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: $\underline{\boldsymbol{X}}_t$
2. Prior probability of the state at time 0: $\underline{\boldsymbol{X}}_0$
3. Evidence variables: $\underline{\boldsymbol{E}}_t$
4. Transition model: $\Pr(\underline{\boldsymbol{X}}_t | \underline{\boldsymbol{X}}_{0:t-1})$
   - How the world evolves
   - Specifies the probability distribution of the state $\underline{\boldsymbol{X}}_t$, 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 $\underline{\boldsymbol{X}}_t$ (hidden)
    - Other RVs are observable $\underline{\boldsymbol{E}}_t$ (evidence)
    - $\underline{\boldsymbol{X}}_{a:b}$ 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 $\underline{\boldsymbol{X}}_t$ 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

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

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

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

  - 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 $\underline{\boldsymbol{X}}_t$ is conditionally dependent only on $\underline{\boldsymbol{X}}_{t-1}$ and $\underline{\boldsymbol{X}}_{t-2}$ and no other earlier state

Time-homogeneous process

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

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

  - 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

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

  - 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., $\underline{\boldsymbol{X}}_t \rightarrow \underline{\boldsymbol{E}}_t$ since the world causes the sensor to take on particular values

Sensor model: rain example

- In a Bayesian network, $\underline{\boldsymbol{X}}_t \rightarrow \underline{\boldsymbol{E}}_t$ 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, $\Pr(\underline{\boldsymbol{X}}_0)$
  - 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.,
  - $\underline{\boldsymbol{X}}_0$ represents the position and velocity of a moving object
  - $\Pr(\underline{\boldsymbol{X}}_0)$ 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 $\underline{\boldsymbol{X}}_0, \underline{\boldsymbol{X}}_1, ..., \underline{\boldsymbol{X}}_t$ and observations $\underline{\boldsymbol{E}}_1, ..., \underline{\boldsymbol{E}}_t$ over time, with the simplifying assumptions:
  - First-order Markov assumption: $\Pr(\underline{\boldsymbol{X}}_i | \underline{\boldsymbol{X}}_{0:i-1}) = \Pr(\underline{\boldsymbol{X}}_i | \underline{\boldsymbol{X}}_{i-1})$
  - 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:

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

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

$$\begin{aligned} \Pr(\underline{\boldsymbol{X}}_{0:t}, \underline{\boldsymbol{E}}_{1:t}) &= \Pr(\underline{\boldsymbol{X}}_0) \prod_{i=1}^{t} \Pr(\underline{\boldsymbol{X}}_i | \underline{\boldsymbol{X}}_{i-1}) \Pr(\underline{\boldsymbol{E}}_i | \underline{\boldsymbol{X}}_i) \\ &= \text{prior} \times \prod_{i} \text{transition model} \times \text{sensor model} \end{aligned}$$

First-order Markov process: intuition

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

$$\Pr(\underline{\boldsymbol{X}}_{0:t}, \underline{\boldsymbol{E}}_{1:t}) = \Pr(\underline{\boldsymbol{X}}_0) \prod_{i=1}^{t} \Pr(\underline{\boldsymbol{X}}_i | \underline{\boldsymbol{X}}_{i-1}) \Pr(\underline{\boldsymbol{E}}_i | \underline{\boldsymbol{X}}_i)$$
$$= \text{prior} \times \prod_{i} \text{transition model} \times \text{sensor model}$$

- 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 $\Pr(Rain_t|Rain_{t-1}, Rain_{t-2})$
  2. Increase the set of state variables
     - E.g., add $Season_t$ to incorporate the historical records
     - This makes the transition model more complicated
  3. Increase the number of sensor variables
     - E.g., $Location_t$, $Temperature_t$, $Humidity_t$, $Pressure_t$
     - 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	Estimate *current* state given past / current obs	$\Pr(\underline{\boldsymbol{X}}_t \mid \underline{\boldsymbol{E}}_{1:t})$
Prediction	Estimate *future* state given past / current obs	$\Pr(\underline{\boldsymbol{X}}\_t + k \mid \underline{\boldsymbol{E}}_{1:t})$ for $k > 0$
Smoothing	Estimate *past* state given past, current, and *future* obs	$\Pr(\underline{\boldsymbol{X}}_k \mid \underline{\boldsymbol{E}}_{1:T})$ for $k < T$
Most Likely Explanation	Find most probable sequence of states given the evidence	$\text{argmax}_{\underline{x}_{1:T}} \Pr(\underline{\boldsymbol{X}}_{1:t} \mid \underline{\boldsymbol{E}}_{1:t})$
Learning	Learn model parameters or structure from data	θ 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 $\Pr(Rain_t | Umbrella_{1:t})$
- Filtering is needed by a rational agent to track the current state of the world
  - The agent has a belief about the current state $\Pr(\underline{\boldsymbol{X}}_{t-1})$ at time $t-1$
  - New evidence $\underline{\boldsymbol{e}}_t$ arrives for time t
  - The agent updates its belief about the current state $\Pr(\underline{\boldsymbol{X}}_t)$ 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:

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

  - 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:

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

  - 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 $\underline{\boldsymbol{x}}_{1:t}$ most likely to have generated observations $\underline{\boldsymbol{e}}_{1:t}$:

$$\text{argmax}_{\underline{\boldsymbol{x}}_{1:t}} \Pr(\underline{\boldsymbol{x}}_{1:t} | \underline{\boldsymbol{e}}_{1:t})$$

  - 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 $\Pr(\underline{\boldsymbol{X}}_t|\underline{\boldsymbol{X}}_{0:t-1})$ and the sensor model $\Pr(\underline{\boldsymbol{E}}_i|\underline{\boldsymbol{X}}_i)$ 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

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

$$\mathit{NextState} = f(\mathit{PreviousState}, e_{t+1})$$

- **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: $\Pr(X_{t+1}|e_{1:t+1})$

$$
\begin{aligned}
&\text{Divide up the evidence} && = \Pr(X_{t+1}|e_{1:t}, e_{t+1}) \\
&\text{Bayes rule given } e_{1:t} && = \alpha \Pr(e_{t+1}|X_{t+1}, e_{1:t}) \Pr(X_{t+1}|e_{1:t}) \\
&\text{Markov sensor assumption} && = \alpha \Pr(e_{t+1}|X_{t+1}) \Pr(X_{t+1}|e_{1:t}) \\
&\text{Condition on current state} && = \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t, e_{1:t}) \Pr(x_t|e_{1:t}) \\
&\text{Markov assumption} && = \alpha \Pr(e_{t+1}|X_{t+1}) \sum_{x_t} \Pr(X_{t+1}|x_t) \Pr(x_t|e_{1:t})
\end{aligned}
$$

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

- 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

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

1. **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:

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

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

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

  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 $\underline{\boldsymbol{X}}_{t+k+1}$ given state $\underline{\boldsymbol{X}}_{t+k}$ and evidence $\underline{\boldsymbol{E}}_{1:t}$ is:

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

- 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!)

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

- 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:

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

  - 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

$$\text{argmax}_{x_{1:t}} \Pr(x_{1:t}|e_{1:t}) = \textit{argmax}_{Weather_{1:t}} \Pr(Weather_{1:t}|Umbrella_{1:t})$$

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: $S = \{\text{Sunny}, \text{Rainy}\}$ (weather)
  - Observations: $O = \{\text{Yes}, \text{No}\}$ (umbrella)
- Initial Probabilities:

$$\Pr(\text{Sunny}) = 0.6, \quad \Pr(\text{Rainy}) = 0.4$$

- Transition Probabilities:

$$\Pr(\text{Sunny} \to \text{Sunny}) = 0.7, \quad \Pr(\text{Sunny} \to \text{Rainy}) = 0.3$$
$$\Pr(\text{Rainy} \to \text{Sunny}) = 0.4, \quad \Pr(\text{Rainy} \to \text{Rainy}) = 0.6$$

- Observation (Emission) Probabilities:

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

Viterbi algorithm: example 2/2

- Viterbi table

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

- Final most probable state: **Sunny** (Day 3)
- Find the most likely sequence: *Rainy* $\rightarrow$ Rainy $\rightarrow$ 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 $\underline{\boldsymbol{T}}$ 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 $\underline{\boldsymbol{O}}$ (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}	$\Pr(R_t \mid R_{t-1})$
T	0.7
F	0.3

becomes the transition model

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

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

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

Hidden Markov Model: algorithms

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

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

- 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

Markov random fields

- 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

Markov logic network

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State space models and Kalman filter

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- **State space models and Kalman filter**
  - g-h filter
  - One dimensional Kalman filters
  - Multivariate Gaussians
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Reference

- 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
  - 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:**

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

  - 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:

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

- 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** $\mathbf{x}$: current values you are interested in
  - E.g., weight
  - Part of the state might be hidden (i.e., not observable)
  - You cannot observe the entire state directly, only measure it indirectly
- **Measurement** $\mathbf{z}$: the measured value of the system
  - It is observable
  - It can be inaccurate
    - E.g., 99.3kg instead of 100kg
- **State estimate** $\mathbf{x\_est}$: 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:

$$\text{posterior} = \text{normalized}(\text{prior} \times \text{likelihood})$$

- 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

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

  is a Gaussian $\mathit{Normal}(\mu, \sigma^2)$ 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
  - 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 $\sim \mathit{Normal}(\underline{\boldsymbol{\mu}}_i, \underline{\underline{\boldsymbol{\Sigma}}}_i)$
- The product of the Gaussians is still Gaussian $\sim \mathit{Normal}(\underline{\boldsymbol{\mu}}, \underline{\underline{\boldsymbol{\Sigma}}})$

$$\underline{\boldsymbol{\mu}} = \underline{\underline{\boldsymbol{\Sigma}}}_2(\underline{\underline{\boldsymbol{\Sigma}}}_1 + \underline{\underline{\boldsymbol{\Sigma}}}_2)^{-1}\underline{\boldsymbol{\mu}}_1 + \underline{\underline{\boldsymbol{\Sigma}}}_1(\underline{\underline{\boldsymbol{\Sigma}}}_1 + \underline{\underline{\boldsymbol{\Sigma}}}_2)^{-1}\underline{\boldsymbol{\mu}}_2$$
$$\underline{\underline{\boldsymbol{\Sigma}}} = \underline{\underline{\boldsymbol{\Sigma}}}_1(\underline{\underline{\boldsymbol{\Sigma}}}_1 + \underline{\underline{\boldsymbol{\Sigma}}}_2)^{-1}\underline{\underline{\boldsymbol{\Sigma}}}_2$$

- **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:

- σ^2 with covariance matrix $\underline{\underline{\boldsymbol{\Sigma}}}$
- 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 $\hat{\underline{\boldsymbol{x}}}_{t|t-1}$, since you know only the information at time $t-1$, i.e., the previous state
  - The posterior is $\hat{\underline{\boldsymbol{x}}}_{t|t}$, 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., $\overline{x}$, $\overline{\boldsymbol{x}}$, $\overline{\boldsymbol{X}}$)
  - 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: $\overline{\boldsymbol{x}} = \boldsymbol{F}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}$
  - State uncertainty: $\overline{\boldsymbol{P}} = \boldsymbol{F}\boldsymbol{P}\boldsymbol{F}^T + \boldsymbol{Q}$
  - Residual: $\boldsymbol{y} = \boldsymbol{z} - \boldsymbol{H}\overline{\boldsymbol{x}}$
  - Kalman gain: $\boldsymbol{K} = \overline{\boldsymbol{P}}\boldsymbol{H}^T(\boldsymbol{H}\overline{\boldsymbol{P}}\boldsymbol{H}^T + \boldsymbol{R})^{-1}$
  - Updated state: $\boldsymbol{x} = \overline{\boldsymbol{x}} + \boldsymbol{K}\boldsymbol{y}$
  - Update state uncertainty: $\boldsymbol{P} = (\boldsymbol{I} - \boldsymbol{K}\boldsymbol{H})\overline{\boldsymbol{P}}$
- Where
  - $\boldsymbol{x}$ and $\boldsymbol{P}$ are the state mean and covariance
  - $\boldsymbol{F}$ is the state transition function
  - $\boldsymbol{Q}$ is the system error (i.e., the noise in the model assessment)
  - $\boldsymbol{B}$ and $\boldsymbol{u}$ model the control inputs to the system
  - $\boldsymbol{H}$ is the measurement function
  - $\boldsymbol{z}$ and $\boldsymbol{R}$ are the measurement mean and covariance
  - $\boldsymbol{y}$ is the residual
  - $\boldsymbol{K}$ is the Kalman gain
- Use the system model to predict the next state
  - When we multiply $\boldsymbol{F}$ to $\boldsymbol{x}$ 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	$\overline{\mu} = \mu + \mu_f$	$\overline{x} = x + dx$	$\overline{\boldsymbol{x}} = \boldsymbol{F}\boldsymbol{x} + \boldsymbol{B}\boldsymbol{u}$
State uncertainty	$\overline{\sigma}^2 = \sigma^2 + \sigma_f^2$	$\overline{P} = P + Q$	$\overline{\boldsymbol{P}} = \boldsymbol{F}\boldsymbol{P}\boldsymbol{F}^T + \boldsymbol{Q}$
Residual		$y = z - \overline{x}$	$\boldsymbol{y} = \boldsymbol{z} - \boldsymbol{H}\overline{\boldsymbol{x}}$
Kalman gain		$K = \frac{\overline{P}}{\overline{P}+R}$	$\boldsymbol{K} = \overline{\boldsymbol{P}}\boldsymbol{H}^T(\boldsymbol{H}\overline{\boldsymbol{P}}\boldsymbol{H}^T + \boldsymbol{R})^{-1}$
Updated state	$\hat{\mu} = \frac{\overline{\sigma}^2\mu_z + \sigma_z^2\overline{\mu}}{\overline{\sigma}^2+\sigma_z^2}$	$x = \overline{x} + Ky$	$\boldsymbol{x} = \overline{\boldsymbol{x}} + \boldsymbol{K}\boldsymbol{y}$
Upd. state uncertainty	$\sigma^2 = \frac{\overline{\sigma}^2\sigma_z^2}{\overline{\sigma}^2+\sigma_z^2}$	$P = (1-K)\overline{P}$	$\boldsymbol{P} = (\boldsymbol{I} - \boldsymbol{K}\boldsymbol{H})\overline{\boldsymbol{P}}$

Designing a Kalman filter

- The designer of the model needs to design:
  - The form of the state $\underline{\boldsymbol{x}}$ and $\underline{\underline{\boldsymbol{P}}}$
  - The system model $\underline{\underline{\boldsymbol{F}}}$ and $\underline{\underline{\boldsymbol{Q}}}$
  - The measurement $\underline{\boldsymbol{z}}$ and $\underline{\underline{\boldsymbol{R}}}$
  - The measurement function $\underline{\underline{\boldsymbol{H}}}$
  - The control inputs $\underline{\underline{\boldsymbol{B}}}$ and $\underline{\boldsymbol{u}}$ 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., $\sigma_{position} = 500m$ due to uncertainty about initial position
  - Top speed for a dog is 21m/s, so set $3\sigma_{velocity} = 21$
  - Assume covariances to be zero due to unknown initial correlation between position and velocity
  - $\underline{\underline{\boldsymbol{P}}}$ 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 $\underline{\boldsymbol{x}}_{t+1} = \underline{\underline{\boldsymbol{F}}}\underline{\boldsymbol{x}}_t$

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 $\underline{\underline{\boldsymbol{Q}}} = \mathbb{E}[\underline{\boldsymbol{w}} \cdot \underline{\boldsymbol{w}}^T]$:
  - 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

$$\Delta \underline{\overline{x}} = \underline{\underline{B}} \underline{u}$$

- 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:

$$\text{residual} = \text{measured position - predicted position}$$

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

$$\text{measure voltage - predicted position}$$

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

$$\underline{\boldsymbol{y}} = \underline{\boldsymbol{z}} - \underline{\underline{\boldsymbol{H}}}\,\underline{\bar{\boldsymbol{x}}}$$

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 $\underline{\boldsymbol{z}}$ is easy since it just contains the measurements from the sensor
- The measurement noise matrix $\underline{\underline{\boldsymbol{R}}}$ 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:

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

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

Extended Kalman Filter

- Aka EKF
- 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

- Assume you have a distribution X and a non-linearity ϕ
- For every measurement:
  - Generate many points from X
  - Pass them through the non-linear function ϕ
  - 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 $\underline{\boldsymbol{\mu}}$ and covariance $\underline{\underline{\boldsymbol{\Sigma}}}$
  - Encode mean and covariance in a set of points (sigma points) that represent a discrete PMF D with the same mean $\underline{\boldsymbol{\mu}}$ and covariance $\underline{\underline{\boldsymbol{\Sigma}}}$
  - Propagate the discrete PMF D by applying the non-linear function $\underline{\underline{\phi}}$ 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

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

$$\sum_i w_i^m = 1$$

$$\sum_i w_i^c = 1$$

$$\mu(\phi) = \sum_i w_i^m \phi(\underline{\boldsymbol{x}}_i)$$

$$\Sigma(\phi) = \sum_i w_i^c (\phi(\underline{\boldsymbol{x}}_i) - \mu(\phi))(\phi(\underline{\boldsymbol{x}}_i) - \mu(\phi))^T$$

- 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

5. 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_t
  - Evidence variables E_t
- 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 $\underline{\boldsymbol{X}}_t$
- **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:**
  - $S_t = (X_t, \dot{X}_t, \text{BatteryLevel}_t)$
  - $E_t = (\text{GPS}_t, \text{BMeter}_t)$

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_t influences velocity $\dot{X}_t$
  - Battery_{t+1} depends on Battery_t and $\dot{X}_t$
  - BMeter_t depends on Battery_t
  - 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_t

DBN example: Tracking a robot (3/3)

- **Replicate for Multiple Time Slices**:
  - Create slices for $t = 0, 1, 2, \ldots$ 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

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

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- **Variational Inference**
  - Expectation-Maximization (EM) Algorithm

Expectation-Maximization (EM) Algorithm

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- 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 $p_{ij} = P(C = i \mid x_j)$ using Bayes' rule
  - $p_{ij} \propto P(x_j \mid C = i)P(C = i)$
  - Calculate effective count: $n_i = \sum_j p_{ij}$
- **M-step**:
  - Update means: $\mu_i \leftarrow \sum_j p_{ij} x_j / n_i$
  - Update covariances: $\Sigma_i \leftarrow \sum_j p_{ij}(x_j - \mu_i)(x_j - \mu_i)^T / n_i$
  - 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 (θ)**: 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 $\boldsymbol{\theta}^{(0)}$
- **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:
    - $Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)}) = \mathbb{E}_{\mathbf{Z}|\mathbf{X},\boldsymbol{\theta}^{(t)}}[\log p(\mathbf{X}, \mathbf{Z}|\boldsymbol{\theta})]$
- **M-Step (Maximization Step)**
  - Maximize the expected log-likelihood found in the E-step to update the parameters:
    - $\boldsymbol{\theta}^{(t+1)} = \arg\max_{\boldsymbol{\theta}} Q(\boldsymbol{\theta}|\boldsymbol{\theta}^{(t)})$
- **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:
    - $p(\mathbf{X}|\theta) = \int p(\mathbf{X}, \mathbf{Z}|\theta) d\mathbf{Z}$
- **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