

LTAT.02.004 MACHINE LEARNING II

Sequence models

Sven Laur
University of Tartu

Discrete random variables

- ▷ A *random variable* X with possible *outcomes* $x \in \text{supp}(X)$
- ▷ 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

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

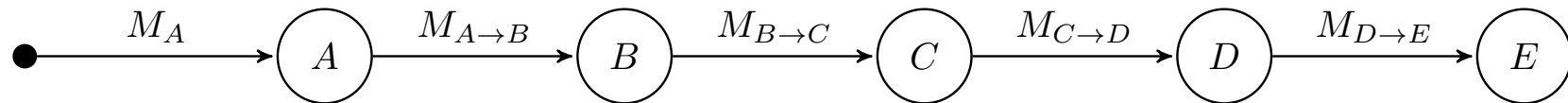
- ▷ Independence of random variables $X_1 \dots X_m \perp Y_1, \dots Y_n$:

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

- ▷ Marginalisation over variables Y_1, \dots, Y_n :

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

Markov chain



Definition. Let X_1, X_2, \dots 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 $\mathcal{S}_1 \dots, \mathcal{S}_n$
- ▷ initial probabilities $\Pr[x_1]$ given as vectors
- ▷ state transition probabilities $\Pr[x_{i+1}|x_i]$ given as matrices

What questions can we ask?

Sampling: What are typical outcomes of the chain?

- ▷ Synthesis of time-series, textures, sounds, games movements.

Stationary distribution: What happens if we run the chain infinitely long?

- ▷ Getting samples from an unnormalised posterior, optimisation tasks.

Likelihood estimation: What is a probability of an observation x_1, \dots, x_n ?

- ▷ Reasoning about probabilities and clustering sequences.

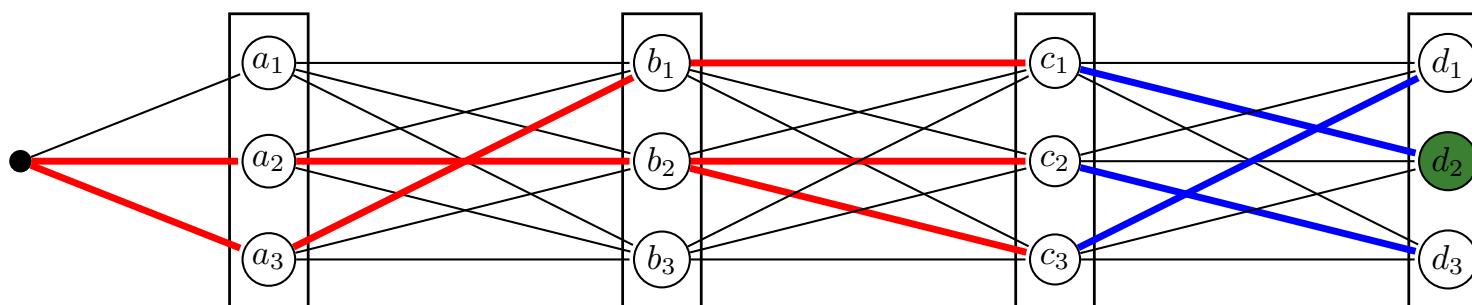
Decoding: What is the most probable outcome x_1, \dots, x_n ?

- ▷ Imputing missing values. Rudimentary logical reasoning.

Parameter estimation: What are the model parameters?

- ▷ Machine learning – finding parameters based on observations.

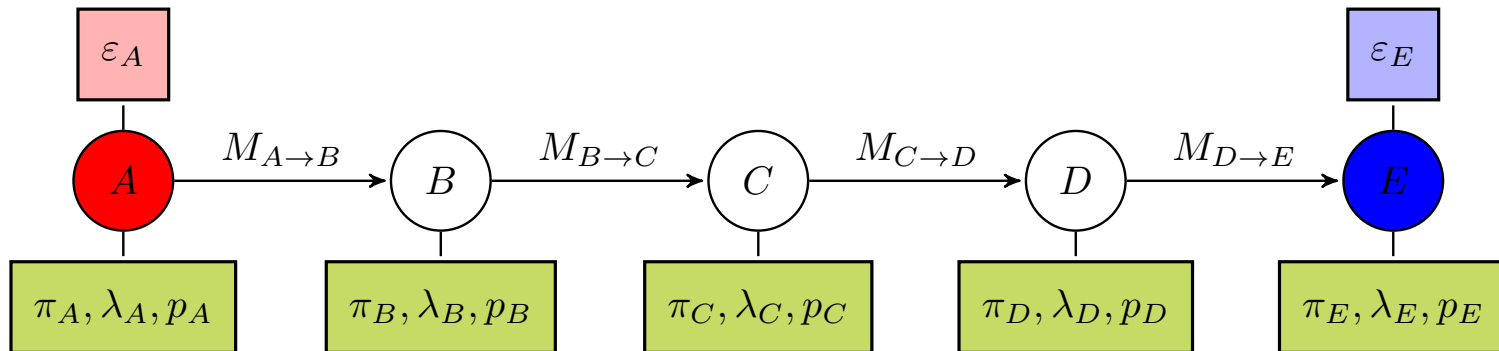
Posterior maximisation in a chain



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

- ▷ The log-posterior $\log \Pr[x|\text{evidence}]$ 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.

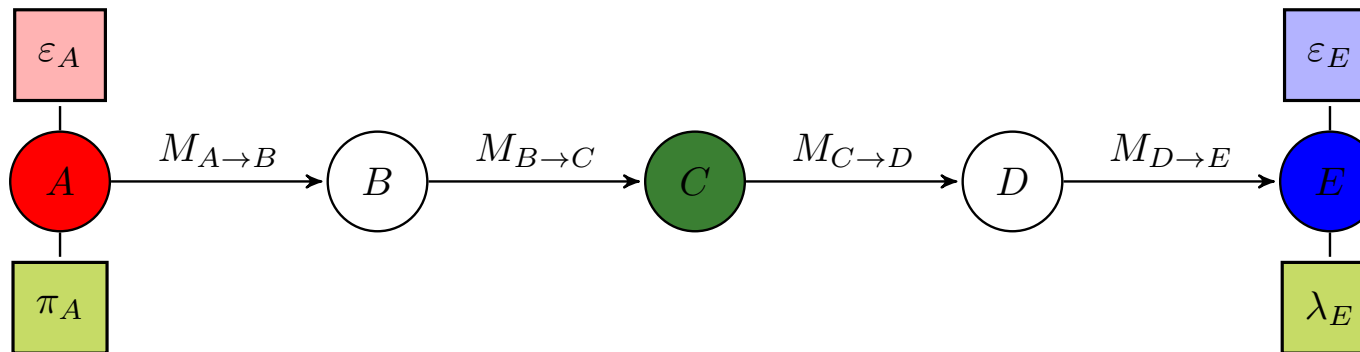
Belief propagation in a chain



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 beginning of chain.
- ▷ Downstream **evidence⁻** is the evidence at the end of chain.
- ▷ Attributes π_V, λ_V, p_V are needed to compute marginal distributions.

Initialisation

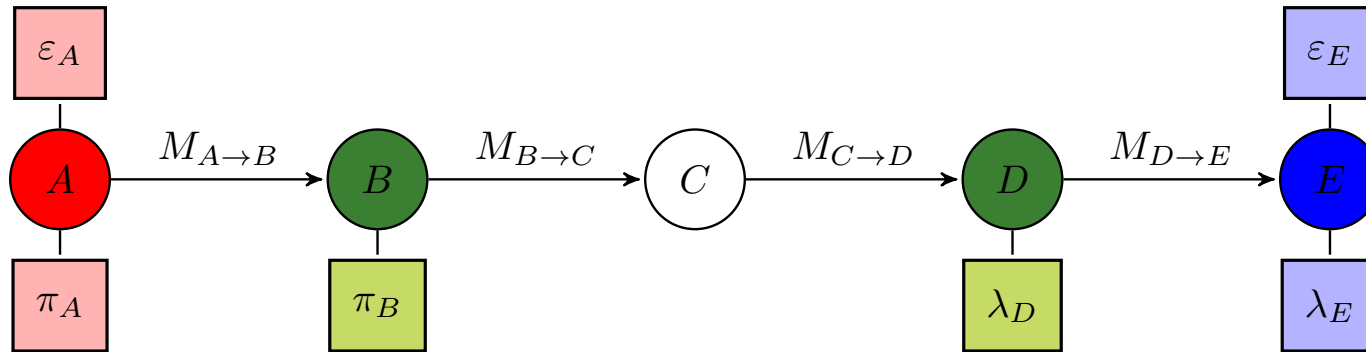


- ▷ Direct evidence ε_V determines the value of V .
- ▷ Indirect evidence ε_V determines the value distribution for V .
- ▷ We can assign the prior for the first and likelihood for the last node

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

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

Belief propagation



Inference goal

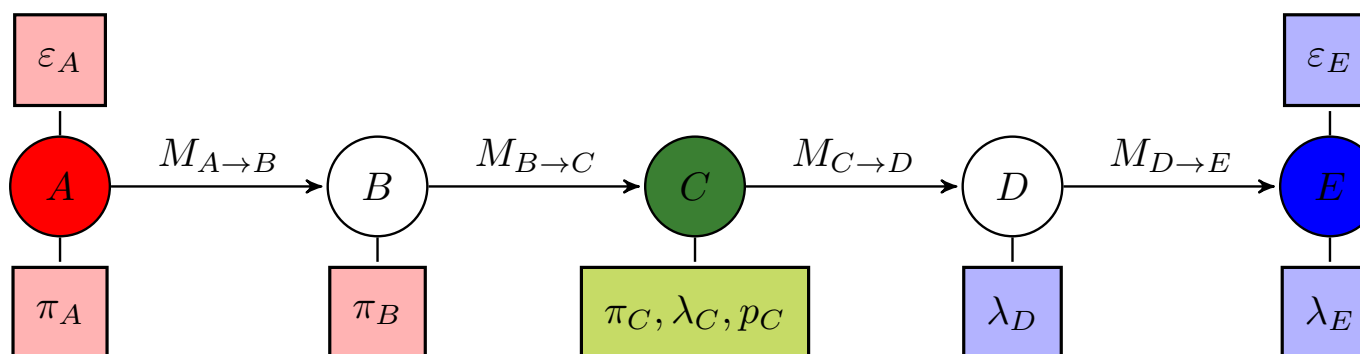
$$\pi_B(b) = \Pr [b | \text{evidence}^+]$$

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

Iterative propagation rules

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

Belief propagation



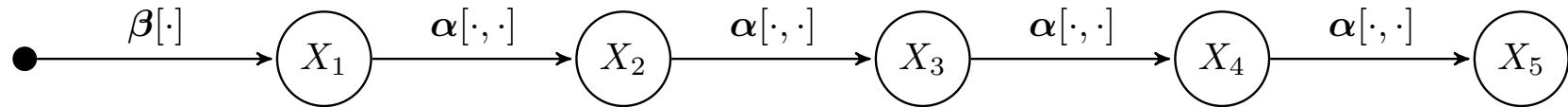
Inference goal

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

Iterative update rule

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

Parameter inference for homogenous case



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

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

where $k(u_1, u_2)$ is the count of bigrams u_1, u_2 in the sequence \mathbf{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

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

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

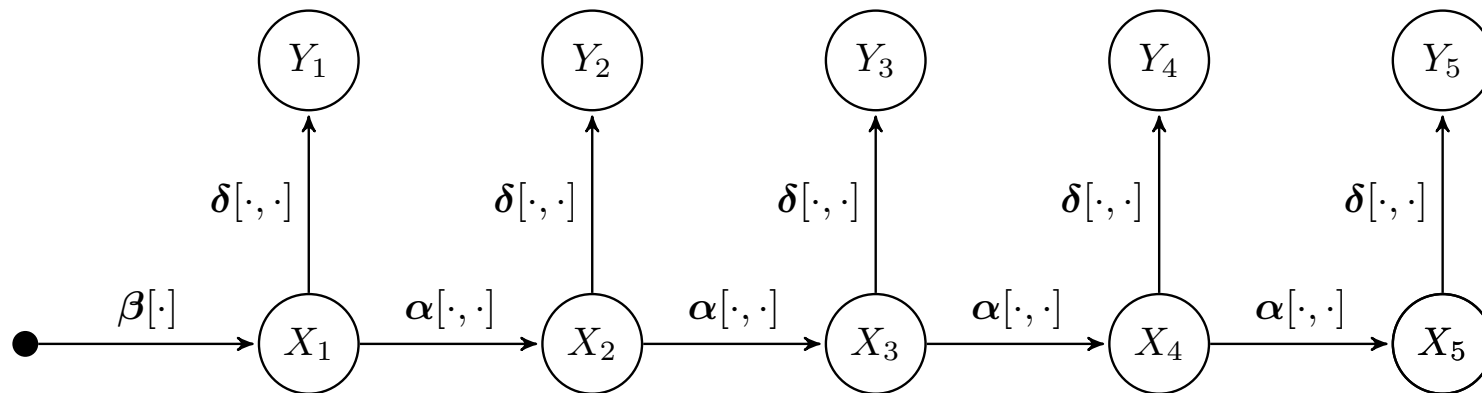
where each of these is equivalent to optimisation of dice throwing posterior. Thus Maximum A posteriori estimates for parameters are

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

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, \dots be hidden states that form a Markov chain and let Y_1, Y_2, \dots 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

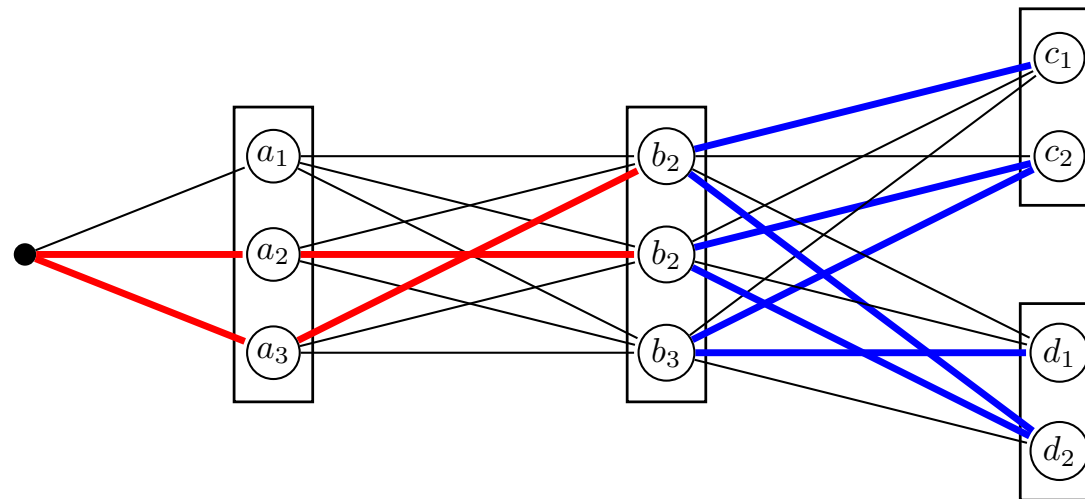
Sequence annotation

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

Decoding

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

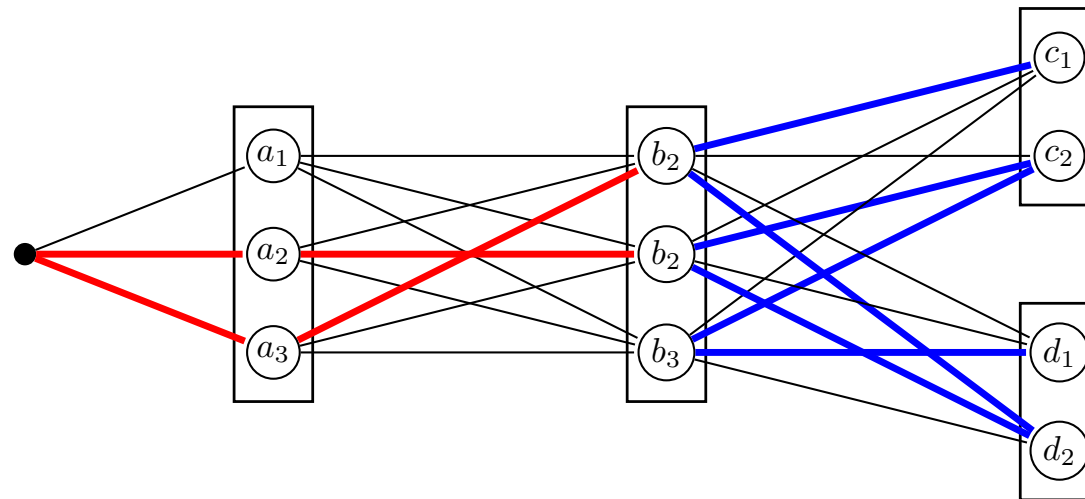
Posterior maximisation in a tree



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

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

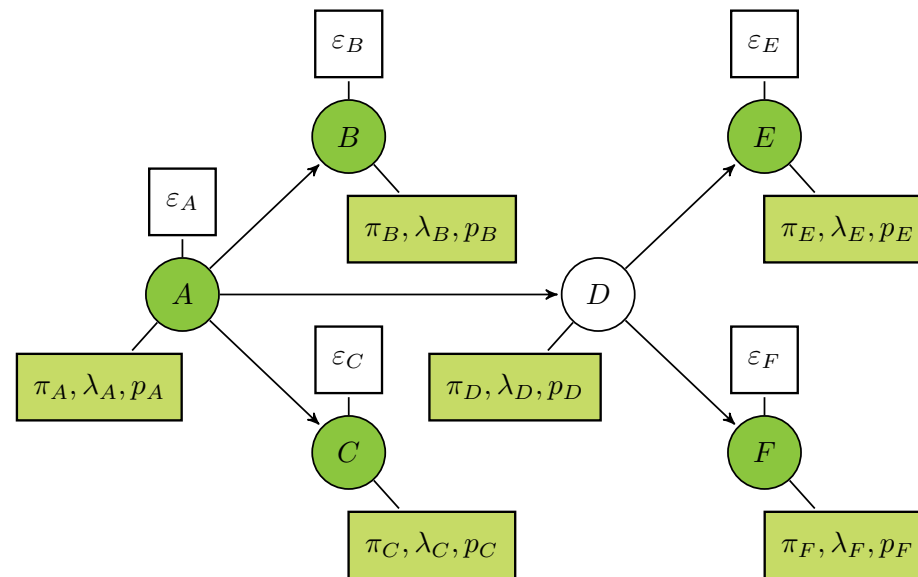
Decomposition into subtasks



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

- ▷ We can build chains with maximum weight from 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.

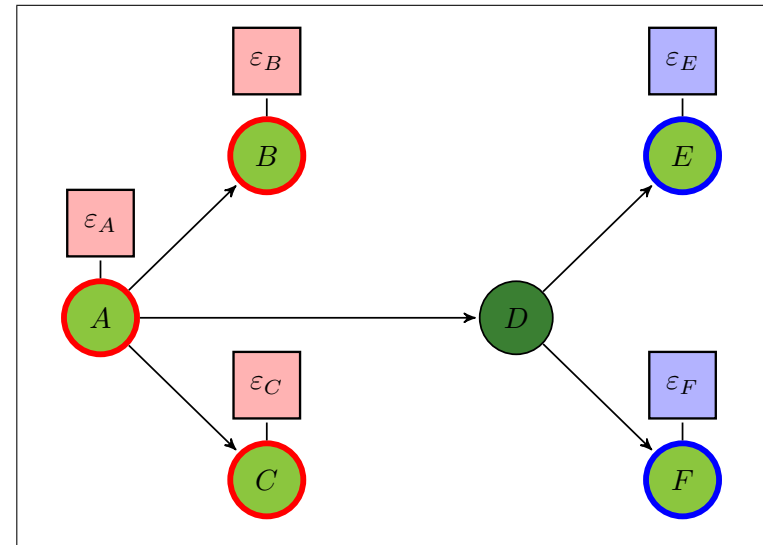
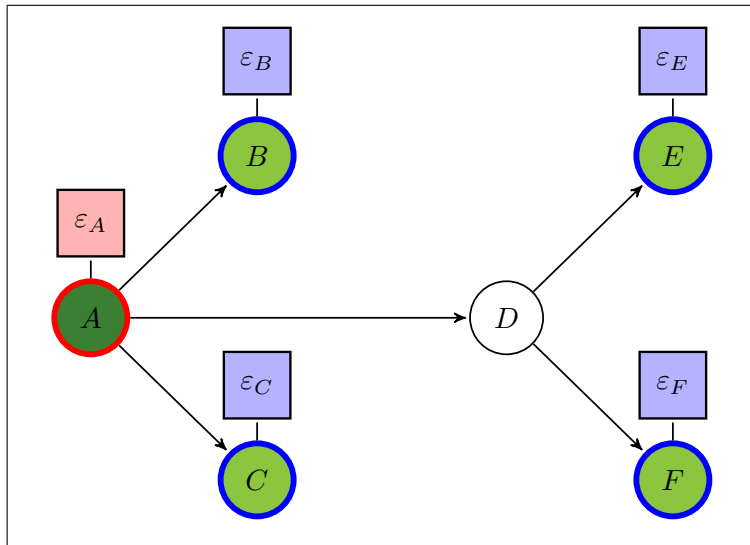
Belief propagation in a tree



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.

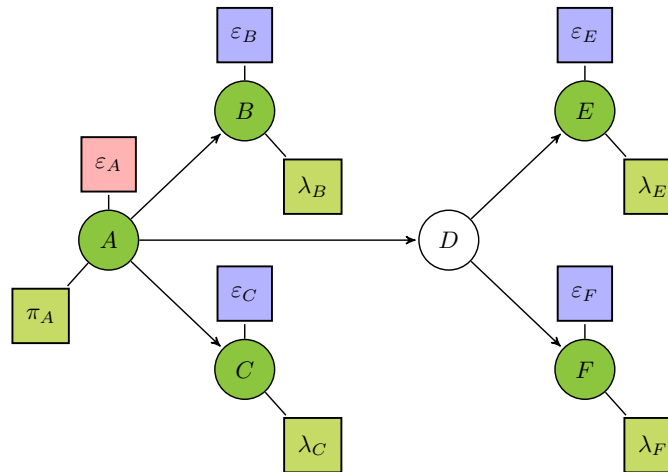
- ▷ Evidence ε_V is an observational data associated with the node V .
- ▷ Attributes π_V, λ_V, p_V are needed to compute marginal distributions.

Evidence decomposition



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

Initialisation



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

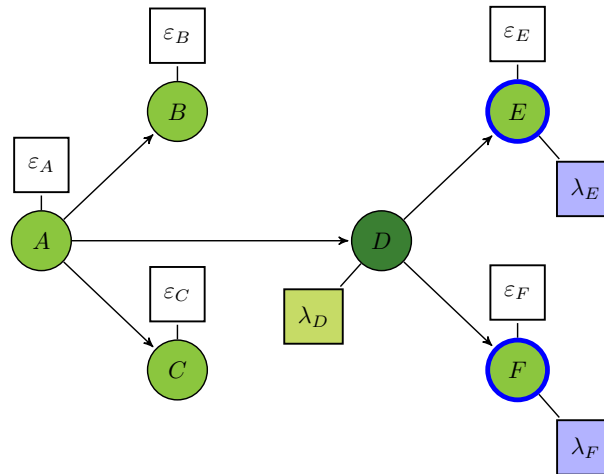
$$\pi_A(a) = \Pr [A = a | \text{evidence}^+(A)] = \Pr [A = a | \epsilon_A]$$

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

...

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

Likelihood propagation



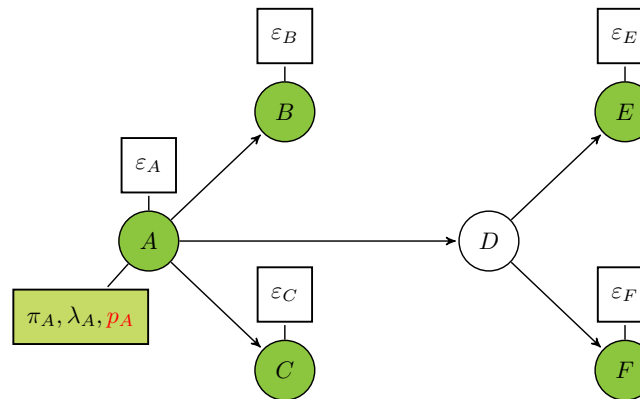
Inference goal

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

Iterative propagation rules

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

Posterior propagation



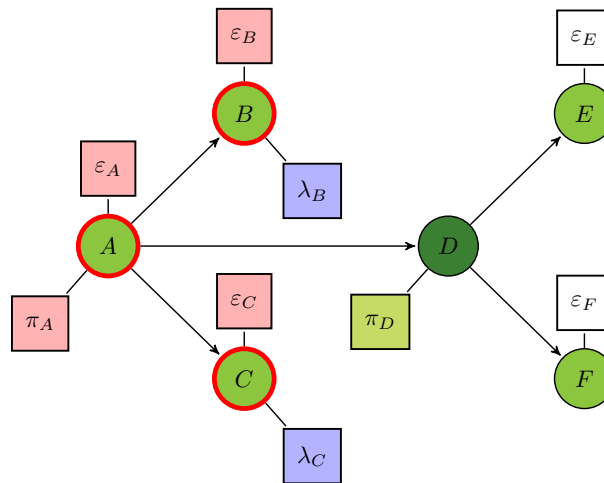
Inference goal

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

Iterative propagation rule

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

Prior propagation



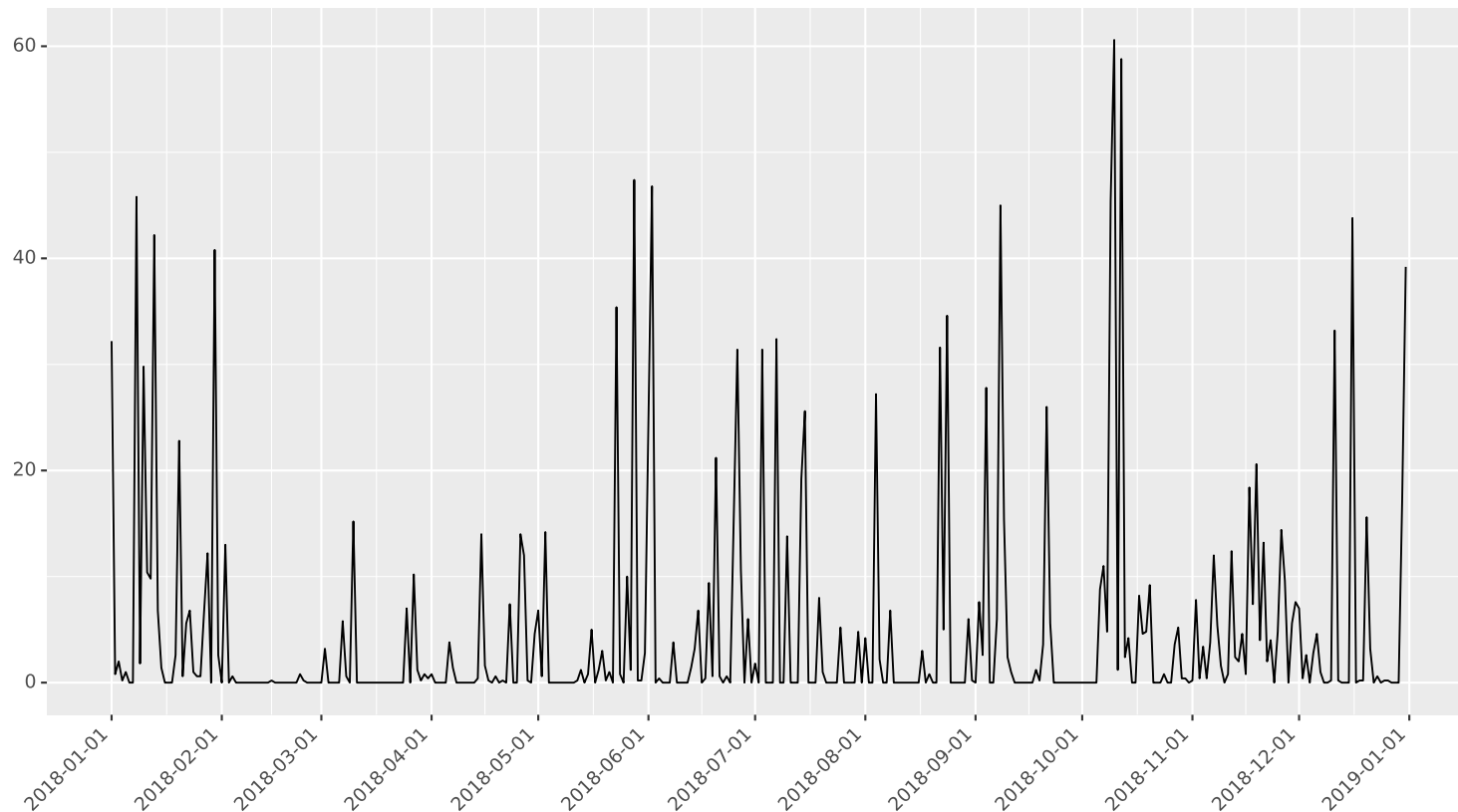
Inference goal

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

Iterative propagation rule

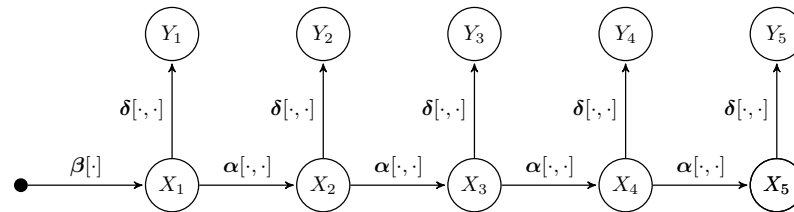
▷ Prior can be computed as $\pi_D \propto \pi_A M_{A \rightarrow D} \otimes M_{A \rightarrow B} \lambda_B \otimes M_{A \rightarrow C} \lambda_C$.

Application on 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

$$\beta = (0.5, 0.5)$$

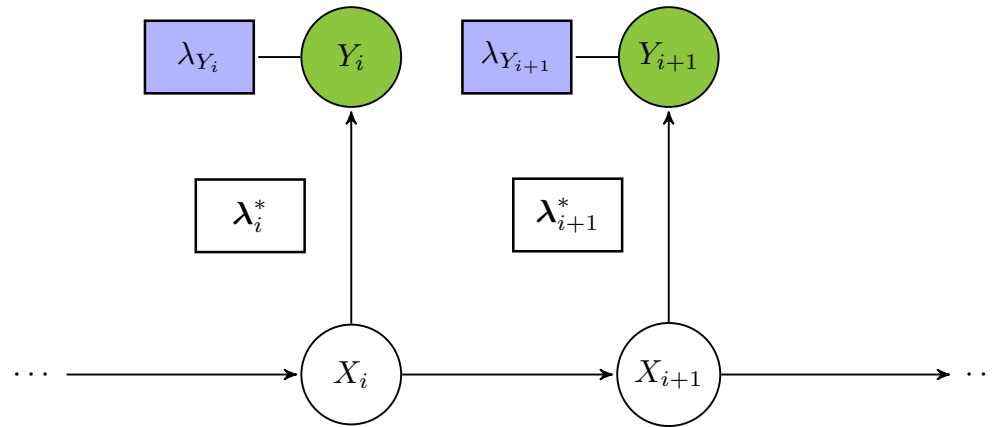
$$\alpha = \begin{pmatrix} 0.95 & 0.05 \\ 0.05 & 0.95 \end{pmatrix}$$

Emission distributions

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

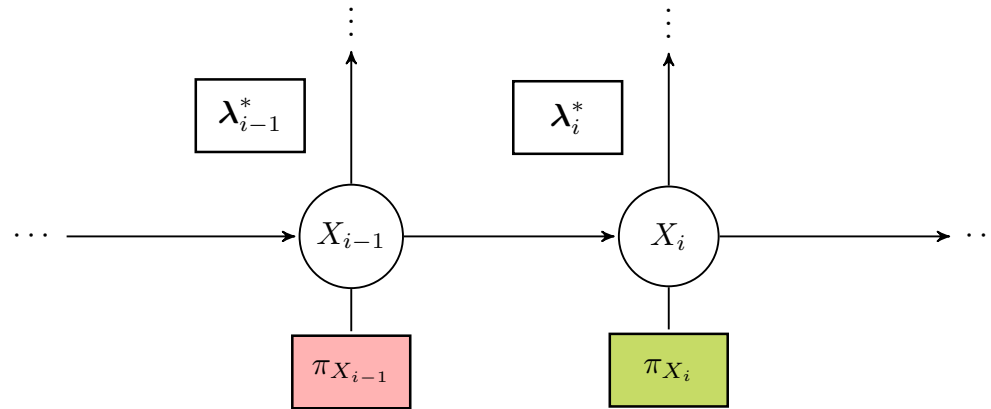
$$Y_i | X_i = 1 \sim \mathcal{N}(\mu_1, \sigma_1)$$

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



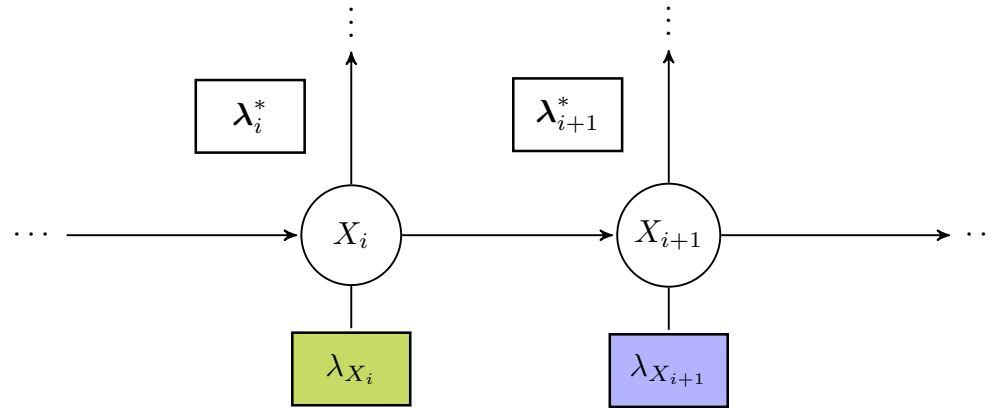
Prior propagation rule yields

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

Now we can do filtering

$$\Pr[x_i | y_1, \dots, y_i] \propto \pi_{X_i}(x_i) \cdot \lambda_i^*(x_i)$$

Likelihood propagation. Smoothing



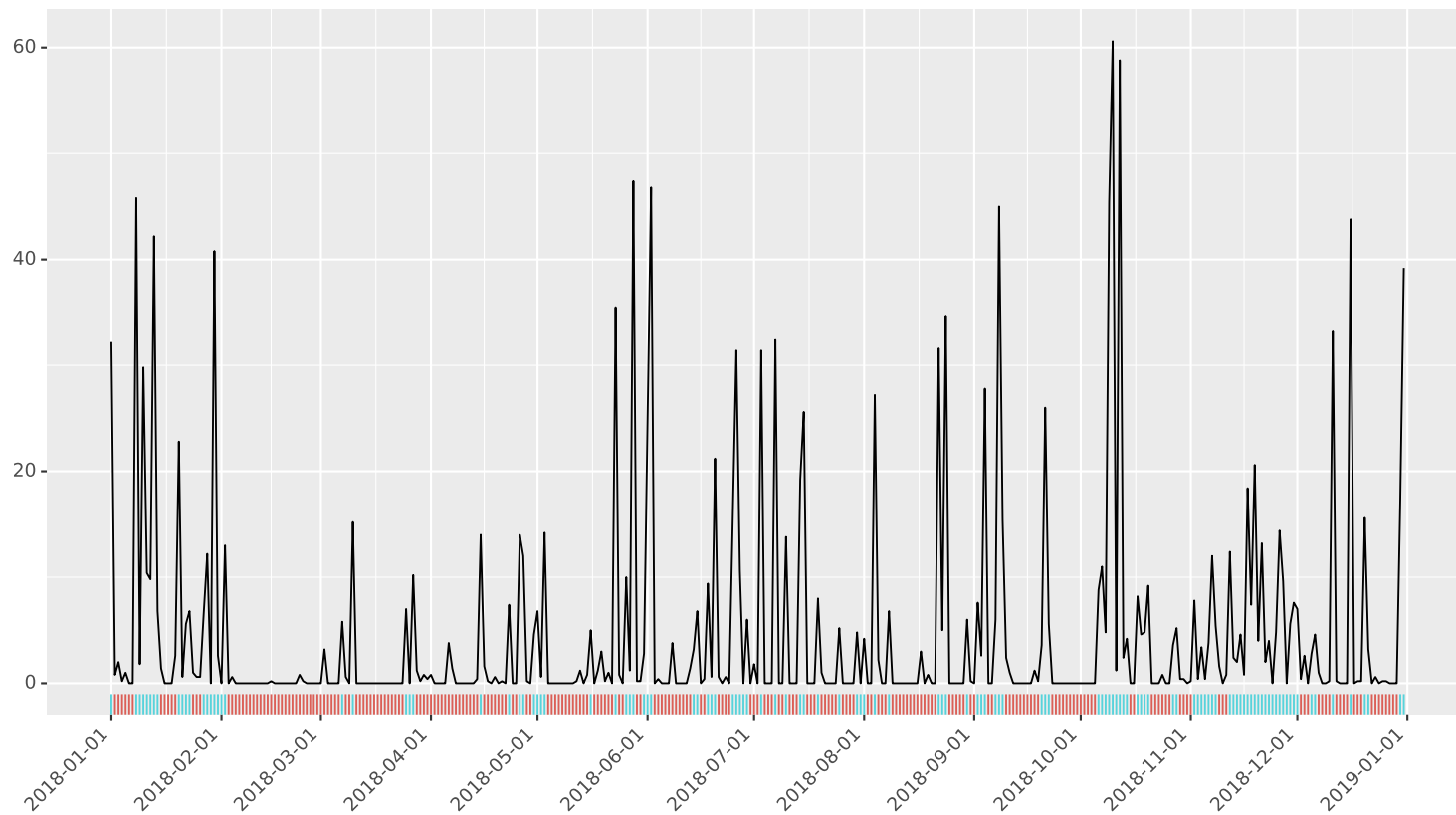
Likelihood propagation rule yields

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

Now we can do smoothing

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

Annotated rainfall data



Sensor fusion problem. Kalman filter

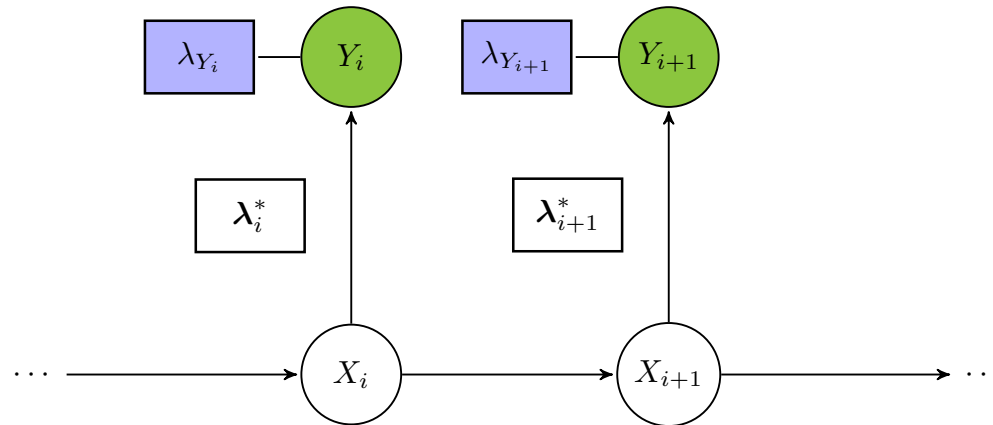
Several sensors measure a physical system

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

Unknown quantities in the system

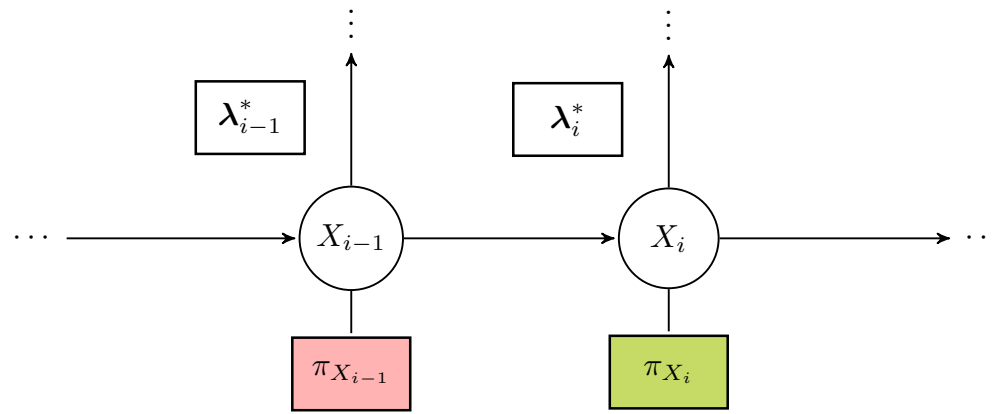
- ▷ Measurement noise \mathbf{v}_t is modelled with a normal distribution.
- ▷ Unknown control signal \mathbf{w}_i is modelled with a normal distribution.
- ▷ Unknown initial state \mathbf{x}_0 is modelled with a normal distribution.
- ▷ Quantities $\mathbf{x}_0, \mathbf{v}_i, \mathbf{w}_i$ are assumed 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 $\mathbf{y}_i = C\mathbf{x}_i + \mathbf{v}_i$ assures that $\mathbf{y}_i | \mathbf{x}_i$ is normal distribution.
- ▷ The local likelihood λ_i^* has a finite description.

Prior propagation. Filtering

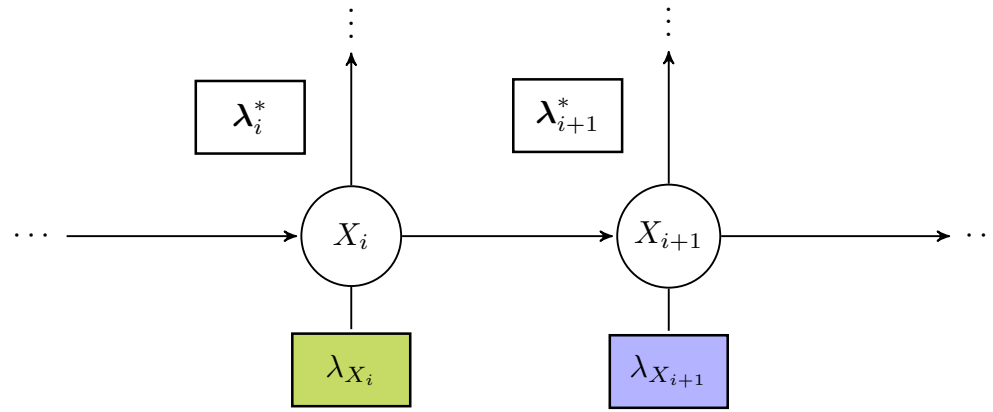


Prior propagation rule

$$\pi_{X_i}(\mathbf{x}_i) \propto \int_{\mathbf{x}_{i-1}} \alpha[\mathbf{x}_{i-1}, \mathbf{x}_i] \cdot \lambda_{i-1}^*(\mathbf{x}_{i-1}) \cdot \pi_{X_{i-1}}(\mathbf{x}_{i-1}) d\mathbf{x}_{i-1}$$

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

Likelihood propagation. Smoothing



Likelihood propagation rule

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

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