce the same color histograms.

Images can be compared, indexed and classified based on their color histogram representation.

Can be computed with OpenCV in Python.

**Describing Local Image Properties** We need something less global, on a local level. Capturing information on image regions, extract **multiple local descriptors**: different location, different scale...

Several approaches, typically performing convolution between a filter and the image region. Using filters sensitive to specific features we can extract many kind of information.

## Localized Descriptors

**Intensity Vector** The simplest form of localized descriptor: a vector  $n \cdot m$  of the pixels of a single patch of the image with dimensions n, m. The vector can be normalized to make it invariant to intensity variations. But rotating gives a different vector. A more robust representation is an histogram of this vector.

**Distribution-Based Descriptors** Represent local patches by histograms describing properties of the pixels in the patch. The simplest is an histogram of intensity values, but it's not invariant enough even if normalized. We want a descriptor invariant to illumination (normalization), scale (captured at multiple scale) and geometric transformations (rotation invariant). We want locality, histogram based and invariant to geometric transformation.

#### SIFT Scale Invariant Feature Transform

- 1. Center the image patch on a pixel x, y of the image I
- 2. Represent image at scale  $\sigma$  (controls how close to look at the image)

Convolve the image with a Gaussian filter with standard variation  $\sigma$ , basically computing average of pixels with the coefficient taken from a Gaussian distribution. With a smooth Gaussian, we artificially smooth the object, and vice versa. We can compute different versions of the image.

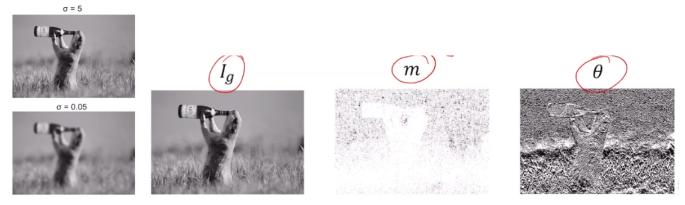
$$L_{\sigma}(x,y) = G(x,y,\sigma) * I(x,y)$$

$$G(x, y, \sigma) = \exp\left(-\frac{x^2 + y^2}{2\sigma^2}\right)$$

3. Compute the **gradient of intensity** in the patch, extracting magnitude m and orientation  $\Theta$  using finite differences.

#### Gaussian Filter of an Image

Iscale = imgaussfilt (I, sigma);



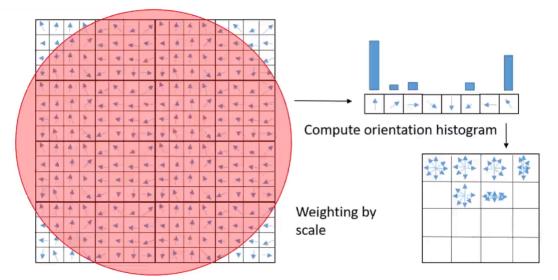
## 4. Create gradient histogram

4×4 gradient window

Histogram of  $4\times4$  per window on 8 orientation bins

Gaussian weighting on center keypoint (width =  $1.5\sigma$ )

 $4 \times 4 \times 8 = 128$  descriptor size



#### **Detectors**

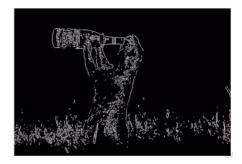
## Visual Feature Detector Properties

Repeatability Detect the same feature in different image portions and different images, under different conditions (color, luminance...). So with respect to translation, photometric changes, rotation, scaling and affine transformations (non-isotropic changes, for example the relative position of the camera)...

**Edge Detection** We need to find interesting points, talking about fundamental elements, basic components. One possible example are the edges of the image.

Reasoning in changes of intensity: edges are those points where the intensity changes.





Typically using an edge detector filter on each pixel and turning pixels white or black by thresholding

Edges and Gradients The image gradient (graylevel) is

$$\nabla I = \left[ \frac{\partial I}{\partial x}, \frac{\partial I}{\partial y} \right]$$

which is basically two images, gradient in both x and y directions. Edge are pixel regions where intensity gradient changes abruptly. The return of finite difference methods:

$$G_x = \frac{\partial I}{\partial x} \simeq I(x+1,y) - I(x-1,y)$$

$$G_y = \frac{\partial I}{\partial y} \simeq I(x, y+1) - I(x, y-1)$$

Edge detectors build on this idea combining with some smoothing: average on multiple pixels.

## Prewitt operators

$$G_x = \left[ \begin{array}{ccc} +1 & 0 & -1 \\ +1 & 0 & -1 \\ +1 & 0 & -1 \end{array} \right] \quad G_y = \left[ \begin{array}{ccc} +1 & +1 & +1 \\ 0 & 0 & 0 \\ -1 & -1 & -1 \end{array} \right]$$



Magnitude





## **Sobel Operator**

$$G_x = \left[ \begin{array}{ccc} +1 & 0 & -1 \\ +2 & 0 & -2 \\ +1 & 0 & -1 \end{array} \right] \quad G_y = \left[ \begin{array}{ccc} +1 & +2 & +1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{array} \right]$$

Often with a constant  $c \simeq \frac{1}{8}$  for scaling.





Blob Detection Pixel regions with little gradient variability.

 $g_{\sigma}(x,y)$  has maximum response when centered on a circle of radius  $\sqrt{2}\sigma$ , with  $\sigma$  being the scale of the gaussian. Laplace of Gaussian (LoG):

$$\nabla^2 g_{\sigma}(x,y) = \frac{\partial^2 g_{\sigma}}{\partial x^2} + \frac{\partial^2 g_{\sigma}}{\partial y^2}$$

Typically using a scale normalized response

$$\nabla_{norm}^2 g_{\sigma}(x, y) = \sigma^2 \left( \frac{\partial^2 g_{\sigma}}{\partial x^2} + \frac{\partial^2 g_{\sigma}}{\partial y^2} \right)$$

- 1. Convolve image with a LoG filter at different scales  $\sigma = k\sigma_0$  by varying k with a starting  $\sigma_0$
- 2. Find maxima of squared LoG responses:

Find maxima on space-scale: focus on a scale and find maxima

Find maxima between scales: do the same for all the scales and pick the maxima

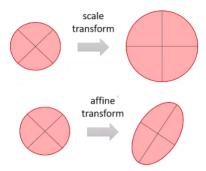
Threshold

The LoG can be approximated by the Difference of Gaussians (DoG) for efficiency, so to reuse part of the computations.

$$g_{k\sigma_0}(x,y) - g_{\sigma_0}(x,y) \simeq (k-1)\sigma_0^2 \nabla^2 g_{(k-1)\sigma_0}$$

SIFT uses LoG.

Affine Detectors Laplacia-based detectors are invariant to scale thanks to the maximization in scale-space. Still not invariant to affine-transformation.



#### MSER Maximally Stable Extremal Regions

Extract covariant regions (blobs) that are stable connected components of intensity sets of the image. Interesting areas stay the same at different thresholds: stable with respect to variations in luminance, not scale dependent and doesn't assume circular regions. The key idea is to take the blobs (extremal regions) which are nearly the same through a wide range of intensity thresholds.

Blobs are generated (locally) by binarizing the image over a large number of thresholds:

Invariance to affine transformation of image intensities

Stability (they are stable on multiple thresholds)

Multi-scale (connected components are identified by intensity stability not by scale)

Sensitive to local lightning effects, shadows...

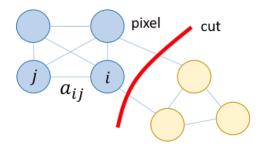
**Intuitions on MSER** Generate frames from the image by thresholding it on all graylevels.

Capture those regions that from a small seed of pixel grow to a stably connected region. Stability is assessed by looking at derivatives of region masks in time (most stable  $\Rightarrow$  minima of connected region variation).

**Image Segmentation** The process of partitioning an image into a set of homogeneous pixels, hoping to match objects or their subparts.

A naive approach: straighten the image in a  $N \cdot M$  vector and use it as a dataset for K-means.

Ncut Normalized cuts



With each node being a pixel: an image is a graph.  $a_{ij}$  is the affinity between pixels at a certain scale  $\sigma$ . A cut of G is the set of edges such whose removal makes G a disconnected graph. Breaking the graph into pieces by cutting edges of low affinity.

The normalized cut problem is NP-hard, approximate solution as an eigenvalue problem. But the eigenvalue decomposition it's really intractable with big images. We need to reduce the number of pixels. We can use  $\mathbf{superpixels}$ : clustering the pixels with K-means (perhaps with different K) and using the clusters as nodes for segmentation algorithms (Ncut, Markov Random Fields...). We can do multiscale superpixeling and segmenting at different scales, different policies...

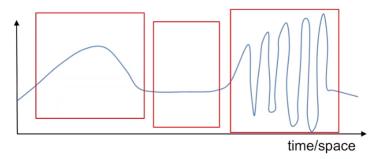
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### Conclusion

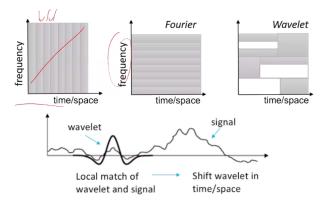
Image processing is a lot about convolutions: linear masks to perform gradient operations, gaussian functions to apply scale changes (zooming in and out). Computational efficiency is a driving factor: convolution in Fourier domain, superpixel, lightweight feature detectors...

#### 0.2.3 Wavelets

Limitations of DFT Sometimes we might need localized frequencies rather than global frequency analysis.



We slice the signal in "time slots" in time analysis and "frequency slots" in frequency analysis. In wavelet analysis you do both.



- 1. Scale and shift original signal
- 2. Compare signal to a wavelet
- 3. Compute coefficient of similarity

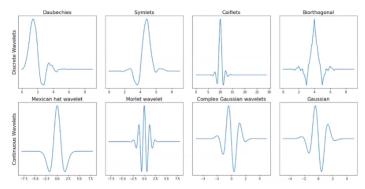
Split the signal with an orthonormal basis generate by translation and dilation of a mother wavelet

$$\sum_{t} \mathbf{x}(t) \phi_{j,k}(t)$$

Terms k, j regulate scaling and shifting of the wavelet

$$\phi_{t,k}(\mathbf{x}) = 2^{\frac{k}{2}} \phi\left(\frac{t - j2^k}{2^k}\right)$$

With many different options for the mother wavelet  $\phi$ 



Scaling and dilation is akin to a sort of frequency: high scale mean stretched wavelet with slowly changing coarse feature and low frequency, while low scale compressed wavelet with rapidly changing details and high frequency.

**DWT** Discrete Wavelet Transform: uses a finite set of scales and shifts rather than "any possible value" as in the continuous wavelet transform.

## 0.3 Generative and Graphical Models

Generative referring to the probability we learn: if we know the distribution probability of data we can generate new data

Graphical referring to graphical formalisms that describe in a syntetic way the structures we'll see.

Generative Learning ML models that represent knowledge inferred from data under the form of probabilities:

Probabilities can be sample: new data can be generated

Supervised, unsupervised, weakly supervised tasks

More easily incorporate prior knowledge on data and tasks

Interpretable knowledge (how data is generated)

The majority of modern tasks comprises large number of variables

Modeling the joint distribution of all variables can become impractical

Exponential size of the parameter space

Computationally impractical to train and predict

**Representation** Graphical models are a compact way to represent exponentially large probability distributions. Encode conditional independence assumptions, and different classes of graph structures imply different assumptions/capabilities.

**Inference** How to query (predict with) a graphical model? Probability of unknown X given observations d, P(X|d), the **most likely hypothesis** (parameters) X.

**Learning** Find the right model parameters.

**Representation** A graph whose nodes are random variables and edges represent probabilistic relationships between the variables.

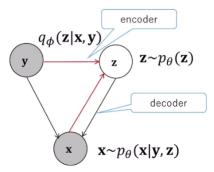
Different classes of graphs:

Directed edges express causal relationships

Undirected edges express soft constraints, values cannot change independently

**Dynamic models**, graphs subject to structure changes to reflect dynamic processes. For example RNNs: recurrent neural networks are unfolded using weight sharing, producing a dynamic model.

In Deep Learning Bayesian learning necessary to understand Variational Deep Learning.



Generate new knowledge Complex data can be generated if the model is powerful enough to capture its distribution.

## 0.3.1 Probability Refresher

todo

#### Inference

Bayesian: consider all hypothesis weighted by their probabilities

$$P(X \mid d) = \sum_{i} P(X \mid h_i) P(h_i \mid d)$$

MAP (Maximum a-Posteriori): infer X from  $P(X | h_{MAP})$  where  $h_{MAP}$  is the maximum a-posteriori hypothesys given d

$$h_{MAP} = \arg\max_{h \in H} P(h \mid d) = \arg\max_{h \in H} P(d \mid h)P(h)$$

ML assuming uniform prioris  $P(h_i) = P(h_j)$  yields the maximum likelihood (ML) estimate  $P(X \mid h_{ML})$ 

$$h_{ML} = \arg\max_{h \in H} P(d \mid h)$$

Any probability can be obtained from the Joint Probability Distribution  $P(X_1, ..., X_n)$  by marginalization but at an exponential cost (e.g.  $2^{n-1}$  for a marginal distribution from binary RV)

## 0.3.2 Graphical Models

Compact graphical representation for exponentially large joint distributions: simplifies marginalization and inference algorithms, allowing to **incorporate prior knowledge** concerning causal relationships and associations between random variables.

Directed graphical models (Bayesian Networks)

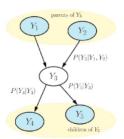
Undirected graphical models (Markov Random Fields)

#### Bayesian Networks

Directed Acyclic Graphs (DAG) G = (V, E)

Nodes  $v \in V$  represent random variables Shaded  $\Rightarrow$  observed, empty (like  $Y_3$ )  $\Rightarrow$  unobserved

Edges  $e \in E$  describe the conditional independence relationships

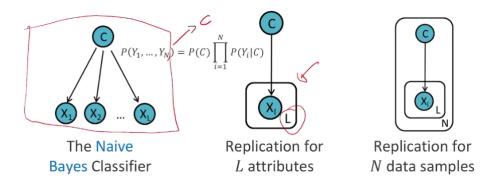


Conditional Probability Tables CPTs are local to each node and describe the probability distribution given its parents.

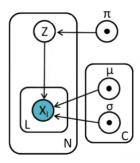
$$P(Y_1, \dots, Y_n) = \prod_{i=1}^{N} P(Y_i \mid \text{Parents}(Y_i))$$

**Plate notation** If the same causal relationship is replicated for a number of variables, we can compactly represent it with plate notation.

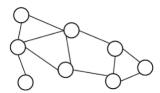
$$P(Y_1, ..., Y_N, C) = P(C) \prod_{i=1}^{N} P(Y_i \mid C)$$



**Full-Plate Notation** Boxes denote replication for a number of times (denoted by the letter in the corner). Shaded nodes are observed variables, empty nodes are unobserved latent variables. Black dots (optional) identify model parameters.



#### Markov Random Fields



Undirected graph G = (V, E) (a.k.a. Markov Networks). Also with shaded/empty nodes to denote observed/unobserved variables.

Edges  $e \in E$  represent bidirectional dependencies between variables (constraints).

Often arranged in a structure that is coherent with the data/constraint we want to model.

Often used in image processing to impose spatial constraints (e.g. smoothness)

### 0.3.3 Conditional Independence and Causality

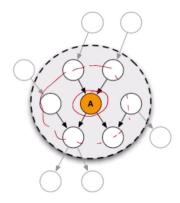
Can we reason on the structure of the graph to infer direct/indirect relationships between random variables?

**Local Markov Property** Each node (random variable) is conditionally independent of all its non-descendants given a joint state of its parents.

$$Y_v \perp Y_{V \setminus \text{Children(v)}} \text{ given } Y_{\text{Parent(v)}} \ \forall \ v \in V$$

There are substructures in the Bayesian networks with which we can build everything.

**Markov Blanket** A Markov blanket Mb(A) of a node A is the minimal set of vertices that isolates/shields the node from the rest of the Bayesian network. If I know the variables in Mb(A) then I know everything I need to know about A



Taking only the parents it's not sufficient, we need also the children and the co-parents (nodes that are parents of one of my children). So it contains parents, children and children's parents.

$$P(A \mid Mb(A), Z) = P(A \mid Mb(A)) \ \forall \ Z \notin Mb(A)$$

**Joint Probability Factorization** An application of the chain rule and local Markov property.

- 1. Pick a topological ordering of the nodes
- 2. Apply chain rule following the order

Sampling of a Bayesian Network A BN describes a generative process for observations.

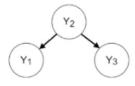
- 1. Pick a topological ordering of the nodes
- 2. Generate data by sampling from the local condition probabilities following this order

Generate ith sample for each variable, example  $s_i \simeq P(S)$ ,  $h_i \simeq P(H \mid S = s_i)$ 

#### 0.3.4Fundamental Bayesian Network Structures

Three fundamental substructures that determine the conditional independence relationships in a Bayesian network.

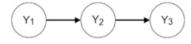
Tail to Tail Common cause



$$P(Y_1, Y_3 \mid Y_2) = P(Y_1 \mid Y_2)P(Y_3 \mid Y_2)$$

If  $Y_2$  is unobserved, then  $Y_1, Y_3$  are marginally dependent  $Y_1 \not\perp Y_3$ If  $Y_2$  is observed,  $Y_1, Y_3$  become conditionally independent  $Y_1 \perp Y_3 \mid Y_2$  (the path between  $Y_1, Y_3$  is blocked by the observed (shaded)  $Y_2$ )

## Head to Tail Causal Effect

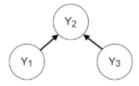


$$P(Y_1, Y_3 \mid Y_2) = P(Y_1)P(Y_2 \mid Y_1)P(Y_3 \mid Y_2) = P(Y_1 \mid Y_2)P(Y_3 \mid Y_2)$$

Same behavior as before!

If  $Y_2$  is unobserved, then  $Y_1, Y_3$  are marginally dependent  $Y_1 \not\perp Y_3$ If  $Y_2$  is observed,  $Y_1, Y_3$  become conditionally independent  $Y_1 \perp Y_3 \mid Y_2$  ( $Y_2$  again blocks the path)

### Heat to Head Common effect

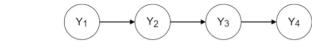


$$P(Y_1, Y_2, Y_3) = P(Y_1)P(Y_3)P(Y_2 \mid Y_1, Y_3)$$

If  $Y_2$  is unobserved, then  $Y_1, Y_3$  are marginally independent  $Y_1 \perp Y_3$  If  $Y_2$  is observed, then  $Y_1, Y_3$  are conditionally dependent  $Y_1 \not\perp Y_3 \mid Y_2$  If any  $Y_2$  descendants is observed it unlocks the path.

**Derived Conditional Independence Relationships** A Bayesian network represent the local relationship encoded by the 3 basic structures plus the derived relationships.

Given the same distribution I can have two different Bayesian Networks, which implies the same factorization.



Local Markov Relationships

$$Y_1 \perp Y_3 | Y_2$$
  
 $Y_4 \perp Y_1, Y_2 | Y_3$ 

Derived Relationship

$$Y_1 \perp Y_4 | Y_2$$

**d-separation** Let  $r = Y_1 \leftrightarrow \ldots \leftrightarrow Y_2$  be un undirected path between  $Y_1, Y_2, r$  is d-separated by Z if there exist at least one node  $Y_c \in Z$  for which path r is blocked. With Z being the set of variable for which we're assessing this separation.

So it holds if at least one of the following holds:

- r contains an head-to-tail structure  $Y_i \to Y_c \to Y_j$  and  $Y_c \in Z$
- r contains a tail-to-tail  $Y_i \leftarrow Y_c \rightarrow Y_j$  and  $Y_c \in Z$
- r contains head-to-head  $Y_i \leftarrow Y_c \leftrightarrow Y_j$  and neither  $Y_c$  nor its descendants are in Z

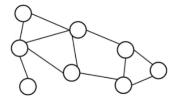
Two nodes  $Y_i, Y_j$  in a BN G are d-separated by  $Z \subset V$  if and only if all undirected paths between  $Y_i, Y_j$  are d-separated by Z (denoted by  $Dsep_F(Y_i, Y_j \mid Z)$ 

**Markov Blanket** The Markov Blanket Mb(Y) is the minimal set of nodes which d-separates a node Y from all other nodes (i.e. makes Y conditionally independent

**Are Directed Models Enough?** Bayesian Networks are used to model asymmetric dependencies. But the answer is no, Directed Models cannot express all conditional dependence relationships: expressing some precludes the expressions of others.

What if we want to model symmetric dependencies: bidirectional effects, spatial dependencies... need undirected approaches. Directed models cannot represent some bidirectional dependencies in the distributions.

### 0.3.5 Markov Random Fields



What is the undirected equivalent of d-separation in directed models? It's based on node separation: the two nodes in the middle separate the two parts.

Node subsets  $A, B \subset V$  are conditionally independent given  $C \subset V \setminus \{A, B\}$  if all paths

**Joint Probability Factorization** What is the undirected equivalent? We seek a product of functions defined over a set of nodes associated with some local properties of the graph. Markov blanket tells that nodes that are not neighbors are conditionally independent given the remainer of the nodes.

Clique Subset of nodes that contain an edge between all pair of nodes. Maximal if you cannot add more nodes.

**Maximal Clique Factorization** Define  $X = X_1, \dots, X_n$  as the random variables associated to the N nodes of the undirected graph G

$$P(X) = \frac{1}{Z} \prod_{C} \psi(X_C)$$

 $X_C$  are the random variables in the maximal clique C,  $\psi(X_C)$  is the potential function over the maximal clique C and Z is the partition function ensuring normalization.

$$Z =$$

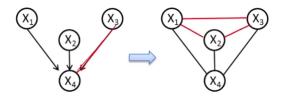
Potential functions are not probabilities, they express which configuration of the local variables are preferred. For example  $\psi(X_1, X_2) = 1$  if  $X_1 = X_2$ , 4 if  $x_2 = 2X_1$  and 0 otherwise You can hand-engineer feature functions. If we restrict to strictly positive potential function the Hammersley-Clifford theorem provides guarantees on the distribution that can be represented by the clique factorization.

#### Boltzmann Distribution A conven

#### From Directed to Undirected

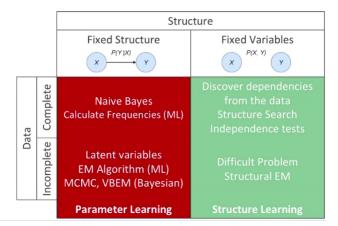
Straightforward when is linear.

Requires some work with v-structures, e.g. moralization (a.k.a. marrying of the parents).



### 0.3.6 Learning Causation from Data

#### Learning with Bayesian Network



**Structure Learning Problem** Observations are given for a set of fixed random variables, and network structure is not specified:

Determine which arcs exist in the network (causal relationships)

Compute Bayesian network parameters (conditional probability tables)

Determining causal relationships between variables entails deciding on arc presence and directing edges.

## Structure Finding Approaches

**Search and Score**: model selection approach, a search in the space of the graphs **Scoring function**: two fundamental properties:

Consistency: same score for graphs in the same equivalence class

Decomposability: can be locally computed

### Two approaches:

Information theoretic: based on data likelihood plus some model-complexity penalization terms Bayesian: score the structures using a graph posterior (likelihood plus proper prior choice

### Search strategy:

Finding maximal scoring structures is NP complete

Constrain search strategy: starting from a candidate structure we modify iteratively by local operations (edge/node addition/deletion). Each operation has a cost, so a cost optimization problem.

#### Constrain search space can be

Known node order: can reduce the search space to the parents of each node (Markov Blankets)

Search in the space of structure equivalence classes

Search in the space of node ordering

Constraint Based: use tests of conditional independence, constraining the network

Hybrid: model selection of constrained structures