



Overview



- 1. Bayesian Probabilities and Conjugacy
- 2. Graphical Models
- 3. The Sum-Product Algorithm
- 4. Bayesian Ranking: TrueSkill
- **5.** Information Theory
- **6.** Arithmetic Coding

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Overview

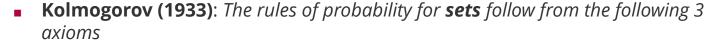


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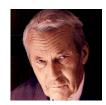
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Frequentist vs. Subjective Probabilities





- 1. $P(A) \ge 0$ for all $A \subseteq S$
- 2. P(S) = 1
- 3. $P(\bigcup_i A_i) = \sum_i P(A_i)$ if for all $i \neq j$: $A_i \cap A_j = \emptyset$
- Cox (1944): The rules of probability for **logic** follow from the following 3 axioms
 - 1. $P(A) \in [0,1]$ for all logical statements A
 - 2. P(A) is independent of how the statement is represented
 - 3. If P(A|C') > P(A|C) and $P(B|A \wedge C') = P(B|A \wedge C)$ then $P(A \wedge B|C') \ge P(A \wedge B|C)$



Andrey Kolmogorov (1903 - 1987)



Richard Threlkeld Cox (1898 - 1991)

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Frequentist vs. Subjectivist Interpretation



Frequentist Interpretation

- Probability is a property of the event ("it rains tomorrow in Bangalore")
- Is operationalized by repeated experiments
- Typically used by scientists and engineers

Subjective Interpretation

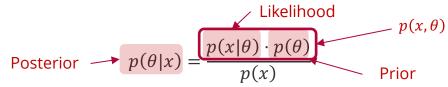
- Probability is an expression of belief of the person makes a statement
- Is subjective and people-dependent: Two people with identical data can come to different probabilities
- Typically used by philosophers and economists
- 1. Probability is not a physical measure but a thought model for randomness!
- 2. The mathematical rules for probability are **identical** for both interpretations!

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Probability Distributions: Conjugacy



■ Bayes Rule for Random Variables. For any probability distribution p over two random variables X and Θ , it holds



Conjugacy. A family $\{p(x,\theta)\}_{x,\theta}$ is conjugate if the posterior $p(\theta|x)$ is part of the same family as the prior $p(\theta)$ for any value of x.

Likelihood $p(x \theta)$	Model Parameter	Conjugate Prior $p(heta)$
$Ber(x;\pi)$	π	Beta $(\pi; \alpha, \beta)$
$Bin(x; n, \pi)$	π	Beta $(\pi; \alpha, \beta)$
$\mathcal{N}(x;\mu,\sigma^2)$	μ , σ^2	$\mathcal{N}(\mu; m, s^2)$



Howard Raiffa (1924 - 2016)



Robert Osher Schlaifer (1914 – 1994)

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Unit 13a – Bayesianische Statistik

■ **Big Advantage**: Computing the exact posterior is computationally efficient!

Probability Distributions: Normal



 Normal Distribution. A continuous random variable X is said to have a normal distribution if the density is given by

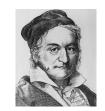
$$p_X(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

$$E[X] = \mu$$

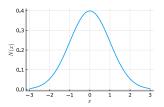
$$var[X] = \sigma^2$$

Properties:

- Importance. The Normal distribution plays a fundamental role in ML!
 - Data Modelling: The limit distribution for the sum of a large number of indepedent and identically distributed random variables.
 - Machine Learning: The most common prior distribution for the parameters of prediction functions!
 - Information Theory: The distribution function with the most uncertainty ("entropy") when fixing mean and variance of the random variable.



Carl Friedrich Gauss (1777 - 1855)



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Normal Distribution: Representations



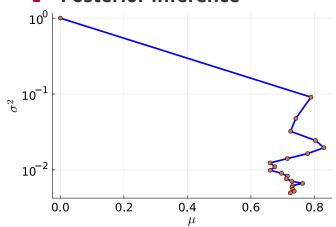
Scale-Location Parameters

$$\mathcal{N}(x; \mu, \sigma^2) = \frac{1}{\sqrt{2\pi}\sigma} \cdot \exp\left(-\frac{(x-\mu)^2}{2\sigma^2}\right)$$

Conversions

$$\mathcal{N}(x; \mu, \sigma^2) = \mathcal{G}\left(x; \frac{\mu}{\sigma^2}, \frac{1}{\sigma^2}\right)$$

Posterior Inference



Natural Parameters

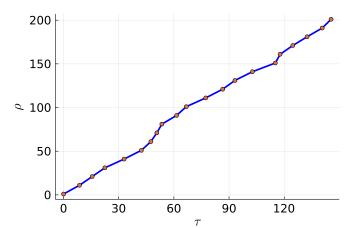
$$G(x; \tau, \rho) = \sqrt{\frac{\rho}{2\pi}} \cdot \exp\left(-\frac{\tau^2}{2\rho}\right) \cdot \exp\left(\tau \cdot x - \rho \cdot \frac{x^2}{2}\right)$$

Conversions

Two divisions only!

$$G(x; \tau, \rho) = \mathcal{N}\left(\mathbf{x}; \frac{\tau}{\rho}, \frac{1}{\rho}\right)$$

Posterior Inference



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Normal Distributions: Efficient Products & Divisions



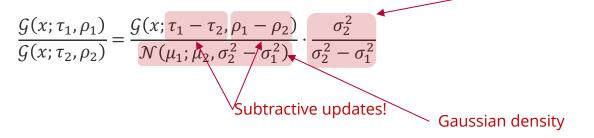
Theorem (Multiplication). Given two one-dimensional Gaussian distributions $G(x; \tau_1, \rho_1)$ and $G(x; \tau_2, \rho_2)$ we have

Gaussian density

$$\mathcal{G}(x;\tau_1,\rho_1)\cdot\mathcal{G}(x;\tau_2,\rho_2)=\mathcal{G}(x;\tau_1+\tau_2,\rho_1+\rho_2)\cdot\mathcal{N}(\mu_1;\mu_2,\sigma_1^2+\sigma_2^2)$$
Additive updates!

■ **Theorem (Division)**. Given two one-dimensional Gaussian distributions $G(x; \tau_1, \rho_1)$ and $G(x; \tau_2, \rho_2)$ where $\rho_1 \ge \rho_2$ we have

Correction factor

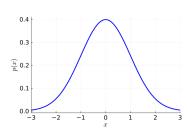


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Limit Normal Distributions: Dirac Delta and Uniform

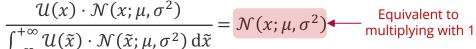


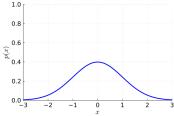
- **Dirac Delta**. The Dirac delta function $\delta(\cdot)$ is defined as the limit $\sigma^2 \to 0$ $\delta(x) = \lim_{\sigma^2 \to 0} \mathcal{N}(x; 0, \sigma^2)$
- **Gaussian Uniform**. The Gaussian uniform $\mathcal{U}(\cdot)$ is defined as the limit $\sigma^2 \to \infty$ $\mathcal{U}(x) = \lim_{\sigma^2 \to +\infty} \mathcal{N}(x; 0, \sigma^2)$



Theorem (Convolution of Normal with Dirac). For any $\mu \in \mathbb{R}$ and $\sigma^2 \in \mathbb{R}^+$ $\int_{\mathbb{R}}^{+\infty} \delta(x) \cdot \mathcal{N}(x; \mu, \sigma^2) \, \mathrm{d}x = \mathcal{N}(0; \mu, \sigma^2) \longrightarrow \text{Gaussian density at } x = 0$







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Overview



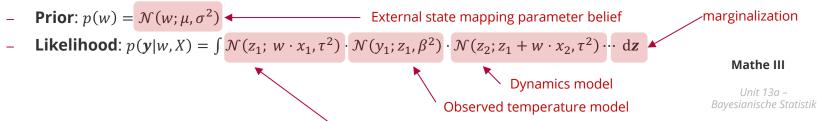
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Graphical Models



- **Challenge**: How to formulate complex likelihoods/data models & priors for *actual* data?
 - **Example 1**: Match outcomes $y \in \{-1,1\}$ (data) for a head-to-head match between two players
 - **Prior**: $p(s) = \mathcal{N}(s_1; \mu_1, \sigma_1^2) \cdot \mathcal{N}(s_2; \mu_2, \sigma_2^2)$ skill belief
 - **Likelihood**: $p(y|s) = \int \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(y(p_1 p_2) > 0)$ d p_1 d p_2 marginalization Match outcome
 - Example 2: Time series y of temperatures



Conditional hidden state model

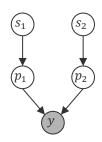
Graphical Models

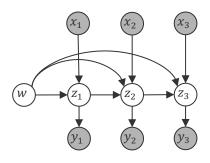


- Observation: The product structure of the probabilities seems crucial
- **Idea**: Define a graph where each of the variables are nodes and edges indicate factor relationships between variables

$$\mathcal{N}(s_1; \mu_1, \sigma_1^2) \cdot \mathcal{N}(s_2; \mu_2, \sigma_2^2) \cdot \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(y(p_1 - p_2) > 0)$$

$$\mathcal{N}(w;\mu,\sigma^2)\cdot\mathcal{N}(z_1;\,w\cdot x_1,\tau^2)\cdot\mathcal{N}(y_1;z_1,\beta^2)\cdot\mathcal{N}(z_2;z_1+w\cdot x_2,\tau^2)\cdot\mathcal{N}(y_2;z_2,\beta^2)\cdots$$





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- Advantages: Simple way to visualize factor structure of the joint probability
 - Bayesian Networks: Insights into (conditional) independence based on graph properties
 - Factor Graphs: Insights into efficient inference and approximation algorithms

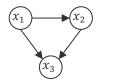
Bayesian Networks



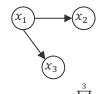
Observation. Any joint distribution $p(x_1, ..., x_n)$ can be written as

$$p(x_1, ..., x_n) = \prod_{i=1}^{n} p(x_i | x_1, ..., x_{i-1})$$

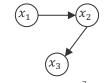
- **Bayesian Network**. Given a joint distribution as a product of conditional distributions, $p(x_1, ..., x_n) = \prod_{i=1}^n p(x_i | \text{parents}_i)$, a Bayesian network is a graph with a node for every variable x_i , and a directed edge from every variable $x \in parent_i$ to x_i . If the variable is independent of all other variables, it has no incoming edges.
- **Examples**: For 3 variables, we have these four generic Bayesian networks



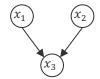
$$p(x_1, x_2, x_3) = p(x_1) \cdot p(x_2|x_1) \cdot p(x_3|x_1, x_2)$$



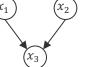
$$p(x_1, x_2, x_3) = p(x_1) \cdot \prod_{i=2}^{3} p(x_i | x_1)$$



$$p(x_1, x_2, x_3) = p(x_1) \cdot \prod_{i=2}^{3} p(x_i)$$



$$p(x_1, x_2, x_3) = p(x_3 | x_1, x_2) \cdot \prod_{i=1}^{n}$$



Bayesianische Statistik

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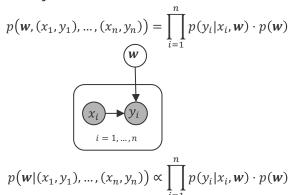
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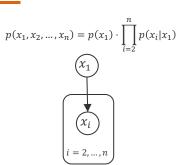
full mesh

Bayesian Network Models



- **Plate**. If a subset of variables has the same relation only differing in their index, we use a "plate" to collapse them into a single graphical element.
 - Increase readability of models for large amounts of parameters and data
- A Bayesian network must always be a directed acyclic graph because only those have a topological order corresponding to a variable order.
- **Observed Variables**. If a subset of variables has been observed ("data"), the variable nodes are usually shaded ("clamped").
 - Example: Discriminatory Models





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Sampling a Bayesian Network



• One advantage of a Bayesian network is the ability to sample $p(x_1, ..., x_n)$

Ancestral Sampling

- 1. Topologically sort all variables $x_1, ..., x_n$ into $x_{(1)}, ..., x_{(n)}$
- 2. Sample each variable $x_{(i)}$ using distribution $p(x_{(i)}|x_{(1)},...,x_{(i-1)})$

Assumption

- 1. Sampling from the conditional distributions is simpler than from the joint distribution
- 2. There are no clamped nodes, that is, we do not condition on any variable

Problems

- 1. Sampling is *sequential* one variable at the time
- 2. Conditioning happens only on frequent events because for samples $x_{j,1},...,x_{j,n}$

$$\frac{\left|\left\{\left(x_{j,1}, \dots, x_{j,n}\right) \mid x_{j,1} = x_1 \land \dots \land x_{j,n} = x_n\right\}\right|}{\left|\left\{x_{j,n} = x_n\right\}\right|} \approx \frac{p(x_1, \dots, x_n)}{p(x_n)} = p(x_1, \dots, x_{n-1} | x_n)$$

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Unit 13a – Bayesianische Statistik

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Sampling a Bayesian Network: Example

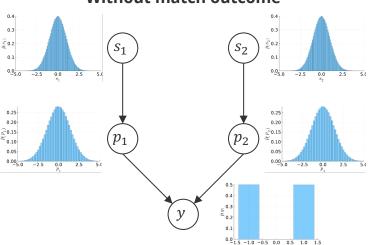


```
\mathcal{N}(s_1; \mu_1, \sigma_1^2) \cdot \mathcal{N}(s_2; \mu_2, \sigma_2^2) \cdot \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(y(p_1 - p_2) > 0)
```

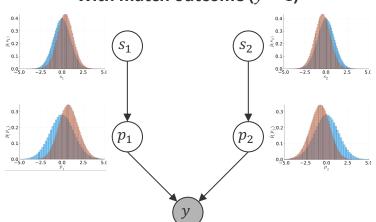
```
\mu_1 = \mu_2
```

```
# samples from the TrueSkill graphical model
function sample(; n = 100000, μ1=0.0, σ1=1.0, μ2=0.0, σ2=1.0, β=1.0)
    samples = Vector{Vector{Float64}} (undef, n)
    for i in 1:n
        s1 = rand(Normal(μ1, σ1))
        s2 = rand(Normal(μ2, σ2))
        p1 = rand(Normal(s1, β))
        p2 = rand(Normal(s2, β))
        y = p1 > p2 ? 1.0 : -1.0
        samples[i] = [s1, s2, p1, p2, y]
    end
    return samples
end
```

Without match outcome



With match outcome (y = 1)



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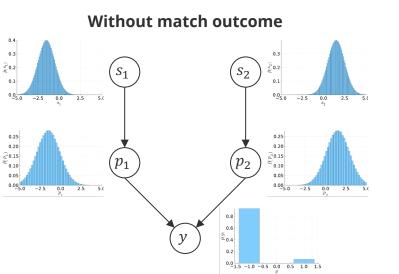
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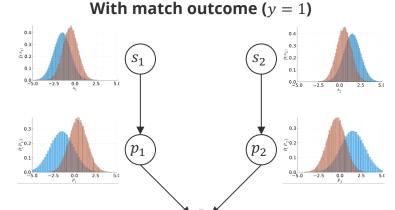
Sampling a Bayesian Network: Example (ctd)



$$\mathcal{N}(s_1; \mu_1, \sigma_1^2) \cdot \mathcal{N}(s_2; \mu_2, \sigma_2^2) \cdot \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(y(p_1 - p_2) > 0)$$

 $\mu_1 \ll \mu_2$





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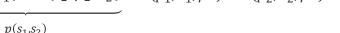
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Inference in Probabilistic Models



- **Inference**: In order to learn from data we follow a three-step procedure
 - **1. Modelling**: Formulate a joint model $p(\theta, D)$ of parameters $\theta = \theta_1, ..., \theta_n$ and data D
 - **2. Conditioning**: Clamp the variables that represent data *D* (as they are observed)
 - **3. Marginalize**: Sum-out all variables that we are not interested in (latent parameters)
- **Example**: Two player game with one winner
 - **1. Modelling**: Parameters $\theta = (s_1, s_2, p_1, p_2)$ are skills and performances; data is $y \in \{0,1\}$

$$p(s_1, s_2, p_1, p_2, y) = \mathcal{N}(s_1; \mu_1, \sigma_1^2) \cdot \mathcal{N}(s_2; \mu_2, \sigma_2^2) \cdot \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(y(p_1 - p_2) > 0)$$

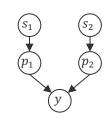


2. Conditioning: Player 1 wins (y = 1)

$$p(s_1, s_2, p_1, p_2 | y = 1) \propto p(s_1, s_2) \cdot \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(p_1 - p_2 > 0)$$

3. Marginalize: We are only interested in the skills and need to sum-out p_1 and p_2

$$p(s_1, s_2 | y = 1) \propto p(s_1, s_2) \cdot \int \int \mathcal{N}(p_1; s_1, \beta^2) \cdot \mathcal{N}(p_2; s_2, \beta^2) \cdot \mathbb{I}(p_1 - p_2 > 0) \, \mathrm{d}p_1 \mathrm{d}p_2$$



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Factors, Variables and Probabilistic Inference



- **Observation I**: The joint probability model of data and parameters is a *product* of conditional probabilities and has many factors with (few) variables!
- Observation II: Conditioning does not reduce factors; it removes variables!
- Problem: Naïve summation scales exponentially because we have a sum of products (i.e., product of conditional disitrubtions of all latent variables)!
 - **Example:** Consider an example of n Bernoulli variables $x_1, ..., x_n$

$$p(x_1) = \sum_{x_2=0}^{1} \sum_{x_3=0}^{1} \cdots \sum_{x_n=0}^{1} p(x_1, x_2, \dots, x_n)$$

$$2^{n-1} \text{ summations}$$

- **Idea**: We exploit the product structure of the probabilisitic model of our data and parameters because not every variable depends on all other variables
 - **Example (ctd)**. Consider $p(x_1, x_2, ..., x_n) = \prod_i p(x_i)$: then there are only O(n) sums and n-1 sum to one!

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Marginalization using the Distributive Law



 Observation 1: The marginal of a factor graph is a sum (over all values of all hidden variables) of a product (of factor functions).

$$p(x_1) = \sum_{x_2=0}^{1} \sum_{x_3=0}^{1} \cdots \sum_{x_n=0}^{1} f_1(x_1, x_2, \dots, x_n) \cdot \cdots \cdot f_m(x_1, x_2, \dots, x_n)$$

Observation 2: Turning a sum of products with a common factor into a product of sums using the distributive law saves computation!

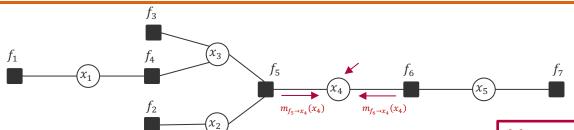
$$a \cdot b + a \cdot c = a \cdot (b + c)$$
3 operations 2 operations

 Observation 3: In a typical factor graph, functions only depend on a small number of variables.

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Sum-Product Algorithm: Marginals





Message $m_{f_j \to x_i}(x_i)$ is the sum over all variables in the subtree rooted at f_j

$$p(x_4) = \sum_{\{x_1\}} \sum_{\{x_2\}} \sum_{\{x_3\}} \sum_{\{x_5\}} f_1(x_1) \cdot f_2(x_2) \cdot f_3(x_3) \cdot f_4(x_1, x_3) \cdot f_5(x_2, x_3, x_4) \cdot f_6(x_4, x_5) \cdot f_7(x_5)$$

$$= \left[\sum_{\{x_1\}} \sum_{\{x_2\}} \sum_{\{x_3\}} f_1(x_1) \cdot f_2(x_2) \cdot f_3(x_3) \cdot f_4(x_1, x_3) \cdot f_5(x_2, x_3, x_4) \right] \cdot \left[\sum_{\{x_5\}} f_6(x_4, x_5) \cdot f_7(x_5) \right]$$

$$m_{f_5 \to x_4}(x_4)$$

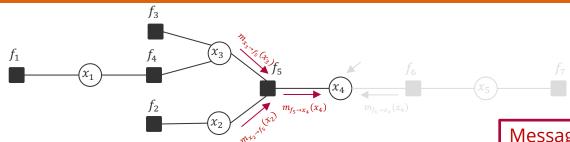
$$m_{f_6 \to x_4}(x_4)$$

Marginals are the product of all incoming messages from neighbouring factors!

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Sum-Product Algorithm: Message from Factor to Variable





Message $m_{x_i \to f_j}(x_i)$ is the sum over all variables in the subtree rooted at x_i

$$m_{f_5 \to x_4}(x_4) = \sum_{\{x_1\}} \sum_{\{x_2\}} \sum_{\{x_3\}} f_1(x_1) \cdot f_2(x_2) \cdot f_3(x_3) \cdot f_4(x_1, x_3) \cdot f_5(x_2, x_3, x_4)$$

$$= \sum_{\{x_2\}} \sum_{\{x_3\}} f_5(x_2, x_3, x_4) \cdot \left[f_2(x_2)\right] \cdot \left[\sum_{\{x_1\}} f_1(x_1) \cdot f_3(x_3) \cdot f_4(x_1, x_3)\right]$$

$$m_{x_2 \to f_5}(x_2) \qquad m_{x_3 \to f_5}(x_3)$$

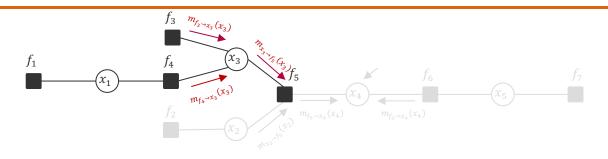
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Messages from a factor to a variable sum out all neighboring variables weighted by their incoming message

Sum-Product Algorithm: Message from Variable to Factor





$$m_{x_3 \to f_5}(x_3) = \sum_{\{x_1\}} f_1(x_1) \cdot f_3(x_3) \cdot f_4(x_1, x_3)$$

$$= [f_3(x_3)] \cdot \left[\sum_{\{x_1\}} f_1(x_1) \cdot f_4(x_1, x_3) \right]$$

$$m_{f_3 \to x_3}(x_3) \qquad m_{f_4 \to x_3}(x_3)$$

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Sum-Product Algorithm



■ Sum-Product Algorithm (Aji-McEliece, 1997). Putting it all together, we have

$$p(x) = \prod_{f \in ne(x)} m_{f \to x}(x)$$

$$m_{f \to x}(x) = \sum_{\{x' \in ne(f) \setminus \{x\}\}} \cdots \sum_{\{x'' \in ne(f) \setminus \{x\}\}} f(x, x', \dots, x'') \prod_{x' \in ne(f) \setminus \{x\}} m_{x' \to f}(x')$$

$$m_{x \to f}(x) = \prod_{f' \in ne(x) \setminus \{f\}} m_{f' \to x}(x)$$

- Basis: Generalized distributive law (which also holds for max-product)
- **Efficiency**: By storing messages, we
 - Only have to compute local summations in $O(2^T)$ where degree $T = \max_f |ne(f)|!$
 - All marginals can be computed recursively in $O(E \cdot 2^T)$ vs $O(2^n)$ (where E is the number of edges of the factor graph)!



Robert McEliece (1942 – 2019)

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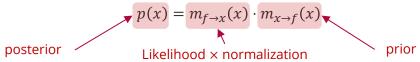
Even more efficiency



Redundancies. By the very definition of messages and marginals

$$p(x) = \prod_{f \in ne(x)} m_{f \to x}(x) = m_{f' \to x}(x) \cdot \prod_{f \in ne(x) \setminus \{f'\}} m_{f \to x}(x)$$

Interpretation. Application of Bayes' rule at a variable x at factor f



Storage Efficiency. We only store the marginals p(x) and $m_{f\to x}(x)$ because

$$m_{x \to f}(x) = \frac{p(x)}{m_{f \to x}(x)}$$

Exponential Family. If all the messages from factors to variables are in the exponential family, then the marginals and messages from the variable to factors are simply additions and subtraction of natural parameters!

Example: If $p(x) = \mathcal{G}(x; \tau_1, \rho_1)$ and $m_{f \to x}(x) = \mathcal{G}(x; \tau_2, \rho_2)$ then $m_{x \to f}(x) \propto \mathcal{G}(x; \tau_1 - \tau_2, \rho_1 - \rho_2)$

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Sum-Product Algorithm Revisited



• The key operation for factor $f(x_1, x_2, ..., x_n)$ and variable x_1 is

$$m_{f \to x_1}(x_1) = \sum_{\{x_2\}} \cdots \sum_{\{x_n\}} f(x_1, x_2, \dots, x_n) \prod_{j=2}^n m_{x_j \to f}(x_j)$$
If all $m_{x_j \to f}(x_j)$ are Gaussian, the result might not be Gaussian!

■ Based on outgoing messages, we can compute both marginals p(x) and $m_{x\to f}(x)$

$$p(x) = \prod_{f \in ne(x)} m_{f \to x}(x) \qquad m_{x \to f}(x) = \frac{p(x)}{m_{f \to x}(x)}$$

If all $m_{x_j \to f}(x_j)$ are Gaussian, the result **must be** Gaussian!

- Idea:
 - 1. We approximate all outgoing messages $m_{f\to x}(\cdot)$ by a Gaussian $\widehat{m}_{f\to x}(\cdot)=\mathcal{N}(\cdot;\mu,\sigma^2)$
 - 2. We measure the approximation quality in the marginal, **not** the outgoing message

$$\hat{p}(\cdot) = \arg\min_{\mathcal{N}(\cdot;\mu,\sigma^2)} \text{KL} \left[\frac{m_{f \to x}(\cdot) \cdot \hat{m}_{x \to f}(\cdot)}{\int_{-\infty}^{+\infty} m_{f \to x}(\tilde{x}) \cdot \hat{m}_{x \to f}(\tilde{x}) \; \mathrm{d}\tilde{x}}, \frac{\mathcal{N}(\cdot;\mu,\sigma^2) \cdot \hat{m}_{x \to f}(\cdot)}{\int_{-\infty}^{+\infty} \mathcal{N}(\tilde{x};\mu,\sigma^2) \cdot \hat{m}_{x \to f}(\tilde{x}) \; \mathrm{d}\tilde{x}} \right]$$

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Unit 13a – Bayesianische Statistik

True marginal with approximate incoming message

Approximate marginal with approximate incoming message

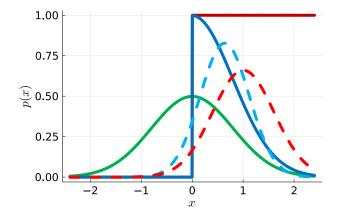
Approximate Message Passing: Example



$$f(x) = \mathbb{I}(x > 0)$$

$$\widehat{m}_{x \to f}(x) \propto \frac{\widehat{p}(x)}{\widehat{m}_{f \to x}(x)} \longrightarrow p(x) \propto f(x) \cdot \widehat{m}_{x \to f}(x) \qquad \widehat{m}_{f \to x}(x) \propto \frac{\widehat{p}(x)}{\widehat{m}_{x \to f}(x)}$$

$$\widehat{p}(x) = \mathcal{N}(x; E_{X \sim p(x)}[X], \text{var}_{X \sim p(x)}[X])$$



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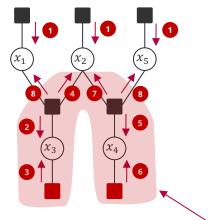
Expectation Propagation



- **Idea**: If we have factors in the factor graph that require approximate messages, we keep iterating on the whole path between them until convergence minimizing $\mathrm{KL}\big(p(\cdot)|\mathcal{N}(\cdot;\mu,\sigma^2)\big)$ locally for the affected marginals of the approximate factor.
- **Theorem (Minka, 2003)**: Approximate message passing will converge if the approximating distribution is in the exponential family!



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Viel Spaß bis zur nächsten Vorlesung!