C19 : Lecture 1 : Graphical Models

Frank Wood

University of Oxford

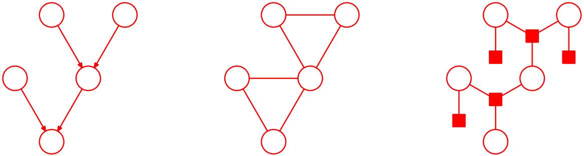
January, 2015

Many figures from PRML [Bishop, 2006]

Graphical Models

- Correspond to a subset of probability models
- Visualisation of structure of probability model
- Useful for model design and development
- Encode properties (some explicitly, others via inspection)
    - Conditional independence (inspection)
- Inference and learning can be formulated in terms of computational operations on the graph

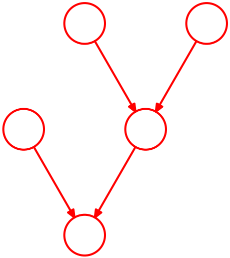
The Graphs of Graphical Models



Graphs consist of

- Vertices
  - Correspond to random variables (and factors)
  - Have types
  - Can represent structured object like vectors, arrays, distributions, infinite sequences, embedded graphical models, etc.
- Edges
  - These will correspond to *d*ependencies
  - Can be directed (arrow) or undirected
  - Usually are associated with conditional density functions or compatibility functions

Directed Graphical Models



Such models are known as

- Generative graphical models
- Bayes nets

Vertices

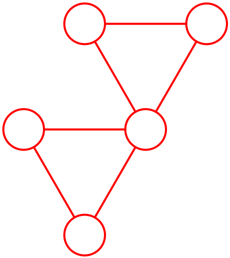
- Variables

Edges

- Conditional probabilities

Good for generative descriptions of data. Conditional probability statements of the form "if A then B with some probability."

Undirected Graphical Models



Such models are known as

- Markov random fields
- Ising models

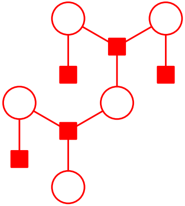
Vertices

- Variables

Edges

- “Compatibility functions”

Good for specifying constraints between variables where generative relationships aren’t obvious (i.e. neighbouring pixel similarity in images)



Generalisation of the undirected and directed graphical models.

Vertices

- Circles : variables
- Squares : "Compatibility functions"

Edges

- Indicate variable is argument of compatibility function

Good for writing down and thinking about message-passing inference algorithms.

Generative Models and Joint Distributions

Consider an arbitrary joint distribution over three variables a, b, and c, $p(a, b, c)$. Recall that

$$p(a, b, c) = p(c|a, b)p(a, b) = p(c|a, b)p(b|a)p(a)$$

Note : This decomposition always holds

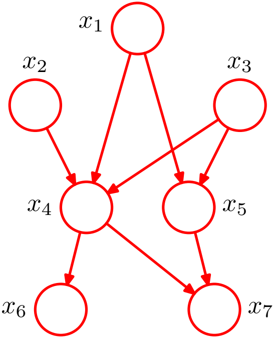
Also

- Corresponds to a generative scheme
  - Generate (sample) a
  - Then generate (sample) b conditioned on a
  - ...
- Dropping conditioning terms restricts the expressivity of the model

Directed Graphical Models

Graphical representation can directly be translated into joint

$$p(\mathbf{x}) = p(x_1)p(x_2)p(x_3)p(x_4|x_1,x_2,x_3)p(x_5|x_1,x_3)p(x_6|x_4)p(x_7|x_4,x_5)$$



More generally

- There is a distribution (term) for each vertex
- The variables which appear in each terms' condition are connected via inbound edges

In math

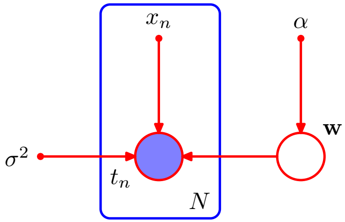
$$p(\mathbf{x}) = \prod_k p(x_k|\mathrm{pa}_k)$$

If each term normalises (i.e. is a proper density or distribution), what value does the following expression take?

$$\int p(\mathbf{x})d\mathbf{x} = \int\int\int\int\int\int\int p(x_1)p(x_2)p(x_3)\ldots p(x_7|x_4,x_5)dx_1\ldots dx_7$$

Note for discrete variables integrals may be interchanged for sums.

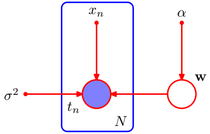
Notational Shorthand for Products and Constants



- Squares indicate multiplied replication
- Filled circles indicate "observed" variables
- Small dots (or no dots) indicate fixed quantities

In math

$$p(\mathbf{t}, \mathbf{x}, \sigma^2, \mathbf{w}, \alpha) = \prod_{n=1}^{N} p(t_n|\mathbf{w}, x_n, \sigma^2)p(\mathbf{w}|\alpha)$$



$$t_n|\mathbf{w}, x_n, \sigma^2 \sim \text{Normal}(\mathbf{w}^T x_n, \sigma^2)$$

$$\mathbf{w}|\alpha \sim \prod_{d=1}^{D} \text{Normal}(0, \alpha) = \text{Normal}(\mathbf{0}, \alpha \mathbf{I})$$

Homework :

- To what well known model does this correspond?
- Is this a supervised or unsupervised model?

Inference = Learning = Prediction = ...

One Goal : Posterior distribution of parameters given data

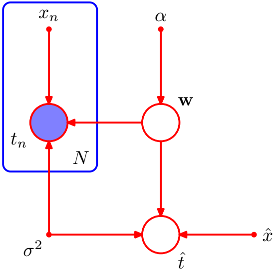
$$p(\mathbf{w}|\mathbf{t}) \propto p(\mathbf{w}) \prod_{n=1}^{N} p(t_n|\mathbf{w})$$

Fixed quantities often are dropped because they always appear on conditioning side of equation(s)

Quiz :

- Why is this a proportionality ($\propto$)? (hint : use Bayes rule)
- Can this be read from the directed graphical model? (hint : be very careful and think about conditional *in*dependence)
- *Important concept!* Why do we want $p(\mathbf{w}|\mathbf{t})$? What are its uses?

Another goal : out of sample predictions



With

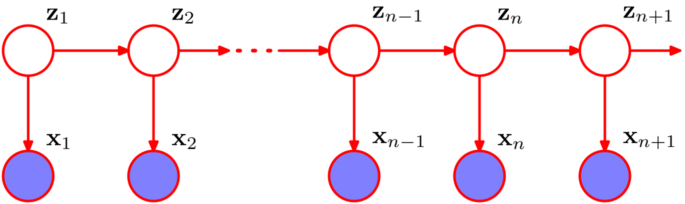
$$\hat{t}|\mathbf{w},\hat{x},\sigma^2 \sim \mathrm{Normal}(\mathbf{w}^T\hat{x},\sigma^2)$$

then

$$\begin{aligned} p(\hat{t}|\mathbf{x},\mathbf{t},\alpha,\sigma^2) &= \int p(\hat{t},\mathbf{w}|\mathbf{x},\hat{x},\mathbf{t},\alpha,\sigma^2)d\mathbf{w} \\ &= \int p(\hat{t}|\mathbf{w},\hat{x})p(\mathbf{w}|\mathbf{t})d\mathbf{w} \end{aligned}$$

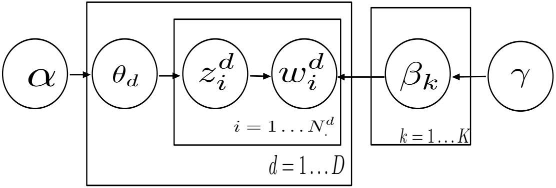
Quiz :

- How do you compute this integral?
- What does it mean to integrate out **w**?



$$
\begin{aligned}
p(\mathbf{z}_n|\mathbf{z}_{n-1}, \mathbf{A}) &= \prod_{k=1}^{K}\prod_{j=1}^{K} A_{jk}^{z_{(n-1)j} z_{nk}} \\
p(\mathbf{z}_1|\boldsymbol{\pi}) &= \prod_{k=1}^{K} \pi_k^{z_{1k}} \\
\mathbf{x}_n | z_{nk} = 1 &\sim \mathrm{F}(\boldsymbol{\theta}_k)
\end{aligned}
$$

Latent Dirichlet Allocation



$$
\begin{aligned}
\theta_d &\sim \mathrm{Dir}_K(\alpha\vec{1}) \\
\beta_k &\sim \mathrm{Dir}_M(\gamma\vec{1}) \\
z_i^d &\sim \mathrm{Discrete}(\theta_d) \\
w_i^d &\sim \mathrm{Discrete}(\beta_{z_i^d})
\end{aligned}
$$

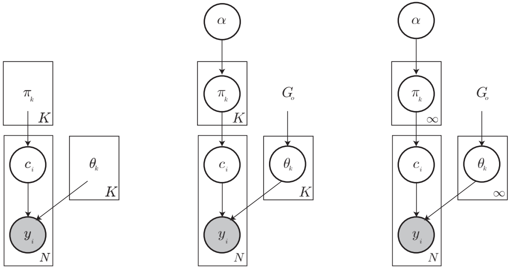
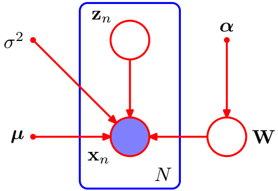


Figure : From left to right: graphical models for a finite Gaussian mixture model (GMM), a Bayesian GMM, and an infinite GMM

$$
\begin{aligned}
c_i|\vec{\pi} &\sim \text{Discrete}(\vec{\pi}) \\
\vec{y}_i|c_i = k; \Theta &\sim \text{Gaussian}(\cdot|\theta_k). \\
\vec{\pi}|\alpha &\sim \text{Dirichlet}(\cdot|\frac{\alpha}{K}, \ldots, \frac{\alpha}{K}) \\
\Theta &\sim \mathcal{G}_0
\end{aligned}
$$

Probabilistic Principal Component Analysis



$$
\begin{aligned}
p(\mathbf{W}|\boldsymbol{\alpha}) &= \prod_{i=1}^{M} \left(\frac{\alpha_i}{2\pi}\right)^{D/2} \exp\left\{-\frac{1}{2}\alpha_i \mathbf{w}_i^T \mathbf{w}\right\} \\
p(\mathbf{z}) &= \mathcal{N}(\mathbf{z}|\mathbf{0}, \mathbf{I}) \\
p(\mathbf{x}_n|\mathbf{z})n) &= \mathcal{N}(\mathbf{x}_n|\mathbf{W}\mathbf{z}_n, \sigma^2\mathbf{I})
\end{aligned}
$$

Study Suggestions

- Distributions, PDFs, Sampling
  - Dirichlet
  - Discrete / Multinomial
  - Multivariate Normal
- Vector Algebra
- Procedures for determining conditional independence(s) given a graphical model

Bibliography I

C M Bishop. *Pattern Recognition and Machine Learning*. Springer, 2006.