# Graphical Models 

## Zoubin Ghahramani

Department of Engineering University of Cambridge, UK

zoubin@eng.cam.ac.uk<br>http://learning.eng.cam.ac.uk/zoubin/

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## Representing knowledge through graphical models



- Nodes correspond to random variables
- Edges represent statistical dependencies between the variables


## Why do we need graphical models?

- Graphs are an intuitive way of representing and visualising the relationships between many variables. (Examples: family trees, electric circuit diagrams, neural networks)
- A graph allows us to abstract out the conditional independence relationships between the variables from the details of their parametric forms. Thus we can answer questions like: "Is $A$ dependent on $B$ given that we know the value of $C$ ?" just by looking at the graph.
- Graphical models allow us to define general message-passing algorithms that implement probabilistic inference efficiently. Thus we can answer queries like "What is $p(A \mid C=c)$ ?" without enumerating all settings of all variables in the model.

Graphical models $=$ statistics $\times$ graph theory $\times$ computer science.

## Directed Acyclic Graphical Models (Bayesian Networks)



A DAG Model / Bayesian network ${ }^{1]}$ corresponds to a factorization of the joint probability distribution:

$$
p(A, B, C, D, E)=p(A) p(B) p(C \mid A, B) p(D \mid B, C) p(E \mid C, D)
$$

In general:

$$
p\left(X_{1}, \ldots, X_{n}\right)=\prod_{i=1}^{n} p\left(X_{i} \mid X_{\mathrm{pa}(i)}\right)
$$

where $\mathrm{pa}(i)$ are the parents of node $i$.

[^0]
## Directed Acyclic Graphical Models (Bayesian Networks)

Semantics: $X \Perp Y \mid \mathcal{V}$ if $\mathcal{V}$ d-separates $X$ from $Y$
 Definition: $\mathcal{V}$ d-separates $X$ from $Y$ if every undirected path ${ }^{2}$ between $X$ and $Y$ is blocked by $\mathcal{V}$. A path is blocked by $\mathcal{V}$ if there is a node $W$ on the path such that either:

1. $W$ has converging arrows along the path $(\rightarrow W \leftarrow)^{3}$ and neither $W$ nor its descendants are observed (in $\mathcal{V}$ ), or
2. $W$ does not have converging arrows along the path ( $\rightarrow W \rightarrow$ or $\leftarrow W \rightarrow$ ) and $W$ is observed $(W \in \mathcal{V})$.

Corollary: Markov Boundary for $X: \quad\{$ parents $(X) \cup$ children $(X) \cup$ parents-of-children $(X)$ \}.

[^1]
## Directed Graphs for Statistical Models: Plate Notation

Consider the following simple model. A data set of $N$ points is generated i.i.d. from a Gaussian with mean $\mu$ and standard deviation $\sigma$ :

$$
p\left(x_{1}, \ldots, x_{N}, \mu, \sigma\right)=p(\mu) p(\sigma) \prod_{n=1}^{N} p\left(x_{n} \mid \mu, \sigma\right)
$$

This can be represented graphically as follows:


## Inference in a graphical model

Consider the following graph:


$$
p(A, B, C, D, E)=p(A) p(B) p(C \mid A, B) p(D \mid B, C) p(E \mid C, D)
$$

Inference: evaluate the probability distribution over some set of variables, given the values of another set of variables.

For example, how can we compute $p(A \mid C=c)$ ? Assume each variable is binary.
Naive method:

$$
\begin{align*}
p(A, C=c) & =\sum_{B, D, E} p(A, B, C=c, D, E)  \tag{16terms}\\
p(C=c) & =\sum_{A} p(A, C=c) \quad[2 \text { terms }] \\
p(A \mid C=c) & =\frac{p(A, C=c)}{p(C=c)} \quad[2 \text { terms }]
\end{align*}
$$

Total: $16+2+2=20$ terms have to be computed and summed

## Inference in a graphical model

Consider the following graph:
 which represents:

$$
p(A, B, C, D, E)=p(A) p(B) p(C \mid A, B) p(D \mid B, C) p(E \mid C, D)
$$

Computing $p(A \mid C=c)$.
More efficient method:

$$
\begin{aligned}
p(A, C=c) & =\sum_{B, D, E} p(A) p(B) p(C=c \mid A, B) p(D \mid B, C=c) p(E \mid C=c, D) \\
& =\sum_{B} p(A) p(B) p(C=c \mid A, B) \sum_{D} p(D \mid B, C=c) \sum_{E} p(E \mid C=c, D) \\
& =\sum_{B} p(A) p(B) p(C=c \mid A, B) \quad \quad[4 \text { terms }]
\end{aligned}
$$

Total: $4+2+2=8$ terms
Belief propagation methods use the conditional independence relationships in a graph to do efficient inference (for singly connected graphs, exponential gains in efficiency!).

## Factor graph propagation

Algorithmically and implementationally, it's often easier to convert directed and undirected graphs into factor graphs, and run factor graph propagation.

$$
\begin{aligned}
p(\mathbf{x}) & =p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{2}\right) p\left(x_{4} \mid x_{2}\right) \\
& \equiv f_{1}\left(x_{1}, x_{2}\right) f_{2}\left(x_{2}, x_{3}\right) f_{3}\left(x_{2}, x_{4}\right)
\end{aligned}
$$

Singly connected


Multiply connected factor graphs:


## Factor Graphs

In a factor graph, the joint probability distribution is written as a product of factors. Consider a vector of variables $\mathbf{x}=\left(x_{1}, \ldots, x_{n}\right)$

$$
p(\mathbf{x})=p\left(x_{1}, \ldots, x_{n}\right)=\frac{1}{Z} \prod_{j} f_{j}\left(\mathbf{x}_{S_{j}}\right)
$$

where $Z$ is the normalisation constant, $S_{j}$ denotes the subset of $\{1, \ldots, n\}$ which participate in factor $f_{j}$ and $\mathbf{x}_{S_{j}}=\left\{x_{i}: i \in S_{j}\right\}$.

variables nodes: we draw open circles for each variable $x_{i}$ in the distribution. factor nodes: we draw filled dots for each factor $f_{j}$ in the distribution.

## Propagation in Factor Graphs

Let $\mathrm{n}(x)$ denote the set of factor nodes that are neighbors of $x$.
Let $\mathrm{n}(f)$ denote the set of variable nodes that are neighbors of $f$.

We can compute probabilities in a factor graph by propagating messages from variable nodes to factor nodes and viceversa.
message from variable $x$ to factor $f$ :

$$
\mu_{x \rightarrow f}(x)=\prod_{h \in \mathrm{n}(x) \backslash\{f\}} \mu_{h \rightarrow x}(x)
$$

message from factor $f$ to variable $x$ :

$$
\mu_{f \rightarrow x}(x)=\sum_{\mathbf{x} \backslash x}\left(f(\mathbf{x}) \prod_{y \in \mathrm{n}(f) \backslash\{x\}} \mu_{y \rightarrow f}(y)\right)
$$

where $\mathbf{x}$ are the variables that factor $f$ depends on, and $\sum_{\mathbf{x} \backslash x}$ is a sum over all variables neighboring factor $f$ except $x$.

## Propagation in Factor Graphs

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message from variable $x$ to factor $f$ :

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$$

message from factor $f$ to variable $x$ :

$$
\mu_{f \rightarrow x}(x)=\sum_{\mathbf{x} \backslash x}\left(f(\mathbf{x}) \prod_{y \in \mathrm{n}(f) \backslash\{x\}} \mu_{y \rightarrow f}(y)\right)
$$

If a variable has only one factor as a neighbor, it can initiate message propagation.

Once a variable has received all messages from its neighboring factor nodes, one can compute the probability of that variable by multiplying all the messages and renormalising:

$$
p(x) \propto \prod_{h \in \mathrm{n}(x)} \mu_{h \rightarrow x}(x)
$$

## Inference in Hidden markov models and Linear Gaussian state-space models



- In HMMs, the states $X_{t}$ are discrete.
- In linear Gaussian SSMs, the states are real Gaussian vectors.
- Both HMMs and SSMs can be represented as singly connected DAGs.
- The forward-backward algorithm in hidden Markov models (HMMs), and the Kalman smoothing algorithm in SSMs are both instances of belief propagation / factor graph propagation.


## Software for Graphical Models

- BUGS and WinBUGS: inference via Gibbs sampling, not very scalable
- HUGIN: widely used, commercial, focus on exact inference
- Kevin Murphy's Bayes Net Toolbox: Matlab, widely used
- Microsoft's Infer.NET: advanced scalable libraries implementing factor graph propagation, EP, and variational message passing.
- Jeff Bilmes' GMTK: very good at HMMs and related time series models
- many others, see http://people.cs.ubc.ca/~murphyk/Software/bnsoft.html


## Summary

- inference consists of the problem of computing $p$ (variables of interest|observed variables)
- for singly connected graphs, belief propagation / factor graph propagation solves this problem exactly.
- well-known algorithms such as Kalman smoothing and forward-backward are special cases these general propagation algorithms.
- for multiply connected graphs, the junction tree algorithm solves the exact inference problem, but can be very slow (exponential in the cardinality of the largest clique).
- one approximate inference algorithm is "loopy belief propagation"-run propagation as if graph is simply connected; often works well in practice.


## Learning parameters



$$
p\left(x_{1}\right) p\left(x_{2} \mid x_{1}\right) p\left(x_{3} \mid x_{1}\right) p\left(x_{4} \mid x_{2}\right)
$$



Assume each variable $x_{i}$ is discrete and can take on $K_{i}$ values.

The parameters of this model can be represented as 4 tables: $\theta_{1}$ has $K_{1}$ entries, $\theta_{2}$ has $K_{1} \times K_{2}$ entries, etc.

These are called conditional probability tables (CPTs) with the following semantics:

$$
p\left(x_{1}=k\right)=\theta_{1, k} \quad p\left(x_{2}=k^{\prime} \mid x_{1}=k\right)=\theta_{2, k, k^{\prime}}
$$

If node $i$ has $M$ parents, $\theta_{i}$ can be represented either as an $M+1$ dimensional table, or as a 2-dimensional table with $\left(\prod_{j \in \mathrm{pa}(i)} K_{j}\right) \times K_{i}$ entries by collapsing all the states of the parents of node $i$. Note that $\sum_{k^{\prime}} \theta_{i, k, k^{\prime}}=1$.

Assume a data set $\mathcal{D}=\left\{\mathbf{x}^{(n)}\right\}_{n=1}^{N}$.

## Learning parameters

Assume a data set $\mathcal{D}=\left\{\mathbf{x}^{(n)}\right\}_{n=1}^{N}$. How do we learn $\boldsymbol{\theta}$ from $\mathcal{D}$ ?


$$
p(\mathbf{x} \mid \boldsymbol{\theta})=p\left(x_{1} \mid \theta_{1}\right) p\left(x_{2} \mid x_{1}, \theta_{2}\right) p\left(x_{3} \mid x_{1}, \theta_{3}\right) p\left(x_{4} \mid x_{2}, \theta_{4}\right)
$$

Likelihood:

$$
p(\mathcal{D} \mid \boldsymbol{\theta})=\prod_{n=1}^{N} p\left(\mathbf{x}^{(n)} \mid \boldsymbol{\theta}\right)
$$

Log Likelihood:

$$
\log p(\mathcal{D} \mid \boldsymbol{\theta})=\sum_{n=1}^{N} \sum_{i} \log p\left(x_{i}^{(n)} \mid x_{\mathrm{pa}(i)}^{(n)}, \theta_{i}\right)
$$

This decomposes into sum of functions of $\theta_{i}$. Each $\theta_{i}$ can be optimized separately:

$$
\hat{\theta}_{i, k, k^{\prime}}=\frac{n_{i, k, k^{\prime}}}{\sum_{k^{\prime \prime}} n_{i, k, k^{\prime \prime}}}
$$

where $n_{i, k, k^{\prime}}$ is the number of times in $\mathcal{D}$ where $x_{i}=k^{\prime}$ and $x_{\mathrm{pa}(i)}=k$, where $k$ represents a joint configuration of all the parents of $i$ (i.e. takes on one of $\prod_{j \in \operatorname{pa}(i)} K_{j}$ values)

ML solution: Simply calculate frequencies!


## Maximum Likelihood Learning with Hidden Variables: The EM Algorithm

Goal: maximise parameter log likelihood given observables.

$$
\mathcal{L}(\theta)=\log p(Y \mid \theta)=\log \sum_{X} p(Y, X \mid \theta)
$$

The Expectation Maximization (EM) algorithm (intuition):


Iterate between applying the following two steps:

- The E step: fill-in the hidden/missing variables
- The M step: apply complete data learning to filled-in data.


## Bayesian Learning

Apply the basic rules of probability to learning from data.

Data set: $\mathcal{D}=\left\{x_{1}, \ldots, x_{n}\right\} \quad$ Models: $m, m^{\prime}$ etc. $\quad$ Model parameters: $\theta$

Prior probability of models: $P(m), P\left(m^{\prime}\right)$ etc.
Prior probabilities of model parameters: $P(\theta \mid m)$
Model of data given parameters (likelihood model): $P(x \mid \theta, m)$

If the data are independently and identically distributed then:

$$
P(\mathcal{D} \mid \theta, m)=\prod_{i=1}^{n} P\left(x_{i} \mid \theta, m\right)
$$

Posterior probability of model parameters:

$$
P(\theta \mid \mathcal{D}, m)=\frac{P(\mathcal{D} \mid \theta, m) P(\theta \mid m)}{P(\mathcal{D} \mid m)}
$$

Posterior probability of models:

$$
P(m \mid \mathcal{D})=\frac{P(m) P(\mathcal{D} \mid m)}{P(\mathcal{D})}
$$

## Summary of parameter learning

|  | Complete (fully observed) data | Incomplete (hidden /missing) data |
| :--- | :--- | :--- |
| ML | calculate frequencies | EM |
| Bayesian | update Dirichlet distributions | MCMC / Viterbi / VB |

- For complete data Bayesian learning is not more costly than ML
- For incomplete data $V B \approx E M$ time complexity
- Other parameter priors are possible but Dirichlet is pretty flexible and intuitive.
- For non-discrete data, similar ideas but generally harder inference and learning.


## Structure learning in graphical models

Given a data set of observations of $(A, B, C, D, E)$ can we learn the structure of the graphical model?


Let $G$ denote the graph structure $=$ the set of edges.

## Structure learning



Constraint-Based Learning: Use statistical tests of marginal and conditional independence. Find the set of DAGs whose d-separation relations match the results of conditional independence tests.

Score-Based Learning: Use a global score such as the BIC score or Bayesian marginal likelihood. Find the structures that maximize this score.

## Bayesian Methods

## Everything follows from two simple rules:

Sum rule: $P(x)=\sum_{y} P(x, y)$
Product rule: $P(x, y)=P(x) P(y \mid x)$

$$
P(\theta \mid \mathcal{D})=\frac{P(\mathcal{D} \mid \theta) P(\theta)}{P(\mathcal{D})}
$$

$P(\mathcal{D} \mid \theta) \quad$ likelihood of $\theta$
$P(\theta) \quad$ prior probability of $\theta$
$P(\theta \mid \mathcal{D}) \quad$ posterior of $\theta$ given $\mathcal{D}$

## Prediction:

$$
P(x \mid \mathcal{D}, m)=\int P(x \mid \theta, \mathcal{D}, m) P(\theta \mid \mathcal{D}, m) d \theta
$$

Model Comparison:

$$
\begin{aligned}
P(m \mid \mathcal{D}) & =\frac{P(\mathcal{D} \mid m) P(m)}{P(\mathcal{D})} \\
P(\mathcal{D} \mid m) & =\int P(\mathcal{D} \mid \theta, m) P(\theta \mid m) d \theta
\end{aligned}
$$

## Score-based structure learning for complete data

Consider a graphical model with structure $m$, discrete observed data $\mathcal{D}$, and parameters $\theta$. Assume Dirichlet priors.

The Bayesian marginal likelihood score is easy to compute:

$$
\operatorname{score}(m)=\log p(\mathcal{D} \mid m)=\log \int p(\mathcal{D} \mid \theta, m) p(\theta \mid m) d \theta
$$

$\operatorname{score}(m)=\sum_{i} \sum_{j}\left[\log \Gamma\left(\sum_{k} \alpha_{i j k}\right)-\sum_{k} \log \Gamma\left(\alpha_{i j k}\right)-\log \Gamma\left(\sum_{k} \tilde{\alpha}_{i j k}\right)+\sum_{k} \log \Gamma\left(\tilde{\alpha}_{i j k}\right)\right]$
where $\tilde{\alpha}_{i j k}=\alpha_{i j k}+n_{i j k}$. Note that the score decomposes over $i$.
One can incorporate structure prior information $p(m)$ as well:

$$
\operatorname{score}(m)=\log p(\mathcal{D} \mid m)+\log p(m)
$$

Greedy search algorithm: Start with $m$. Consider modifications $m \rightarrow m^{\prime}$ (edge deletions, additions, reversals). Accept $m^{\prime}$ if $\operatorname{score}\left(m^{\prime}\right)>\operatorname{score}(m)$. Repeat.

Bayesian inference of model structure: Run MCMC on $m$.

## Bayesian Structural EM for incomplete data

Consider a graphical model with structure $m$, observed data $\mathcal{D}$, hidden variables $\mathcal{X}$ and parameters $\theta$

The Bayesian score is generally intractable to compute:

$$
\operatorname{score}(m)=p(\mathcal{D} \mid m)=\int \sum_{\mathcal{X}} p(\mathcal{X}, \theta, \mathcal{D} \mid m) d \theta
$$

Bayesian Structure EM (Friedman, 1998):

1. compute MAP parameters $\hat{\theta}$ for current model $m$ using EM
2. find hidden variable distribution $p(\mathcal{X} \mid \mathcal{D}, \hat{\theta})$
3. for a small set of candidate structures compute or approximate

$$
\operatorname{score}\left(m^{\prime}\right)=\sum_{\mathcal{X}} p(\mathcal{X} \mid \mathcal{D}, \hat{\theta}) \log p\left(\mathcal{D}, \mathcal{X} \mid m^{\prime}\right)
$$

4. $m \leftarrow m^{\prime}$ with highest score

## Variational Bayesian Learning of Graph Structures

## A case study for discrete directed graphs

- Bipartite structure: only hidden variables can be parents of observed variables.
- Two binary hidden variables, and four five-valued discrete observed variables.

- Conjugate prior is Dirichlet, Conjugate-Exponential model, so VB-EM algorithm is a straightforward modification of EM.
- Experiment: There are 136 distinct structures (out of 256) with 2 latent variables as potential parents of 4 conditionally independent observed vars.
- Score each structure for twenty varying size data sets:

$$
n \in\{10,20,40,80,110,160,230,320,400,430,480,560,640,800,960,1120,1280,2560,5120,10240\}
$$

using 3 methods: BIC, VB, and a gold standard Annealed Importance Sampling AIS

- 2720 graph scores computed, times for each: BIC (1.5s), VB (4s), AIS (400s).


## Results, averaged over about 100 parameter draws




VB is also more accurate than Cheeseman-Stutz (CS) approximation to the marginal likelihood. In fact we can prove than $\mathrm{VB} \geq \mathrm{CS}$ (Beal and Ghahramani, Bayesian Analysis, 2006).

## How tight is VB bound?



About $10^{4}$ sweeps of sampling needed to achieve VB lower bound.

## How many latent variables should there be?



Y - latent factors (e.g. diseases)
Z - graph structure (binary adjacency matrix)
$\mathbf{X}$ - observed binary features (e.g. symptoms)
Solution 1: Do model comparison for $m=1, m=2, \ldots$
Solution 2: Assume potentially $m=\infty$ of which we only observe a finite number.

Note: this is analogous to the question of how many mixture components to use (model selection for finite mixture model vs infinite mixture model using Dirichlet processs mixtures).

## Graphical models with infinitely many latent variables

"A Non-Parametric Bayesian Method for Inferring Hidden Causes" (Frank Wood, Tom Griffiths, \& Ghahramani, Uncertainty in Artificial Intelligence, 2006)


Y - binary latent factors (diseases)
Z - graph structure
X - observed binary features (symptoms)
"Noisy-or" observations: $P\left(x_{i t}=1 \mid \mathbf{Z}, \mathbf{Y}, \lambda, \epsilon\right)=1-(1-\lambda)^{\sum_{k} z_{i k} y_{k t}}(1-\epsilon)$

## What should we use as $P(\mathbf{Z})$ ?

The matrix $\mathbf{Z}$ is a binary matrix of size ( $N=$ number of observed variables) $\times(K$ $=$ number of latent variables).

But $K \rightarrow \infty$.

We can define a consistent distribution over such infinite sparse binary matrices using the "Indian Buffet Process"
(IBP) (cf Chinese restaurant process, Aldous 1985; Pitman sparse binary matrices using the "Indian Buffet Process"
(IBP) (cf Chinese restaurant process, Aldous 1985; Pitman 2002).

A sample from prior shown on right.
Note "rich get richer" property.
We can derive a Gibbs sampler for this model.
Prior sample from IBP with $\alpha=10$


## Graphical models with infinitely many latent variables



Figure 5: Trace plots and histograms for the Gibbs sampler applied to the signs exhibited by 50 stroke patients. The left column shows the current value of $\epsilon, \lambda, p, \alpha$, and $K_{+}$as the sampler progressed, where $K_{+}$ is obtained by examining the current $\mathbf{Z}$ sample. The right column shows histograms of the same variables computed over the samples.

Comparison to RJMCMC


Figure 3: Learning the number of hidden causes using both RJMCMC and Gibbs sampling. Each line show the mean and standard deviation of the expected value of the dimensionality of the model ( $K$ for RJMCMC, and $K_{+}$for Gibbs) taken over 500 iterations of sampling for each of 10 datasets.

Seems to work reliably, and mixed better than RJMCMC.

## Graphical models with infinitely many latent variables

(with Frank Wood and Tom Griffiths)
Inferring stroke localization from patient symptoms:


Figure 6: Causal structure with highest posterior probability. Two grouping of signs are highlighted. In solid black, we find a grouping of poor optokinetic nystagmus, lack of facial control, weakness, decreased rapid alternating movements, abnormal deep tendon reflexes, Babinski sign, and double simultaneous stimulation neglect, all on the left side, consistent with a right frontal/parietal infarct. In dashed black, we find a grouping of comprehension deficit, non-fluency, repetition, anomia, visual field deficit, facial weakness, and general weakness, with the latter three on the right side, generally consistent with a left temporal infarct.
(50 stroke patients, 56 symptoms/signs)

## Directed Graphical Models and Causality

Causal relationships are a fundamental component of cognition and scientific discovery.

Even though the independence relations are identical, there is a causal difference between

- "smoking" $\rightarrow$ "yellow teeth"
- "yellow teeth" $\rightarrow$ "smoking"

Key idea: interventions and the do-calculus:

$$
\begin{aligned}
& p(S \mid Y=y) \neq p(S \mid \operatorname{do}(Y=y)) \\
& p(Y \mid S=s)=p(Y \mid \operatorname{do}(S=s))
\end{aligned}
$$

Causal relationships are robust to interventions on the parents.
The key difficulty in learning causal relationships from observational data is the presence of hidden common causes:

$$
(A) \rightarrow(B)(A)-(B)
$$

## Learning parameters and structure in undirected graphs


$p(\mathbf{x} \mid \boldsymbol{\theta})=\frac{1}{Z(\boldsymbol{\theta})} \prod_{j} g_{j}\left(\mathbf{x}_{C_{j}} ; \boldsymbol{\theta}_{j}\right)$ where $Z(\boldsymbol{\theta})=\sum_{\mathbf{x}} \prod_{j} g_{j}\left(\mathbf{x}_{C_{j}} ; \boldsymbol{\theta}_{j}\right)$.
Problem: computing $Z(\boldsymbol{\theta})$ is computationally intractable for general (non-tree-structured) undirected models. Therefore, maximum-likelihood learning of parameters is generally intractable, Bayesian scoring of structures is intractable, etc.

## Solutions:

- directly approximate $Z(\boldsymbol{\theta})$ and/or its derivatives (cf. Boltzmann machine learning; contrastive divergence; pseudo-likelihood)
- use approx inference methods (e.g. loopy belief propagation, bounding methods, EP).

See: (Murray and Ghahramani, 2004; Murray et al, 2006) for Bayesian learning in undirected models.

## Scaling Bayesian Methods

Case Studies:

- Microsoft XBox Live TrueSkill
- Microsoft AdPredictor
- Netflix Bayesian PMF

Approaches:


- Approximate inference
- Parallel (MPI) and cloud / distributed (Hadoop, MapReduce) data and inference
- Subsample data


## Summary

- Probabilistic modelling and Bayesian inference are two sides of the same coin
- Bayesian machine learning treats learning as a probabilistic inference problem
- Themes:
- Graphical models: an intuitive and computationally useful representation for probabilistic modelling.

$$
\begin{gathered}
\text { http://learning.eng.cam.ac.uk/zoubin } \\
\text { zoubin@eng.cam.ac.uk }
\end{gathered}
$$

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## Appendix

## Propagation in Factor Graphs


initialise all messages to be constant functions
an example schedule of messages resulting in computing $p\left(x_{4}\right)$ :

| message direction | message value |
| :--- | :--- |
| $x_{1} \rightarrow f_{1}$ | $1\left(x_{1}\right)$ |
| $x_{3} \rightarrow f_{2}$ | $1\left(x_{3}\right)$ |
| $f_{1} \rightarrow x_{2}$ | $\sum_{x_{1}} f_{1}\left(x_{1}, x_{2}\right) 1\left(x_{1}\right)$ |
| $f_{2} \rightarrow x_{2}$ | $\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right) 1\left(x_{3}\right)$ |
| $x_{2} \rightarrow f_{3}$ | $\left(\sum_{x_{1}} f_{1}\left(x_{1}, x_{2}\right)\right)\left(\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right)\right)$ |
| $f_{3} \rightarrow x_{4}$ | $\sum_{x_{2}} f_{3}\left(x_{2}, x_{4}\right)\left(\sum_{x_{1}} f_{1}\left(x_{1}, x_{2}\right)\right)\left(\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right)\right)$ |

where $1(x)$ is a constant uniform function of $x$

## Propagation in Factor Graphs


an example schedule of messages resulting in computing $p\left(x_{4} \mid x_{1}=a\right)$ :

| message direction | message value |
| :--- | :--- |
| $x_{1} \rightarrow f_{1}$ | $\delta\left(x_{1}=a\right)$ |
| $x_{3} \rightarrow f_{2}$ | $1\left(x_{3}\right)$ |
| $f_{1} \rightarrow x_{2}$ | $\sum_{x_{1}} f_{1}\left(x_{1}, x_{2}\right) \delta\left(x_{1}=a\right)=f_{1}\left(x_{1}=a, x_{2}\right)$ |
| $f_{2} \rightarrow x_{2}$ | $\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right) 1\left(x_{3}\right)$ |
| $x_{2} \rightarrow f_{3}$ | $f_{1}\left(x_{1}=a, x_{2}\right)\left(\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right)\right)$ |
| $f_{3} \rightarrow x_{4}$ | $\sum_{x_{2}} f_{3}\left(x_{2}, x_{4}\right) f_{1}\left(x_{1}=a, x_{2}\right)\left(\sum_{x_{3}} f_{2}\left(x_{3}, x_{2}\right)\right)$ |

where $\delta(x=a)$ is a delta function


[^0]:    1 "Bayesian networks" can and often are learned using non-Bayesian (i.e. frequentist) methods; Bayesian networks (i.e. DAGs) do not require parameter or structure learning using Bayesian methods. Also called "belief networks".

[^1]:    ${ }^{2} \mathrm{An}$ undirected path ignores the direction of the edges.
    ${ }^{3}$ Note that converging arrows along the path only refers to what happens on that path. Also called a collider.

