LTAT.02.004 Machine Learning II

Graphical models

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Discrete random variables

- A *random variable* X with possible *outcomes* $x \in \operatorname{supp}(X)$
- Compact notation for probabilities

$$\Pr[x_1] := \Pr[\xi \leftarrow X_1 : \xi = x_1]$$

$$\Pr[x_1 \wedge x_2] := \Pr[\xi_1 \leftarrow X_1, \xi_2 \leftarrow X_2 : \xi_1 = x_1 \wedge \xi_2 = x_2]$$

- Bayes formula

$$\Pr[a|b] = \frac{\Pr[a \wedge b]}{\Pr[b]} = \frac{\Pr[b|a]\Pr[a]}{\Pr[b]}$$

- Independence of random variables $X_1 \ldots X_m \perp Y_1, \ldots Y_n$:

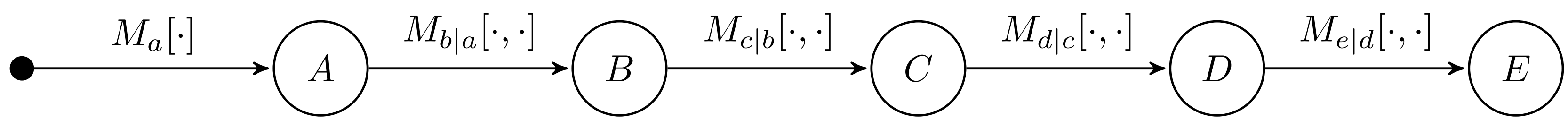
$$\Pr[x_1 \wedge \ldots \wedge x_m \wedge y_1 \wedge \ldots \wedge y_n] = \Pr[x_1 \wedge \ldots \wedge x_m] \cdot \Pr[y_1 \wedge \ldots \wedge y_n]$$

- Marginalisation over variables $Y_1, \ldots, Y_n$:

$$\Pr[x_1 \wedge \ldots \wedge x_m] = \sum_{y_1, \ldots, y_n} \Pr[x_1 \wedge \ldots \wedge x_m \wedge y_1 \wedge \ldots \wedge y_n]$$

Common models

Markov chain



Definition. Let $X_1, X_2, \ldots$ be correlated random variables such that the probability of the observation x_{i+1} depends only on the observation x_i. Then the entire process is known as Markov chain.

Parametrisation. Markov chain is determined by specifying

- ▷ state spaces $\mathcal{S}_1 \ldots, \mathcal{S}_n$
- ▷ initial probabilities $\Pr[x_1]$
- ▷ state transition probabilities $\Pr[x_{i+1}|x_i]$

What questions can we ask?

Sampling: What are typical outcomes of the chain?
$\triangleright$ Synthesis of time-series, textures, sounds, games movements.

Stationary distribution: What happens if we run the chain infinitely long?
$\triangleright$ Getting samples from an unnormalised posterior, optimisation tasks.

Likelihood estimation: What is a probability of an observation $x_1, \ldots, x_n$?
$\triangleright$ Reasoning about probabilities and clustering sequences.

Decoding: What is the most probable outcome $x_1, \ldots, x_n$?
$\triangleright$ Imputing missing values. Rudimentary logical reasoning.

Parameter estimation: What is are the model parameters?
$\triangleright$ Machine learning – finding parameters based on observations.

Parameter inference for homogenous case

$$\bullet \xrightarrow{\boldsymbol{\beta}[\cdot]} X_1 \xrightarrow{\boldsymbol{\alpha}[\cdot,\cdot]} X_2 \xrightarrow{\boldsymbol{\alpha}[\cdot,\cdot]} X_3 \xrightarrow{\boldsymbol{\alpha}[\cdot,\cdot]} X_4 \xrightarrow{\boldsymbol{\alpha}[\cdot,\cdot]} X_5$$

For a sequence of observations $\boldsymbol{x} = (x_1, \ldots, x_n)$ the log-likelihood is

$$\begin{aligned}\ell[\boldsymbol{x}] &= \log \underbrace{\Pr\left[x_1\right]}_{\beta[x_1]} + \sum_{i=1}^{n-1} \log \underbrace{\Pr\left[x_{i+1}|x_i\right]}_{\alpha[x_i,x_{i+1}]} \\ &= \log \beta[x_1] + \sum_{u_1,u_2} k(u_1,u_2) \log \alpha[u_1,u_2]\end{aligned}$$

where $k(u_1, u_2)$ is the count of bigrams u_1, u_2 in the sequence $\boldsymbol{x}$.

Posterior decomposition

As a result the log-likelihood of unnormalised posterior decomposes into the sum of independent terms

$$\begin{aligned}\log p[\boldsymbol{\alpha},\boldsymbol{\beta}|\boldsymbol{x}] =& \sum_{u_1} k(u_1)\log\beta[u_1] + \log p(\boldsymbol{\beta})\\ &+\sum_{u_1,u_2} k(u_1,u_2)\log\alpha[u_1,u_2] + \sum_{u_1}\log p(\boldsymbol{\alpha}[u_1,\cdot])\end{aligned}$$

where

- ▷ $k(u_1)$ is the count u_1 at the beginning of the observed sequences
- ▷ $k(u_1,u_2)$ is the count of bigrams u_1,u_2 in the observed sequences.
- ▷ $p(\boldsymbol{\beta})$ is the prior for an entire vector of initial probabilities
- ▷ $p(\boldsymbol{\alpha}[u_1,\cdot])$ is the prior for the transition probabilities from u_1

Reduction to the dice throwing experiment

Posterior decomposition leads to many independent optimisation tasks

$$\sum_{u_1} k(u_1)\log\beta[u_1] + \log p(\boldsymbol{\beta}) \to \max$$

$$\sum_{u_2} k(u_1,u_2)\log\alpha[u_1,u_2] + \log p(\boldsymbol{\alpha}[u_1,\cdot]) \to \max$$

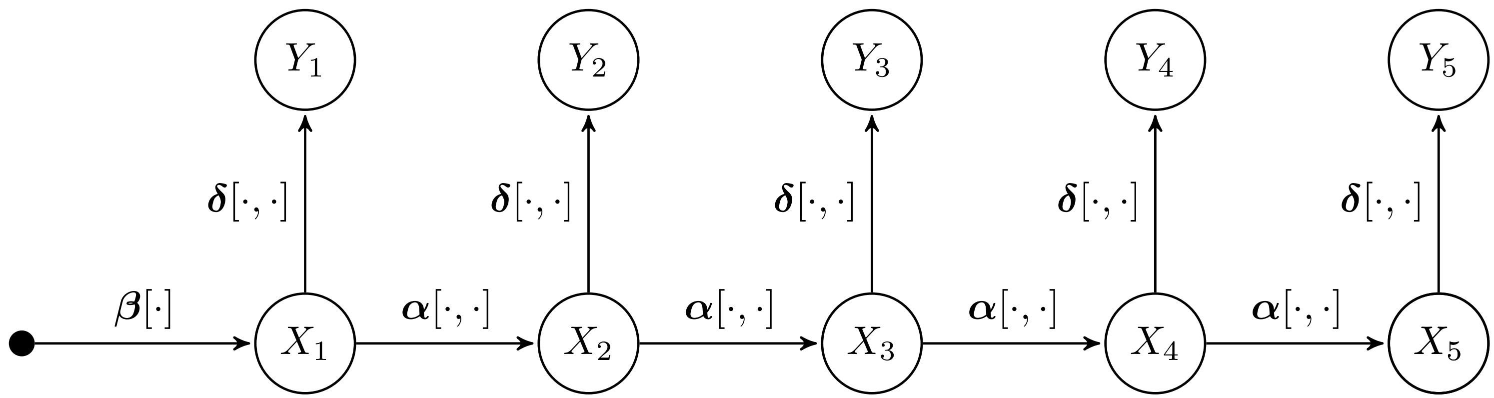
where each of these is equivalent to optimisation of dice throwing posterior. Thus Maximum Aposteriori estimates for parameters are

$$\beta[u_1] = \frac{k(u_1)+c}{k(*)+mc} \qquad\qquad \alpha[u_1,u_2] = \frac{k(u_1,u_2)+c}{k(u_1,*)+mc}$$

where

- ▷ $*$ is a wildcard symbol in the count queries
- ▷ m is the number of states and c is a constant for Laplacian smoothing.

Hidden Markov Model



Definition. Let $X_1, X_2, \ldots$ be hidden states that form a Markov chain and let $Y_1, Y_2, \ldots$ be observations that the probability of y_i depends only on the state x_i. Then the entire process is known as Hidden Markov Model.

Common tasks

- parameter estimation
- filtering, smoothing, prediction

Applications

Modelling and prediction

- stock prices
- linear control algorithms

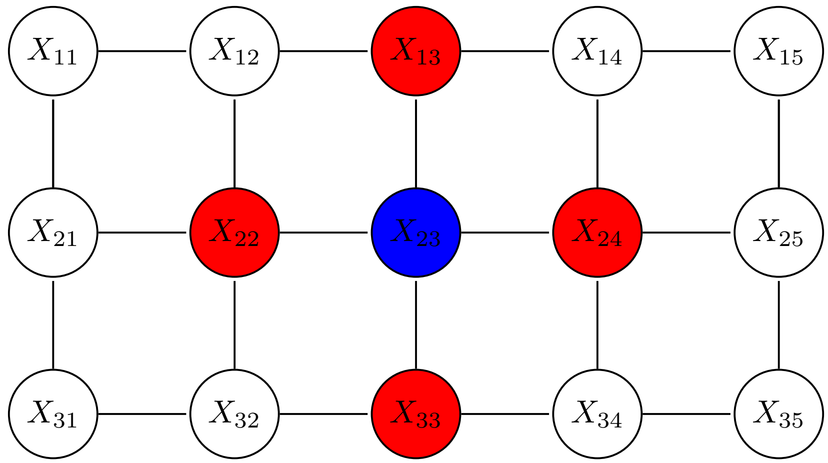
Sequence annotation

- fraud detection
- change detection
- functional motifs of DNA sequences

Decoding

- speech recognition
- communication over a nosy channels
- object tracking and data fusion

Random Markov Fields



Definition. Markov random field is specified by undirected graph connecting random variables $X_1, X_2, \ldots$ such that for any node X_i

$$\Pr\left[x_i | (x_j)_{j \neq i}\right] = \Pr\left[x_i | (x_j)_{j \in \mathcal{N}(X_i)}\right]$$

where the set of neighbours $\mathcal{N}(X_i)$ is also known as *Markov blanket* for X_i.

Hammersley-Clifford theorem

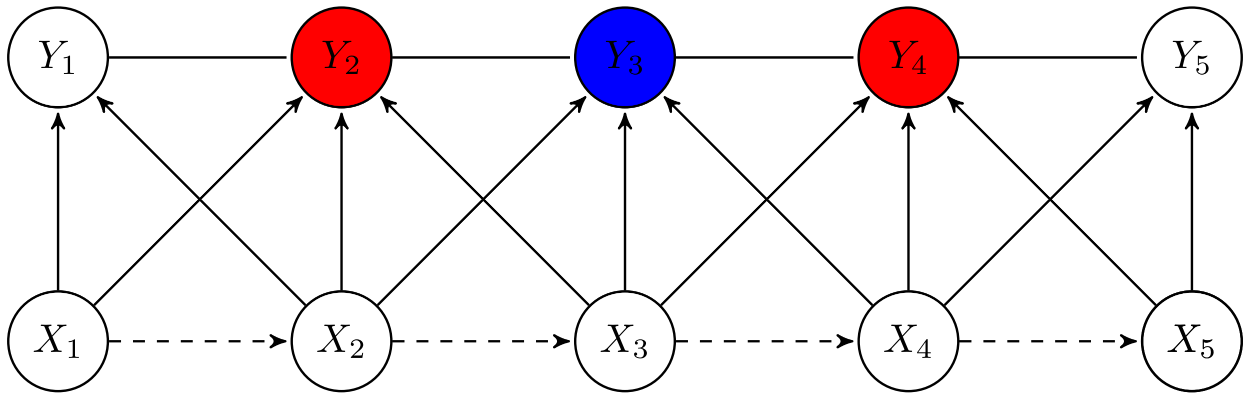
The probability of an observation $\boldsymbol{x} = (x_1, x_2, \ldots)$ generated by a Markov random field can be expressed in the form

$$\Pr\left[\boldsymbol{x}\right] = \frac{1}{Z(\omega)} \cdot \exp\left(-\sum_{c \in \mathsf{MaxClique}} \Psi_c(\boldsymbol{x}_c, \omega)\right)$$

where

- $Z(\omega)$ is a normalising constant
- MaxClique is the set of maximal cliques in the Markov random field
- Ψ_c is defined on the variables in the clique c

Conditional Random Fields



Definition. Let $X_1, X_2, \ldots$ and $Y_1, Y_2, \ldots$ be random variables. The entire process is conditional random field if random variables $Y_1, Y_2, \ldots$ conditioned for any sequence of observations $x_1, x_2, \ldots$ form a Markov random field

$$\Pr\left[y_i|(x_k)_{k=1}^{\infty}, (y_j)_{j\neq i}\right] = \Pr\left[y_i|(x_k)_{k=1}^{\infty}, (y_j)_{j\in\mathcal{N}(Y_i)}\right]$$

where the set of neighbours $\mathcal{N}(Y_i)$ is a *conditional Markov blanket* for Y_i.

Applications

Standard setting

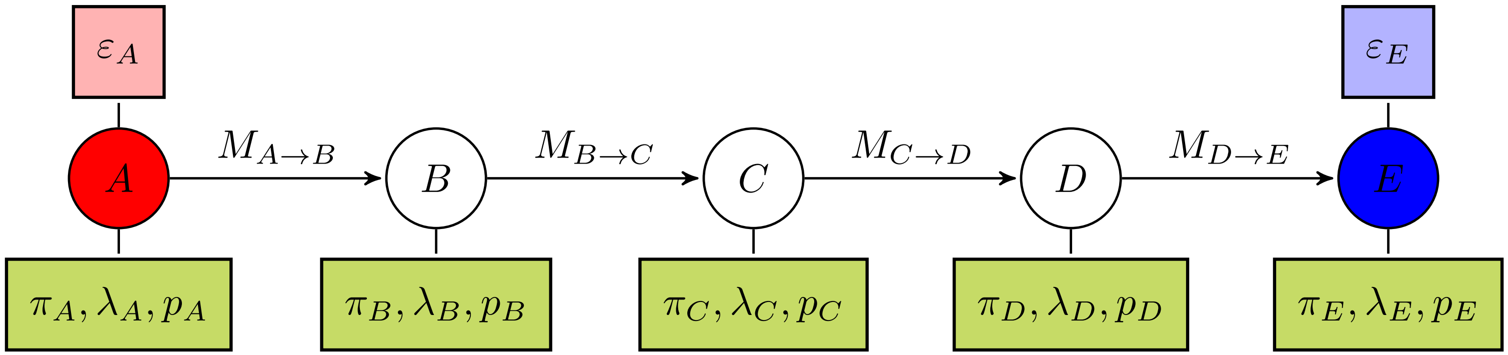
- ▷ The input $\boldsymbol{x}$ is used to predict labels $y_1, y_2, \ldots$.
- ▷ A correct label sequence must satisfy possibly unknown restrictions.
- ▷ These restrictions are captured by conditional random random field.

Instantiation

- ▷ Hammersley-Clifford theorem prescribes the format of $\Pr[\boldsymbol{y}|\boldsymbol{x}]$
- ▷ Clique features Ψ_c can depend on $(y_i)_{i\in c}$, $(x_i)_{i=1}^{\infty}$
- ▷ Features can be defined as linear combination of vertex and edge features.
- ▷ A vertex feature looks only variable y_i associated with the vertex.
- ▷ An edge feature looks only variables y_i, y_j associated with the edge.

Belief propagation

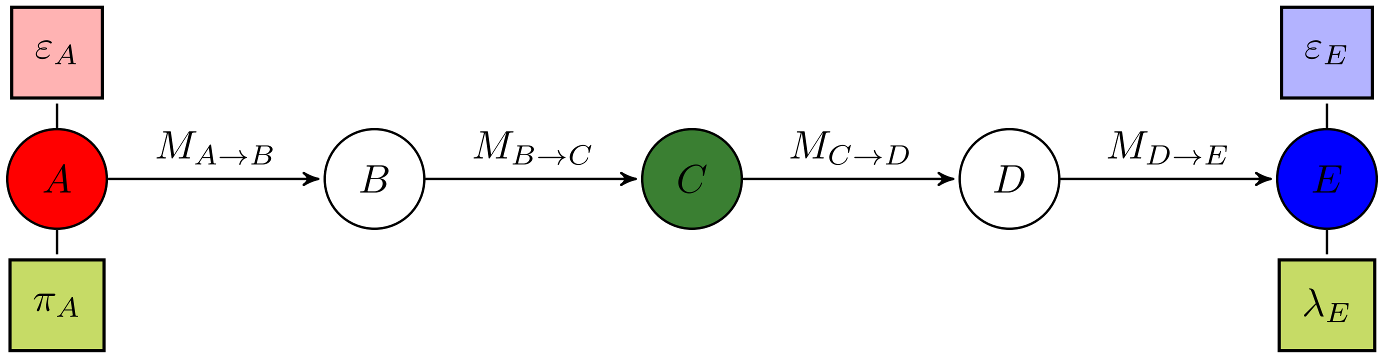
Belief propagation in a simple chain



Inference goal. Given evidence at the ends of the chain find marginal posterior probabilities for each node in the chain.

- Evidence ε_V is an observational data associated with the node V.
- Upstream evidence$^-$ is the evidence at the end of chain.
- Downstream evidence$^+$ is the evidence at the beginning of chain.
- Attributes π_V, λ_V, p_V are needed to compute marginal distributions.

Initialisation

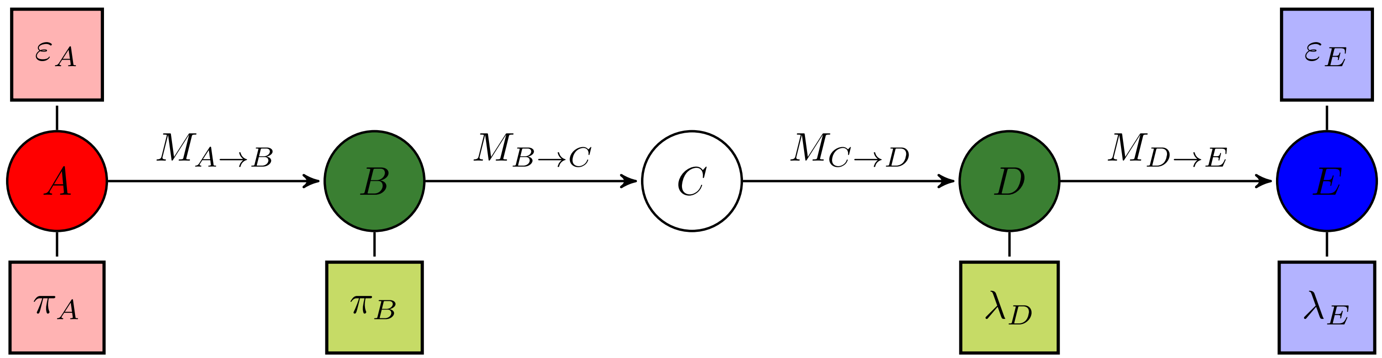


- Direct evidence ε_V determines the value of V.
- Indirect evidence ε_V determines the value distribution for V.
- We can assign the prior for the first and likelihood for the last node

$$\pi_A(a) = \Pr\left[A = a|\text{evidence}^+\right] = \Pr\left[A = a|\varepsilon_A\right]$$

$$\lambda_E(e) = \Pr\left[\text{evidence}^-|E = e\right] = \Pr\left[\varepsilon_E|E = e\right]$$

Belief propagation



Inference goal

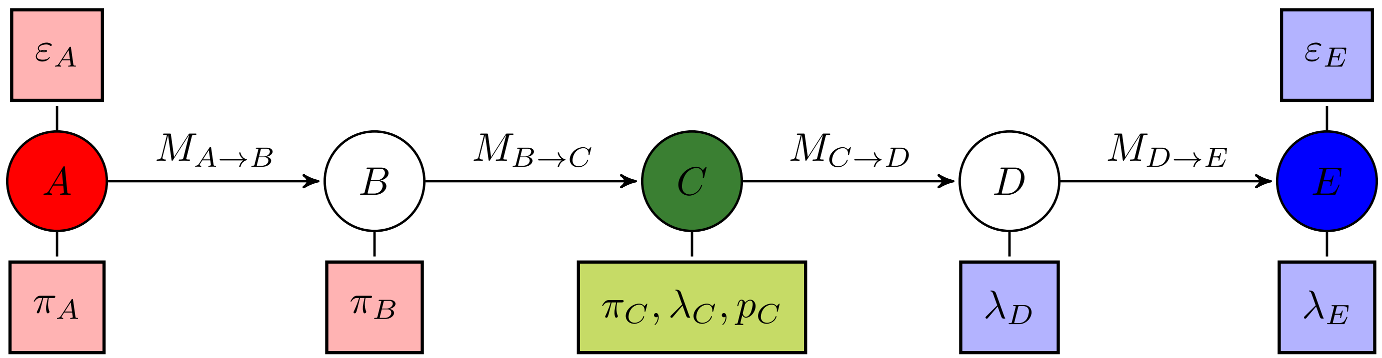
$$\pi_B(b) = \Pr\left[b|\text{evidence}^{+}\right]$$

$$\lambda_D(d) = \Pr\left[\text{evidence}^{-}|d\right]$$

Iterative propagation rules

- ▷ Marginalisation gives an update rule $\lambda_D = M_{D\to E}\lambda_E$.
- ▷ Marginalisation gives an update rule $\pi_B \propto \pi_A M_{A\to B}$.

Belief propagation



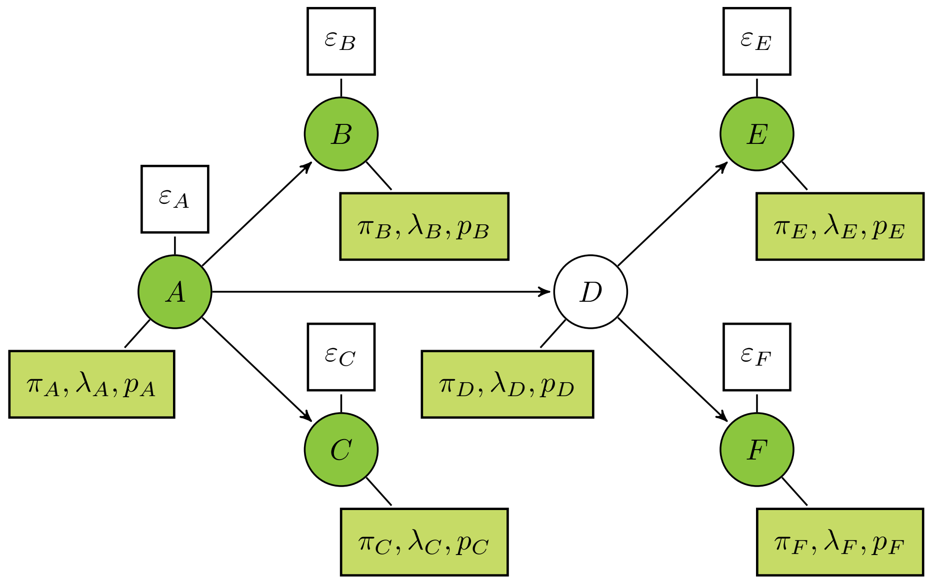
Inference goal

$$p_C(c) = \Pr\left[c|\text{evidence}^+, \text{evidence}^-\right]$$

Iterative update rule

▷ Bayes formula gives $p_C \propto \pi_C \otimes \lambda_C$.

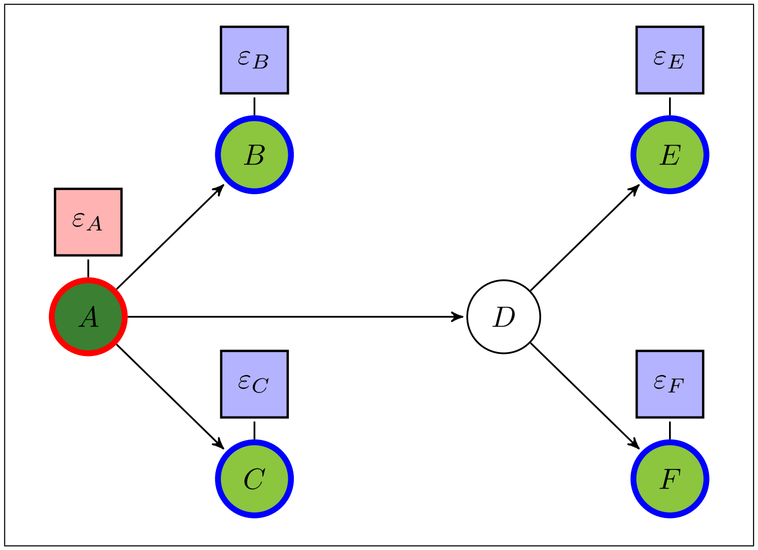
Belief propagation in a simple tree

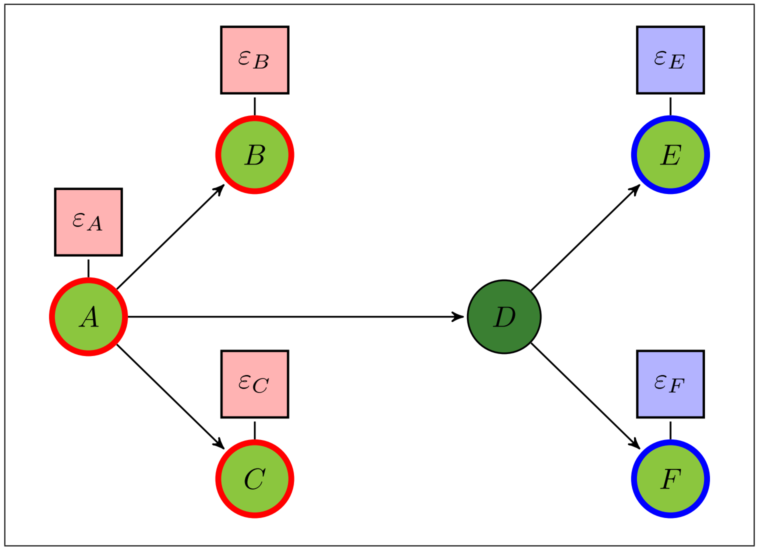


Inference goal. Given evidence at the ends of the leafs and the root of tree find marginal posterior probabilities for each node in the tree.

- Evidence ε_V is an observational data associated with the node V.
- Attributes π_V, λ_V, p_V are needed to compute marginal distributions.

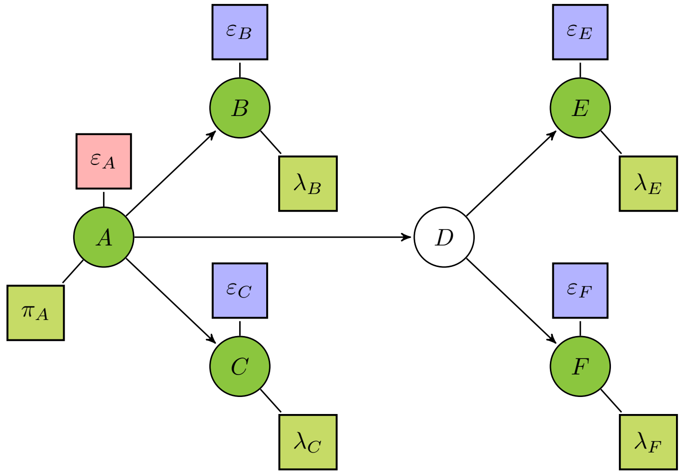
Evidence decomposition





- Evidence decomposes into up- and downstream evidence
- Downstream evidence$^{-}(V)$ is reachable through child nodes.
- Upstream evidence$^{+}(V)$ is reachable through the predessesor node.
- Different nodes have totally different decompositions.

Initialisation



Goal. Assign prior to the root node and likelihood to the leaf nodes.

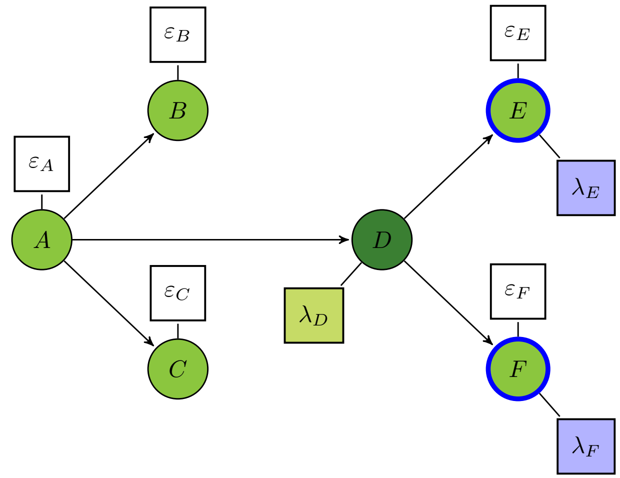
$$\pi_A(a) = \Pr\left[A = a|\text{evidence}^+(A)\right] = \Pr\left[A = a|\varepsilon_A\right]$$

$$\lambda_B(b) = \Pr\left[\text{evidence}^-(B)|F = f\right] = \Pr\left[\varepsilon_B|B = b\right]$$

$$\dots$$

$$\lambda_F(f) = \Pr\left[\text{evidence}^-(F)|F = f\right] = \Pr\left[\varepsilon_F|F = f\right]$$

Likelihood propagation



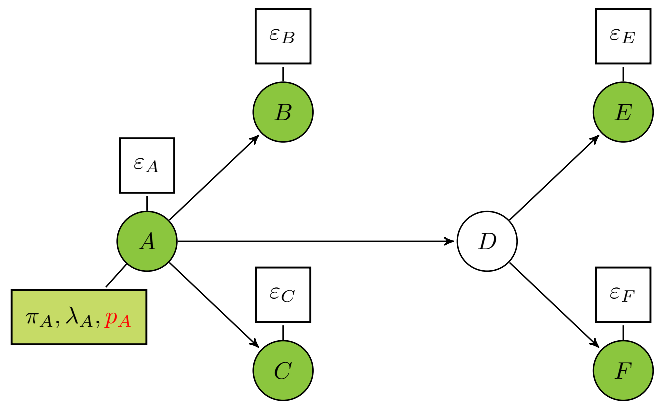
Inference goal

$$\lambda_D(d) = \Pr\left[\text{evidence}^-(D)|D = d\right]$$

Iterative propagation rules

- Independence gives a pooling rule $\lambda_D = \lambda_1 \otimes \lambda_2$
- Marginalisation gives rules $\lambda_1 = M_{D\to E}\lambda_E$ and $\lambda_2 = M_{D\to F}\lambda_F$.

Posterior propagation



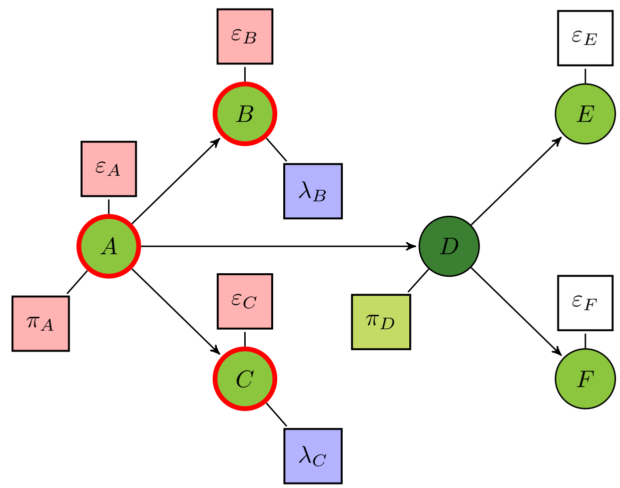
Inference goal

$$p_A(a) = \Pr\left[A = a | \text{evidence}^+(A), \text{evidence}^-(A)\right]$$

Iterative propagation rule

▷ Marginal conditional probability $p_A \propto \pi_A \otimes \lambda_A$

Prior propagation



Inference goal

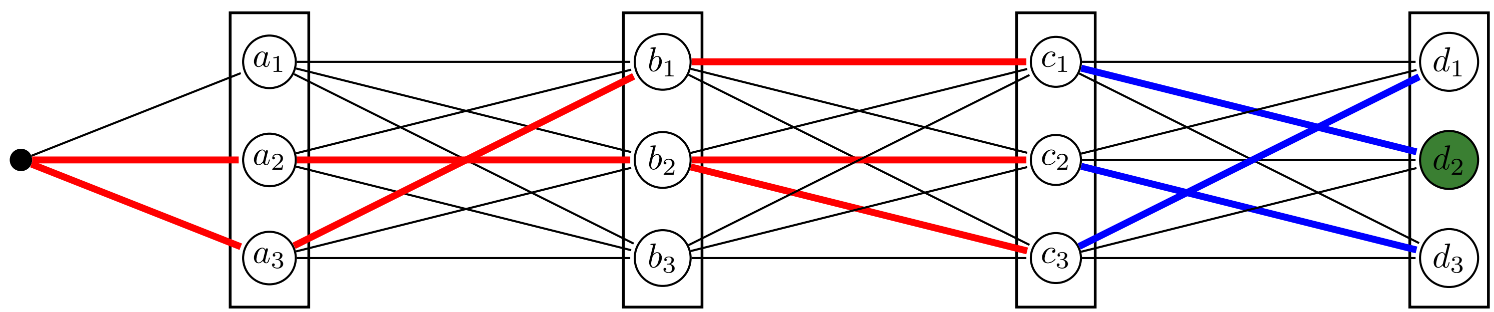
$$
\begin{aligned}
\pi_D(d) &= \Pr\left[D = d \middle| \text{evidence}^+(D)\right] \\
&= \Pr\left[D = d \middle| \text{evidence}^+(A), \text{evidence}^-(B), \text{evidence}^-(C)\right]
\end{aligned}
$$

Iterative propagation rule

▷ Prior can be computed as $\pi_D \propto \pi_A M_{A\to D} \otimes M_{A\to B}\lambda_B \otimes M_{A\to C}\lambda_C$.

Posterior Maximisation

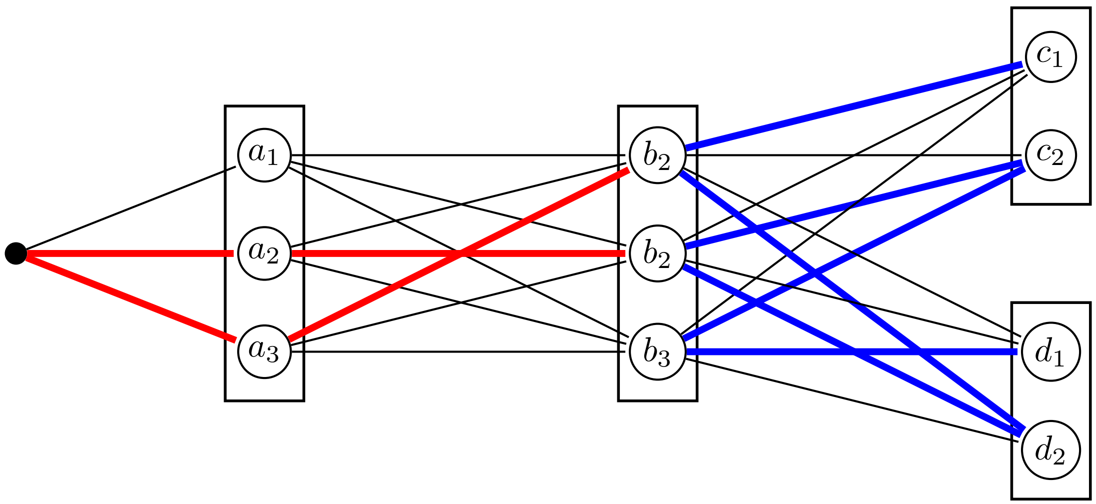
Posterior maximisation in a simple chain



Inference goal. Given evidence at the ends of the chain find the sequence of states $\boldsymbol{x}$ that maximise the posterior probability $\Pr[\boldsymbol{x}|\text{evidence}]$.

- ▷ The log-posterior $\log \Pr[\boldsymbol{x}|\text{evidence}]$ decomposes into a sum.
- ▷ We must find a sequence with maximal weight.
- ▷ The task can be split into subtask as all subpaths of the path with maximal weight must have maximal weight.
- ▷ The corresponding iterative algorithm is known as Viterbi algorithm.

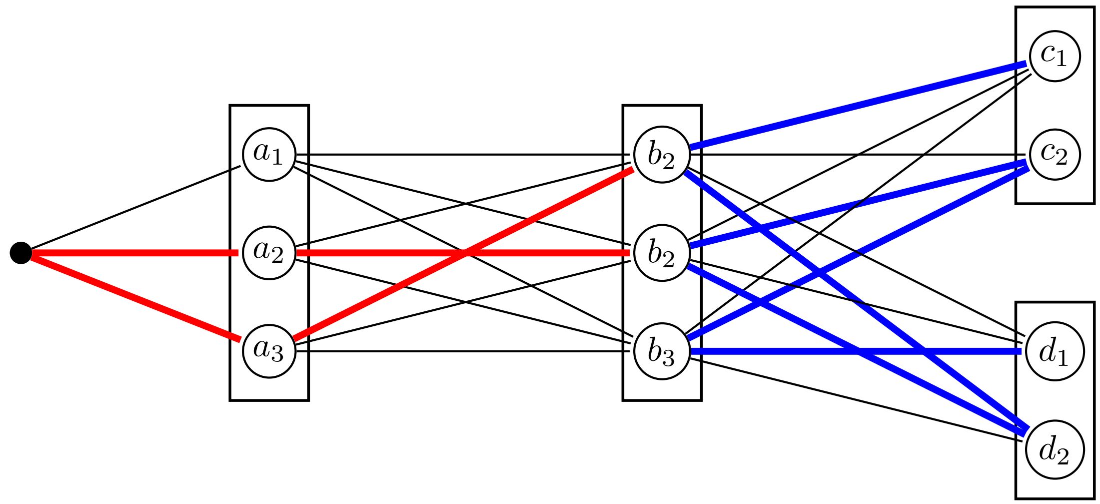
Posterior maximisation in a simple tree



Inference goal. Given evidence at the ends of the chain find the sequence of states $\boldsymbol{x}$ that maximise the posterior probability $\Pr[\boldsymbol{x}|\text{evidence}]$.

- ▷ The log-posterior $\log \Pr[\boldsymbol{x}|\text{evidence}]$ decomposes into a sum.
- ▷ We must find a tree with maximal weight.

Decomposition into subtasks

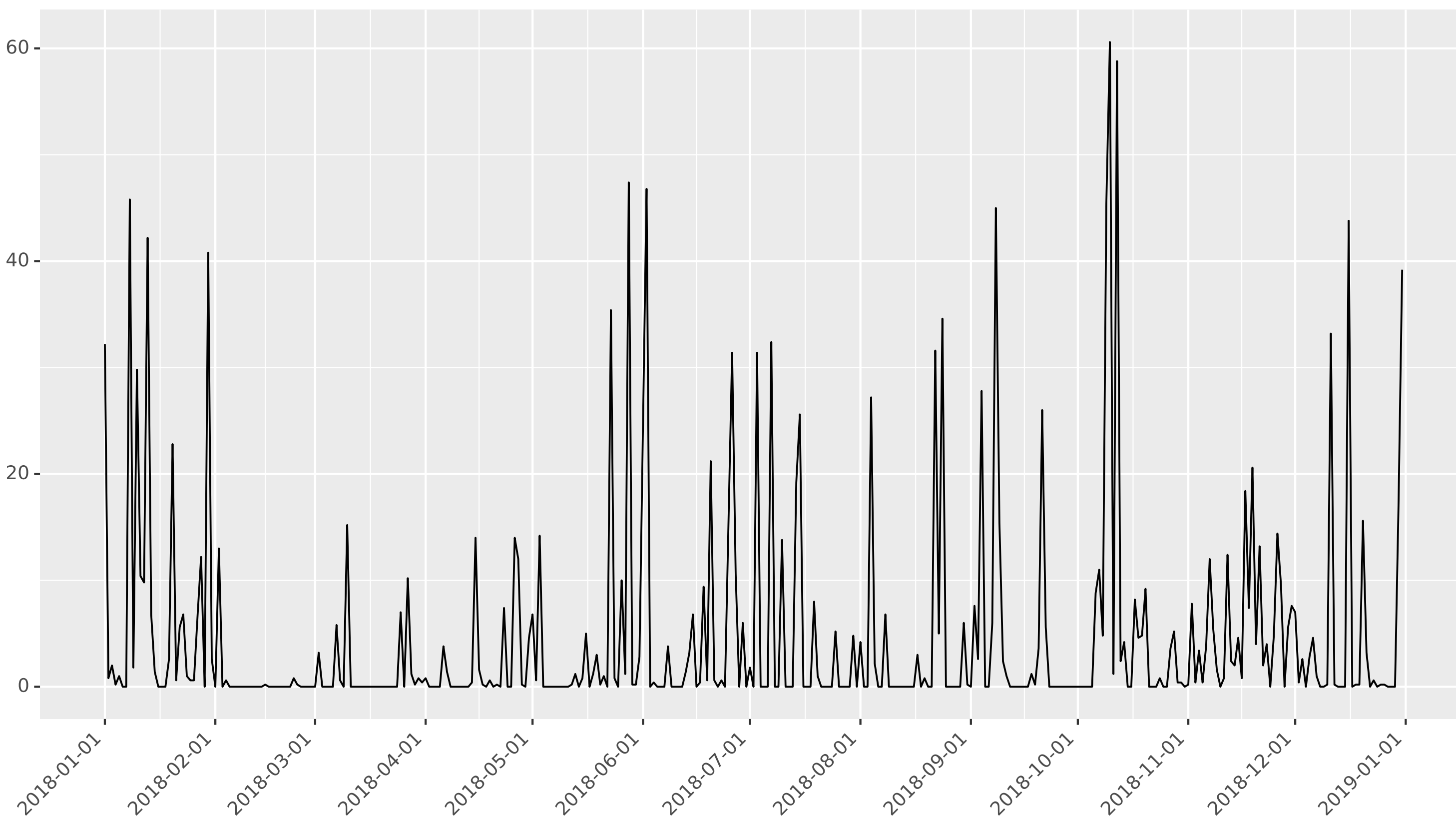


All subtrees of the tree with maximal weight must have maximal weight.

- ▷ We can build chains with maximum weight form leafs
- ▷ We can merge subtrees with maximum weight to maximise the weight.
- ▷ The algorithm works from leafs to the root node.
- ▷ The corresponding iterative algorithm is known as Viterbi algorithm.

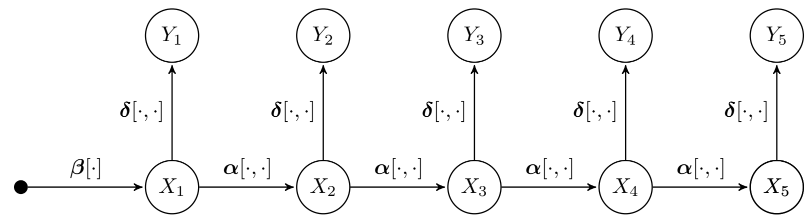
Applications

Rainfall data



There are two monsoon seasons in Singapore: dry and wet phase.

Modelling with Hidden Markov Model



Markov chain with states $\mathcal{S} = \{0, 1\}$ and parameters

$$\boldsymbol{\beta} = (0.5, 0.5)$$

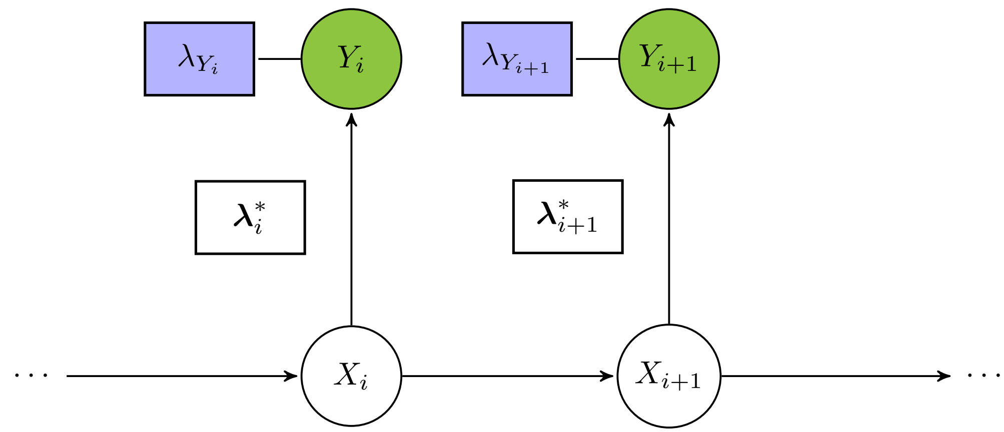
$$\boldsymbol{\alpha} = \begin{pmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{pmatrix}$$

Emission distributions

$$Y_i | X_i = 0 \sim \mathcal{N}(\mu_0, \sigma_0)$$

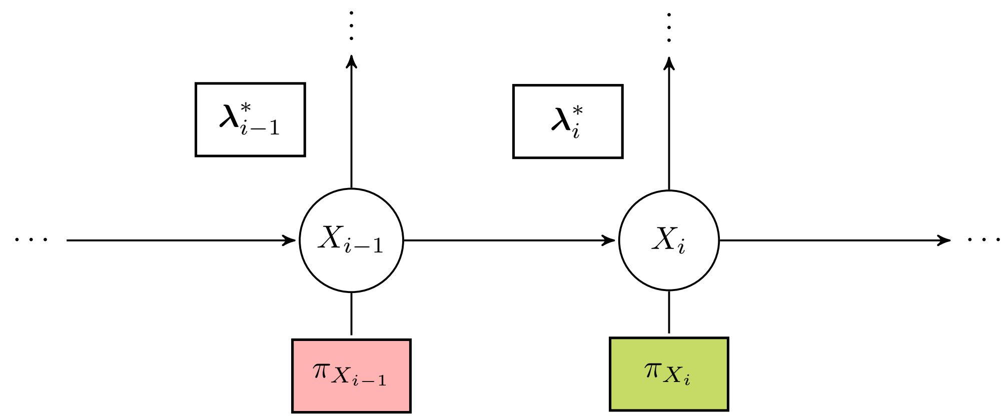
$$Y_i | X_i = 1 \sim \mathcal{N}(\mu_1, \sigma_1)$$

Belief propagation. Initialisation



- ▷ We have a direct evidence $Y_i = y_i$ for each node Y_i.
- ▷ The likelihood vector is infinite and captured by $\lambda_{Y_i} = \delta_{y_i}$.
- ▷ The local likelihood $\lambda_i^*(x_i) = \Pr[Y_i = y_i | x_i]$ is a finite vector.

Prior propagation. Filtering



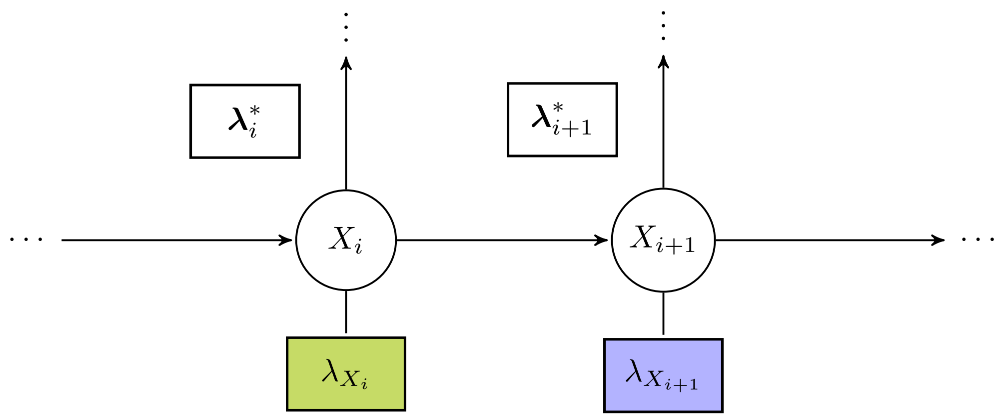
Prior propagation rule yields

$$\pi_{X_i}(x_i) \propto \sum_{x_{i-1}\in\mathcal{S}} \alpha[x_{i-1}, x_i] \cdot \lambda^*_{i-1}(x_{i-1}) \cdot \pi_{X_{i-1}}(x_{i-1})$$

Now we can do filtering

$$\Pr\left[x_i | y_1, \ldots, y_i\right] \propto \pi_{X_i}(x_i) \cdot \lambda^*_i(x_i)$$

Likelihood propagation. Smoothing



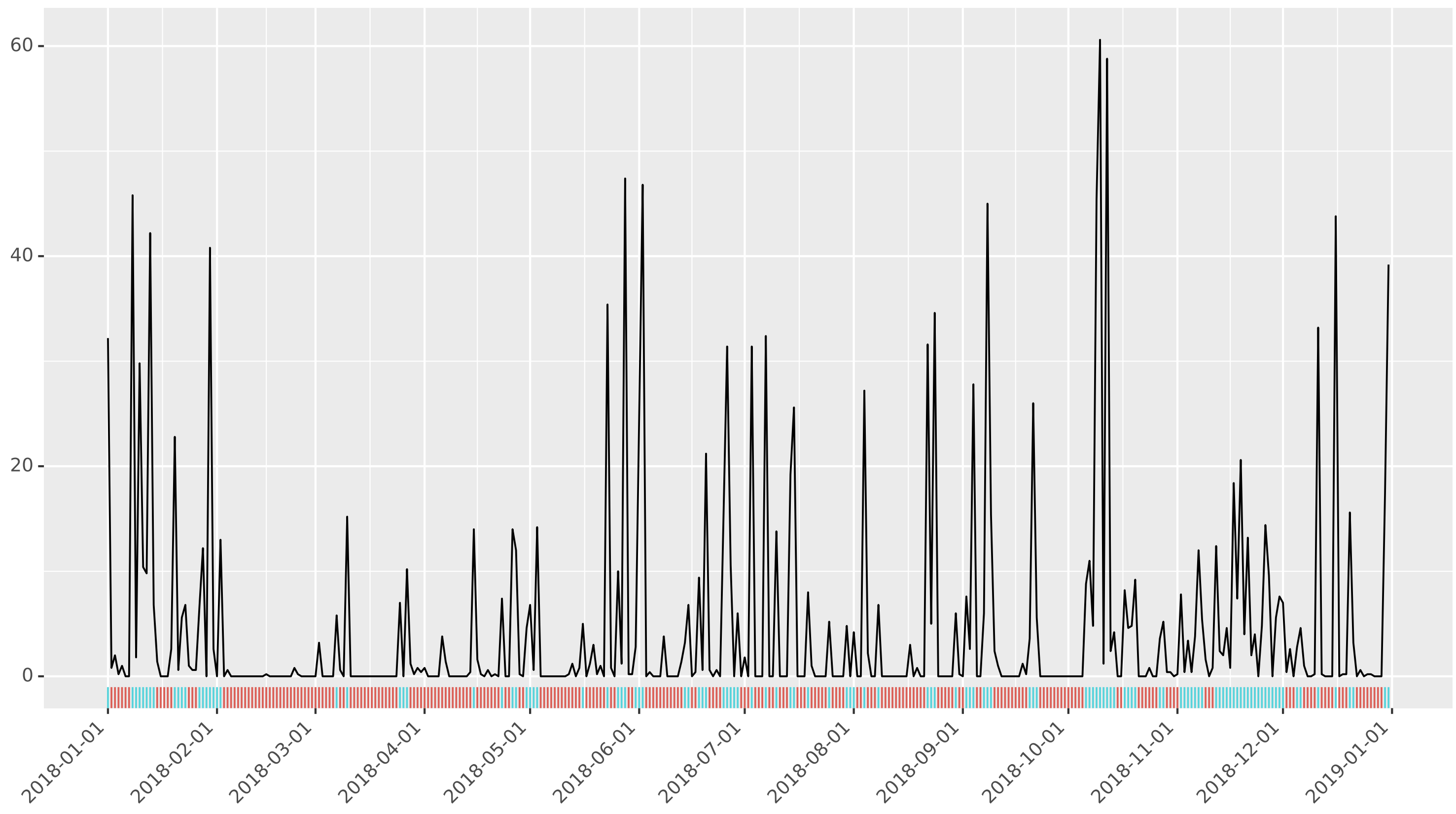
Likelihood propagation rule yields

$$\lambda_{X_i}(x_i) \propto \sum_{x_{i+1}\in\mathcal{S}} \alpha[x_i, x_{i+1}] \cdot \lambda_{X_{i+1}}(x_{i+1}) \cdot \lambda_i^*(x_i)$$

Now we can do smoothing

$$\Pr\left[x_i | y_1, \ldots, y_n\right] \propto \pi_{X_i}(x_i) \cdot \lambda_{X_i}(x_i)$$

Annotated rainfall data



Sensor fusion problem. Kalman filter

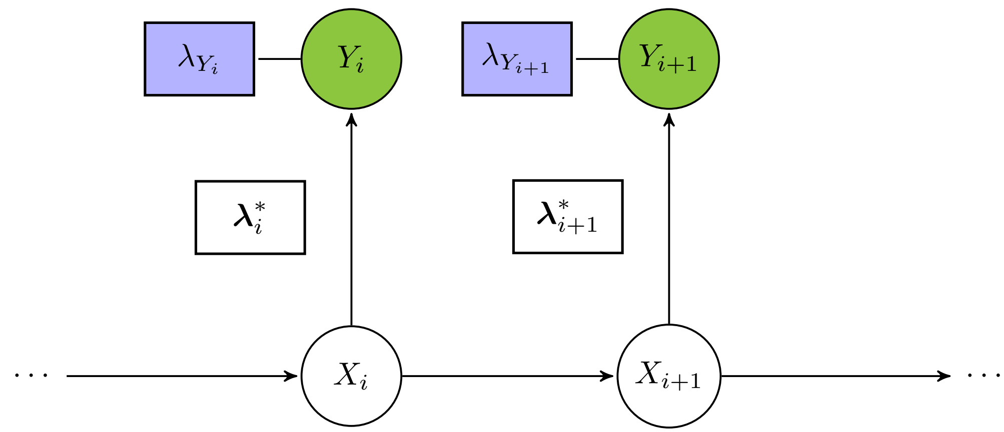
Several sensors measure a physical system

- ▷ Measurements are observable as $\boldsymbol{y} \in \mathbb{R}^p$.
- ▷ Physical system has an hidden state $\boldsymbol{x} \in \mathbb{R}^n$.
- ▷ Physical system evolves linearly $\boldsymbol{x}_{i+1} = A\boldsymbol{x}_i + \boldsymbol{w}_i$.
- ▷ Measurements are linear from the state $\boldsymbol{y}_i = C\boldsymbol{x}_i + \boldsymbol{v}_i$.

Unknown quantities in the system

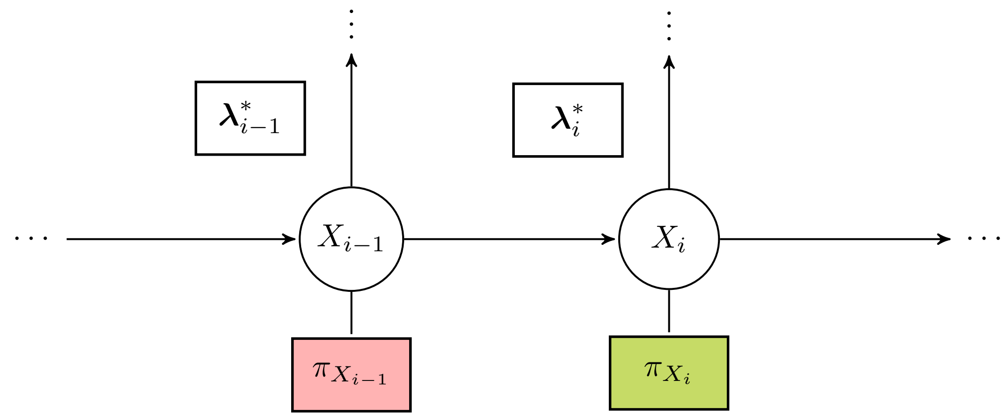
- ▷ Measurement noise $\boldsymbol{v}_t$ is modelled with a normal distribution.
- ▷ Unknown control signal $\boldsymbol{w}_i$ is modelled with a normal distribution.
- ▷ Unknown initial state $\boldsymbol{x}_0$ is modelled with a normal distribution.
- ▷ Quantities $\boldsymbol{x}_0, \boldsymbol{v}_i, \boldsymbol{w}_i$ are assumed to be independent.
- ▷ All normal distributions can have complex correlation structure.

Belief propagation. Initialisation



- We have a direct evidence $Y_i = y_i$ for each node Y_i.
- The likelihood vector is infinite and captured by $\lambda_{Y_i} = \delta_{y_i}$.
- The local likelihood $\lambda_i^*(x_i) = p[Y_i = y_i|x_i]$ is an infinite vector.
- The form $\boldsymbol{y}_i = C\boldsymbol{x}_i + \boldsymbol{v}_i$ assures that $\boldsymbol{y}_i|\boldsymbol{x}_i$ is normal distribution.
- The local likelihood λ_i^* has a finite description.

Prior propagation. Filtering

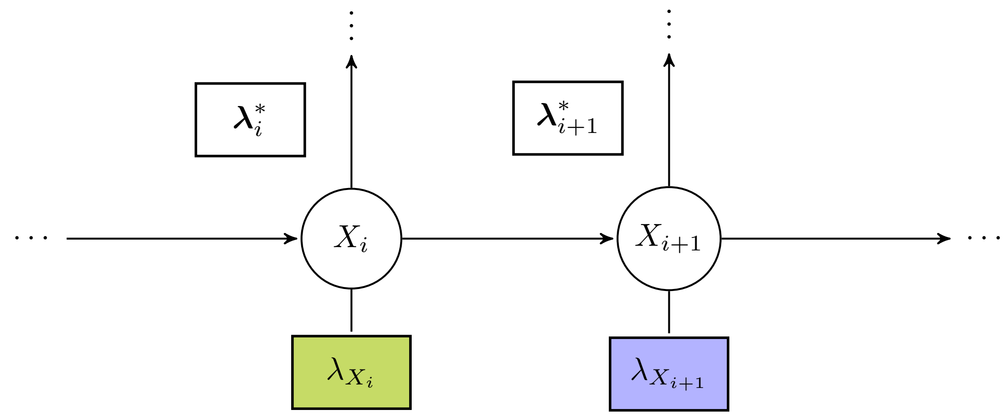


Prior propagation rule

$$\pi_{X_i}(\boldsymbol{x}_i) \propto \int\limits_{\boldsymbol{x}_{i-1}} \alpha[\boldsymbol{x}_{i-1}, \boldsymbol{x}_i] \cdot \lambda^*_{i-1}(\boldsymbol{x}_{i-1}) \cdot \pi_{X_{i-1}}(\boldsymbol{x}_{i-1}) d\boldsymbol{x}_{i-1}$$

leads to a finite description because on the right is a normal distribution.

Likelihood propagation. Smoothing



Likelihood propagation rule

$$\lambda_{X_i}(x_i) \propto \int\limits_{\boldsymbol{x}_{i+1}} \alpha[\boldsymbol{x}_i, \boldsymbol{x}_{i+1}] \cdot \lambda_{X_{i+1}}(\boldsymbol{x}_{i+1}) \cdot \lambda_i^*(\boldsymbol{x}_i) d\boldsymbol{x}_{i+1}$$

leads to a finite description because on the right is a normal distribution.