Variational Inference Introduction: Bayesian networks

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^{*}Some of the introductory slides are stolen from Manfred Jaeger, Aalborg University.

People involved



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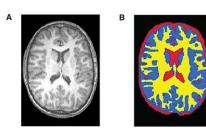
Helge Langseth

Example 1: SLAM



Simultaneous Localization and Mapping: learn a map of the environment and locate current position

Example 2: Image Segmentation



(source: http://pubs.niaaa.nih.gov/publications/arh313/243-246.htm)

Divide image into small number of regions representing structurally similar areas

Example 3: Statistical Semantics

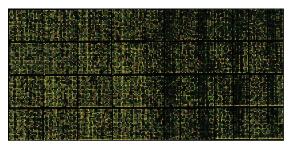
Given a collection of texts:



Goal: automatically learn semantic descriptors for documents and words, that support document clustering, text understanding, information retrieval ...

Example 4: Bioinformatics

Micro-array gene expression data:



Which genes are expressed under which conditions? Which are co-regulated, or functionally dependent?

Statistical Machine Learning

Common ground in 4 examples:

- Use a probabilistic model, typically learned from data (using statistical learning techniques)
- Apply probabilistic inference algorithms to use models for prediction (classification, regression), structure analysis (clustering, segmentation)

Advantages of probabilistic/statistical methods:

- Principled quantification of prediction uncertainties
- Robust and principled techniques to deal with incomplete information, missing data.

Probabilistic Graphical Models

Need: probabilistic models that ...

- can represent models for high-dimensional state spaces
- support efficient learning and inference techniques

Probabilistic Graphical Models ...

- support a structured specification of high-dimensional distributions in terms of low-dimensional factors
- structured representation can be exploited for efficient learning and inference algorithms (sometimes ...)
- graphical representation gives human-friendly design and description possibilities

This seminar series is about efficient inference and learning for Bayesian networks using "Variational inference".

Plan for this weeks

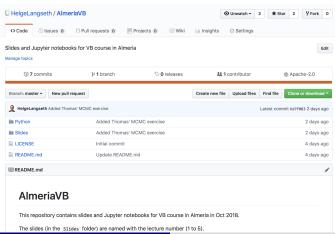
- Day 1: Bayesian networks Definition and inference
 - Definition of Bayesian networks: Syntax and semantics
 - Exact inference
 - Approximate inference using MCMC
- Day 2: Variational inference Introduction and basis
 - Approximate inference through the Kullback-Leibler divergence
 - Variational Bayes
 - The mean-field approach to Variational Bayes
- Day 3: Variational Bayes cont'd
 - Solving the VB equations
 - Introducing Exponential families
- Day 4: Scalable Variational Bayes
 - Variational message passing
 - Stochastic gradient ascent
 - Stochastic variational inference
- Day 5: Current approaches and extensions
 - Variational Auto Encoders
 - Black Box variational inference
 - Probabilistic Programming Languages

Information about the course

Online repository

Materials for the course, including (almost last-version of) the slides, and description of implementation-tasks are available at

https://github.com/HelgeLangseth/AlmeriaVB



Starting-point

I will assume that these topics are (well) known:

- Probabilities, P(X = x); conditional probabilities, P(X = x | Y = y).
- $\bullet \ \ \text{Independence}, \mathbf{X} \perp \!\!\! \perp \mathbf{Y}; \text{conditional independence} \ \mathbf{X} \perp \!\!\! \perp \mathbf{Y} \, | \, \mathbf{Z}.$
- "Standard" probability calculus:

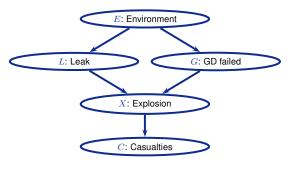
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Product: P(x,y) = P(x \mid y) \cdot P(y) = P(x) \cdot P(y \mid x). Sum-rule: P(x \lor y) = P(x) + P(y) = P(x) - P(y \land x). Total probability: P(Y = y) = \sum_{x'} P(y \mid X = x') \cdot P(X = x'). Bayes rule: P(x \mid y) = P(x) \cdot P(y \mid x) / P(y).
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I will assume that these topics are (somewhat) known:

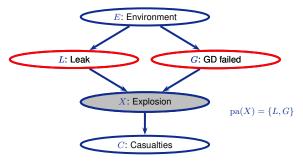
- Bayesian network syntax and semantics.
- Exact inference in Bayesian networks.
- Approximate inference using MCMC.

Implementation tasks:

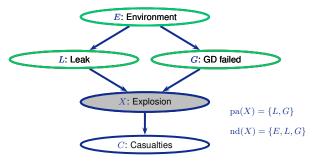
- We will get some implementation tasks as we move along.
- You will be supplied partly running Python-code (in the form of Jupyter notebooks).
- You will need to have Python 3.x on your computer (https://www.python.org/downloads/), and a set of packages (numpy, scipy, matplotlib, jupyter).



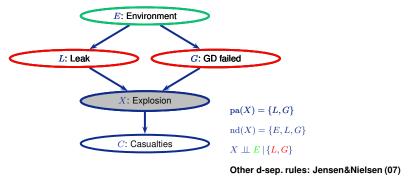
P(E, L, G, X, C)



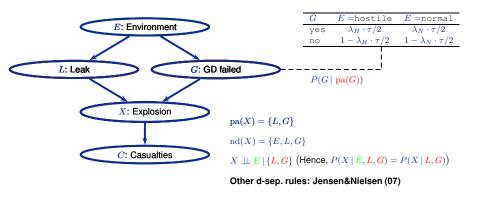
P(E, L, G, X, C)



P(E, L, G, X, C)



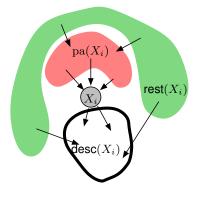
P(E, L, G, X, C)



$$P(E, L, G, X, C) = P(E) \cdot P(L \mid E) \cdot P(G \mid E, L) \cdot P(X \mid E, L, G) \cdot P(C \mid E, L, G, X)$$
$$= P(E) \cdot P(L \mid E) \cdot P(G \mid E) \quad \cdot P(X \mid L, G) \quad \cdot P(C \mid X)$$

Markov properties ⇔ Factorisation property

Nondescendant Criterion



In the distribution P defined by the BN the following independence relation holds:

$$P(X_i \mid pa(X_i), rest(X_i)) = P(X_i \mid pa(X_i))$$

" X_i is independent of its non-descendants given its parents"

"rest" are all nodes except:

- \bullet X_i itself
- X_i's parents
- X_i's descendants

Syntax and semantics formalized

Bayesian network syntax

Let X_1, \ldots, X_n be a collection of random variables. A Bayesian network over X_1, \ldots, X_n consists of

- ullet a directed acyclic graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ whose nodes \mathcal{V} are the variables X_1, \dots, X_n
- a set of local conditional distributions, $\mathcal{P} = \{p(X_i \mid \operatorname{pa}(X_i)), X_i \in \mathcal{V}\}$, where $\operatorname{pa}(X_i)$ are the parents of X_i in \mathcal{G} as defined by the edges \mathcal{E} .

Bayesian network semantics

A Bayesian network $\mathcal N$ with nodes X_1,\dots,X_n defines a joint distribution

$$p_{\mathcal{N}}(X_1,\ldots,X_n) = \prod_{i=1}^n p(X_i \mid pa(X_i))$$

Exact inference

Probabilistic Inference

Bayesian network inference

Inference in the Bayesian network amounts to calculating $p(\mathbf{Z} = \mathbf{z} \mid \mathbf{X} = \mathbf{x})$, where

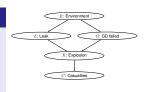
- ullet $\mathbf{X}\subset\mathcal{V}$ are the observed variables, currently taking the configuration $\mathbf{X}=\mathbf{x}.$
- ullet $\mathbf{Z} \subseteq \mathcal{V} \setminus \mathbf{X}$ are our variables of interest.

Inference is therefore the tool to answer any probabilistic query we may have in our domain, given a partial (or empty) observation from the domain

- "What is the chance that Almería will move back to La Liga before 2020, given that they didn't win during the first four games of this campaign?"
- "What is the probability of Google going bankrupt before you are done with your education?"

Probability propagation

$$\left. \begin{array}{c} \mathsf{Bayesian} \ \mathsf{network} \\ + \\ \mathsf{Evidence:} \ \mathbf{X}_E = \mathbf{x}_e \end{array} \right\} \Rightarrow P(\mathbf{X}_Q | \mathbf{x}_e) ?$$

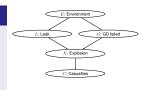


Example: Calculate P(X = x | G = g)

$$\begin{split} P(x,g) &= \sum_{e} \sum_{l} \sum_{c} P(E=e, L=l, g, X=x, C=c) \\ &= \sum_{e} \sum_{l} \sum_{c} P(e) \cdot P(l \, | \, e) \cdot P(g \, | \, e) \cdot P(x \, | \, l, g) \cdot P(c \, | \, x) \\ &= \sum_{e} P(e) \cdot P(g \, | \, e) \sum_{l} P(l \, | \, e) \cdot P(x \, | \, l, g) \sum_{c} P(c \, | \, x) \end{split}$$

Probability propagation

$$\left. \begin{array}{c} \mathsf{Bayesian} \ \mathsf{network} \\ + \\ \mathsf{Evidence:} \ \mathbf{X}_E = \mathbf{x}_e \end{array} \right\} \Rightarrow P(\mathbf{X}_Q | \mathbf{x}_e) ?$$

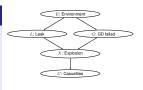


Example: Calculate P(X = x | G = g)

$$\begin{split} P(x,g) &= \sum_{e} P(e) \cdot P(g \mid e) \sum_{l} P(l \mid e) \cdot P(x \mid l,g) \\ P(X=x \mid G=g) &= \frac{P(x,g)}{\sum_{x'} P(X=x',g)} \propto P(x,g) \end{split}$$

Probability propagation

$$\left. \begin{array}{c} \mathsf{Bayesian} \ \mathsf{network} \\ + \\ \mathsf{Evidence:} \ \mathbf{X}_E = \mathbf{x}_e \end{array} \right\} \Rightarrow P(\mathbf{X}_Q | \mathbf{x}_e) ?$$



Operations to calculate $P(\mathbf{X}_Q \mid \mathbf{x}_e)$

Restriction: Restrict domain of a potential (e.g., P(g|E) from P(G|E))

Combination: Multiplication of potentials (e.g., $P(l \mid e) \cdot P(X \mid l, g)$)

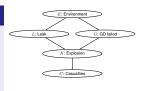
Marginalisation: Sum/integrate out a variable form a potential, e.g., the operation $\sum P(I|g) \cdot P(x|I|g)$ which removes I from the potential over

 $\sum_{l} P(l \mid e) \cdot P(x \mid l, g)$, which removes L from the potential over $\{L, X, E, G\}$ and results in $P(x \mid e, g)$ over $\{X, E, G\}$.

 $\{L,X,E,G\}$ and results in $P(x\,|\,e,g)$ over $\{X,E,G\}$

Probability propagation

$$\left. \begin{array}{c} \text{Bayesian network} \\ + \\ \text{Evidence: } \mathbf{X}_E = \mathbf{x}_e \end{array} \right\} \Rightarrow P(\mathbf{X}_Q | \mathbf{x}_e) ?$$



Requirements for efficient calculation of $P(\mathbf{X}_Q \mid \mathbf{x}_e)$

- Constraints wrt. structure:
 - Size of combined potentials
- Constraints wrt. distributions:
 - Ability to perform operations
 - Ability to represent results of operations

Inference in discrete BNs - Formalized

Computation of conditional distributions

Given $\mathbf{X} = X_1, \dots, X_k \subset \mathcal{V}, x_i \in dom(X_i), \mathbf{Z} = Z_1, \dots, Z_l \subset \mathcal{V}$, compute

$$p(\mathbf{Z} \mid \mathbf{X} = \mathbf{x})$$

Especially: Single variable posterior distributions: for each $Z \notin \mathbf{X}$ compute $p(Z \mid \mathbf{X} = \mathbf{x})$.

Problem reduction

This problem can be reduced to the computation of partial distributions, i.e., functions

$$p(\mathbf{Z}, \mathbf{X} = \mathbf{x})$$

(function defined on $dom(\mathbf{Z})$) because

$$p(\mathbf{Z} \mid \mathbf{X} = \mathbf{x}) = p(\mathbf{Z}, \mathbf{X} = \mathbf{x})/p(\mathbf{X} = \mathbf{x})$$

Variable Elimination

Direct approach: Denote $V(=V_1,\ldots,V_m):=\mathcal{V}\setminus (\mathbf{X}\cup\mathbf{Z})$, and let \mathbf{v} range over $dom(\mathbf{V})$. Then for $\mathbf{z}\in dom(\mathbf{Z})$:

$$p(\mathbf{Z} = \mathbf{z}, \mathbf{X} = \mathbf{x}) = \sum_{\mathbf{v}} p(\mathbf{Z} = \mathbf{z}, \mathbf{X} = \mathbf{x}, \mathbf{V} = \mathbf{v})$$

$$= \sum_{\mathbf{v}} \prod_{i} p(Y_{i} \mid pa(Y_{i}))(\mathbf{z}, \mathbf{x}, \mathbf{v})$$

$$= \sum_{v_{1} \in dom(V_{1})} \dots \sum_{v_{m} \in dom(V_{m})} \prod_{i} p(Y_{i} \mid pa(Y_{i}))(\mathbf{z}, \mathbf{x}, \mathbf{v})$$

"Algorithm": Sum out the v_j one by one, move factors $p(Y_i \mid \operatorname{pa}(Y_i))(\mathbf{z}, \mathbf{x}, \mathbf{v})$ that do not depend on current v_j (because $V_j \notin \{Y_i\} \cup \operatorname{pa}(Y_i)$) out of the sum.

Advantage: Can be used to compute conditional distributions for arbitrary set ${\bf Z}$ of query variables.

Variable Elimination: Example

Example



	t X	f
	.5	.5

	X	-2
X_1	t	f
t	.7	ċ
f	.1	.9

	X	-3
X_1	t	f
t	.7	.3
f	.2	.8

$$p(X_2 = x_2, X_4 = f) = \sum_{x_1, x_3 \in \{t, f\}} p(X_1 = x_1, X_2 = x_2, X_3 = x_3, X_4 = f)$$

$$= \sum_{x_1, x_3} \left[p(X_1 = x_1) p(X_2 = x_2 \mid X_1 = x_1) p(X_3 = x_3 \mid X_1 = x_1) \right]$$

$$p(X_4 = f \mid X_2 = x_2, X_3 = x_3)$$

Variable Elimination: Example

$$p(X_2 = x_2, X_4 = f)$$

$$= \sum_{x_1} p(X_1 = x_1) p(X_2 = x_2 \mid X_1 = x_1) \left[\sum_{x_3} p(X_3 = x_3 \mid X_1 = x_1) \right]$$

$$p(X_4 = f \mid X_2 = x_2, X_3 = x_3)$$

$$= \sum_{x_1} p(X_1 = x_1) p(X_2 = x_2 \mid X_1 = x_1) F_1(X_1 = x_1, X_2 = x_2) = F_2(X_2 = x_2)$$

where

		,	X_3
_	X_1	t	f
_	t	.7	.3
	f	.2	.8

			,	7
X_2	X_3	t	K_4 f	
t	t	.9	.1	١,
t	f	.7	.2	ľ
f	t	.7 .8 .4	.2	
f	f	.4	.6	

	x_1	x_2	$F_1(X_1, X_2)$
	t	t	.7· .1 + .3· .3 = .16
•	t	f	$.7 \cdot .2 + .3 \cdot .6 = .32$
	f	t	$.2 \cdot .1 + .8 \cdot .3 = .26$
	f	f	$.2 \cdot .2 + .8 \cdot .6 = .52$

and

	λ	1
t	t	f
	.5	.5

	X_2		ı
X_1	t	f	ŀ
t	.7	.3	I
f	.1	.9	I

x_1	x_2	$F_1(X_1, X_2)$	
t	t	.16	H
-			

	x_2	$F_2(X_2)$
\rightarrow	t	
	f	

Complexity

- Variable elimination is exponential in maximal number of arguments of factors $p(\ldots | \ldots)$ resp. $F_i(\ldots)$ that appear in the summation process.
- This number depends strongly on the network structure
- ... and can also depend strongly on the order in which we sum out the variables!

Approximate inference using sampling

Approximate Inference using sampling

Problem Structure

Input: Evidence X = x, random variable Z, value $z \in dom(Z)$.

Output: Find approximation q for $p := P(Z = z \mid \mathbf{X} = \mathbf{x})$.

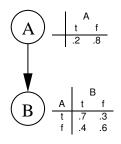
Grand plan

- Somehow sample instantiations from the domain Y; $X \cup Z \subseteq Y$.
- Somehow use the samples $\{y_1, \dots, y_N\}$ to find the approximation q.

Forward Sampling

Observation: can use Bayesian network as random generator that produces full instantiations $\mathbf{Y} = \mathbf{y}$ according to distribution $P(\mathbf{Y})$.

Example:



- Generate random numbers r_1, r_2 uniformly from [0,1].
- Set A = t if $r_1 \leq .2$ and A = f else.
- Depending on the value of A and r₂ set B to t or f.

Generation of one random instantiation: linear in size of network.

Sample Estimate

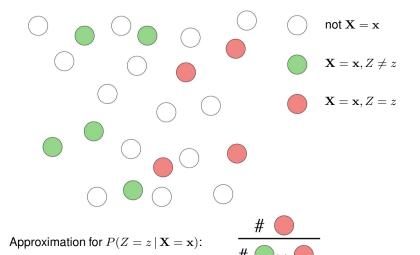
• Given a sample y_1, \dots, y_N of complete instantiations generated (independently) by the sampling algorithm, approximate P(X = x) as

$$q^* := \frac{1}{N} |\{i \in 1, \dots, N \mid \mathbf{X} = \mathbf{x} \text{ in } \mathbf{y}_i\}|$$

- Similarly, the sample provides an estimate for $P(Z = z, \mathbf{X} = \mathbf{x})$.
- Put together, we can estimate

$$P(Z = z \mid \mathbf{X} = \mathbf{x}) = P(Z = z, \mathbf{X} = \mathbf{x})/P(\mathbf{X} = \mathbf{x}).$$

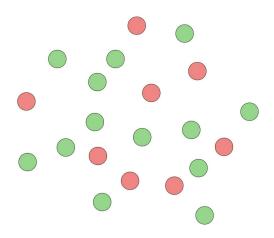
Forward Sampling: Illustration



Sampling from the Conditional

Problem of forward sampling: samples with $\mathbf{X} \neq \mathbf{x}$ are useless!

Goal: find algorithm that samples according to $P(\mathbf{Z} \mid \mathbf{X} = \mathbf{z})$:



Approximate inference – Gibbs Sampling

- **Principle:** obtain new sample from previous sample by randomly changing the value of only one selected variable.
- \bullet Notation: Let $\mathbf{Y}=(\mathbf{Z},\mathbf{X})$ denote all variables in the domain, where $\mathbf{X}=\mathbf{x}$ is observed.

Gibbs sampling

```
\begin{aligned} \mathbf{z}_0 &:= \text{arbitrary instantiation of } \mathbf{Z}. \\ \mathbf{y}_0 &:= (\mathbf{z}_0, \mathbf{x}). \\ t &:= 1. \\ \text{repeat forever} \\ &\quad \text{choose } Z_k \in \mathbf{Z} \\ &\quad \text{set } y_{t,j} := y_{t-1,j} \text{ for all } Y_j \text{ except the chosen } Z_k. \\ &\quad \text{generate randomly } z_{t,k} \text{ according to } P\left(Z_k \,|\, \mathbf{Y} \setminus \{Z_k\} = \mathbf{y}_t^{\downarrow \mathbf{Y} \setminus \{Z_k\}}\right) \\ &\quad \text{Store the sampled value in } Z_k' \text{s location in } \mathbf{y}_t. \\ &\quad t := t+1. \end{aligned}
```

Resampling Z_k

$$P(Z_{k} = z_{k} \mid \mathbf{Y} \setminus \{Z_{k}\} = \mathbf{y}_{t}^{\downarrow \mathbf{Y} \setminus \{Z_{k}\}})$$

$$\propto P(Z_{k} = z_{k}, \mathbf{Y} \setminus \{Z_{k}\} = \mathbf{y}_{t}^{\downarrow \mathbf{Y} \setminus \{Z_{k}\}})$$

$$\propto P(Z_{k} = z_{k} \mid \operatorname{pa}(Z_{k}) = \mathbf{y}_{t}^{\downarrow \operatorname{pa}(Z_{k})}).$$

$$\prod_{i: Y_{i} \in \operatorname{ch}(Z_{k})} P(Y_{i} = y_{t,i} \mid \operatorname{pa}(Y_{i}) \setminus \{Z_{k}\} = \mathbf{y}_{t}^{\downarrow \operatorname{pa}(Y_{i}) \setminus \{Z_{k}\}}, Z_{k} = z_{k}) \quad (*),$$

where \propto means: equals up to a constant that does not depend on z_k .

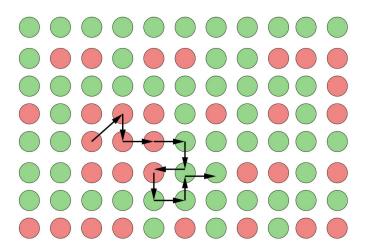
 \rightsquigarrow **Note:** To sample a value we only need to consider the **Markov blanket** for $Z_k!$

To sample $Z_{t,k}$

- $\bullet \ \, \mathsf{Normalize} \ (*) \ \, \mathsf{to} \ \, \mathsf{obtain} \ \, P\left(Z_k \, | \, \mathbf{Y} \setminus \{Z_k\} = \mathbf{y}_t^{\downarrow \mathbf{Y} \setminus \{Z_k\}}\right)$
 - $P\left(Z_k = z_k \mid \mathbf{Y} \setminus \{Z_k\} = \mathbf{y}_t^{\downarrow \mathbf{Y} \setminus \{Z_k\}}\right)$ is called the *full conditional* for Z_k .
- ullet Sample value $z_{t,k}$ according to the resulting distribution

Gibbs Random Walk

The process of Gibbs sampling can be understood as a *random walk* in the space of all instantiations with X = x:

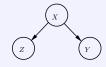


Reachable in one step: instantiations that differ from current one by value assignment to at most one variable (assume randomized choice of variable \mathbb{Z}_k).

Code task: Exact and approximate inference in a simple Gaussian model

Code Task: Exact and approximate inference

In this exercise you should implement a Gibbs sampler for the linear Gaussian model



where the distributions are given as

$$f(x) = \mathcal{N}(x|\mu_x, \sigma_x^2)$$
 $f(y|x) = \mathcal{N}(y|x, \sigma^2)$ $f(z|x) = \mathcal{N}(z|x, \sigma^2)$.

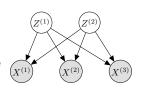
Start with the partial implementation

Things to try out:

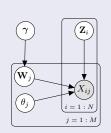
- How does changing the number of samples affect the accuracy of the approximation?
- Try experimenting with different values for the initial parameters.
- Are your results sensitive wrt. the starting position? Why (not)?

A more elaborate example: Factor analysis

- Factor analysis is a statistical model used to summarize
 a high-dimensional observation X of correlated
 variables by a smaller set Z of factors that a priori are
 assumed independent.
- **Example:** X is a set of scores a subject gets from some intelligence-test, Z models different types of intelligence (e.g., sense of logics, verbal skills, . . .).



Mathematical formulation:



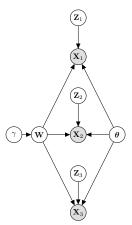
- $\mathbf{Z}_i \sim \mathcal{N}(\mathbf{0}, \mathbf{I})$.
- $X_{i,j} | \{\mathbf{z}_i, \mathbf{w}_j, \theta_j\} \sim \mathcal{N}(\mathbf{w}_j^\mathsf{T} \mathbf{z}_i, 1/\theta_j).$
- Bayesian setting: Add W_j 's and θ as r.v.'s with priors.

Relevant questions given a dataset $\mathcal{D} = \{\mathbf{x}_1, \dots, \mathbf{x}_N\}$:

- Learning: $p(\mathbf{w}, \boldsymbol{\theta}, \gamma \mid \mathcal{D})$.
- "Understanding" a new example \mathbf{x}^* : $p(\mathbf{z} \mid \mathbf{X} = \mathbf{x}^*, \mathcal{D})$.
- ...

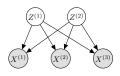
Analysis of FA inference

Unfolded model



FA model "unfolded" for three data instances $(\mathbf{X}_1, \mathbf{X}_2, \mathbf{X}_3)$

Recall local model



Observations

Inspecting the independence properties of unfolded model we see that the

- number of variables (W and θ) in "separating factor" are manageable.
- posterior cannot be calculated in closed-form because the priors (assumed a priori independent) are not conjugate. (More on this later.)
- → Approximate inference required.

Gibbs sampling: Example

Full conditional for
$$p(\mathbf{w}_j | \mathbf{w}_{-j}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}, \gamma)$$

Let $\mathbf{w}_{-j}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}, \gamma$ be a configuration over all variables except \mathbf{w}_j . Then

$$p(\mathbf{w}_j | \mathbf{w}_{-j}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}, \gamma) \propto p(\mathbf{w}_j | \gamma) \prod_{i=1}^{N} p(x_{ij} | \mathbf{W}_j, \mathbf{z}_i, \boldsymbol{\theta}_j)$$

With a bit of pencil pushing we find that:

$$p(\mathbf{w}_j | \mathbf{w}_{-j}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}, \gamma) = \mathcal{N}(\mathbf{w}_j | \boldsymbol{\mu}, \mathbf{Q}^{-1}),$$

where

$$\mathbf{Q} \leftarrow \gamma \mathbf{I} + \theta_j \sum_{i=1}^N \mathbf{z}_i \mathbf{z}_i^\mathsf{T}$$

$$\bullet \ \boldsymbol{\mu} \leftarrow \mathbf{Q}^{-1} \theta_j \sum_{i=1}^N x_{ij} \mathbf{z}_i$$

Gibbs sampling: Example

Full conditional for $p(\gamma \,|\, \mathbf{w}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z})$

$$p(\gamma \mid \mathbf{w}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}) \propto p(\gamma) \prod_{j=1}^{M} p(\mathbf{w}_j \mid \gamma)$$

We find that

$$p(\gamma \,|\, \mathbf{w}, \boldsymbol{\theta}, \mathbf{x}, \mathbf{z}) = \mathsf{Gamma}(\gamma \,|\, shape, rate),$$

where

- $shape \leftarrow prior_shape + \frac{M \cdot D}{2}$
- $rate \leftarrow prior_rate + \frac{1}{2} \sum_{j=1}^{M} \mathbf{w}_{j}^{\mathsf{T}} \mathbf{w}_{j}$