

### MSML610: Advanced Machine Learning

### **Reasoning Over Time**

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References: - AIMA 14: Probabilistic reasoning over time

# Reasoning over time

- Reasoning over time
- HMMs
- Markov random fields
- Markov logic network
- State space models and Kalman filter
- Multivariate Kalman filters
- Dynamic Bayesian networks
- State space model
- Variational Inference

### Reference

• AIMA: 14

# **Agents**

- Agents in partially observable environments track the current state using sensor information
  - 1. Belief state
    - Store possible world states (by enumeration or logical formulas)
    - Use probability theory to quantify belief
    - Belief state is the posterior distribution of the current state given all evidence so far
  - 2. Belief state + Transition model
    - Predict how the world might evolve in the next step
  - 3. Sensor model + Percepts
    - Update belief state
- Time is handled by making each quantity a function of time

# Static vs dynamic probabilistic reasoning: example

### Static probabilistic reasoning

- Each random variable has a single fixed value over time
- E.g., when repairing a car:
  - Whatever is broken stays broken during the diagnosis
  - · Observed evidence remains fixed

### Dynamic probabilistic reasoning

- Random variables change over time
- E.g.,
  - Tracking the location of a plane
  - Tracking the economic activity of a nation
- E.g., treating a diabetic patient
  - Goal: assess the state of the patient and decide on insulin dose
  - Evidence: previous insulin doses, food intake, blood sugar (which change over time)
  - Dependency on time (e.g., metabolic activity and time of day)

# **Model components**

- 1. State of the world:  $X_t$
- 2. Prior probability of the state at time 0:  $\underline{\mathbf{X}}_0$
- 3. Evidence variables:  $\underline{\boldsymbol{E}}_t$
- 4. Transition model:  $Pr(\underline{X}_t | \underline{X}_{0:t-1})$ 
  - How the world evolves
  - Specifies the probability distribution of the state <u>X</u><sub>t</sub>, given all previous values
- 5. Sensor model:  $Pr(\underline{\boldsymbol{E}}_t|\underline{\boldsymbol{X}}_{0:t},\underline{\boldsymbol{E}}_{0:t-1})$ 
  - How the evidence variables  $\underline{\boldsymbol{E}}_t$  are generated

### Discrete vs continuous time models

#### Discrete time models

- View the world as a series of time slices ("snapshots")
  - Assume time intervals are equal, so samples are equispaced
  - Label times t = 0, 1, 2, ...
- Each time slice contains random variables:
  - Some RVs are not observable  $X_t$  (hidden)
  - Other RVs are observable  $\underline{\boldsymbol{E}}_t$  (evidence)
  - $\underline{X}_{a:b}$  represents variables in [a, b]

#### Continuous time models

- Uncertainty over continuous time can be modeled by stochastic differential equations (SDEs)
- Discrete time models can be discrete approximations to SDEs

### Markov property

• In general, the current state  $\underline{X}_t$  depends on a growing number of past states:

$$\Pr(\underline{\boldsymbol{X}}_t|\textit{history}) = \Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_0,\underline{\boldsymbol{X}}_1,...,\underline{\boldsymbol{X}}_{t-1})$$

 Markov property: the current state (conditionally) depends only on a finite fixed number of k previous states:

$$\Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_0,\underline{\boldsymbol{X}}_1,...,\underline{\boldsymbol{X}}_{t-k-1},\underline{\boldsymbol{X}}_{t-k},...,\underline{\boldsymbol{X}}_{t-1}) = \Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_{t-1:t-k})$$

## Markov process

Markov processes (aka Markov chains) have the Markov property

$$\Pr(\underline{\boldsymbol{X}}_t|history) = \Pr(\underline{\boldsymbol{X}}_t|\underline{\underline{\boldsymbol{X}}}_{t-1:t-k})$$

• First-order Markov process: the current state depends only on the previous state (and no other earlier state):

$$\Pr(\underline{\boldsymbol{X}}_t|history) = \Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_{t-1})$$

- E.g., the probability of rain today depends only on what happened yesterday  $\Pr(R_t|R_{t-1}) \ \forall t$
- The Bayesian network for a first-order Markov process looks like:
- Second-order Markov process: the current state  $\underline{X}_t$  is conditionally dependent only on  $\underline{X}_{t-1}$  and  $\underline{X}_{t-2}$  and no other earlier state

### Time-homogeneous process

- Even with the Markov assumption, there are infinite probability distributions  $Pr(\underline{X}_t | \underline{X}_{t-1})$ , one for every value of t
- Stationarity: the transition probability doesn't change over time

$$\Pr(\underline{X}_t | \underline{X}_{0:t-1}) = \Pr(\underline{X}_{t-k} | \underline{X}_{0:t-k-1}) \ \forall k, t$$

- The process evolves over time, but the governing laws don't change
- First-order time-homogeneous: only one conditional probability table is needed

$$\Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_{t-1}) = \Pr(\underline{\boldsymbol{X}}_{t-k}|\underline{\boldsymbol{X}}_{t-k-1}) \ \forall k,t$$

• E.g., the probability of rain depends on what happened yesterday and is the same every day:  $\Pr(R_t|R_{t-1}) = f(R_{t-1}) \ \forall t$ 

### Sensor model

- Aka "observation model"
- In general, the evidence variables  $\underline{\boldsymbol{E}}_t$  could depend on previous  $\underline{\boldsymbol{X}}$  (state of the world) and  $\underline{\boldsymbol{E}}$  (sensor value) variables:

$$\Pr(\underline{\boldsymbol{E}}_t|\underline{\boldsymbol{X}}_{0:t},\underline{\boldsymbol{E}}_{0:t-1})$$

- Sensor Markov property
  - We assume that the sensor value  $\underline{\boldsymbol{E}}_t$  depends only on the current state of the world  $\underline{\boldsymbol{X}}_t$ , not on previous sensor values

$$\Pr(\underline{\boldsymbol{\mathcal{E}}}_t|\underline{\boldsymbol{\mathcal{X}}}_{0:t},\underline{\boldsymbol{\mathcal{E}}}_{0:t-1}) = \Pr(\underline{\boldsymbol{\mathcal{E}}}_t|\underline{\boldsymbol{\mathcal{X}}}_t)$$

• In a Bayesian network, even if  $vX_t$  and  $\underline{\boldsymbol{E}}_t$  are contemporaneous in the time step, the arrow goes from the state of the world  $\underline{\boldsymbol{X}}_t$  to the sensor value  $\underline{\boldsymbol{E}}_t$ , i.e.,  $\underline{\boldsymbol{X}}_t \to \underline{\boldsymbol{E}}_t$  since the world causes the sensor to take on particular values

### Sensor model: rain example

- In a Bayesian network,  $\underline{X}_t \to \underline{E}_t$  since the world causes the sensor to take on particular values
  - E.g., the rain "causes" the umbrella to appear
  - The inference goes in the other direction: we see the umbrella and need to guess if it's raining
- E.g.,
  - The transition model is  $Pr(Rain_t|Rain_{t-1})$ 
    - $Pr(R_t|R_{t-1} = T) = 0.7$
    - $Pr(R_t|R_{t-1}=F)=0.3$
    - The sum doesn't have to be 1 since it's a conditional probability
  - The sensor model is  $Pr(Umbrella_t|Rain_t)$ 
    - $Pr(U_t|R_t = T) = 0.9$
    - $Pr(U_t|R_t = F) = 0.2$

### **Prior probability**

- To complete the system specification, we need the prior probability of the state variables at time 0,  $Pr(\underline{X}_0)$ 
  - Represents the initial belief about the state of the system before any observations are made
  - It is crucial for initializing the state estimation process
- E.g.,
  - $X_0$  represents the position and velocity of a moving object
  - $Pr(\underline{X}_0)$  could be a Gaussian distribution centered around an initial guess of the object's position and velocity with some uncertainty

# First-order Markov process: Joint Distribution

- Model a sequence of states  $\underline{X}_0, \underline{X}_1, ..., \underline{X}_t$  and observations  $\underline{E}_1, ..., \underline{E}_t$  over time, with the simplifying assumptions:
  - First-order Markov assumption:  $Pr(\underline{X}_i | \underline{X}_{0:i-1}) = Pr(\underline{X}_i | \underline{X}_{i-1})$
  - Sensor model:  $\Pr(\underline{\boldsymbol{E}}_i|\underline{\boldsymbol{X}}_{0:i},\underline{\boldsymbol{E}}_{1:i-1}) = \Pr(\underline{\boldsymbol{E}}_i|\underline{\boldsymbol{X}}_i)$
- The joint distribution of *n* random variables:

$$\Pr(X_1,...,X_n) = \prod_{i=1}^n \Pr(X_i|parents(X_i))$$

• The joint distribution probability can be written for any t:

$$\Pr(\underline{\boldsymbol{X}}_{0:t},\underline{\boldsymbol{E}}_{1:t}) = \Pr(\underline{\boldsymbol{X}}_{0}) \prod_{i=1}^{t} \Pr(\underline{\boldsymbol{X}}_{i} | \underline{\boldsymbol{X}}_{i-1}) \Pr(\underline{\boldsymbol{E}}_{i} | \underline{\boldsymbol{X}}_{i})$$

$$= \operatorname{prior} \times \prod_{i} \operatorname{transition model} \times \operatorname{sensor model}$$

### First-order Markov process: intuition

 The joint distribution probability for a time-homogeneous first-order Markov process can be written, for any t:

$$\Pr(\underline{\boldsymbol{X}}_{0:t},\underline{\boldsymbol{E}}_{1:t}) = \Pr(\underline{\boldsymbol{X}}_{0}) \prod_{i=1}^{t} \Pr(\underline{\boldsymbol{X}}_{i}|\underline{\boldsymbol{X}}_{i-1}) \Pr(\underline{\boldsymbol{E}}_{i}|\underline{\boldsymbol{X}}_{i})$$

$$= \operatorname{prior} \times \prod_{i} \operatorname{transition model} \times \operatorname{sensor model}$$

- Intuition:
  - Each observation depends only on the current state (sensor model)
  - The state evolves probabilistically from the previous state (transition model)
  - This structure reduces complexity and enables tractable inference
- How to represent this process?
  - A Bayesian network can represent a temporal model by modeling time with indices t, i.e., "unrolling the model"
  - Problem: There are infinite t, even assuming the Markov property

# Improving approximation of real-world systems

- A first-order Markov process can be reasonable or not, e.g.,
  - A particle following a random walk is well represented by Markov process (by definition)
  - In the umbrella example the rain depends only on what happened the previous day
- How to improve the approximation
  - 1. Increase the order of the Markov process model
    - E.g., to model "rarely rains more than two days in a row", we need a second-order Markov model Pr(Rain<sub>t</sub>|Rain<sub>t-1</sub>, Rain<sub>t-2</sub>)
  - 2. Increase the set of state variables
    - E.g., add Seasont to incorporate the historical records
    - This makes the transition model more complicated
  - 3. Increase the number of sensor variables
    - E.g., Locationt, Temperaturet, Humidityt, Pressuret
    - This can simplify modeling of the state

## Inference tasks in temporal models

• There are several possible applications that we will consider in details

Task	Description	Estimate
Filtering Prediction Smoothing	Estimate <i>current</i> state given past / current obs Estimate <i>future</i> state given past / current obs Estimate <i>past</i> state given past, current, and	$ \begin{array}{l} \Pr(\underline{X}_t   \underline{E}_{1:t}) \\ \Pr(\underline{X} t + k   \underline{E}_{1:t}) \text{ for } k > 0 \\ \Pr(\underline{X}_k   \underline{E}_{1:T}) \text{ for } k < T \end{array} $
Most Likely Explanation	future obs Find most probable sequence of states given the evidence	$\operatorname{argmax}_{\underline{\mathbf{x}}_{1:T}} \operatorname{Pr}(\underline{\mathbf{X}}_{1:t}   \underline{\mathbf{E}}_{1:t})$
Learning	Learn model parameters or structure from data	heta of a model

### Task 1: Filtering

- Aka "state estimation"
- Filtering computes the posterior distribution of the current state (belief state) given all evidence to date:

$$\Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{E}}_{1:t}=\underline{\boldsymbol{e}}_{1:t})$$

- E.g., estimate the probability of rain today, given all umbrella observations so far Pr(Raint | Umbrella1:t)
- Filtering is needed by a rational agent to track the current state of the world
  - The agent has a belief about the current state  $\Pr(\underline{X}_{t-1})$  at time t-1
  - New evidence  $\underline{e}_t$  arrives for time t
  - ullet The agent updates its belief about the current state  $\Pr(\underline{X}_t)$  at time t
- The term "filtering" refers to the problem in signal processing of filtering out noise in a signal by estimating system parameters

### **Task 2: Prediction**

• **Prediction** involves predicting the posterior distribution over a *future* state, given all evidence to date:

$$\Pr(\underline{\boldsymbol{X}}_{t+k}|\underline{\boldsymbol{e}}_{1:t})$$
 with  $k>0$ 

• E.g., compute the probability of rain three days from now:

$$Pr(Rain_{t+3}|Umbrella_{0:t})$$

 Prediction helps a rational agent evaluate possible actions based on expected outcomes

## Task 3: Smoothing

• **Smoothing** is the task of computing the posterior distribution over a *past* state given *all* the past, present, and future evidence:

$$\Pr(\underline{\boldsymbol{X}}_{k}|\underline{\boldsymbol{e}}_{1:t})$$
 with  $0 \leq k < t$ 

- Note: you have information about the "future" of the evidence, but you
  don't know the state
- Smoothing provides a better estimate of the state since it incorporates more evidence about the future
- E.g., compute the probability that it rained last Wednesday, given all the observations made up to today
- The name "smoothing" refers to the fact that the state estimate is smoother than filtering

## Task 4: Most-likely explanation

• Most-likely explanation finds the sequence of states  $\underline{x}_{1:t}$  most likely to have generated observations  $\underline{e}_{1:t}$ :

$$\mathsf{argmax}_{\underline{\pmb{x}}_{1:t}} \mathsf{Pr}\big(\underline{\pmb{x}}_{1:t} | \underline{\pmb{e}}_{1:t} \big)$$

- E.g.,
  - Umbrella appeared on 3 days, not on the fourth
  - Most likely explanation: rained for 3 days, then stopped
- Applications
  - Speech recognition: most likely sequence of words given sounds
  - Digital processing: reconstruct bit strings over a noisy channel

### Task 5: Learning

- Learning involves estimating the transition model  $\Pr(\underline{X}_t|\underline{X}_{0:t-1})$  and the sensor model  $\Pr(\underline{E}_i|\underline{X}_i)$  from observations
- Learning:
  - Can be a byproduct of inference
  - Requires smoothing rather than filtering for better state estimates
    - Smoothing uses all available data to estimate states, leading to more accurate models
    - E.g., in a weather prediction system, smoothing might use past, present, and future data to better estimate the current weather state

# Task 1: Recursive filtering: goal

- Aka "recursive state estimation"
- A practical filtering algorithm updates the current state estimate  $\underline{\boldsymbol{X}}_{t+1}$  using the previous state  $\underline{\boldsymbol{X}}_t$  and the new evidence  $\underline{\boldsymbol{e}}_{t+1}$ , rather than recomputing it by going over the entire history of the percepts

$$\Pr(\underline{X}_{t+1}|\underline{e}_{1:t+1}) = f(\Pr(\underline{X}_t|\underline{e}_{1:t}),\underline{e}_{t+1})$$
 $NextState = f(PreviousState, e_{t+1})$ 

- Why?
  - Time and space requirements for updating must be constant if a (finite) agent needs to keep track of current state indefinitively
- Is it possible?
  - What is the formula f(...)?

### Task 1: Recursive filtering: update formula

- Compute the state at time t+1 with all the evidence up to that time
- Assume that state and evidence are scalar and not vector:  $Pr(X_{t+1}|e_{1:t+1})$

$$\begin{array}{ll} \text{Divide up the evidence} &= \Pr(X_{t+1}|e_{1:t},e_{t+1}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1},e_{1:t}) \Pr(X_{t+1}|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1},e_{1:t}) \Pr(X_{t+1}|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1}) \Pr(X_{t+1}|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t,e_{1:t}) \Pr(x_t|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t,e_{1:t}) \Pr(x_t|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t) \Pr(x_t|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{t+1}) \Pr(x_t|e_{1:t}) \\ &= \alpha \Pr(e_{t+1}|X_{$$

$$Pr(X_{t+1}|e_{1:t+1}) = f(Pr(X_t|e_{1:t}), e_{t+1})$$

- The next state is "Sensor model x Transition model x Recursive state"
  - Sensor model:  $Pr(e_{t+1}|X_{t+1})$
  - Transition model:  $Pr(X_{t+1}|x_t)$
  - Recursive term:  $Pr(x_t|e_{1:t})$

### Task 1: Recursive filtering: intuition

 Recursive state estimation updates in two steps the belief about a system's state over time as new evidence arrives

$$\Pr(X_{t+1}|e_{1:t+1}) = \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t) \Pr(x_t|e_{1:t})$$

 Prediction step: Use the transition model to predict the next state based on the current belief

$$\Pr(X_{t+1}|e_{1:t}) = \sum_{x_t} \Pr(X_{t+1}|x_t) \Pr(x_t|e_{1:t})$$

- Intuition: Project the current belief forward using the model of system evolution
- 2. Update step: Incorporate the new observation to refine the prediction

$$\Pr(X_{t+1}|e_{1:t+1}) = \alpha \Pr(e_{t+1}|X_{t+1})\Pr(X_{t+1}|e_{1:t})$$

- Intuition: Correct the prediction using the likelihood of the new evidence
- Maintain  $Pr(X_t|e_{1:t})$ , the probability of the current state given all past evidence
  - E.g., in a weather model, if it was likely to rain today and rain usually continues, the prediction leans toward rain tomorrow
  - Seeing an umbrella supports this and updates the belief accordingly

### Task 1: Forward update

We achieved:

$$\begin{aligned} \Pr(\underline{\boldsymbol{X}}_{t+1}|\underline{\boldsymbol{e}}_{1:t+1}) &= \alpha \Pr(\underline{\boldsymbol{e}}_{t+1}|\underline{\boldsymbol{X}}_{t+1}) \sum_{\boldsymbol{x}_t} \Pr(\underline{\boldsymbol{X}}_{t+1}|\underline{\boldsymbol{x}}_t) \Pr(\underline{\boldsymbol{x}}_t|\underline{\boldsymbol{e}}_{1:t}) \\ &= f(\Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{e}}_{1:t}),\underline{\boldsymbol{e}}_{t+1}) \end{aligned}$$

• The filtered estimate  $\underline{f}_{1:t} = \Pr(\underline{X}_t | \underline{e}_{1:t})$  is propagated forward and updated by each transition and new observation

$$\underline{\mathbf{f}}_{1:t+1} = Forward(\underline{\mathbf{f}}_{1:t}, \underline{\mathbf{e}}_{t+1})$$

starting with the initial condition  $\underline{\boldsymbol{f}}_{1:0} = \Pr(\underline{\boldsymbol{X}}_0)$ 

- This is called "forward update"
- This process allows efficient online inference without storing the full history
  - Time and space requirements for updating is constant
  - A (finite) agent can keep track of current state indefinitively

### Task 2: Prediction: update formula

- Prediction is equivalent to filtering without updating the state with new evidence (since we lack evidence)
  - Only the transition model is needed, not the sensor model
- The rule predicting state  $\underline{X}_{t+k+1}$  given state  $\underline{X}_{t+k}$  and evidence  $\underline{E}_{1:t}$  is:

$$\Pr(\underline{\boldsymbol{X}}_{t+k+1}|\underline{\boldsymbol{e}}_{1:t}) = \sum_{\boldsymbol{x}_{t+k}} \Pr(\underline{\boldsymbol{X}}_{t+k+1}|\underline{\boldsymbol{x}}_{t+k}) \Pr(\underline{\boldsymbol{x}}_{t+k}|\underline{\boldsymbol{e}}_{1:t})$$

- This equation can be used recursively to advance over time
  - Predicting even a few steps ahead generally incurs large uncertainty

## **Task 3: Smoothing: intuition**

 We want to calculate the probability distribution over the hidden state at time k, given all evidence up to time t (in the future!)

$$\Pr(X_k | e_{1:t})$$
 where  $0 \le k < t$ 

- Filtering gives  $Pr(X_k|e_{1:k})$  using past and present evidence
- Smoothing refines the estimate of past states using later evidence
- E.g.,
  - You're tracking whether it was raining yesterday
  - You had some evidence up to yesterday (e.g., a cloudy sky)
  - Today you see puddles on the ground
  - That new observation supports the idea that it was raining

# Task 3: Smoothing: update formula

- Using the same math as for filtering and the two key assumptions of Markov process and Markov sensor
- Forward Pass (aka filtering):
  - Move forward through time, using the filtering algorithm to compute:

$$f_{1:k} = \Pr(X_k|e_{1:k})$$

- This gives you a "best guess" of the state at time k, based only on evidence up to k
- Backward Pass (aka smoothing):
  - Move backward through time from time t, computing:

$$b_{k+1:t} = P(e_{k+1:t}|X_k)$$

- ullet This captures how likely the future evidence is, given a particular value of  $X_{k}$
- Combine them:
  - Multiply forward and backward messages to get:

$$P(X_k|e_{1:t}) \propto f_{1:k} \times b_{k+1:t}$$

## Task 4: Most likely explanation: Intuition 1/2

- You are tracking the weather (sunny or rainy) based on whether someone carries an umbrella
- You can't see Weather directly (hidden state), but you observe umbrellas (which is a noisy observation)
  - You have 5 observations Umbrella = [T, T, F, T, T]
- Question: what is the most likely sequence of Weather states that explains the Umbrella observations?
  - You know something about the transition model (i.e., "it tends to rain several days in a row") and the sensor model (i.e., "people often forget the umbrella")
- Mathematically

$$\mathsf{argmax}_{\mathsf{X}_{1:t}} \mathsf{Pr}(\mathsf{X}_{1:t}|e_{1:t}) = \mathit{argmax}_{\mathit{Weather}_{1:t}} \mathsf{Pr}(\mathit{Weather}_{1:t}|\mathit{Umbrella}_{1:t})$$

## Task 4: Most likely explanation: Intuition 2/2

- Naive approach: Use smoothing to choose the most likely state at each time step
  - Cons
    - Might lead to an implausible overall path
    - Suboptimal since the question addresses joint probability and we are not using all the information (only one step at the time!)
- Viterbi algorithm:
  - Constructs a path through a state-time graph with states as nodes and transitions as edges
  - Finds the most likely entire path through the hidden states
- Key difference:
  - E.g., in speech recognition, find the most likely word sequence behind a noisy audio signal
  - Smoothing: Best guess per time step (may not find words that are not English and / or suboptimal sequence)
  - Viterbi: Best overall path (maximizes joint probability of the entire sequence)

### Viterbi algorithm: Intuition

- Objective: Find the most likely sequence of hidden states given observations
- 1. Initialization
  - At t = 1, estimate the probability of starting in each state using the initial state distribution and observation likelihood
- 2. Recursion via dynamic programming
  - At each time t > 1, for each state  $x_t$ :
  - Compute the maximum probability path to  $x_t$  from any previous state
  - Use:
    - $Pr(x_t|x_{t-1})$ : transition model
    - $Pr(e_t|x_t)$ : sensor model
    - Best path probability to  $x_{t-1}$  from prior step
  - Store the probability and the corresponding back-pointer to  $x_{t-1}$
- 3. Termination and backtrace
  - At final time t = T, identify the state with the highest final probability
  - Trace back through the stored pointers to reconstruct the optimal path

# Viterbi algorithm: Example 1/2

- You observe a friend carrying an umbrella over 3 days: Umbrella = [Yes, Yes, No]
- You want to infer the most likely sequence of hidden Weather states
  - States:  $S = \{Sunny, Rainy\}$  (weather)
  - Observations:  $O = \{Yes, No\}$  (umbrella)
- Initial Probabilities:

$$Pr(Sunny) = 0.6$$
,  $Pr(Rainy) = 0.4$ 

Transition Probabilities:

$$\begin{aligned} & \mathsf{Pr}(\mathsf{Sunny} \to \mathsf{Sunny}) = 0.7, & \mathsf{Pr}(\mathsf{Sunny} \to \mathsf{Rainy}) = 0.3 \\ & \mathsf{Pr}(\mathsf{Rainy} \to \mathsf{Sunny}) = 0.4, & \mathsf{Pr}(\mathsf{Rainy} \to \mathsf{Rainy}) = 0.6 \end{aligned}$$

Observation (Emission) Probabilities:

$$\begin{split} & \text{Pr}(\text{Yes}|\text{Sunny}) = 0.1, \quad \text{Pr}(\text{No}|\text{Sunny}) = 0.9 \\ & \text{Pr}(\text{Yes}|\text{Rainy}) = 0.8, \quad \text{Pr}(\text{No}|\text{Rainy}) = 0.2 \end{split}$$

# Viterbi algorithm: example 2/2

#### • Viterbi table

Day	State	Probability	Backpointer
1	Sunny	$0.6 \times 0.1 = 0.06$	
	Rainy	$0.4 \times 0.8 = 0.32$	_
2	Sunny	$max(0.06 \times 0.7, 0.32 \times 0.4) \times 0.1 = 0.0128$	Rainy
	Rainy	$\max(0.06 \times 0.3, \ 0.32 \times 0.6) \times 0.8 = 0.1536$	Rainy
3	Sunny	$\max(0.0128 \times 0.7, \ 0.1536 \times 0.4) \times 0.9 = 0.0553$	Rainy
	Rainy	$\max(0.0128 \times 0.3, \ 0.1536 \times 0.6) \times 0.2 = 0.0184$	Rainy

- Final most probable state: Sunny (Day 3)
- Find the most likely sequence:
   Rainy → Rainy → Sunny

### **HMMs**

- Reasoning over time
- HMMs
- Markov random fields
- Markov logic network
- State space models and Kalman filter
- Multivariate Kalman filters
- Dynamic Bayesian networks
- State space model
- Variational Inference

## Algorithms for Specific Models

- General temporal probabilistic reasoning makes minimal assumptions:
  - Markov property for transitions
  - Sensor model depends only on current state
  - No constraints on:
    - Mathematical form of transition/sensor models
    - Nature of state and evidence variables (discrete or continuous)
- Efficiency and accuracy can improve by exploiting specific model structures:
  - Hidden Markov Models (HMMs):
    - State is a single discrete variable
    - Transition and observation models are discrete probability tables
    - Enables fast algorithms like the Viterbi algorithm, forward-backward, etc
  - Kalman Filters (for continuous domains):
    - State variables are continuous and normally distributed
    - Linear-Gaussian models for transitions and observations
    - · Allows exact, efficient updates using matrix operations
- Tailored algorithms can be orders of magnitude faster and more accurate than general methods

# Hidden Markov Model: State and Transition Model

- Hidden Markov Model (HMM): A temporal model with simplified structure for efficiency
  - State model:
    - The system state at time t is a discrete random variable  $X_t \in \{1,\ldots,S\}$
    - E.g., in the umbrella domain,  $X_t = Rain_t$  with states  $\{rain, no rain\}$
    - Generality: Multiple variables can be combined into one "mega-state" variable
  - Transition model  $Pr(X_t|X_{t-1})$ :
    - Described by a transition matrix  $\underline{T}$  of size  $S \times S$
    - Entry  $T_{ij} = \Pr(X_t = j | X_{t-1} = i)$ : probability of transitioning from state i to j
  - Sensor model:
    - Defined as  $Pr(E_t|X_t=i)$  for each state i
    - Representable as a vector (discrete observations) or a diagonal matrix  $\underline{O}$  (for convenience)
    - No assumptions about the number or type (discrete / continuous) of observation variables
- Benefit
  - This structure enables efficient algorithms like forward, backward, and Viterbi

# Hidden Markov Model: umbrella example

• E.g., if Rain = T is state 1 and Rain = F is state 2, then the transition matrix for the umbrella world

$$R_{t-1}$$
  $Pr(R_t|R_{t-1})$   $T$  0.7  $F$  0.3

becomes the transition model

$$\underline{\underline{T}} = \begin{pmatrix} 0.7 & 0.3 \\ 0.3 & 0.7 \end{pmatrix}$$

• On day 1 we observe  $U_1 = T$  and on day 3,  $U_3 = F$ , we have the observation matrices

$$\underline{\mathbf{O}}_1 = \begin{pmatrix} 0.9 & 0 \\ 0 & 0.2 \end{pmatrix} \quad \underline{\mathbf{O}}_3 = \begin{pmatrix} 0.1 & 0 \\ 0 & 0.8 \end{pmatrix}$$

# Hidden Markov Model: algorithms

 Using the matrix representation all the forward / backward computations become matrix operations:

$$\mathbf{f}_{1:t+1} = \alpha \mathbf{O}_{t+1} \mathbf{T}^{\mathsf{T}} \mathbf{f}_{1:t}$$
  $\mathbf{b}_{k+1:t} = \mathbf{TO}_{k+1} \mathbf{b}_{k+2:t}$ 

- So all the inference tasks (e.g., filtering, smoothing) can be expressed as matrix multiplication which are typically efficient
- There are several improvements that can be done to reduce time and space complexity
  - Baum-Welch
    - Special case of Expectation-Maximization (EM) algorithm
    - Pros: Converge to a local maximum of the likelihood
    - Cons: Only point-estimation of params, no uncertainty estimation
  - Viterbi
    - · Find the most likely sequence of hidden states
    - Pros: Fast approximation of BW
    - Cons: returns a local optimum
  - Gradient-based methods
    - For more complex models with differentiable form
    - Use gradient descent to optimize parameter

# Hidden Markov Model: applications

- HMMs are very versatile to model systems that have hidden states which produce observable outputs
- Audio / speech
  - Speech recognition: map audio to phonemes, words
  - Speaker identification: model vocal traits to recognize a speaker
  - Music generation and transcription
- Biology / genomics
  - Gene prediction: find regions of DNA
  - Protein structure prediction
- Finance / economics
  - Market regime detection: e.g., bull/bear markets, volatility regimes
  - Credit scoring: observe purchases and estimate financial health (hidden variable)
- Security / anomaly detection
  - User behavior modeling: detect anomalous login patterns or usage activities
  - Intrusion detection: model normal traffic patterns to spot attacks

#### **HMMs: limitations**

- Short memory
  - Markov assumption, i.e., current state depends only on the previous state
  - Inefficient for capturing long-range dependencies or context
- Predefined and fixed number of states
  - Underestimating / overestimating the number of states can lead to underfitting or overfitting
- Stationarity assumption
  - Transition and sensor probabilities are assumed to be constant over time
- Use an atomic representation
  - The states have no internal structure and are simply labels
- Training is computationally expensive for large datasets
- Struggles with sparse data
- Hard to interpret when there is a lot of states or states don't have a clean meaning

Alternatives

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### Markov random fields

- Reasoning over time
- HMMs
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- Markov logic network
- State space models and Kalman filter
- Multivariate Kalman filters
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# Markov logic network

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# State space models and Kalman filter

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- Markov logic network
- State space models and Kalman filter
  - g-h filter
  - One dimensional Kalman filters
  - Multivariate Gaussians
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#### Reference

 $\bullet \ https://github.com/rlabbe/Kalman-and-Bayesian-Filters-in-Python$ 

# **Tracking objects**

- Many problems can be formulated as "tracking objects", e.g.,
  - Navigation of aircraft, drones, autonomous cars
  - Robotics: arm kinematics to predict the position of joints
  - Sensor fusion: merge multiple sensor readings
  - Finance: predict economic variables (e.g., stock prices)
  - Computer vision: track moving objects across video
  - Aerospace: radar tracking, missile, satellite
- Kalman filter is widely used for state estimation in dynamic systems, when measurements are noisy and uncertain
  - Track something over time using a combination of predictions (i.e., a model) and observations

# Some guiding principles

- The world is noisy
  - A car might swerve around a pothole or brake for a pedestrian
  - Wind or ice might change the car's path
- Sensors are noisy
  - E.g., a kitchen scale gives different readings for the same object
- Data is better than a guess
  - · Even if noisy
- Knowledge is uncertain
  - We alter beliefs based on evidence strength
- Use past information and system knowledge to estimate future information
  - ullet E.g., if a car moves at a certain speed at time t, the speed at time t+1 is likely close to the previous speed
- Never discard information, no matter how poor
  - E.g., two sensors, even if one is less accurate, are better than one

# g-h filter

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# Example of weight: blending predictions and measurements

- Imagine going to the gym to gain muscle mass
  - Estimate your weight over time
- You could:
  - 1. Predict your weight
    - Track calorie intake and energy expense
    - Compute expected weight gain
    - Cons: Difficult to track food intake and exercise accurately
  - 2. Measure your weight
    - Use a scale
    - Cons: Scale is noisy, water weight fluctuates, different clothes
- Prediction doesn't match measurements
  - At time *t* − 1
    - Estimate:  $\hat{x}_{t-1} = 158$
  - At time *t*:
    - Scale measures 164
    - Estimate  $\hat{x}_{t|t-1} = 159$  based on calorie intake
- What's your real weight?
  - You need to blend prediction and measurement

# **Example of weight: correct gain\_rate**

Blend the estimates like:

estimate = 
$$0.6 \times prediction + (1 - 0.6) \times measurement$$

• You believe the prediction is more likely correct than the measurement

#### Algorithm

- 1. Start with an initial guess
  - Assume it's correct for now
- 2. Predict the next weight based on the model
- 3. Measure the weight
- 4. Estimate the next weight by merging values:
  - The prediction is always between the prediction and the measurement
- 5. Go back to first step

## **Example of weight:**

- The black line is the actual weight, i.e., ground truth
- The initial guess is 160 lbs
- The red line is the prediction from previous day's weight
- The measurements are the circles
- The blue line is the estimate from the filter
  - Always falls between measurement and prediction
- It's not impressive since the prediction model describes the ground truth, so you don't need the measurements

# **Example of weight: learning gain\_rate**

- Consider when the model predicts a gain of -10lb/day, which is incorrect
  - Estimates diverge from measurements
- The filter needs a correct guess of the weight change rate
  - Also the rate of change can vary over time
- Solution: estimate the rate of change from measurements
  - "Data is better than a guess, even if it's noisy"
  - Refine the estimate of the gain rate:

```
\mathsf{new} \ \mathsf{gain} = \mathsf{old} \ \mathsf{gain} + 0.3 \ \mathsf{(measurement - prediction)} \ / \ 1 \ \mathsf{day}
```

 The "state" is given by weight and gain\_rate, so you need to predict and update both

### g-h filter

- The previous algorithm is called g-h filter
  - g: scaling used to blend predicted state and measurement
  - h: scaling used to update the parameter of the system model based on the measurements
- g-h filters have different values of g and h to achieve different properties
  - E.g., pick g to minimize the transient error when the derivative of the signal has a step (i.e., a discontinuity of the slope)
  - Many filters (including Kalman filter) are just generalizations of a g-h filter

# **Control theory nomenclature**

- State space models were developed in control theory, so there is a different nomenclature
- System: object you want to estimate/track
- Filter: algorithm to estimate the state of the system
- State of the system x: current values you are interested in
  - E.g., weight
  - Part of the state might be hidden (i.e., not observable)
  - $\bullet$  You cannot observe the entire state directly, only measure it indirectly
- Measurement z: the measured value of the system
  - It is observable
  - It can be inaccurate
    - E.g., 99.3kg instead of 100kg
- State estimate x est: filter estimate of the state
- System model: mathematical model of the system
  - E.g., "weight today = weight yesterday + weight gain"
  - The system model is typically imperfect

# g-h filter algorithm: pseudo-code

#### 1. Initialization

- Initialize the state of the filter
- Initialize your belief in the state

#### 2. Predict

- Use system model to predict state at next time step
- Adjust belief to account for uncertainty in prediction

#### 3. Update

- Get measurement and associated belief about its accuracy
- Use as estimate of the next state a point between estimated state and measurement

# Interpretation of g

- If g = 0:
  - The filter follows the system model, ignoring the measurements
- If g increases:
  - The filter follows the measurements more, ignoring the prediction
  - Useful when measurements are accurate and the system model is inaccurate
- If g = 1:
  - The filter follows only the measurements, ignoring the system model

# **Interpretation of** h

- You might need to estimate some model parameters from data, e.g.,
  - The change of weight
  - The rate of change of the measurements
  - The speed of the car on different terrains
- If *h* = 0:
  - The filter follows the previous values of the rate of change of the underlying model
  - I.e., it adapts slowly to the change of the signals
- If *h* = 1:
  - The filter reacts to the transient rapidly if the signal varies significantly with respect to the time step
- Note: an incorrect initial state (e.g., initial value/rate of change) is similar to a changing state

### One dimensional Kalman filters

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# **Updating belief using Gaussians**

The Bayes theorem tells that:

```
posterior = normalized(prior \times likelihood)
```

- If the prior and the likelihood are Gaussian the result is also Gaussian (conjugate prior)
  - The belief and probability are represented as a Gaussian
  - We can encode the PDF in terms of mean and std dev
  - Updating belief is equivalent to sum and multiplication of Gaussians
- Algorithm:

```
# Create prior (using current estimate and system model)
prior = predict(x, process_model)

# Create likelihood (using measurement).
likelihood = gaussian(z, sensor_var)

# Update belief using prior and likelihood
posterior = update(prior, likelihood)
```

#### **Sum of Gaussians**

• The sum of two independent Gaussians

Normal
$$(\mu_1, \sigma_1^2)$$
  
Normal $(\mu_2, \sigma_2^2)$ 

is a Gaussian  $Normal(\mu, \sigma^2)$  with:

$$\mu = \mu_1 + \mu_2$$
$$\sigma^2 = \sigma_1^2 + \sigma_2^2$$

- The mean is the sum of the mean (by linearity)
- The variance always increases

#### **Product of Gaussians**

The product of two independent Gaussians

Normal
$$(\mu_1, \sigma_1^2)$$
  
Normal $(\mu_2, \sigma_2^2)$ 

is a Gaussian  $N(\mu, \sigma^2)$  with:

$$\mu = \frac{\mu_1 \sigma_2^2 + \mu_2 \sigma_1^2}{\sigma_1^2 + \sigma_2^2}$$
$$\sigma^2 = \frac{\sigma_1^2 \sigma_2^2}{\sigma_1^2 + \sigma_2^2}$$

#### • Interpretation:

- The variance may be reduced as more information is incorporated
- If one Gaussian  $N_1$  is much narrower than the other (i.e., one measure is more accurate), the result is pushed towards  $N_1$
- If two Gaussians are similar (i.e., two measures corroborate each other),
   the result becomes more certain

#### Kalman Gain

- Assume that:
  - x is the model prediction
  - z indicates the measurements
- The mean of the posterior is:

$$\mu = \frac{\sigma_x^2 \mu_z + \sigma_z^2 \mu_x}{\sigma_x^2 + \sigma_z^2} = \frac{\sigma_x^2}{\sigma_x^2 + \sigma_z^2} \mu_z + \frac{\sigma_z^2}{\sigma_x^2 + \sigma_z^2} \mu_x = K \mu_z + (1 - K) \mu_x$$

- The Kalman Gain K:
  - Is the scaling term that mixes the prediction and the measurement
  - Depends on the ratio of uncertainty of prior and measurement

## Kalman pseudo-algorithm

- The typical formulation of the Kalman filter is in terms of the "orthogonal projection" approach to minimize mean squared error
  - Instead of a Bayesian formulation
- Typical symbols used in Kalman literature:
  - x: state
  - P: variance of state (uncertainty, belief)
  - f(): system model
  - Q: system model error
  - z: measurement
  - R: measurement noise
- Initialization
  - Initialize state of filter  $x = x_0$
  - Initialize belief in the state  $P = P_0$
- Predict
  - Use system model to predict state at the next time step x = f(x)
  - Adjust belief to account for uncertainty in prediction P = P + Q
- Update
  - Get measurement z and belief about its accuracy R
  - Compute residual between estimated state x and z: y = z x
  - Compute scaling factor (Kalman K) based on accuracy of prediction P and measurement R

#### **Multivariate Gaussians**

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#### Multivariate state

- Often the state variable is multivariate, e.g.,
  - Position and velocity of a dog (probably uncorrelated)
  - Height and weight of an adult (correlated)
- Variance is a measure of how a population varies, e.g.,
  - Variance = 0 means constant
  - Large variance means lots of variation
- Covariance are correlated variances
  - E.g., height and weight are generally positively correlated
- Covariance matrix
  - The diagonal contains the variance for each variable
  - ullet The off-diagonal elements contain the covariance between i and j variables
  - The covariance matrix is symmetric
- Correlation allows prediction
  - E.g., "as winter comes you predict you will spend more on heating your house"

#### Multivariate Gaussian

- The marginal of a multivariate Gaussian is 1-d Gaussian
- Consider a contour plot (i.e., the intersection of a 2-d Gaussian z = f(x, y) with a plane z = c)
  - The contour plot is always an ellipses

# Multiplying two multivariate Gaussians

- Given two multivariate Gaussians  $\sim Normal(\underline{\mu}_i, \underline{\underline{\Sigma}}_i)$
- The product of the Gaussians is still Gaussian  $\sim Normal(\mu, \underline{\Sigma})$

$$\begin{split} &\underline{\mu} = \underline{\underline{\Sigma}}_2 (\underline{\underline{\Sigma}}_1 + \underline{\underline{\Sigma}}_2)^{-1} \underline{\mu}_1 + \underline{\underline{\Sigma}}_1 (\underline{\underline{\Sigma}}_1 + \underline{\underline{\Sigma}}_2)^{-1} \underline{\mu}_2 \\ &\underline{\underline{\Sigma}} = \underline{\underline{\Sigma}}_1 (\underline{\underline{\Sigma}}_1 + \underline{\underline{\Sigma}}_2)^{-1} \underline{\underline{\Sigma}}_2 \end{split}$$

Note: this is a generalization of the 1-d case to multivariate

$$\mu = \frac{\mu_1 \sigma_2^2 + \mu_2 \sigma_1^2}{\sigma_1^2 + \sigma_2^2}$$
$$\sigma^2 = \frac{\sigma_1^2 \sigma_2^2}{\sigma_1^2 + \sigma_2^2}$$

#### replacing:

- $\sigma^2$  with covariance matrix  $\Sigma$
- Division with matrix inversion

# Multivariate filtering

- Covariance structure helps improve the estimate, e.g.,
  - You know an airplane direction can't change quickly
  - Knowing an approximate value for the velocity helps constrain possible next positions
- E.g., airplane
  - You are tracking a plane moving in a direction (1-d problem)
  - At time 1, you are fairly certain about the position x = 0, but you don't know the velocity
    - You plot position and velocity on an x-y plane
    - The covariance matrix between position and velocity is narrow and tall
    - It is narrow on the x-axis since you know that the position is around x=0
    - It is tall on the y-axis because of your lack of knowledge about velocity
  - After 1 sec, you get a position update of x = 5
    - You can infer that the velocity is 5/s
    - The covariance matrix is then stretched diagonally

#### Multivariate Kalman filters

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#### **Notation**

- A Bayesian notation a|b means "a given the evidence of b"
  - The prior is  $\hat{\underline{x}}_{t|t-1}$ , since you know only the information at time t-1, i.e., the previous state
  - The posterior is  $\hat{\underline{x}}_{t|t}$ , since you know all the information at time t, i.e., the measurement
- A simpler notation:
  - Indicate the "prior" version of the variables (i.e., after the system update) with an overline (E.g.,  $\overline{x}$ ,  $\overline{x}$ ,  $\overline{X}$ )
  - Omit the indices t+1 and t and use an assignment notation (representing "update in place" of a variable):

$$x = x + 1$$

instead of the mathematical notation using a different variable for each time step:

$$x_{t+1} = x_t + 1$$

- With this notation:
  - The prior is  $\overline{x} = \hat{x}_{t|t-1}$
  - The posterior is  $x = \hat{x}_{t|t}$

#### Multivariate Kalman filter

- With the previous notation:
  - State update:  $\overline{x} = Fx + Bu$
  - State uncertainty:  $\overline{P} = FPF^T + Q$
  - Residual:  $y = z H\overline{x}$
  - Kalman gain:  $\mathbf{K} = \overline{\mathbf{P}} \mathbf{H}^T (\mathbf{H} \overline{\mathbf{P}} \mathbf{H}^T + \mathbf{R})^{-1}$
  - Updated state:  $\mathbf{x} = \overline{\mathbf{x}} + \mathbf{K}\mathbf{y}$
  - Update state uncertainty:  $P = (I KH)\overline{P}$
- Where
  - x and P are the state mean and covariance
  - F is the state transition function
  - Q is the system error (i.e., the noise in the model assessment)
  - B and u model the control inputs to the system
  - **H** is the measurement function
  - z and R are the measurement mean and covariance
  - y is the residual
  - K is the Kalman gain
- Use the system model to predict the next state
  - When we multiply F to x we get the prior (i.e., the state before seeing any measurement)
- Form an estimate between the prior and the measurement

### From univariate to multivariate Kalman filter

#### • Let's compare

Definition	Univariate (Bayesian)	Univariate (Kalman)	Multivariate (Kalman)
State update	$\overline{\mu} = \mu + \mu_f$	$\overline{x} = x + dx$	$\overline{x} = Fx + Bu$
State uncertainty	$\overline{\sigma}^2 = \sigma^2 + \sigma_f^2$	$\overline{P} = P + Q$	$\overline{P} = FPF^T + Q$
Residual		$y=z-\overline{x}$	$y = z - H\overline{x}$
Kalman gain		$K = \frac{\overline{P}}{\overline{P} + R}$	$K = \overline{P}H^T(H\overline{P}H^T + R)^{-1}$
Updated state	$\hat{\mu} = \frac{\overline{\sigma}^2 \mu_z + \sigma_z^2 \overline{\mu}}{\overline{\sigma}^2 + \sigma_z^2}$	$x = \overline{x} + Ky$	$x = \overline{x} + Ky$
Upd. state uncertainty	$\sigma^2 = \frac{\overline{\sigma}^2 \sigma_z^2}{\overline{\sigma}^2 + \sigma_z^2}$	$P = (1 - K)\overline{P}$	$P = (I - KH)\overline{P}$

## Designing a Kalman filter

- The designer of the model needs to design:
  - The form of the state  $\underline{x}$  and  $\underline{P}$
  - ullet The system model  $\underline{\underline{F}}$  and  $\underline{\underline{Q}}$
  - The measurement  $\underline{z}$  and  $\underline{R}$
  - The measurement function <u>H</u>
  - The control inputs  $\underline{\underline{B}}$  and  $\underline{\underline{u}}$  if there are control inputs

# Tracking a dog with a Kalman filter

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# Tracking 1d dog: Problem formulation

- There is a dog moving on a 1-d track
- The dog moves approximately 1 meter per step
  - The velocity has variance due to noise/imperfect model specification
- There is a sensor that measures the position of the dog
  - The sensor has a certain error
- Time is discrete



(Nuvolo)

## Tracking dog: Predict step

- At each step, the position is described with a Gaussian distribution  $\mathit{Normal}(\mu, \sigma^2)$
- The position is part of the system's state, along with the velocity
  - The position is "observed" by a sensor
  - The velocity is a "hidden" variable
  - You could use more variables (E.g., acceleration, jerk, etc.)

# Tracking dog: Design state covariance

- Initialize variances to reasonable values
  - E.g.,  $\sigma_{position} = 500 m$  due to uncertainty about initial position
  - Top speed for a dog is 21 m/s, so set  $3\sigma_{velocitv} = 21$
  - Assume covariances to be zero due to unknown initial correlation between position and velocity
  - **P** is diagonal

## Tracking dog: Design system model

Describe mathematically the behavior of the system

$$x_{t+1} = x_t + v\Delta t$$

- No model to predict how dog velocity changes over time
  - Assume it remains constant

$$\dot{x}_{t+1} = \dot{x}_t$$

- This is not correct, but if velocity doesn't change much, the filter will perform well
- Put the model in matrix form  $\underline{\mathbf{x}}_{t+1} = \underline{\underline{\mathbf{F}}}\underline{\mathbf{x}}_t$

## Tracking dog: Predicting the system

- If we predict the system without measurements:
  - The state follows the system model
  - The state uncertainty grows
    - This is true even without system error (noise)

## Tracking dog: Design system noise

- Consider a car driving on a road with cruise control on
- It should travel at constant speed:

$$x_t = \dot{x}_{t-1} \Delta t + x_{t-1}$$

- In reality, it is affected by unknown factors:
  - The cruise control is not perfect
  - Wind, hills, potholes affect the car
  - Passengers roll down windows, changing the drag profile of the car
- Model this as:

$$\dot{x}_t = \dot{x}_{t-1} + w$$

- Model all of this with a covariance matrix  $\underline{\boldsymbol{Q}} = \mathbb{E}[\underline{\boldsymbol{w}} \cdot \underline{\boldsymbol{w}}^T]$ :
  - Assume the noise is iid, has zero mean, and is independent from the system
  - For these reasons, you don't have to change the position, only the velocity

# Tracking dog: Design the control function

Incorporate control inputs to predict state based on this information

$$\Delta \underline{\overline{x}} = \underline{\underline{Bu}}$$

- E.g., in the case of the car
  - Steering
  - Acceleration
- E.g., in the case of the dog, control inputs can be
  - The voice of its master
  - Seeing a squirrel

# Tracking dog: Design the measurement function

- Kalman filter computes the update step in the measurement space
- If the measurement is in the same units as the state, the residual is simple to compute:

residual = measured position - predicted position

- E.g., assume we are tracking the position of the dog using a sensor that outputs a voltage
  - We cannot compute the residual as:

measure voltage - predicted position

- We need to convert the position into voltage
- The Kalman space allows to have a measurement matrix  $\underline{\underline{H}}$  to convert the state into a measurement

$$\underline{y} = \underline{z} - \underline{\underline{H}}\overline{x}$$

# Why working in measurement and not in state space?

- The problem is that it is possible to convert state into measurement, but not vice versa because of the hidden variables
  - E.g., transform position (discarding velocity) into voltage
  - If the sensor doesn't read velocity how do we estimate the measured velocity

# Tracking dog: Design the measurement

- Typically  $\underline{z}$  is easy since it just contains the measurements from the sensor
- The measurement noise matrix  $\underline{R}$  can be difficult to estimate
  - Noise can be not Gaussian
  - There can be a bias in the sensor
  - The error can be not symmetrical (e.g., temperature sensor is less precise as the temperature increases)

# Non-linear filtering

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## **Optimality**

#### Assumptions:

- Everything is linear
- System and sensor noise is Gaussian
- Under these assumptions, the Kalman filter is optimal in a least square sense
- The Kalman filter is a mathematical model of the world
  - The output is only as accurate as the model of the world

## The world is non-linear

- The Kalman filter uses linear equations and can only handle linear problems
- The world is non-linear:
  - System model can be non-linear:
    - Many physical systems are described by non-linear differential equations
    - E.g., a ball flying through air is affected by drag, leading to non-linear behaviors
  - Measurements can be non-linear:
    - To measure the height on a plane, you can measure the distance of the plane from the radar. Given the Pythagorean theorem, you get:

$$x = \sqrt{\mathsf{dist}^2 - \mathsf{height}^2}$$

 Rarely does a physical system have equations that can be solved analytically

## **Extended Kalman Filter**

- Aka FKF
- EKF is a nonlinear version of the Kalman filter
  - Linearize the differential equations to compute the Jacobian (i.e., matrix of partial derivatives) at the point of the current estimate
  - Used for estimating the state of a nonlinear dynamic system
- Pros
  - Use the linear Kalman machinery
- Cons:
  - Analytical solution:
    - Difficult or impossible
  - Numerical solution:
    - Expensive computationally
    - Errors can compound forcing the filter to diverge (unstable)

## **Unscented Kalman filter**

- Aka UKF
- It is superior to EKF in almost every way

## Intuition of sampling techniques

- ullet Assume you have a distribution X and a non-linearity  $\phi$
- For every measurement:
  - Generate many points from X
  - Pass them through the non-linear function  $\phi$
  - Approximate the result (E.g., compute mean and variance)

#### Problem:

- "How many points are needed to build an accurate output distribution"?
- Even if n=500,000 points are enough for 1 dimension, for k dimensions you might need  $n^k$  points (curse of dimensionality)

## **Unscented transform**

- Unscented transform estimates the result of applying a non-linear transformation to a probability distribution characterized by a finite number of moments (e.g., mean and covariance)
  - E.g., compute the non-linear transform of a distribution, given mean and covariance estimate
  - Called "unscented" since "it doesn't stink."

#### Intuition

- Given a PDF C with mean  $\mu$  and covariance  $\Sigma$
- Encode mean and covariance in a set of points (sigma points) that represent a discrete PMF D with the same mean  $\underline{\mu}$  and covariance  $\underline{\Sigma}$
- $\bullet$  Propagate the discrete PMF D by applying the non-linear function  $\overline{\phi}$  to each point of the PMF
- The mean and covariance of  $\phi(D)$  approximate the mean and covariance of  $\phi(C)$

## Unscented transform: 1d case

- The idea is that we need 3 sigma points for a 1-d Gaussian
  - One point for the mean
  - Two points around the mean
- Each point has a weight

# Unscented transform: sigma points

- ullet Consider a distribution F and a non-linearity  $\phi$
- There are algorithms to generate points and weights (given the mean and covariance of F) to evaluate mean and covariance of F transformed through  $\phi$
- In *n* dimensions, we need 2n+1 points  $\underline{x}_i$  and weights  $w_i^m$ ,  $w_i^c$

$$\sum_{i} w_{i}^{m} = 1$$

$$\sum_{i} w_{i}^{c} = 1$$

$$\mu(\phi) = \sum_{i} w_{i}^{m} \phi(\underline{x}_{i})$$

$$\Sigma(\phi) = \sum_{i} w_{i}^{c} (\phi(\underline{x}_{i}) - \mu(\phi)) (\phi(\underline{x}_{i}) - \mu(\phi))^{T}$$

Note that selecting the sigma points has not a single solution

# Monte Carlo sampling

- Use a finite number of randomly sampled points to represent the problem
- Run the points through the transformation (e.g., non-linear function / system you are modeling)
- Compute the results on the transformed points

## Particle filters

- Aka Sequential Monte Carlo (SMC) methods
- Monte Carlo algorithms to solve problems in Bayesian statistical inference (e.g., in filtering problems)
- The goal is to compute posterior distributions of the states, given some data

## Generic particle filter algorithm

- 1. Randomly generate particle
- Particles have all state variable that needs to be estimated (e.g., position, velocity)
- Each particle has a weight representing the probability that it represents the actual state of the system
- 2. Predict next state of the particles
- 3. Update weighting
- Update the weighting of the particles based on the measurements
- Particles that match closely the measurements are weighted higher
- 4. Resample
- Discard highly improbable particle
- Compute estimate
- Compute weighted mean and covariance of the particles to get an estimate of the state and uncertainty

## **Dynamic Bayesian networks**

- Reasoning over time
- HMMs
- Markov random fields
- Markov logic network
- State space models and Kalman filter
- Multivariate Kalman filters
- Dynamic Bayesian networks
- State space model
- Variational Inference

## Dynamic Bayesian Networks (DBNs)

- DBNs extend Bayesian networks to model temporal processes
- Main idea
  - "Unroll" the model over time
  - Capture intra-slice (within time) and inter-slice (across time) dependencies
- Each time slice includes:
  - State variables X<sub>t</sub>
  - Evidence variables E<sub>t</sub>
- Assumptions
  - First-order Markov process: current state depends only on the previous state
  - First-order sensor Markov process: evidence depends only on current state
  - Stationarity: each time slice is the same, both structure and parameters do not change over time
    - Structure and CPTs (Conditional Probability Tables) are the same across slices (time-homogeneous model)
  - No Gaussian distribution

## **DBNs vs HMMs**

- DBNs generalize Hidden Markov Models (HMMs)
- HMMs are a special case with a single hidden and evidence variable per time step
- DBNs model more complex systems than HMMs by:
  - Using multiple state variables
    - Enables modeling large systems like robot localization with many state components
  - Exploiting sparse connections among variables yielding compact model
    - HMM: transition matrix of size  $O(d^{2n})$
    - DBN: size  $O(nd^k)$  with k bounded parents per variable

## **DBNs vs Kalman filters**

- DBNs generalize Kalman filters
- Every Kalman filter can be represented in a DBN with:
  - Continuous variables
  - Linear / Gaussian conditional distributions
- Not every DBN can be represented by a Kalman filter, since:
  - DBN variables can mix discrete/continuous and non-Gaussian
  - Allow arbitrary conditional dependencies among variables
- Pros of DBNs
  - DBNs are applicable to broader domains including:
    - Fault diagnosis in networks
    - Complex system monitoring
- Pros of Kalman filters:
  - Optimal for linear systems with Gaussian noise
  - Support exact inference, DBNs often require approximate methods

## Constructing a DBN

- Key components of a DBN
  - Prior distribution of state  $Pr(X_0)$
  - Transition model  $Pr(X_{t+1}|X_t)$
  - Sensor model  $Pr(E_t|X_t)$
  - Transition and sensor models are time-homogeneous
- Network topology includes:
  - Intra-slice topology
  - Inter-slice links

# DBN example: Tracking a robot (1/3)

- Problem:
  - Tracking a robot moving randomly on a line X over time
- Initial model:
  - Position  $X_t$  and velocity  $\dot{X}_t$  as state variables
  - Update via Newton's laws
  - Easy to generalize for 2d or 3d by using a  $X_t$
- Issue:
  - Velocity changes over time
  - Battery exhaustion affects velocity systematically
  - Effect depends on cumulative energy use
  - Violates the Markov property (future depends on full history)
- Solution:
  - Include battery level  $Battery_t$  in the state  $X_t$
  - Restores the Markov assumption
  - Allows motion prediction considering energy constraints
  - Enables coherent reasoning about motion and power consumption over time
- New requirement for state:
  - $S_t = (X_t, \dot{X}_t, \mathsf{BatteryLevel}_t)$
  - $E_t = (GPS_t, BMeter_t)$

# DBN example: Tracking a robot (2/3)

- The DBN structure models both intra-slice (within time) and inter-slice (across time) dependencies
- Intra-slice dependencies:
  - Position  $X_t$  influences velocity  $\dot{X}_t$
  - BatteryLevel<sub>t</sub> influences velocity  $\dot{X}_t$
  - Battery $_{t+1}$  depends on Battery $_t$  and  $\dot{X}_t$
  - BMeter<sub>t</sub> depends on Battery<sub>t</sub>
  - GPS $_t$  depends on  $X_t$
- Inter-slice dependencies:
  - Position  $X_{t+1}$  depends on Position  $X_t$  and velocity  $\dot{X}_t$
  - Velocity  $\dot{X}_{t+1}$  depends on  $\dot{X}_t$  and Battery,

# DBN example: Tracking a robot (3/3)

- Replicate for Multiple Time Slices:
  - Create slices for t = 0, 1, 2, ... with the above variables and dependencies
  - Group each time slice vertically or horizontally for clarity
- Unrolling:
  - Visualize the full DBN by unrolling these slices over the desired number of time steps (e.g., three slices for t = 0, 1, 2)

## Inference in DBNs

- DBNs are Bayesian networks and we can use the same inference algorithms
  - "Unroll" the DBN over time (i.e., replicate slices for each time step) and apply standard BN inference
  - We can't unroll "forever", but we limit to a certain number of slices to approximate a fixed amount of time dependency
- Use recursive methods to get a constant time and space update complexity
  - Variable elimination with temporal ordering
  - At time step t+1 add slice t+2 and remove slice t so one has always two slices to do inference
  - Maintains constant memory by keeping only two slices at a time
- Complexity:
  - Exponential in number of state variables  $(O(nd^{n+k}))$
  - More efficient than full HMM representation  $(O(d^{2n}))$
- Even though we can use DBNs to represent very complex temporal processes with many sparsely connected variables, we cannot reason efficiently and exactly about those processes
  - The prior joint distribution over all the variables is factorizable into its constituents CPTs

• The posterior joint distribution conditioned on observation sequence is not 119

# **Approximate Inference in DBNs**

- Particle Filtering:
  - Represent belief state with weighted samples (particles)
  - Steps: propagate, weight, resample
- Benefits:
  - Focuses computation on high-probability regions
  - Maintains manageable memory and time per step
- Challenges:
  - Approximation error
  - Sensitive to transition and observation model assumptions
- Used when exact inference is computationally impractical
- Real-world application: robot localization, speech recognition

## DBN to represent changing model

- We can model the fact that the system can change over time
  - Transient failure: a sensor reads wrong measures
  - Persistent failure model: we can model it with additional variables (e.g., SensorBroken)

## **DBN**: inference

 We can unroll the DBN and get a BayesNet and then perform exact or approximate inference with the known methods (e.g., MCMC)

## **DBN: optimization for inference**

- Many optimizations are possible, e.g.,
  - Instead of running each sample through the entire DBN one can run all the samples evaluating one slice at a time to compute the posterior distribution

# State space model

- Reasoning over time
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- Markov logic network
- State space models and Kalman filter
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- Dynamic Bayesian networks
- State space model
- Variational Inference

## **Variational Inference**

- Reasoning over time
- HMMs
- Markov random fields
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- State space model
- Variational Inference
  - Expectation-Maximization (EM) Algorithm

# **Expectation-Maximization (EM) Algorithm**

- Reasoning over time
- HMMs
- Markov random fields
- Markov logic network
- State space models and Kalman filter
- Multivariate Kalman filters
- Dynamic Bayesian networks
- State space model
- Variational Inference
  - Expectation-Maximization (EM) Algorithm

## **EM Algorithm: Intuition and Applications**

- Expectation-Maximization (EM) is a method for learning with hidden or missing data
  - Useful when some variables influencing the data are not directly observed
  - Works by iteratively improving parameter estimates
  - Alternates between estimating missing data and optimizing parameters
- Two main steps:
  - E-step (Expectation): Estimate distribution over hidden variables using current parameters
  - M-step (Maximization): Update parameters to maximize expected log-likelihood from the E-step
- Used in diverse settings:
  - Unsupervised clustering (e.g., Gaussian Mixture Models)
  - Learning with incomplete data in Bayesian networks
  - Hidden Markov Models (HMMs)
- Key property: EM increases data likelihood at each iteration
- Converges to a local maximum of the likelihood function
- No need for a step size parameter unlike gradient descent

# EM Algorithm: Mechanics and Example in Gaussian Mixture Models

- Goal: Recover parameters of Gaussian components from unlabeled data
- E-step:
  - Compute  $p_{ij} = P(C = i \mid x_i)$  using Bayes' rule
  - $p_{ii} \propto P(x_i \mid C = i)P(C = i)$
  - Calculate effective count:  $n_i = \sum_i p_{ij}$
- M-step:
  - Update means:  $\mu_i \leftarrow \sum_j p_{ij} x_j / n_i$
  - Update covariances:  $\Sigma_i \leftarrow \sum_i p_{ij} (x_j \mu_i) (x_j \mu_i)^T / n_i$
  - Update weights:  $w_i \leftarrow n_i/N$
- Intuition: Softly assign points to components, then re-estimate the components
- Example scenario:
  - 500 data points from a mix of 3 Gaussians
  - EM reconstructs original distribution closely after iterations
- Limitations:
  - Sensitive to initialization
  - May converge to poor local optima
  - Component collapse or merging can occur

# Introduction to the Expectation–Maximization (EM) Algorithm

## Purpose of EM Algorithm

- Iterative method for finding maximum likelihood or maximum a posteriori (MAP) estimates in statistical models with latent variables
- Particularly useful when data is incomplete or has missing values

## Key Concepts

- Observed Data (X): The data we can directly observe
- Latent Variables (Z): Hidden or unobserved variables that influence the observed data
- Parameters  $(\theta)$ : Unknown parameters to be estimated

#### • Challenge Addressed

- Direct maximization of the likelihood function  $p(\mathbf{X}|\theta)$  is often intractable due to the presence of latent variables
- EM Algorithm Overview
  - Alternates between estimating the expected value of the log-likelihood (E-step) and maximizing this expectation (M-step)

## Applications

 Widely used in clustering (e.g., Gaussian Mixture Models), natural language processing, and image reconstruction

## The EM Algorithm: Step-by-Step

- Initialization
  - Start with initial guesses for the parameters  $oldsymbol{ heta}^{(0)}$
- E-Step (Expectation Step)
  - Compute the expected value of the log-likelihood function, with respect to the conditional distribution of the latent variables given the observed data and current parameter estimates:
    - $Q(\theta|\theta^{(t)}) = \mathbb{E}_{\mathbf{Z}|\mathbf{X},\theta^{(t)}}[\log p(\mathbf{X},\mathbf{Z}|\theta)]$
- M-Step (Maximization Step)
  - Maximize the expected log-likelihood found in the E-step to update the parameters:
    - $\theta^{(t+1)} = \arg\max_{\theta} Q(\theta|\theta^{(t)})$
- Iteration
  - Repeat E and M steps until convergence, i.e., until the parameters stabilize or the increase in likelihood is below a threshold

## Mathematical Foundation of EM

#### Likelihood with Latent Variables

- The marginal likelihood of the observed data is:
  - $p(X|\theta) = \int p(X,Z|\theta)dZ$
- Intractability
  - The integral is often difficult to compute due to the complexity introduced by the latent variables
- EM Solution
  - EM circumvents this by iteratively applying the E and M steps to find parameter estimates that locally maximize the likelihood
- Convergence
  - Each iteration of EM is guaranteed to increase the likelihood function, ensuring convergence to a local maximum

# **Example: Gaussian Mixture Models (GMM)**

## Problem Setup

 Data is assumed to be generated from a mixture of Gaussian distributions, each with its own mean and covariance

#### Latent Variables

 Each data point is associated with a latent variable indicating the Gaussian component from which it was generated

## • E-Step in GMM

 Compute the posterior probabilities (responsibilities) that each data point belongs to each Gaussian component

## M-Step in GMM

 Update the parameters (means, covariances, and mixing coefficients) of each Gaussian component using the responsibilities computed in the E-step

#### Iteration

Repeat E and M steps until the parameters converge

## **Properties and Limitations of EM**

#### Advantages

- Can handle missing or incomplete data effectively
- Provides a framework for parameter estimation in complex models

#### Limitations

- Converges to a local maximum, which may not be the global maximum
- Sensitive to initial parameter estimates; poor initialization can lead to suboptimal solutions

#### Extensions and Variants

- Variational Bayes: Provides a fully Bayesian approach by estimating distributions over parameters
- Generalized EM (GEM): Relaxes the requirement of fully maximizing the expected log-likelihood in the M-step
- Expectation Conditional Maximization (ECM): Breaks the M-step into several conditional maximization steps

#### Practical Considerations

- Multiple runs with different initializations can help in finding better solutions
- Monitoring the increase in likelihood can help in determining convergence