Intelligent Agents: Web-mining Agents

Probabilistic Graphical Models

Continuous Space

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Probabilistic Graphical Models (PGMs)

Recap: Propositional modelling

- Factor model, Bayesian network, Markov network
- Semantics, inference tasks
 + algorithms + complexity

2. Probabilistic relational models (PRMs)

- Parameterised models, Markov logic networks
- Semantics, inference tasks

3. Lifted inference

- LVE, LJT, FOKC
- Theoretical analysis

4. Lifted learning

- Recap: propositional learning
- From ground to lifted models
- Direct lifted learning

5. Approximate Inference: Sampling

- Importance sampling
- MCMC methods

Sequential models & inference

- Dynamic PRMs
- Semantics, inference tasks + algorithms + complexity, learning

7. Decision making

- (Dynamic) Decision PRMs
- Semantics, inference tasks
 + algorithms, learning

8. Continuous Space

- Gaussian distributions and Bayesian networks
- Probabilistic soft logic



Models with Continuous Variables

- Discretisation of continuous variables
 - Discrete model again
 - Own set of problems
 - Hard to find good discretisation
 - High granularity might be necessary
 - → large ranges → large factors
 - Lose characteristics of variable
 - Not each value necessarily associated with a probability
 - Nearby values have similar probabilities → hard to capture in a discrete distribution (no notion of closeness between range values)
- Therefore, use models with continuous variables



Outline: 8. Continuous Space

A. Basics

- Continuous variables, probability density function, cumulative probability distribution
- Joint distribution, marginal density, conditional density

B. Gaussian models

- (Multivariate) Gaussian distribution
- (Parameterised) Gaussian Bayesian networks

C. Probabilistic Soft Logic (PSL)

Modelling, semantics, inference task



Probability Density Function

- Continuous randvar R
 - Range $\mathcal{R}(R) = [0,1]$
- Function $p: \mathbb{R} \to \mathbb{R}$ is a probability density function (PDF) for R if it is a non-negative, integrable function s.t.

$$\int_{\mathcal{R}(R)} p(r)dr = 1$$

• For any
$$a$$
 (and b) in event space
$$P(R \le a) = \int_{-\infty}^{b} p(r) dr \qquad P(a \le R \le b) = \int_{a}^{b} p(r) dr$$

- Function P is a cumulative distribution for R
- Intuitively, value of p(r) at point r is the incremental amount that r adds to the cumulative distribution during integration

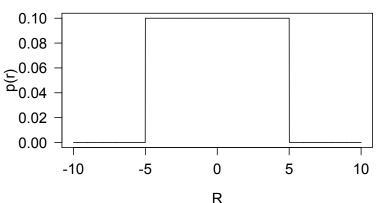


PDFs: Uniform Distribution

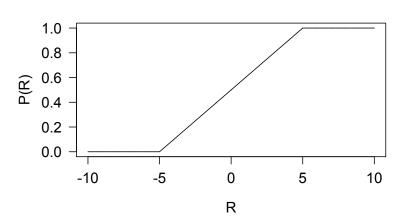
• Continuous randvar R has a uniform distribution over [a,b], denoted $R \sim \mathrm{Unif}[a,b]$, if it has the PDF

$$p(r) = \begin{cases} \frac{1}{b-a} & b \ge r \ge a \\ 0 & \text{otherwise} \end{cases}$$

- Density can be larger than 1 if b-a<1
 - Can be legal if the total area under the pdf is 1



PDF



Cumulative Distribution



Joint/Multivariate Distribution

- Let P be a joint distribution over continuous randvars R_1, \dots, R_n
- Function $p(r_1, ..., r_n)$ is a joint density function of $R_1, ..., R_n$ if
 - $p(r_1, ..., r_n) \ge 0$ for all values $r_1, ..., r_n$ of $R_1, ..., R_n$
 - p is an integrable function
 - For any choice a_1, \ldots, a_n and b_1, \ldots, b_n ,

$$P(a_1 \le R_1 \le b_1, \dots, a_n \le R_n \le b_n)$$

$$= \int_{a_1}^{b_1} \dots \int_{a_n}^{b_n} p(r_1, \dots, r_n) dr_1 \dots r_n$$



Marginal Density

- Given a joint density, integrate out the non-query randvars
 - E.g., given p(r,s) a joint density for randvars R,S, then

$$p(r) = \int_{-\infty}^{\infty} p(r,s) \, ds$$

- Shorthand notations
 - $p_R = p(r)$ marginal density
 - $p_{R.S} = p(r,s)$ joint density

Conditional Density Function

- Discrete case: $P(S|R=r) = \frac{P(S,R=r)}{P(R=r)}$ Problem in continuous case: P(R=r) = 0 $\rightarrow P(S|R=r)$ undefined
- To avoid problem, condition on event $r - \epsilon \le R \le r + \epsilon$ and consider limit when $\epsilon \to 0$ $P(S|r) = \lim_{\epsilon \to 0} P(S|r - \epsilon \le R \le r + \epsilon)$
- If a continuous joint density p(r,s) exists, derive form of this expression:

$$p(s|r) = \frac{p(r,s)}{p(r)}$$

- If p(r) = 0, conditional density undefined
- Chain rule and Bayes' rule hold as well:

$$p(r,s) = p(r)p(s|r) p(s|r) = \frac{p(s)p(r|s)}{p(r)}$$



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B. Gaussian models

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- (Parameterised) Gaussian Bayesian networks

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Modelling, semantics, inference task



Models with Continuous Variables

- Problem: Space of possible parameterisation essentially unbounded
- Special case: (Multivariate) Gaussian distributions
 - Two parameters per variable: mean, variance
 - Strong assumptions, e.g.,
 - Exponential decay away from its mean
 - Linearity of interactions between randvars
 - → Assumptions often invalid but still work as a good approximation for many real-world distributions
 - Many generalisations exist which use Gaussians as a foundation
 - Non-linear interactions
 - Mixture of Gaussians



PDFs: Gaussian/Normal Distribution

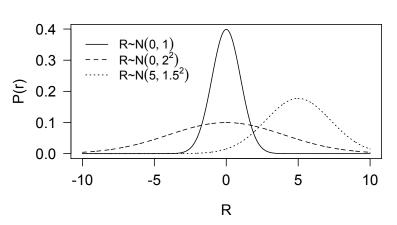
• Continuous randvar R has a Gaussian distribution with mean μ and variance σ^2 , denoted $R \sim \mathcal{N}(\mu, \sigma^2)$, if it has the PDF Standard Gauss

$$p(r) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(r-\mu)^2}{2\sigma^2}}$$

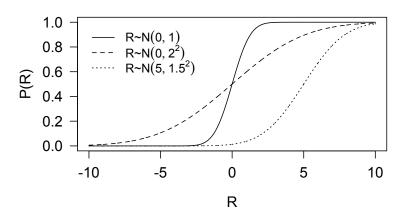
Standard Gaussian $R \sim \mathcal{N}(\mu=0,\sigma^2=1)$: $p(r) = \frac{1}{\sqrt{2\pi}}e^{-\frac{(r)^2}{2}}$

- Expected value and variance of R given by μ and σ^2
 - Standard deviation: σ

PDF



Cumulative Distribution





Multivariate Gaussian

- Univariate Gaussian: two parameters
 - Mean μ and variance σ^2
- Multivariate Gaussian distribution over continuous randvars $R_1, ..., R_n$ characterised by
 - n-dimensional mean vector μ
 - Symmetric $n \times n$ covariance matrix Σ
 - I.e., $\mathcal{N}(\mu; \Sigma)$
- Density function defined as

$$p(\mathbf{r}) = \frac{1}{\sqrt{(2\pi)^n |\Sigma|}} \exp\left[-\frac{1}{2}(\mathbf{r} - \boldsymbol{\mu})^T \Sigma^{-1} (\mathbf{r} - \boldsymbol{\mu})\right]$$

- $\mathbf{r} = (r_1, \dots, r_n)^T$
- $|\Sigma|$ determinant of Σ
- To induce a well-defined density, Σ must be positive-definite
 - For any $r \in \mathbb{R}^n$ s.t. $r \neq 0 : r^T \Sigma r > 0$
 - Guaranteed to be non-singular → non-zero determinant

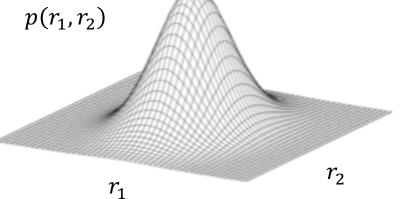
Standard multivariate Gaussian $R_1, ..., R_n$ with

- $\mu = 0$ (all-zero vector)
- $\Sigma = I$ (identity matrix)

Example

• Joint Standard Gaussian distribution over two randvars R_1, R_2 , i.e.,

•
$$\mu = (0 \quad 0)^T$$
, $\Sigma = I_2$



- Joint Gaussian distribution over three randvars R_1, R_2, R_3
 - Mean vector, covariance matrix:

$$\mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

- Covariances $Cov[R_1;R_3]$ and $Cov[R_2;R_3]$ negative, i.e., R_3 negatively correlated with R_1 (and R_2)
 - When R_1 (R_2) goes up, R_3 goes down



Marginalisation

- Trivial with covariance matrix:
 - Compute pairwise covariances, i.e., generating the distribution in its covariance form
 - Given covariance form Σ : Read off from μ , Σ
- Assume a joint Gaussian distribution over $\{R, T\}$ where $R \in \mathbb{R}^n$ and $T \in \mathbb{R}^m$
 - One can decompose mean and covariance:

$$p(\mathbf{r}, \mathbf{t}) = \mathcal{N}\left(\begin{pmatrix} \boldsymbol{\mu}_{R} \\ \boldsymbol{\mu}_{T} \end{pmatrix}; \begin{bmatrix} \boldsymbol{\Sigma}_{RR} & \boldsymbol{\Sigma}_{RT} \\ \boldsymbol{\Sigma}_{TR} & \boldsymbol{\Sigma}_{TT} \end{bmatrix}\right)$$

- where
 - $\mu_R \in \mathbb{R}^n$, $\mu_T \in \mathbb{R}^m$,
 - Σ_{RR} an $n \times n$ matrix, Σ_{RT} an $n \times m$ matrix, $\Sigma_{TR} = \Sigma_{RT}^T$ an $m \times n$ matrix, Σ_{TT} a $m \times m$ matrix
- Then, marginal distribution over T given by Gaussian distribution of $\mathcal{N}(\mu_T; \Sigma_{TT})$



Example

- Given joint Gaussian distribution over three randvars R_1 , R_2 , R_3
 - Mean vector, covariance matrix:

$$\mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$$

• $p(R_1, R_2)$ given by Gaussian distribution with

$$\mu = \begin{pmatrix} 1 \\ -3 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} 4 & 2 \\ 2 & 5 \end{pmatrix}$$



Dual: Information/Precision Form

• Rewrite exp $\left|-\frac{1}{2}(\boldsymbol{r}-\boldsymbol{\mu})^T\Sigma^{-1}(\boldsymbol{r}-\boldsymbol{\mu})\right|$ by setting $\Gamma = \Sigma^{-1}$ and multiplying out: $-\frac{1}{2}(\mathbf{r}-\boldsymbol{\mu})^T \mathbf{\Gamma}(\mathbf{r}-\boldsymbol{\mu}) = -\frac{1}{2}[\mathbf{r}^T \mathbf{\Gamma} \mathbf{r} - 2\mathbf{r}^T \mathbf{\Gamma} \boldsymbol{\mu} + \boldsymbol{\mu}^T \mathbf{\Gamma} \boldsymbol{\mu}]$

• $\mu^T \Gamma \mu$ is constant over the different r, therefore,

$$p(\mathbf{r}) \propto \exp\left(-\frac{1}{2}[\mathbf{r}^T \Gamma \mathbf{r} - 2\mathbf{r}^T \Gamma \boldsymbol{\mu}]\right)$$
$$= \exp\left[-\frac{1}{2}\mathbf{r}^T \Gamma \mathbf{r} + \mathbf{r}^T \Gamma \boldsymbol{\mu}\right]$$
$$= \exp\left[-\frac{1}{2}\mathbf{r}^T \Gamma \mathbf{r} + (\Gamma \boldsymbol{\mu})^T \mathbf{r}\right]$$

• $\Gamma \mu$ called potential vector

$$= \exp\left[-\frac{1}{2}\mathbf{r}^{T}\Gamma\mathbf{r} + (\Gamma\boldsymbol{\mu})^{T}\mathbf{r}\right]$$

$$= \exp\left[-\frac{1}{2}\mathbf{r}^{T}\Gamma\mathbf{r} + (\Gamma\boldsymbol{\mu})^{T}\mathbf{r}\right]$$

$$= \left((\Gamma\boldsymbol{\mu})^{T}\mathbf{r}^{T}\right)^{T} \quad \triangleright A^{T^{T}} = A$$

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Dual: Information/Precision Form

• For a decomposition $\{R,T\}$ where $R\in\mathbb{R}^n$ and $T\in\mathbb{R}^m$:

$$\Gamma = \Sigma^{-1} = \begin{bmatrix} \Sigma_{RR} & \Sigma_{RT} \\ \Sigma_{TR} & \Sigma_{TT} \end{bmatrix}^{-1} = \begin{bmatrix} \Gamma_{RR} & \Gamma_{RT} \\ \Gamma_{TR} & \Gamma_{TT} \end{bmatrix}$$

- Getting to Σ
 - $\Sigma_{RR} = \left(\Gamma_{RR} \Gamma_{RT}\Gamma_{TT}^{-1}\Gamma_{TR}\right)^{-1}$
 - $\Sigma_{TT} = \left(\Gamma_{TT} \Gamma_{TR}\Gamma_{RR}^{-1}\Gamma_{RT}\right)^{-1}$
 - $\Sigma_{RT} = -\Gamma_{RR}^{-1}\Gamma_{RT}(\Gamma_{TT} \Gamma_{TR}\Gamma_{RR}^{-1}\Gamma_{RT})^{-1} = \Sigma_{TR}^{T}$
 - $\Sigma_{TR} = -\Gamma_{TT}^{-1}\Gamma_{TR} \left(\Gamma_{RR} \Gamma_{RT}\Gamma_{TT}^{-1}\Gamma_{TR}\right)^{-1} = \Sigma_{RT}^{T}$
- Getting to Γ
 - $\Gamma_{RR} = \left(\Sigma_{RR} \Sigma_{RT}\Sigma_{TT}^{-1}\Sigma_{TR}\right)^{-1}$
 - $\Gamma_{TT} = \left(\Sigma_{TT} \Sigma_{TR}\Sigma_{RR}^{-1}\Sigma_{RT}\right)^{-1}$
 - $\Gamma_{RT} = -\Sigma_{RR}^{-1} \Sigma_{RT} (\Sigma_{TT} \Sigma_{TR} \Sigma_{RR}^{-1} \Sigma_{RT})^{-1} = \Gamma_{TR}^{T}$
 - $\Gamma_{TR} = -\Sigma_{TT}^{-1}\Sigma_{TR}(\Sigma_{RR} \Sigma_{RT}\Sigma_{TT}^{-1}\Sigma_{TR})^{-1} = \Gamma_{RT}^{T}$



Conditioning

• Conditioning a Gaussian on observations ${\pmb E}={\pmb e}$ easy to perform in the information form by setting ${\pmb E}$ to ${\pmb e}$ in one of the following

$$p(\mathbf{r}) \propto \exp\left[-\frac{1}{2}(\mathbf{r} - \boldsymbol{\mu})^T \Gamma(\mathbf{r} - \boldsymbol{\mu})\right]$$
$$\propto \exp\left[-\frac{1}{2}\mathbf{r}^T \Gamma \mathbf{r} + (\Gamma \boldsymbol{\mu})^T \mathbf{r}\right]$$

• Assuming a decomposition into \boldsymbol{R} and \boldsymbol{E} , i.e.,

$$p(r, e) = \mathcal{N}\left(\begin{pmatrix} \mu_R \\ \mu_E \end{pmatrix}; \begin{bmatrix} \Sigma_{RR} & \Sigma_{RE} \\ \Sigma_{ER} & \Sigma_{EE} \end{bmatrix}\right)$$

$$\propto \exp\left[-\frac{1}{2}\begin{pmatrix} r \\ e \end{pmatrix} - \begin{pmatrix} \mu_R \\ \mu_E \end{pmatrix}\right)^T \begin{bmatrix} \Gamma_{RR} & \Gamma_{RT} \\ \Gamma_{TR} & \Gamma_{TT} \end{bmatrix} \begin{pmatrix} r \\ e \end{pmatrix} - \begin{pmatrix} \mu_R \\ \mu_E \end{pmatrix}\right]$$



In the exponential function:

$$-\frac{1}{2} \left(\begin{pmatrix} \boldsymbol{r} \\ \boldsymbol{e} \end{pmatrix} - \begin{pmatrix} \boldsymbol{\mu}_{\boldsymbol{R}} \\ \boldsymbol{\mu}_{\boldsymbol{E}} \end{pmatrix} \right)^{T} \begin{bmatrix} \Gamma_{\boldsymbol{R}\boldsymbol{R}} & \Gamma_{\boldsymbol{R}\boldsymbol{E}} \\ \Gamma_{\boldsymbol{E}\boldsymbol{R}} & \Gamma_{\boldsymbol{E}\boldsymbol{E}} \end{bmatrix} \left(\begin{pmatrix} \boldsymbol{r} \\ \boldsymbol{e} \end{pmatrix} - \begin{pmatrix} \boldsymbol{\mu}_{\boldsymbol{R}} \\ \boldsymbol{\mu}_{\boldsymbol{E}} \end{pmatrix} \right)$$

$$p(\mathbf{r}) \propto \exp\left[-\frac{1}{2}(\mathbf{r} - \boldsymbol{\mu})^T \boldsymbol{\Sigma}^{-1}(\mathbf{r} - \boldsymbol{\mu})\right]$$
$$= \exp\left[-\frac{1}{2}(\mathbf{r} - \boldsymbol{\mu})^T \boldsymbol{\Gamma}(\mathbf{r} - \boldsymbol{\mu})\right]$$

$$= -\frac{1}{2} \begin{pmatrix} \mathbf{r} - \boldsymbol{\mu}_{R} \\ \mathbf{e} - \boldsymbol{\mu}_{E} \end{pmatrix}^{T} \begin{bmatrix} \Gamma_{RR} & \Gamma_{RE} \\ \Gamma_{ER} & \Gamma_{EE} \end{bmatrix} \begin{pmatrix} \mathbf{r} - \boldsymbol{\mu}_{R} \\ \mathbf{e} - \boldsymbol{\mu}_{E} \end{pmatrix}$$

$$=-\frac{1}{2}(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})^{T}\boldsymbol{\Gamma}_{\boldsymbol{R}\boldsymbol{R}}(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})-\frac{1}{2}2(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})^{T}\boldsymbol{\Gamma}_{\boldsymbol{R}\boldsymbol{E}}(\boldsymbol{e}-\boldsymbol{\mu}_{\boldsymbol{E}})-\frac{1}{2}(\boldsymbol{e}-\boldsymbol{\mu}_{\boldsymbol{E}})^{T}\boldsymbol{\Gamma}_{\boldsymbol{E}\boldsymbol{E}}(\boldsymbol{e}-\boldsymbol{\mu}_{\boldsymbol{E}})$$

$$\propto -\frac{1}{2}(r-\mu_R)^T \Gamma_{RR}(r-\mu_R) - (r-\mu_R)^T \Gamma_{RE}(e-\mu_E)$$
 Does not depend on r

$$=-\frac{1}{2}(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})^{T}\boldsymbol{\Gamma}_{\boldsymbol{R}\boldsymbol{R}}(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})-(\boldsymbol{r}-\boldsymbol{\mu}_{\boldsymbol{R}})^{T}\boldsymbol{\Gamma}_{\boldsymbol{R}\boldsymbol{E}}(\boldsymbol{e}-\boldsymbol{\mu}_{\boldsymbol{E}})-\boldsymbol{A}+\boldsymbol{A}$$

Use -A to get expression into the form $(r - \mu)^T \Gamma(r - \mu)$ by factoring out Γ_{RR}

$$A = \frac{1}{2} (\boldsymbol{e} - \boldsymbol{\mu}_{\boldsymbol{E}}) \Gamma_{\boldsymbol{E}\boldsymbol{R}} \Gamma_{\boldsymbol{R}\boldsymbol{R}}^{-1} \Gamma_{\boldsymbol{R}\boldsymbol{R}} \Gamma_{\boldsymbol{R}\boldsymbol{R}}^{-1} \Gamma_{\boldsymbol{R}\boldsymbol{E}} (\boldsymbol{e} - \boldsymbol{\mu}_{\boldsymbol{E}})$$

$$\exp\left[-\frac{1}{2}\left(\left(r-\mu_R+\Gamma_{RR}^{-1}\Gamma_{ER}(e-\mu_E)\right)^T\Gamma_{RR}\left(r-\mu_R+\Gamma_{RR}^{-1}\Gamma_{RE}(e-\mu_E)\right)\right)\right]\exp[A]$$

$$\propto \exp\left[-\frac{1}{2}\left(\left(r-\mu_R+\Gamma_{RR}^{-1}\Gamma_{ER}(e-\mu_E)\right)^T\Gamma_{RR}\left(r-\mu_R+\Gamma_{RR}^{-1}\Gamma_{ER}(e-\mu_E)\right)\right)\right]$$

$$\mu^* = \mu_R - \Gamma_R^{-1} \Gamma_{ER} (\boldsymbol{e} - \mu_E)$$

$$\Sigma^* = \Gamma_{RR}$$

Conditioning

- Conditioning a Gaussian on observations $m{E}=m{e}$ with remaining randvars R
- Result:

$$R|E = e \sim \mathcal{N}(\mu^*, \Sigma^*)$$

• Information form:

Covariance form:

•
$$\mu^* = \mu_R - \Gamma_R^{-1} \Gamma_{ER} (e - \mu_E)$$

•
$$\mu^* = \mu_R - \Gamma_R^{-1} \Gamma_{ER} (e - \mu_E)$$
 • $\mu^* = \mu_R + \Sigma_{RE} \Sigma_{EE}^{-1} (e - \mu_E)$

•
$$\Sigma^* = \Gamma_{RR}$$

$$\bullet \ \Sigma^* = \Sigma_{RR} - \Sigma_{RE} \Sigma_{EE}^{-1} \Sigma_{ER}$$

- Mean moved from μ_R according to correlation and variance on observations $\Sigma_{RE}\Sigma_{EE}^{-1}(e-\mu_E)$
- Covariance does not depend on observations e



Query Answering: Summary

- For marginalisation, read off parameters in covariance form
 - Marginal query for $T: \mathcal{N}(\mu_T; \Sigma_{TT})$
- For conditioning, one needs to invert the covariance matrix to obtain the information form
 - Conditioning on E = e: $R|E = e \sim \mathcal{N}(\mu^*, \Sigma^*)$
 - In covariance form
 - $\mu^* = \mu_R + \Sigma_{RE} \Sigma_{EE}^{-1} (\boldsymbol{e} \mu_E)$
 - $\Sigma^* = \Sigma_{RR} \Sigma_{RE} \Sigma_{EE}^{-1} \Sigma_{ER}$
 - Matrix inversion can be very costly!



Linear Gaussian Model

- Let S be a continuous randvar with continuous parents R_1, \dots, R_k
- S has a linear Gaussian model if there are parameters $\beta_0, ..., \beta_k$ and σ^2 such that $p(S|r_1, ..., r_k) = \mathcal{N}(\beta_0 + \beta_1 r_1 + \cdots + \beta_k r_k; \sigma^2) = \mathcal{N}(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{r}; \sigma^2) \longleftarrow$ (vector notation)
 - $p(S|r_1,...,r_k)$ a conditional probability distribution (CPD)
 - Interpretations
 - β_0 is an initial mean μ_0 that is moved according to the influences by the parents
 - S is a linear function of $R_1, ..., R_k$ with the addition of Gaussian noise: $S = \beta_0 + \beta_1 r_1 + \cdots + \beta_k r_k + \epsilon$
 - ϵ a Gaussian randvar with mean 0 and variance σ^2 , representing the noise in the system
 - Does not allow σ^2 to depend on parent values
 - But can be a useful approximation



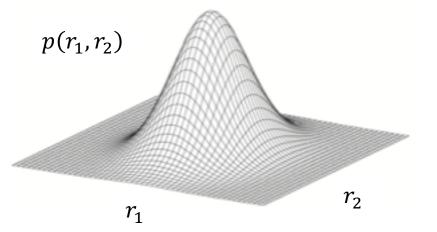
Independencies in Gaussians

- Let randvars R_1, \dots, R_n have a joint distribution $\mathcal{N}(\boldsymbol{\mu}; \Sigma)$
- Then, R_i , R_j independent iff $\Sigma_{ij}=0$
 - Joint distribution needs to be Gaussian for this equivalence to hold
 - If the distribution is not Gaussian, $\Sigma_{ij}=0$ might be the case and there still might be a dependence between R_i , R_j
- Conditional independence can be read of in the inverse of the covariance matrix, Σ^{-1}
 - Given a Gaussian distribution $p(r_1, ..., r_n) = \mathcal{N}(\boldsymbol{\mu}; \boldsymbol{\Sigma})$
 - Then, $\Sigma_{ij}^{-1} = 0$ iff $p \models (R_i \perp R_j | \{R_1, \dots, R_n\} \setminus \{R_i, R_j\})$



Example

- Joint Standard Gaussian distribution over two randvars R_1 , R_2 , i.e.,
 - $\mu = (0 \quad 0)^T$, $\Sigma = I_2$
 - R_1 , R_2 independent as $\Sigma_{ij} = \Sigma_{ji} = 0$



- Gaussian for R_1 , R_2 , R_3 from before
 - Covariance and inverse covariance matrix:

$$\Sigma = \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix} \quad \Sigma^{-1} = \begin{pmatrix} 0.3125 & -0.125 & 0 \\ -0.125 & 0.5833 & 0.3333 \\ 0 & 0.3333 & 0.3333 \end{pmatrix}$$

- R_1 , R_3 conditionally independent given R_2
- $\Sigma_{13}^{-1} = 0$ iff

$$p \models (R_1 \perp R_3 | \{R_1, R_2, R_3\} \setminus \{R_1, R_3\}) = (R_1 \perp R_3 | R_2)$$

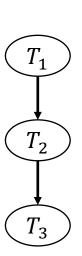


Gaussian Bayesian Network (GBN)

- Factorisation of a joint distribution into factors also possible with linear Gaussians as local CPDs
- A BN is a directed acyclic graph G whose nodes are discrete randvars $\{R_1, \ldots, R_n\}$ and whose full joint P_G factorises according to the local CPTs, i.e.,

$$P_G = \prod_i P(R_i | parents(R_i))$$

- Gaussian BN is a BN where
 - R_i are continuous randvars
 - All CPDs are linear Gaussians
 - E.g., $T_1 \rightarrow T_2 \rightarrow T_3$ (also depicted right)
 - $p(T_1) = \mathcal{N}(1; 4)$
 - $p(T_2|T_1) = \mathcal{N}(-3.5 + 0.5 \cdot T_1; 4)$
 - $p(T_3|T_2) = \mathcal{N}(1 + (-1) \cdot T_2; 3)$





Connection to Multivariate Gaussian

- Linear GBN an alternative representation to multivariate Gaussian distribution
 - A linear Gaussian BN always defines a joint multivariate Gaussian distribution
- Let S be a linear Gaussian of its parents R_1, \dots, R_k
 - $\mathcal{N}(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{r}; \sigma^2) = \mathcal{N}(\beta_0 + \beta_1 r_1 + \dots + \beta_k r_k; \sigma^2)$
 - $R_1, ..., R_k$ jointly Gaussian with $\mathcal{N}(\boldsymbol{\mu}; \boldsymbol{\Sigma})$
- Distribution of S is a Gaussian $p(S) = \mathcal{N}(\mu_S; \sigma_S^2)$ with $\mu_S = \beta_0 + \boldsymbol{\beta}^T \boldsymbol{r}$ $\sigma_S^2 = \sigma^2 + \boldsymbol{\beta}^T \Sigma \boldsymbol{\beta}$
- Joint distribution over $\{R_1, ..., R_k, S\}$ is a Gaussian with

$$Cov[R_i; S] = \sum_{j=1}^{\infty} \beta_j \Sigma_{ij}$$



General Procedure for Conversion

- Let $(R_1, ..., R_n)$ be the randvars of a GBN
 - Each R_i is a Gaussian $\mathcal{N}(\beta_0 + \boldsymbol{\beta}^T \boldsymbol{r}; \sigma^2)$ conditional on its parents $parents(R_i)$
 - $(R_1, ..., R_n)$ follows a topological ordering θ s.t. $\forall R_j \in \{R_1, ..., R_n\} : \forall R_i \in parents(R_j) : R_i \prec_{\theta} R_j$
 - Build a matrix $B^{n \times n}$ that has a non-zero entry β_{ij} if there exists a parent-child relation $R_i \to R_j$ with β_{ij} being the factor for R_i in the β of R_j

$$B = \begin{pmatrix} 0 & \beta_{12} & \dots & \beta_{1n} \\ 0 & 0 & \dots & \beta_{2n} \\ \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix}$$

- i chooses the row(s), j chooses the column(s)
- B is upper-triangular because no loops allowed in BNs
 - Including self-loops $\rightarrow \beta_{ii} = 0$ as well



General Procedure for Conversion

- Joint distribution $p(r_1, ..., r_n)$ given by $\mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$
 - Means

$$\boldsymbol{\mu} = \left(\mu_1, \beta_{0,2} + \boldsymbol{\beta}_2^T \boldsymbol{r}, ..., \beta_{0,n} + \boldsymbol{\beta}_n^T \boldsymbol{r}\right)^T$$

• Covariance (recursive rules): $j \in \{2, ..., n\}, i = 1 ... j - 1$

$$\Sigma_{11} \leftarrow \sigma_1^2$$

$$\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$$

$$\Sigma_{ji} \leftarrow \Sigma_{ij}^T$$

$$\Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij}$$

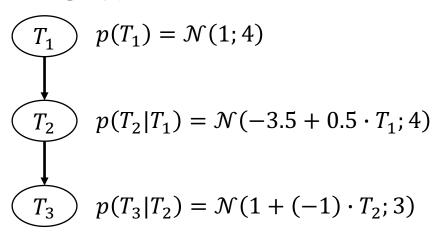
- First index chooses the row(s), second index chooses the column(s)
- given B

filling Σ layer-wise:

$$B = \begin{pmatrix} 0 & \beta_{12} & \dots & \beta_{1n} \\ 0 & 0 & & & \beta_{2n} \\ \vdots & \ddots & \vdots \\ 0 & 0 & \dots & 0 \end{pmatrix} \qquad \Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \dots & \Sigma_{1n} \\ \Sigma_{21} & \Sigma_{22} & & & \Sigma_{2n} \\ \vdots & \ddots & \vdots \\ \Sigma_{n1} & \Sigma_{n2} & \dots & \Sigma_{nn} \end{pmatrix}$$

GBN: Conversion Example

• GBN



Goal: Joint distribution

$$p(t_{1}, t_{2}, t_{3}) = \mathcal{N}(\mu; \Sigma)$$

$$\mu = \begin{pmatrix} \mu_{1} \\ \mu_{2} \\ \mu_{3} \end{pmatrix}$$

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

Matrix B

- B_{12} : $T_1 \to T_2$, $\beta_1 = 0.5$
- B_{23} : $T_2 \to T_3$, $\beta_1 = -1$
- Rest: zeroes
- Result:

$$\bullet \ B = \begin{pmatrix} 0 & 0.5 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

Means

- $\mu_1 = 1$
- $\mu_2 = -3.5 + 0.5 \cdot \mu_1 = -3$
- $\mu_3 = 1 + (-1) \cdot \mu_2 = 4$
- Result:

•
$$\mu = \begin{pmatrix} 1 \\ -3 \\ 4 \end{pmatrix}$$



GBN: Conversion Example

• Filling Σ :

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix} \quad \bullet \quad j = 2, i = 1$$

 Need B and the recursive rules

$$B = \begin{pmatrix} 0 & 0.5 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Sigma_{11} \leftarrow \sigma_1^2$$

$$\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$$

$$\Sigma_{ji} \leftarrow \Sigma_{ij}^T$$

$$\Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij}$$

- First index: row(s)
- Second index: column(s)

•
$$\Sigma_{11} = \sigma_1^2 = 4$$

•
$$j = 2, i = 1$$

•
$$\Sigma_{12}$$

= $\Sigma_{11}B_{12}$
= $4 \cdot 0.5$
= 2

$$\Sigma_{21} = \Sigma_{12}^T$$

$$= 2^T$$

$$= 2$$

•
$$\Sigma_{22}$$

= $\sigma_2^2 + \Sigma_{21}B_{12}$
= $4 + 2 \cdot 0.5$
= 5

$$\begin{pmatrix} 4 & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & \Sigma_{13} \\ 2 & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & \Sigma_{13} \\ 2 & 5 & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$



GBN: Conversion Example

Remaining goal:

$$\Sigma = \begin{pmatrix} \Sigma_{11} & \Sigma_{12} & \Sigma_{13} \\ \Sigma_{21} & \Sigma_{22} & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

 Need B and the recursive rules

$$B = \begin{pmatrix} 0 & 0.5 & 0 \\ 0 & 0 & -1 \\ 0 & 0 & 0 \end{pmatrix}$$

$$\Sigma_{11} \leftarrow \sigma_1^2$$

$$\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$$

$$\Sigma_{ji} \leftarrow \Sigma_{ij}^T$$

$$\Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij}$$

- First index: row(s)
- Second index: column(s)

•
$$j = 3, i = 12$$

•
$$\Sigma_{(12)3}$$

= $\Sigma_{(12)(12)}B_{(12)3}$
= $\binom{4}{2}\binom{0}{-1}$
= $\binom{-2}{-5}$

$$\Sigma_{3(12)} = \Sigma_{(12)3}^{T}$$

$$= \begin{pmatrix} -2 \\ -5 \end{pmatrix}^{T}$$

$$= (-2 -5)$$

•
$$\Sigma_{33}$$

= $\sigma_3^2 + \Sigma_{3(12)} B_{(12)3}$
= $3 + (-2 -5) \begin{pmatrix} 0 \\ -1 \end{pmatrix} \begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & 8 \end{pmatrix}$
= $3 + 5 = 8$

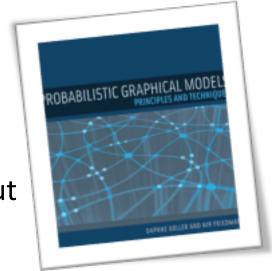
$$\begin{pmatrix} 4 & 2 & \Sigma_{13} \\ 2 & 5 & \Sigma_{23} \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ \Sigma_{31} & \Sigma_{32} & \Sigma_{33} \end{pmatrix}$$

$$\begin{pmatrix} 4 & 2 & -2 \\ 2 & 5 & -5 \\ -2 & -5 & \Sigma_{33} \end{pmatrix}$$

Inference in GBNs

- Inference in linear Gaussians with Variable Elimination
 - Representation through linear Gaussian CPDs instead of CPTs/factors
 - Modified operations for multiply/sum-out
- Message passing formulation
 - Approximate belief propagation
- Sampling in the continuous space
 - Rejection sampling, importance sampling, MCMC methods for GBNs
- Actually using the full joint
 - Marginalisation, conditioning as sketched in Basics



See Ch. 14 of PGM book for further information

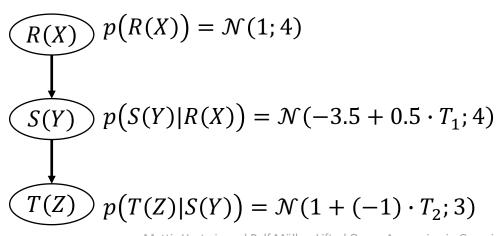


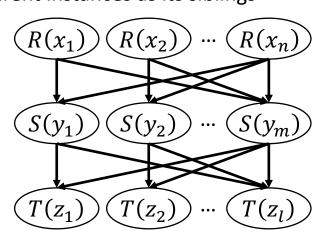
Lifting the Full Joint

- Lifting conversion approach by Shachter and Kenley for parameterised GBNs
 - GBN with PRVs A_1, \dots, A_m as nodes
 - PDF for each A_i applies to each $R \in gr(A_i)$
 - $m \ll n, n = |\bigcup_i gr(A_i)|$
 - Semantics: grounding and forming full joint $p(\bigcup_i gr(A_i))$
 - Simple case for GBNs (general case under review):

For all parent-child relations
$$R(X) \rightarrow S(Y)$$
, it holds that $X \cap Y = \emptyset$

Each child instance has the same parent instances as its siblings





 $\Sigma_{11} \leftarrow \sigma_1^2$

 $\Sigma_{ii} \leftarrow \Sigma_{ii}^T$

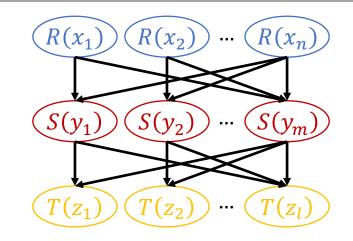
 $\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$

 $\Sigma_{ij} \leftarrow \sigma_i^2 + \Sigma_{ii} B_{ij}$



Lifting the Full Joint: Simple Case

- With PRVs, matrix B and covariance matrix have liftable blocks for each PRV
 - Given the case of no overlaps in logvars: *B*

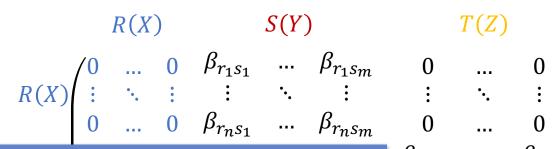


		R(X))	S(Y)			T(Z)		
	/ 0		0	$\beta_{r_1s_1}$		$\beta_{r_1s_m}$	0		0 \
R(X)		•.	•	:	٠.	:	•	•.	: \
	0		0	$\beta_{r_n s_1}$		$\beta_{r_n s_m}$	0		0
	0		0	0		0			$\beta_{s_1t_l}$
S(Y)	:	٠.	:	•	•	:	•	٠.	:
	0	•••	0	0		0	$\beta_{s_m t_1}$	•••	$\beta_{s_m t_l}$
	0		0	0		0	0		0
T(Z)	\ :	٠.	:	•	•.	:		٠.	:]
	/0		0	0		0	0		0 /



Lifting the Full Joint: Simple Case

- With PRVs, matrix B and covariance matrix have liftable blocks for each PRV
 - Given the case of no overlaps in logvars: B

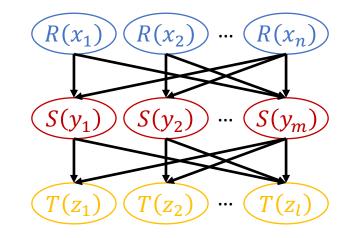


Each $R(x_i)$ has the same influence on each $S(y_i)$. Given $P(s(Y)|r(X)) = \mathcal{N}(\beta_0 + \beta_1 r(X); \sigma^2)$,

$$\beta_{r_i s_j} = \beta_1$$

for all $i \in \{1, ..., n\}, j \in \{1, ..., m\}$.

The same holds for $S(y_i)$ and $T(z_k)$ (as well as $R(x_i)$ and $T(z_k)$, which has $\beta_{r_i t_k} = 0$).



T(Z)

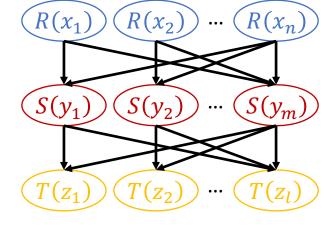
Lifted
$$B'$$

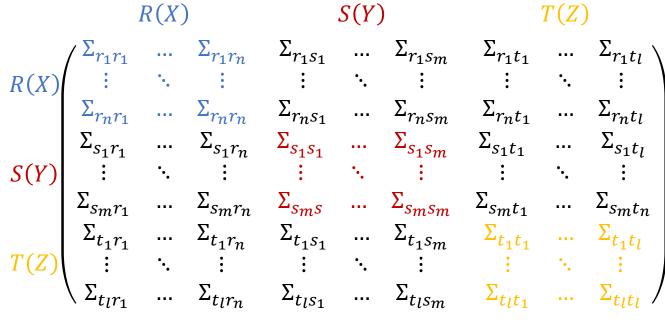
$$\begin{pmatrix} 0 & \beta_{rs} & 0 \\ 0 & 0 & \beta_{st} \\ 0 & 0 & 0 \end{pmatrix}$$

Lifted
$$B'$$

$$\begin{pmatrix}
0 & 0.5 & 0 \\
0 & 0 & -1 \\
0 & 0 & 0
\end{pmatrix}$$

- With PRVs, matrix B and covariance matrix have liftable blocks for each PRV
 - Given the case of no overlaps in logvars: Σ







$$\begin{pmatrix} \Sigma_{r_1r_1} & \dots & \Sigma_{r_1r_n} & \Sigma_{r_1s_1} & \dots & \Sigma_{r_1s_m} & \Sigma_{r_1t_1} & \dots & \Sigma_{r_1t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \Sigma_{r_nr_1} & \dots & \Sigma_{r_nr_n} & \Sigma_{r_ns_1} & \dots & \Sigma_{r_ns_m} & \Sigma_{r_nt_1} & \dots & \Sigma_{r_nt_l} \\ \Sigma_{s_1r_1} & \dots & \Sigma_{s_1r_n} & \Sigma_{s_1s_1} & \dots & \Sigma_{s_1s_m} & \Sigma_{s_1t_1} & \dots & \Sigma_{s_1t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \Sigma_{s_mr_1} & \dots & \Sigma_{s_mr_n} & \Sigma_{s_ms} & \dots & \Sigma_{s_ms_m} & \Sigma_{s_mt_1} & \dots & \Sigma_{s_mt_n} \\ \Sigma_{t_1r_1} & \dots & \Sigma_{t_1r_n} & \Sigma_{t_1s_1} & \dots & \Sigma_{t_1s_m} & \Sigma_{t_1t_1} & \dots & \Sigma_{t_1t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \Sigma_{t_lr_1} & \dots & \Sigma_{t_lr_n} & \Sigma_{t_ls_1} & \dots & \Sigma_{t_ls_m} & \Sigma_{t_lt_1} & \dots & \Sigma_{t_lt_l} \end{pmatrix}$$

$$\Sigma_{r_1 r_1} = \sigma_{R(X)}^2$$

$$\Sigma_{r_1 r_2} = \sigma_{R(X)}^2 B_{r_1 r_2} = \sigma_{R(X)}^2 B'_{11} = \sigma_{R(X)}^2 \cdot 0 = 0$$

$$\Sigma_{r_2 r_1} = 0$$

$$\Sigma_{r_2 r_2} = \sigma_{R(X)}^2 + \Sigma_{r_2 r_1} B_{r_1 r_2} = \sigma_{R(X)}^2 + 0 = \sigma_{R(X)}^2$$
...

$$R(X)$$

$$R(X) \stackrel{\sigma_{R(X)}^{2}}{\vdots} \quad \dots \quad 0 \qquad 4 \quad \dots \quad 0$$

$$R(X) \stackrel{\vdots}{\vdots} \quad \ddots \quad \vdots \quad = \vdots \quad \ddots \quad \vdots \quad \rightarrow \text{on-diagonal: } \sigma_{R(X)}^{2}$$

$$0 \quad \dots \quad \sigma_{R(X)}^{2} \quad 0 \quad \dots \quad 4 \quad \text{off-diagonal: } 0$$

$$\Sigma_{11} \leftarrow \sigma_1^2$$

$$\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$$

$$\Sigma_{ji} \leftarrow \Sigma_{ij}^T$$

$$\Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij}$$

Lifted
$$B'$$

$$\begin{pmatrix} 0 & \beta_{rs} & 0 \\ 0 & 0 & \beta_{st} \\ 0 & 0 & 0 \end{pmatrix}$$



$$\begin{pmatrix} \sigma_{R(X)}^2 & \dots & 0 & \sum_{r_1 S_1} & \dots & \sum_{r_1 S_m} & \sum_{r_1 t_1} & \dots & \sum_{r_1 t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{R(X)}^2 & \sum_{r_n S_1} & \dots & \sum_{r_n S_m} & \sum_{r_n t_1} & \dots & \sum_{r_n t_l} \\ \sum_{S_1 r_1} & \dots & \sum_{S_1 r_n} & \sum_{S_1 S_1} & \dots & \sum_{S_1 S_m} & \sum_{S_1 t_1} & \dots & \sum_{S_1 t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \sum_{S_m r_1} & \dots & \sum_{S_m r_n} & \sum_{S_m S} & \dots & \sum_{S_m S_m} & \sum_{S_m t_1} & \dots & \sum_{S_m t_n} \\ \sum_{t_1 r_1} & \dots & \sum_{t_1 r_n} & \sum_{t_1 s_1} & \dots & \sum_{t_1 s_m} & \sum_{t_1 t_1} & \dots & \sum_{t_1 t_l} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \sum_{t_l r_1} & \dots & \sum_{t_l r_n} & \sum_{t_l s_1} & \dots & \sum_{t_l s_m} & \sum_{t_l t_1} & \dots & \sum_{t_l t_l} \end{pmatrix}$$

$$\begin{split} & \Sigma_{(r_1 \dots r_n)s_1} \\ &= \Sigma_{(r_1 \dots r_n)(r_1 \dots r_n)} B_{(r_1 \dots r_n)s_1} \\ &= \begin{pmatrix} \sigma_{R(X)}^2 & \dots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \dots & \sigma_{R(X)}^2 \end{pmatrix} \begin{pmatrix} \beta_{rs} \\ \vdots \\ \beta_{rs} \end{pmatrix} = \begin{pmatrix} \sigma_{R(X)}^2 \beta_{rs} \\ \vdots \\ \sigma_{R(X)}^2 \beta_{rs} \end{pmatrix} = \begin{pmatrix} 4 \cdot 0.5 \\ \vdots \\ 4 \cdot 0.5 \end{pmatrix} = \begin{pmatrix} 2 \\ \vdots \\ 2 \end{pmatrix} \begin{bmatrix} \Sigma_{11} \leftarrow \sigma_1^2 \\ \Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij} \\ \Sigma_{ji} \leftarrow \Sigma_{ij}^T \\ \Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij} \end{bmatrix} \end{split}$$

$$\Sigma_{11} \leftarrow \sigma_1^2$$

$$\Sigma_{ij} \leftarrow \Sigma_{ii} B_{ij}$$

$$\Sigma_{ji} \leftarrow \Sigma_{ij}^T$$

$$\Sigma_{jj} \leftarrow \sigma_j^2 + \Sigma_{ji} B_{ij}$$

$$\begin{split} & \sum_{S_1 S_1} \\ & = \sigma_{S(Y)}^2 + \sum_{S_1(r_1 \dots r_n)} B_{(r_1 \dots r_n) S_1} \\ & = \sigma_{S(Y)}^2 + \left(\sigma_{R(X)}^2 \beta_{rs} \quad \dots \quad \sigma_{R(X)}^2 \beta_{rs}\right) \begin{pmatrix} \beta_{rs} \\ \vdots \\ \beta_{rs} \end{pmatrix} = \sigma_{S(Y)}^2 + n \sigma_{R(X)}^2 \beta_{rs}^2 \end{split} \qquad \begin{array}{c} \text{Lifted } B' \\ \begin{pmatrix} 0 & \beta_{rs} & 0 \\ 0 & 0 & \beta_{st} \\ 0 & 0 & 0 \end{pmatrix} \\ & = 4 + n \cdot 4 \cdot 0.5^2 = 4 + n \end{split}$$





$$\begin{split} & \Sigma_{(r_1 \dots r_n s_1) s_2} \\ & = \Sigma_{(r_1 \dots r_n s_1) (r_1 \dots r_n s_1) B}(r_1 \dots r_n s_1) s_2 \\ & = \begin{pmatrix} \sigma_{R(X)}^2 & \dots & 0 & \sigma_{R(X)}^2 \beta_{rs} \\ \vdots & \ddots & \vdots & & \vdots \\ 0 & \dots & \sigma_{R(X)}^2 & \sigma_{R(X)}^2 \beta_{rs} \\ \sigma_{R(X)}^2 \beta_{rs} & \dots & \sigma_{R(X)}^2 \beta_{rs} \end{pmatrix} \begin{pmatrix} \beta_{rs} \\ \vdots \\ \beta_{rs} \\ 0 & \dots & \sigma_{R(X)}^2 & \sigma_{S(Y)}^2 + n \sigma_{R(X)}^2 \beta_{rs}^2 \end{pmatrix} \begin{pmatrix} \beta_{rs} \\ \vdots \\ \beta_{rs} \\ 0 \end{pmatrix} = \begin{pmatrix} \sigma_{R(X)}^2 \beta_{rs} & \dots & \sigma_{R(X)}^2 \beta_{rs} & \sigma_{S(Y)}^2 + n \sigma_{R(X)}^2 \beta_{rs}^2 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ \beta_{rs} & \dots & \sum_{r_n s_n} & \sum_{s_n t_1} \dots & \sum_{t_n t_1} \dots & \sum_{t_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n s_n} t_n \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n s_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n s_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n s_n} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_n t_1} \dots & \sum_{s_n t_n} & \sum_{s_n t_1} \dots & \sum_{s_n t_n} \\ \sum_{s_$$

 $= \sigma_{S(Y)}^2 + n\sigma_{R(X)}^2 \beta_{rs}^2 = 4 + n$



```
T(Z) \\ \sigma_{T(Z)}^{2} + m\beta_{st}^{2} \left(\sigma_{S(Y)}^{2} + mn\sigma_{R(X)}^{2}\beta_{rs}^{2}\right) & \dots & m\beta_{st}^{2} \left(\sigma_{S(Y)}^{2} + mn\sigma_{R(X)}^{2}\beta_{rs}^{2}\right) \\ T(Z) & \vdots & \ddots & \vdots \\ m\beta_{st}^{2} \left(\sigma_{S(Y)}^{2} + mn\sigma_{R(X)}^{2}\beta_{rs}^{2}\right) & \dots & \sigma_{T(Z)}^{2} + m\beta_{st}^{2} \left(\sigma_{S(Y)}^{2} + mn\sigma_{R(X)}^{2}\beta_{rs}^{2}\right) \\ \end{pmatrix}
                    on-diagonal: \sigma_{T(Z)}^2 + m\beta_{st}^2 (\sigma_{S(Y)}^2 + mn\sigma_{R(X)}^2 \beta_{rs}^2) = 3 + 4m + m^2n
              \rightarrow off-diagonal: m\beta_{st}^2(\sigma_{S(Y)}^2 + mn\sigma_{R(X)}^2\beta_{rs}^2) = 4m + m^2n
```

Lifted Joint

- Only two structures required for covariance matrix
 - A matrix

$$R(X) \qquad S(Y) \qquad T(Z)$$

$$R(X) \begin{pmatrix} 0 & \sigma_{R(X)}^2 \beta_{rs} & m \sigma_{R(X)}^2 \beta_{rs} \beta_{st} \\ \sigma_{R(X)}^2 \beta_{rs} & n \sigma_{R(X)}^2 \beta_{rs}^2 & (\sigma_{S(Y)}^2 + m n \sigma_{R(X)}^2 \beta_{rs}^2) \beta_{st} \\ T(Z) \begin{pmatrix} m \sigma_{R(X)}^2 \beta_{rs} \beta_{st} & (\sigma_{S(Y)}^2 + m n \sigma_{R(X)}^2 \beta_{rs}^2) \beta_{st} & m \beta_{st}^2 (\sigma_{S(Y)}^2 + m n \sigma_{R(X)}^2 \beta_{rs}^2) \end{pmatrix}$$

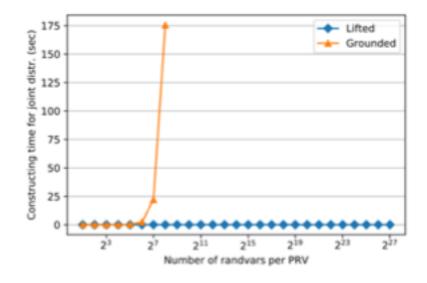
$$= \begin{pmatrix} 4 & 2 & -2m \\ 2 & n & -4 - mn \\ -2m & -4 - mn & 4m + m^2n \end{pmatrix}$$

- A vector for on-diagonal covariance entries
 - Individual variances
 - Have to be stored anyway

$$\begin{array}{l}
R(X) \left(\sigma_{R(X)}^{2}\right) \\
S(Y) \left(\sigma_{S(Y)}^{2}\right) \\
T(Z) \left(\sigma_{T(Z)}^{2}\right)
\end{array} = \begin{pmatrix} 4 \\ 4 \\ 3 \end{pmatrix}$$

Lifted Joint

- Only two structures required for covariance matrix
- Depend only on the number of PRVs, not the domain sizes!

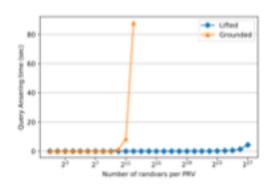


Lifted Query Answering

- Marginal queries
 - Read off values in (lifted) covariance representation
- Conditional queries $R|E=e\sim\mathcal{N}(\mu^*,\Sigma^*)$

•
$$\mu^* = \mu_R + \Sigma_{RE} \Sigma_{EE}^{-1} (e - \mu_E)$$

- $\Sigma^* = \Sigma_{RR} \Sigma_{RE} \Sigma_{EE}^{-1} \Sigma_{ER}$
- Matrix multiplication, inversion required
 - Possible to compute them in a lifted manner due to block structure
 - Proof in paper by Hartwig and Möller (2020)
- Evidence is ground
 - Probably no symmetries in observations with real numbers as range values
 - → unlikely to get identical observations
 - Fig.: 50% of ground instances get random values assigned as evidence





Interim Summary

Linear Gaussian models

- Linear dependency between child and parent randvars
- Full joint given by vector of means and covariance matrix
 - Information form as inverse of covariance form
- Query answering
 - Marginal using covariance matrix
 - Conditional using information form

Gaussian BNs

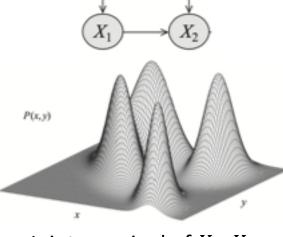
- Explicitly encode independencies in network structure
 - Conditional linear Gaussian
- GBN = multivariate Gaussian distribution
- Lifting for PRVs without an overlap in logvars between parent and child



Hybrid Models

• Models that contain discrete (D_i in fig.) and continuous randvars (X_i in fig.)

- Some general results
 - Even representing the correct marginal distribution in a hybrid network can require space that is exponential in the size of the network
 - Query answering problem is NP-hard even if the GBN is a polytree where all discrete randvars are Boolean-valued and where every continuous randvar has at most one discrete ancestor



Joint marginal of X_1, X_2

 There are not even approximate algorithms to solve the problem in polynomial time with a useful error bound without further restrictions



Outline: 8. Continuous Space

A. Basics

- Continuous variables, probability density function, cumulative probability distribution
- Joint distribution, marginal density, conditional density

B. Gaussian models

- (Multivariate) Gaussian distribution
- (Parameterised) Gaussian Bayesian networks

C. Probabilistic Soft Logic (PSL)

Modelling, semantics, inference task

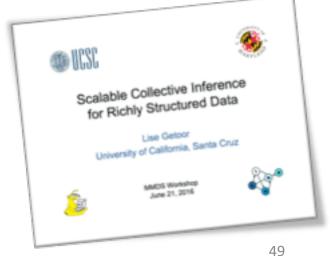


Probabilistic Soft Logic (PSL)

- Logic-based approach
- Probabilistic programming language
 - Predicate = relationship or property
 - Atom = continuous randvar
 - Rule = dependency or constraint
 - Set = define aggregates
- PSL program = rules + input database
- Implementation: https://psl.linqs.org

Based on slides by Lise Getoor, "Scalable Collective Inference for Richly Structured Data", MMDS Workshop 2016.





Syntax & Semantics

• Let ${\bf R}$ be a set of weighted logical rules, each R_j has the form

$$w_j: \bigwedge_{i \in I_j^-} x_i \Rightarrow \bigvee_{i \in I_i^+} x_i$$

- $w_i \geq 0$
- Sets I_i^- , I_i^+ index conjuncted/disjuncted literals
- Equivalent clausal form:

$$\left(\bigvee_{i\in I_j^+} x_i\right) \vee \left(\bigvee_{i\in I_j^-} \neg x_i\right)$$

Probability distribution (compare: MLNs)

$$P(\mathbf{x}) \propto \exp\left(\sum_{R_j \in \mathbf{R}} w_j \left(\bigvee_{i \in I_j^+} x_i\right) \vee \left(\bigvee_{i \in I_j^-} \neg x_i\right)\right)$$



MPE Inference

- MPE: Find the most probable assignment to the unobserved randvars
 - I.e., given a model ground over an input database,

$$\underset{\boldsymbol{x}}{\operatorname{argmax}} \sum_{R_j \in \boldsymbol{R}} w_j \left(\bigvee_{i \in I_j^+} x_i \right) \vee \left(\bigvee_{i \in I_j^-} \neg x_i \right)$$

Combinatorial, NP-hard

Approximation:
 View as optimising rounding probabilities



Expected Score

 Expected score of a clause is the weight times the probability that at least one literal is true:

$$w_j \left(1 - \prod_{i \in I_j^+} (1 - p_i) \prod_{i \in I_j^-} p_i \right)$$

At least one literal true \rightarrow or-semantics \rightarrow trick: Instead of computing $P(A \lor B)$ $= P(A) + P(B) - P(A \land B)$ compute $P(\neg \neg (A \lor B))$ $= 1 - P(\neg A \land \neg B)$

• Then, expected total score is

$$\widehat{W} = \sum_{R_j \in \mathbb{R}} w_j \left(1 - \prod_{i \in I_j^+} (1 - p_i) \prod_{i \in I_j^-} p_i \right)$$

• But, $\underset{p}{\operatorname{argmax}} \widehat{W}$ highly non-convex due to product



Approximate Inference

 Instead: Optimise a linear program that bounds expected score

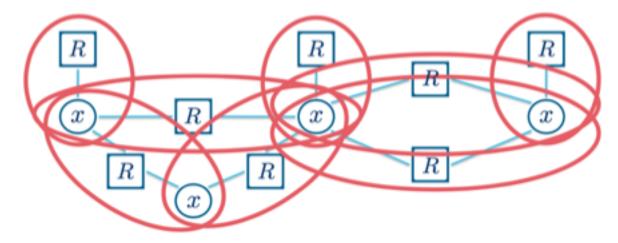
$$\sum_{R_{j} \in \mathbb{R}} w_{j} \left(1 - \prod_{i \in I_{j}^{+}} (1 - p_{i}) \prod_{i \in I_{j}^{-}} p_{i} \right) \geq \left(1 - \frac{1}{e} \right) \sum_{R_{j} \in \mathbb{R}} w_{j} \min \left\{ \sum_{i \in I_{j}^{+}} p_{i} + \sum_{i \in I_{j}^{-}} (1 - p_{i}), 1 \right\}$$

• Can give $\left(1 - \frac{1}{e}\right)$ -optimal *discrete* solution



Scalable Approximate Inference

 Linear programming algorithms do not scale well to big probabilistic models

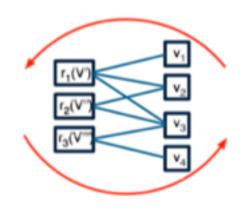


- Instead of solving the problem as one big optimisation, decompose the problem based on its graphical structure
 - Compare: cliques/clusters



Consensus Optimisation

- Decompose problem and solve sub-problems independently (in parallel), then merge results
 - Sub-problems are ground rules
 - Auxiliary variables enforce consensus across sub-problems



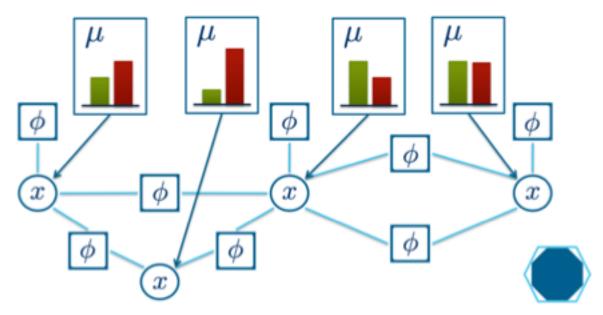
- Framework:
 Alternating direction method of multipliers
 (ADMM) (Boyd, 2011)
 - Guaranteed to converge for convex problems
 - Inference with ADMM fast, scalable, straightforward to implement (Bach et al, 2017)



Local Consistency Relaxation

Relax search over consistent marginals to simpler set

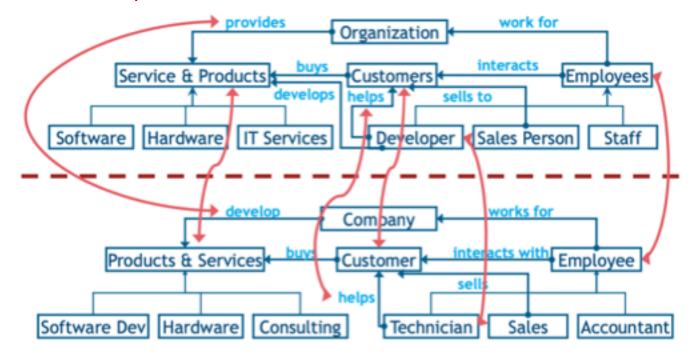
$$\underset{\mu \in [0,1]^n}{\operatorname{argmax}} \sum_{R_j \in R} w_j \min \left\{ \sum_{i \in I_j^+} \mu_i + \sum_{i \in I_j^-} (1 - \mu_i), 1 \right\}$$





Continuous Variables & Similarity

- Continuous values interpreted as similarities
 - E.g., multiple ontologies → alignment
 - Match/Don't match → similar to what extent?



⇒ Soft logic



Soft Logic

- Logical operators defined for continuous values in the $\left[0,1\right]$ interval
 - Interpret as similarities or degree of truth
- Łukasiewicz logic
 - $p \wedge q = \max\{p + q 1, 0\}$
 - $p \lor q = \min\{p + q, 1\}$
 - $\neg p = 1 p$
- PSL: Use Łukasiewicz logic to interpret rules
 - Hinge-loss MNs (or Markov random fields as called in the publications by the PSL team) formalise this



Hinge-loss MNs

- Relaxed, logic-based MNs can reason about both discrete and continuous graph data scalably and accurately
 - General objective $\underset{y \in [0,1]^n}{\operatorname{argmax}} P(y)$ $= \underset{y \in [0,1]^n}{\operatorname{argmax}} \sum_{j=1}^m w_j \min \left\{ \sum_{i \in I_j^+} y_i + \sum_{i \in I_j^-} (1 y_i), 1 \right\}$ $= \underset{y \in [0,1]^n}{\operatorname{argmin}} \sum_{j=1}^m w_j \max \left\{ 1 \sum_{i \in I_j^+} y_i \sum_{i \in I_i^-} (1 y_i), 0 \right\}$
 - Notion of distance to satisfaction

Distance to Satisfaction

$$\underset{y \in [0,1]^n}{\operatorname{argmin}} \sum_{j=1}^m w_j \max \left\{ 1 - \sum_{i \in I_j^+} y_i - \sum_{i \in I_j^-} (1 - y_i), 0 \right\}$$

- Maximum value of any unweighted term is 1
 - Term is satisfied
- Unsatisfied term → distance to satisfaction
 - How far it is from achieving its maximum value
 - Each unweighted objective term measures how far the linear constraint is away from being satisfied:

$$1 - \sum_{i \in I_i^+} y_i - \sum_{i \in I_j^-} (1 - y_i) \le 0$$

Relaxed Linear Constraints

• Instead of requiring logical clauses, each term can be defined using any function $\ell_j(y)$ linear in y

$$\underset{\mathbf{y} \in [0,1]^n}{\operatorname{argmin}} \sum_{j=1}^{n} w_j \max \left\{ \ell_j(\mathbf{y}), 0 \right\}$$

- Each term represents the distance to satisfaction of a linear constraint $\ell_i(y) \leq 0$
 - Can use logical clauses or something else based on domain knowledge
 - Also called hinge losses
 - Sometimes $\max\{\ell_j(y), 0\}$ gets squared to better trade off conflicting objective terms
- Weight indicates how important it is to satisfy a constraint relative to others by scaling the distance to satisfaction



Hinge-loss MNs

- Let $\mathbf{y} = (y_1, ..., y_n)$ be a vector of n randvars and $\mathbf{x} = (x_1, ..., x_{n'})$ be a vector of n' randvars with joint range $\mathbf{D} = [0,1]^{n+n'}$
- Let $\phi = (\phi_1, ..., \phi_m)$ be a vector of m continuous potentials of the form

$$\phi_j(\mathbf{y}, \mathbf{x}) = \left(\max\{\ell_j(\mathbf{y}, \mathbf{x}), 0\}\right)^{p_j}$$

- $\ell_i(y, x)$ linear function of y, x
- $p_i \in \{1,2\}$
- For $(y, x) \in D$ and given a vector of m weights $w = (w_1, ..., w_m)$, constrained hinge-loss energy function f_w is defined as

$$f_{w}(\mathbf{y}, \mathbf{x}) = \sum_{j=1}^{m} w_{j} \phi_{j}(\mathbf{y}, \mathbf{x})$$



Hinge-loss MNs

- Let $c = (c_1, ..., c_r)$ be a vector of linear constraint functions which further restrict the domain \mathbf{D} to \mathbf{D}'
- Hinge-loss MN over randvars y and conditioned on randvars x is a PDF defined as follows
 - if $(y, x) \notin D'$, then P(y|x) = 0
 - if $(y, x) \in D'$, then

$$P(\mathbf{y}|\mathbf{x}) = \frac{1}{Z(\mathbf{w}, \mathbf{x})} \exp(-f_{\mathbf{w}}(\mathbf{y}, \mathbf{x}))$$

where

$$Z(w, x) = \int_{y|(y,x)\in D'} \exp(-f_w(y, x)) dy$$

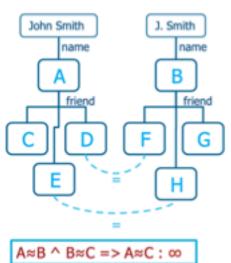
Define hinge-loss MNs using PSL

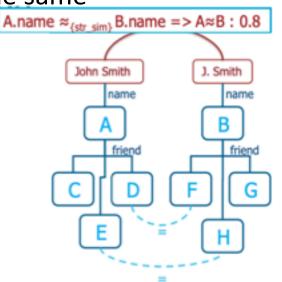


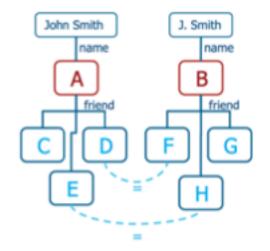
Application: E.g., Entity Resolution

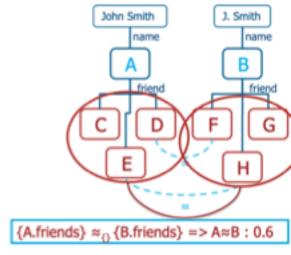
- Goal: Identify references that denote the same person
- Use model to express dependencies
 - "If A=B and B=C, then A and C must also denote the same person"
 - "If two people have similar names, they are probably the same"

 "If two people have similar friends, they are probably the same"











Interim Summary

- PSL
 - Logic programming language
 - Approximations
 - Linear program that bounds MPE solution from below
 - Decomposition of PGM to optimise set of subproblems (consensus optimisation)
 - Local consistency relaxation
 - Soft logic: Łukasiewicz logic
 - Interpret continuous values as similarities/degree of truth
- Hinge-loss MNs
 - Notion of distance to satisfaction
 - Define using PSL



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