# Mathematics and numerics for data assimilation and state estimation - Lecture 6 

Summer semester 2020

## Summary of lecture 5

- Markov property:

$$
\begin{align*}
& \mathbb{P}\left(Z_{n+1}=z_{n+1}, Z_{n}=z_{n}, \ldots, Z_{0}=z_{0}\right) \\
& \quad=\mathbb{P}\left(Z_{n+1}=z_{n+1} \mid Z_{n}=z_{n}\right) \mathbb{P}\left(Z_{n}=z_{n}, \ldots, Z_{0}=z_{0}\right) \tag{1}
\end{align*}
$$

- time-homogeneous chains $\operatorname{Markov}(\pi, p)$ with transition function

$$
\mathbb{P}\left(Z_{n+1}=j \mid Z_{n}=i\right)=p(i, j) \quad \text { whenever } \mathbb{P}\left(Z_{n}=i\right)>0
$$

■ evolution of distributions

$$
\pi^{n}=\pi^{0} p^{n}
$$

and invariant distributions

$$
\pi=\pi p
$$

■ aperiodicity of states and irreduciblity and recurrence of $p$.

## Overview

1 Recurrence and construction of invariant distributions for time-homogeneous finite Markov chains

2 Filtering

3 Prediction

4 Smoothing

## Overview

1 Recurrence and construction of invariant distributions for time-homogeneous finite Markov chains

## 2 Filtering

3 Prediction

4 Smoothing

## Recurrence and construction of invariant distributions

## Definition 1

Consider an irreducible transition function $p$ associated to a state-space $\mathbb{S}$. Then we say that $p$ is recurrent if it for any state $i \in \mathbb{S}$ and Markov chain $\left\{Z_{n}^{i}\right\} \sim \operatorname{Markov}\left(\mathbb{1}_{\{i\}}, p\right)$ holds that

$$
\begin{equation*}
\mathbb{P}\left(Z_{n}^{i}=i \quad \text { for infinitely many } n\right)=1 \tag{2}
\end{equation*}
$$

which for the hitting time $T_{i}:=\inf \left\{n \geq 1 \mid Z_{n}^{i}=i\right\}$ is equivalent to

$$
\mathbb{P}\left(T_{i}<\infty\right)=1
$$

## Lemma 2

If $p$ is irreducible and the state-space is finite, then $p$ is recurrent.

Proof: Let us write $\mathbb{S}=\{1,2, \ldots, d\}$. Since $\mathbb{S}$ is finite, there must be at least one pair of states $i, j \in \mathbb{S}$ satisfying

$$
\begin{equation*}
\mathbb{P}\left(Z_{n}^{i}=j \text { for infinitely many } n\right)>0 \tag{3}
\end{equation*}
$$

since otherwise we reach the contradiction

$$
\begin{aligned}
0 & =b P\left(Z_{n}^{i} \notin \mathbb{S} \quad \text { for infinitely many } n\right) \\
& \geq 1-\sum_{j \in \mathbb{S}} b P\left(Z_{n}^{i}=j \quad \text { for infinitely many } n\right)=1 .
\end{aligned}
$$

And

$$
\begin{align*}
& \mathbb{P}\left(Z_{n}^{j}=j \quad \text { for infinitely many } n\right) \\
& =\mathbb{P}\left(Z_{n}^{i}=j \quad \text { for infinitely many } n \cap\left\{Z_{n}^{i}=j \quad \text { for some } n\right\}\right)  \tag{4}\\
& =\mathbb{P}\left(Z_{n}^{i}=j \quad \text { for infinitely many } n\right)>0 .
\end{align*}
$$

Theorem 9, Lecture 4 extends to the current setting, so by defining

$$
N^{j}:=\sum_{n \in \mathbb{N}} \mathbb{1}_{Z_{n}^{j}=j} \quad(\text { total visits at state } j)
$$

we obtain for $\lambda_{j}:=\mathbb{P}\left(T^{j}<\infty\right)$ that

$$
\mathbb{P}\left(N^{j}=k\right)= \begin{cases}\left(1-\lambda_{j}\right) \lambda_{j}^{k-1} & \text { if } \lambda_{j}<1 \\ \mathbb{1}_{k=\infty} & \text { if } \lambda_{j}=1\end{cases}
$$

Consequently,

$$
0<\mathbb{P}\left(Z_{n}^{j}=j \quad \text { for infinitely many } n\right)=\mathbb{P}\left(N^{j}=\infty\right)= \begin{cases}0 & \text { if } \lambda_{j}<1 \\ 1 & \text { if } \lambda_{j}=1\end{cases}
$$

Conclusion: $\lambda_{j}$ must equal 1 and $j$ is a recurrent state.

It remains to verify that $N^{k}=\infty$ a.s. for all $k \in \mathbb{S} \backslash\{j\}$. Observe first that

$$
\begin{aligned}
\mathbb{P}\left(N^{k}=\infty\right)=1 \Longleftrightarrow \mathbb{P}\left(N^{k}=\right. & \infty)>0 \\
& \Longleftrightarrow \mathbb{E}\left[N^{k}\right]=\infty \Longleftrightarrow \sum_{n \in \mathbb{N}} p_{k k}^{n}=\infty
\end{aligned}
$$

where the last $\Longleftrightarrow$ follows from

$$
\mathbb{E}\left[N^{k}\right]=\sum_{n \in \mathbb{N}} \mathbb{E}\left[\mathbb{1}_{Z_{n}^{k}=k}\right]=\sum_{n \in \mathbb{N}} \mathbb{P}\left(\mathbb{1}_{Z_{n}^{k}=k}\right)=\sum_{n \in \mathbb{N}} p_{k k}^{n}
$$

Since $\mathbb{P}\left(N^{j}=\infty\right)=1$, we know that $\sum_{n \in \mathbb{N}} p_{j j}^{n}=\infty$. And by the irreducibility of $p$, there exist $m_{1}, m_{2} \geq 1$ such that $p_{k j}^{m_{1}} p_{j k}^{m_{2}}>0$. So for any $n \geq m_{1}+m_{2}$,

$$
p_{k k}^{n} \geq p_{k j}^{m_{1}} p_{j j}^{n-\left(m_{1}+m_{2}\right)} p_{j k}^{m_{2}}
$$

and

$$
\sum_{n \in \mathbb{N}} p_{k k}^{n} \geq p_{k j}^{m_{1}} p_{j k}^{m_{2}} \sum_{n \in \mathbb{N}} p_{j j}^{n}=\infty
$$

Q.E.D.

## Construction of invariant measures

For an irreducible transition function $p$ associated to $\mathbb{S}=\{1,2, \ldots, d\}$, we fix a state $k \in \mathbb{S}$, the chain $\left\{Z_{n}^{k}\right\} \sim \operatorname{Markov}\left(\mathbb{1}_{\{k\}}, p\right)$ and introduce

$$
\gamma_{j}^{k}:=\mathbb{E}\left[\sum_{n=0}^{T^{k}-1} \mathbb{1}_{Z_{n}^{k}=j}\right] \quad \text { for } \quad j \in \mathbb{S} .
$$

(the expected number of visits spent at state $j$ in between vists to $k$ ).

Theorem 3 (Theorem 1.7.5, Norris, Markov Chains)
For every $k \in \mathbb{S}$,

$$
\gamma^{k}=\gamma^{k} p
$$

which makes

$$
\pi:=\frac{\gamma^{k}}{\sum_{j \in \mathbb{S}} \gamma_{j}^{k}}
$$

is an invariant distribution.

## Example 4

$$
p=\left(\begin{array}{lll}
0 & 1 & 0 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{array}\right)
$$

Irreducible but periodic chain. $p_{i i}^{n}>0$ only for $n=3,6,9, \ldots$. So Lemma 19 does not apply.
But $\gamma^{1}=\gamma^{2}=\gamma^{3}=[1,1,1]$, giving rise to $\pi=\gamma^{1} / 3$.

## Example 5

$$
p=\left(\begin{array}{ccc}
0 & 1 / 2 & 1 / 2 \\
0 & 0 & 1 \\
1 & 0 & 0
\end{array}\right)
$$



Irreducible chain with aperiodic state 3. So Lemma 19 does apply. But theorem 22 also:

$$
\gamma^{1}=[1,0.5,1], \quad \gamma^{2}=[2,1,2], \quad \gamma^{3}=[1,0.5,1]
$$

## Simulation of a time-homogeneous Markov chain

For $\left\{Z_{n}\right\} \sim \operatorname{Markov}\left(\pi^{0}, p\right)$ on $\mathbb{S}=\{1,2, \ldots, d\}$ the main challenges for simulation are to draw the inital state and the transitions:

1 Draw $Z_{0} \sim \pi^{0}$
2 ...
3 given $Z_{n}=i$, draw $Z_{n+1} \sim\left[p_{i 1}, p_{i, 2}, \ldots, p_{i d}\right]$

Same challenge for every step: draw a sample/new state from a distribution $f=\left[f_{1}, \ldots, f_{d}\right]$.

Sampling method:
1 construct a vector

$$
\bar{f}=\left(\begin{array}{c}
f_{1} \\
f_{1}+f_{2} \\
\vdots \\
\sum_{j=1}^{d-1} f_{j} \\
1
\end{array}\right)
$$

2 Draw a uniformly distributed $\mathrm{rv} U \sim U[0,1]$ and determine new state by:

$$
j(U):=\min \left\{k \in\{1,2, \ldots, d\} \mid \bar{f}_{k}>U\right\} .
$$

Exercise: verify that $\mathbb{P}(j(U)=\ell)=f_{\ell}$.

## Data assimilation of Markov Chains

Let $\left\{Z_{n}\right\}$ with $Z_{n}=\left(X_{n}, Y_{n}\right)$ denote a time-homogeneous Markov chain.
For observations $Y_{0: n}$ related to a signal of interest $X_{0: n}$ we consider the following conditional estimation problems:

- Prediction: $X_{k} \mid Y_{0: j}$ for $j<k$,
- Filtering: $X_{k} \mid Y_{0: k}$,

■ Smoothing $X_{k} \mid Y_{0: T}$ for $T>k$.


Figure: From "Bayesian Filtering and Smoohting" by S. Särrkä.

## Overview

1 Recurrence and construction of invariant distributions for time-homogeneous finite Markov chains

2 Filtering

3 Prediction

## 4 Smoothing

## Filtering setting

Time homogeneous Markov chain $\left\{Z_{n}\right\}=\left\{\left(X_{n}, Y_{n}\right)\right\}$ with

- countable state-space $C$, since

$$
\left(X_{n}, Y_{n}\right): \Omega \rightarrow A \times B=: C
$$

■ and transition function $p: C \times C \rightarrow C$ satisfying

$$
\mathbb{P}\left(Z_{n+1}=c_{n+1} \mid Z_{n}=c_{n}\right)=p\left(c_{n}, c_{n+1}\right) \quad \text { whenever } \mathbb{P}\left(Z_{n}=c_{n}\right)>0
$$

■ For every $n \geq 0$, recall that $Y_{0: n}=\left(Y_{0}, Y_{1}, \ldots, Y_{n}\right)$ is the history of observations

■ and we seek the state of the signal of interest $X_{n}$ given $Y_{0: n}$.

## Examples

■ Random walk $Z_{n}=\left(X_{n}, Y_{n}\right)$ on $\mathbb{Z}^{2}$.
■ Discrete Markov chain $X_{n}$ on $\mathbb{S}=\mathbb{Z}^{d}$ with $Y_{n}=H X_{n}+W_{n}$ for some matrix $H \in \mathbb{Z}^{k \times d}$ and with $W_{n}$ a random walk on $\mathbb{Z}^{k}$.

- Discrete Markov chain $X_{n}$ on $\mathbb{S}$ with $Y_{n}=X_{\lfloor n / 5\rfloor}$ (new observation every fifth time unit).

■ Hidden Markov models: $X_{n}$ a discrete Markov chain and

$$
Y_{n}=\gamma\left(X_{n}, W_{n}\right)
$$

where $\left\{W_{n}\right\}$ are iid and $\left\{X_{n}\right\}$ and $\left\{W_{n}\right\}$ are independent.

Note $Z_{n}$ being a Markov chain does not imply that either of $X_{n}$ or $Y_{n}$ is:

## Example 6

Consider chain $Z_{n}$ on $\{1,2\} \times\{1,2\}$ and $X_{n}$ and $Y_{n}$ discrete processes on $A=B=\{1,2\}$, say with uniformly random initial condition, to make the chain stochastic.
It is then clear that for $n>1$,

$$
\mathbb{P}\left(X_{n}=1 \mid X_{n-1}=2\right)=1 / 2
$$

while


$$
\mathbb{P}\left(X_{n}=1 \mid X_{n-1}=2, X_{n-2}=2\right)=1
$$

## How detailed state-information do we seek?

- Best approximation in mean-square sense:

$$
\tilde{X}_{n}:=\mathbb{E}\left[X_{n} \mid Y_{0: n}\right]=\sum_{a \in A} a \mathbb{P}\left(X_{n}=a \mid Y_{0: n}\right)
$$

■ or perhaps the (more informative) conditional distribution

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: n}\right) \quad \text { for relevant } a \in A
$$

## Example 7 (Comparison of conditional expectation and distribution)

Let the sequence $Z_{n}=\left(X_{n}, Y_{n}\right)$ be a simple symmetric random walk on $\mathbb{Z}^{2}$ with $Z_{0}=(0,0)$. Then for any $n \geq 0$ and observation sequence $b_{0: n}$,

$$
\mathbb{E}\left[X_{n} \mid Y_{0: n}=b_{0: n}\right]=0
$$

since

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: n}=b_{0: n}\right)=\mathbb{P}\left(X_{n}=-a \mid Y_{0: n}=b_{0: n}\right) \quad \forall a \in A
$$

Conclusion: $\mathbb{P}\left(X_{n}=a \mid Y_{0: n}=b_{0: n}\right)$ is not always needed to compute the associated conditional expectation.

## Filtering setting 2

■ We will consider observations of the kind $Y_{0: n}=b_{0: n}$, accumulating as $n \mapsto n+1$.

■ We assume that $\mathbb{P}\left(Y_{0: n}=b_{0: n}\right)>0$ for $n=0,1, \ldots$ (since these observations have occurred).

- Iteratively in time $n=0,1, \ldots$, we seek the conditional distribution

$$
\begin{equation*}
\mathbb{P}\left(X_{n}=a_{n} \mid Y_{0: n}=b_{0: n}\right) \quad \text { for relevant } \quad a_{n} \in A \tag{5}
\end{equation*}
$$

■ For efficiency, we seek a recursive algorithm, using the new measurement $b_{n}$ to update the previous calculations of

$$
\left\{\mathbb{P}\left(X_{n-1}=a_{n-1} \mid Y_{0: n-1}=b_{0: n-1}\right)\right\}_{a_{n-1} \in A}
$$

when computing (5).

## Recursive algorithm

By definition,

$$
\begin{equation*}
\mathbb{P}\left(X_{n}=a \mid Y_{0: n}=b_{0: n}\right)=\frac{\mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}\right)}{\mathbb{P}\left(Y_{0: n}=b_{0: n}\right)} \tag{6}
\end{equation*}
$$

Idea: Apply law of total probability
$\mathbb{P}\left(X_{n}=a_{n}, Y_{0: n}=b_{0: n}\right)=\sum_{a_{0: n-1} \in A^{n}} \mathbb{P}\left(X_{n}=a_{n}, X_{0: n-1}=a_{0: n-1}, Y_{0: n}=b_{0: n}\right)$
and use the Markov property to render every summand computable

$$
\begin{aligned}
& \mathbb{P}\left(X_{0: n}=a_{0: n}, Y_{0: n}=b_{0: n}\right) \\
& =\mathbb{P}\left(X_{n}=a_{n}, Y_{n}=b_{n} \mid X_{n-1}=a_{n-1}, Y_{n-1}=b_{n-1}\right) \\
& \\
& \quad \times \mathbb{P}\left(X_{0: n-1}=a_{0: n-1}, Y_{0: n-1}=b_{0: n-1}\right)=\ldots
\end{aligned}
$$

## Simplification of idea

By the law of total probability and Markovianity [FJK Corrollary 2.2.7] yields

$$
\begin{aligned}
& \mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}\right) \\
& \quad=\sum_{r \in A} \mathbb{P}\left(X_{n}=a, X_{n-1}=r, Y_{0: n}=b_{0: n}\right) \\
& \begin{array}{r}
=\sum_{r \in A} \mathbb{P}\left(\left(X_{n}, Y_{n}\right)=\left(a, b_{n}\right),\left(X_{n-1}, Y_{n-1}\right)=\left(r, b_{n-1}\right), Y_{0: n-2}=b_{0: n-2}\right) \\
=\sum_{r \in A} \mathbb{P}\left(\left(X_{n}, Y_{n}\right)=\left(a, b_{n}\right) \mid\left(X_{n-1}, Y_{n-1}\right)=\left(r, b_{n-1}\right)\right) \\
\\
\quad \times \mathbb{P}\left(\left(X_{n-1}, Y_{n-1}\right)=\left(r, b_{n-1}\right), Y_{0: n-2}=b_{0: n-2}\right)
\end{array}
\end{aligned}
$$

Motivation last equality?

## Recursive algorithm

Recalling that on positive probability conditioned events,

$$
\begin{aligned}
\mathbb{P}\left(\left(X_{n}, Y_{n}\right)\right. & \left.=\left(a, b_{n}\right) \mid\left(X_{n-1}, Y_{n-1}\right)=\left(r, b_{n-1}\right)\right)=p\left(\left(r, b_{n-1}\right),\left(a, b_{n}\right)\right) \\
& =: q^{r a}\left(b_{n-1}, b_{n}\right)
\end{aligned}
$$

we have that

$$
\begin{equation*}
\mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}\right)=\sum_{r \in A} q^{r a}\left(b_{n-1}, b_{n}\right) \mathbb{P}\left(X_{n-1}=r, Y_{0: n-1}=b_{0: n-1}\right) \tag{7}
\end{equation*}
$$

## Algorithm 1: Recursive relationship joint density

Let $\varphi_{n}^{a}\left(b_{0: n}\right):=\mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}\right)$. Then (7) yields

$$
\varphi_{n}^{a}\left(b_{0: n}\right)=\sum_{r \in A} q^{r a}\left(b_{n-1}, b_{n}\right) \varphi_{n-1}^{r}\left(b_{0: n-1}\right)
$$

Algorithm 1 continued
Moreover,

$$
\mathbb{P}\left(Y_{0: n}=b_{0: n}\right)=\sum_{r \in A} \varphi_{n}^{r}\left(b_{0: n}\right)
$$

and thus

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: n}=b_{0: n}\right)=\frac{\varphi_{n}^{a}\left(b_{0: n}\right)}{\sum_{r \in A} \varphi_{n}^{r}\left(b_{0: n}\right)}
$$

## Verification:

## Iterations

■ Compute $\varphi_{0}^{a}\left(b_{0}\right):=\mathbb{P}\left(X_{0}=a, Y_{0}=b_{0}\right)$ for relevant non-zero probability outcomes $a \in A$.

- When observation $b_{1}$ is obtained, compute $\varphi_{1}^{a}\left(b_{0: 1}\right)$ for all relevant outcomes $a \in A$ using Algorithm 1 and the pre-computed values $\left\{\varphi_{0}^{a}\left(b_{0}\right)\right\}_{a}$.
- Similar iteration " $\left\{\varphi_{n}^{r}\left(b_{1: n}\right)\right\}_{r} \mapsto\left\{\varphi_{n+1}^{r}\left(b_{1: n+1}\right)\right\}_{r}$ " for each $n \mapsto n+1$.

The iterations based on Alg 1 are called online learning, here meaning that you recursively update your estimate for every new observation.

An alternative would be offline/batch learning, here meaning to learn/precompute $\varphi_{n}^{a}\left(\tilde{b}_{0: n}\right)$ for all relevant $n \geq 0, a \in A$ and $\tilde{b}_{0: n} \in B^{n+1}$ before filtering.

## Remarks

■ If instead of conditioning on the observation $b_{0: n}$, we condition on $Y_{0: n}$, then we get the following rv associated to filtering:

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: n}\right)(\omega)=\frac{\varphi_{n}^{a}\left(Y_{0: n}(\omega)\right)}{\sum_{r \in A} \varphi_{n}^{r}\left(Y_{0: n}(\omega)\right)}
$$

- Extension of Alg 1 to when $\left\{Z_{n}\right\}$ is not a time-homogeneous Markov chain is straightforward. Replace time-independent transition functions by the time-dependent ones

$$
q^{r a}\left(n, b_{n}, b_{n+1}\right):=p\left(n,\left(r, b_{n}\right),\left(a, b_{n+1}\right)\right)
$$

■ Given a finite state-space $A$, we may view $\left\{q^{r a}\left(b_{n}, b_{n+1}\right)\right\}_{(r, a) \in A^{2}}$ as a matrix $q_{n}$ and $\left\{\varphi_{n}^{a}\left(b_{0: n}\right)\right\}_{a}=\varphi_{n}$ as a column vector. The iterations in Alg 1 then becomes

$$
\varphi_{n+1}=q_{n}^{T} \varphi_{n}
$$

## Example 8 ( Hidden Markov model)

Let $X_{n}$ be a simple symmetric RW on $\mathbb{Z}$ and $Y_{n}=X_{n}+W_{n}$, where $\left\{W_{n}\right\}$ is iid and independent of $\left\{X_{n}\right\}$ with $\mathbb{P}\left(W_{n}=k\right)=1 / 5$ for all $|k| \leq 2$. Assume $X_{0}=0$. Compute $\mathbb{P}\left(X_{2}=0 \mid Y_{0: 2}=(0,2,1)\right)$.

## Some steps in the solution:

1. Identify transition function

$$
\begin{aligned}
q^{r a}(c, d) & =\mathbb{P}\left(\left(X_{n}, Y_{n}\right)=(a, d) \mid\left(X_{n-1}, Y_{n-1}\right)=(r, c)\right) \\
& = \\
& =\mathbb{P}\left(X_{n}=a \mid X_{n-1}=r\right) \mathbb{P}\left(W_{n}=d-a\right)
\end{aligned}
$$

(above eq holds $\left.\mathbb{P}\left(\left(X_{n-1}, Y_{n-1}\right)=(r, c)\right)>0\right)$.
2. Observe that $\left\{\varphi_{n}^{a}\left(b_{0: n}\right)\right\}_{a}$ is only possibly non-zero for
$a \in\{-n,-n+1, \ldots, n\}$
3. Use Alg 1.

## Overview

1 Recurrence and construction of invariant distributions for time-homogeneous finite Markov chains

2 Filtering

3 Prediction

## 4 Smoothing

## Prediction problem

The prediction problem is to estimate

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right)
$$

for some $n>m \geq 0$.
Derivation of recursive algorithm:

$$
\begin{aligned}
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right) & =\frac{\mathbb{P}\left(X_{n}=a, Y_{0: m}=b_{0: m}\right)}{\mathbb{P}\left(Y_{0: m}=b_{0: m}\right)} \\
& =\frac{\sum_{\bar{b} \in B} \mathbb{P}\left(X_{n}=a, Y_{n}=\bar{b}, Y_{0: m}=b_{0: m}\right)}{\mathbb{P}\left(Y_{0: m}=b_{0: m}\right)}
\end{aligned}
$$

Idea for obtaining computable terms:

For $n \geq m$, introduce

$$
\varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right):=\mathbb{P}\left(X_{n}=a, Y_{n}=\bar{b}, Y_{0: m}=b_{0: m}\right)
$$

Then, for $n=m$,

$$
\varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right)=\varphi_{n}^{a}\left(b_{0: m}\right) \mathbb{1}_{b_{m}}(\bar{b})
$$

## Verification

And, for $n>m$,

$$
\begin{aligned}
\varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right) & =\sum_{r \in A, s \in B} \mathbb{P}\left(X_{n}=a, Y_{n}=\bar{b}, X_{n-1}=r, Y_{n-1}=s, Y_{0: m}=b_{0: m}\right) \\
& =
\end{aligned}
$$

$$
=\sum_{r \in A, s \in B} \mathbb{P}\left(X_{n}=a, Y_{n}=\bar{b} \mid X_{n-1}=r, Y_{n-1}=s\right) \varphi_{n-1}^{r, s}\left(b_{0: m}\right)
$$

$$
=\sum_{r \in A, s \in B} q^{r a}(s, \bar{b}) \varphi_{n-1}^{r, s}\left(b_{0: m}\right)
$$

## Summary

We seek a recursive algorithm for

$$
\begin{aligned}
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right) & =\frac{\sum_{\bar{b} \in B} \mathbb{P}\left(X_{n}=a, Y_{n}=\bar{b}, Y_{0: m}=b_{0: m}\right)}{\mathbb{P}\left(Y_{0: m}=b_{0: m}\right)} \\
& =\frac{\sum_{\bar{b} \in B} \varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right)}{\sum_{r \in A} \varphi_{m}^{r}\left(b_{0: m}\right)}
\end{aligned}
$$

Every summand in the numerator satisfies recursive equation

$$
\begin{equation*}
\varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right)=\sum_{r \in A, s \in B} q^{r a}(s, \bar{b}) \varphi_{n-1}^{r, s}\left(b_{0: m}\right) \quad n>m \tag{8}
\end{equation*}
$$

with "initial condition"

$$
\varphi_{m}^{r, s}\left(b_{0: m}\right)=\varphi_{m}^{r}\left(b_{0: m}\right) \mathbb{1}_{b_{m}}(s)
$$

## Algorithm 2 - Prediction

1 Compute $\left\{\varphi_{m}^{r}\left(b_{0: m}\right)\right\}_{r \in A}$ by Algorithm 1.
2 "Initialize" $\varphi_{m}^{r, s}\left(b_{0: m}\right)=\varphi_{m}^{r}\left(b_{0: m}\right) \mathbb{1}_{b_{m}}(s)$ for relevant $(r, s) \in A \times B$.
3 Compute $\left\{\varphi_{k}^{r, s}\left(b_{0: m}\right)\right\}_{r \in A, s \in B}$ for $k=m+1, m+2, \ldots, n-1$ by the recursive formula (8).
4 Compute $\left\{\varphi_{n}^{a, \bar{b}}\left(b_{0: n}\right)\right\}_{\bar{b} \in B}$ by (8) (i.e., for the fixed state $a \in A$ only).
5 Output:

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right)=\frac{\sum_{\bar{b} \in B} \varphi_{n}^{a, \bar{b}}\left(b_{0: m}\right)}{\sum_{r \in A} \varphi_{m}^{r}\left(b_{0: m}\right)}
$$

Remark: Algorithm 2 simplifies in many settings, e.g., hidden Markov models [FJK 3.4.3].

Exercise Simplify the "recursive" equation predictions when $n=m+1$.

## Overview

1 Recurrence and construction of invariant distributions for time-homogeneous finite Markov chains

2 Filtering

3 Prediction

4 Smoothing

## Smoothing problem

The smoothing/interpolation problem is to estimate

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right)
$$

for some $m>n \geq 0$.

Property: More information leads to improved approximations: for $m>n>k \geq 0$
$\underbrace{\mathbb{E}\left[\left|X-\mathbb{E}\left[X_{n} \mid Y_{0: m}\right]\right|^{2}\right]}_{\text {smoothing }} \leq \underbrace{\mathbb{E}\left[\left|X-\mathbb{E}\left[X_{n} \mid Y_{0: n}\right]\right|^{2}\right]}_{\text {filtering }} \leq \underbrace{\mathbb{E}\left[\left|X-\mathbb{E}\left[X_{n} \mid Y_{0: k}\right]\right|^{2}\right]}_{\text {prediction }}$

## Derivation of a recursive algorithm:

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right)=\frac{\mathbb{P}\left(X_{n}=a, Y_{0: m}=b_{0: m}\right)}{\mathbb{P}\left(Y_{0: m}=b_{0: m}\right)}=\frac{\varphi_{n}^{a}\left(b_{0: m}\right)}{\sum_{r \in A} \varphi_{m}^{r}\left(b_{0: m}\right)}
$$

Using the Markov property [FJK 2.2.7]

$$
\begin{align*}
\varphi_{n}^{a}\left(b_{0: m}\right) & =\mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}, Y_{n+1: m}=b_{n+1: m}\right) \\
& =\mathbb{P}\left(Y_{n+1: m}=b_{n+1: m} \mid X_{n}=a, Y_{0: n}=b_{0: n}\right) \mathbb{P}\left(X_{n}=a, Y_{0: n}=b_{0: n}\right) \\
& =\mathbb{P}\left(Y_{n+1: m}=b_{n+1: m} \mid X_{n}=a, Y_{n}=b_{n}\right) \varphi_{n}^{a}\left(b_{0: n}\right) \tag{9}
\end{align*}
$$

Next seek to obtain recursive formula for first factor when $\mathbb{P}\left(X_{n}=a, Y_{n}=b_{n}\right)>0$.

Otherwise, also $\varphi_{n}^{a}\left(b_{0: n}\right)=0$, and the value of the first-factor value is not needed.

By the law of total probability,

$$
\begin{aligned}
& \mathbb{P}\left(Y_{n+1: m}=b_{n+1: m} \mid X_{n}=a, Y_{n}=b_{n}\right) \\
& =\sum_{\bar{a}_{n+1: m} \in A^{m-n}} \mathbb{P}\left(X_{n+1: m}=\bar{a}_{n+1: m}, Y_{n+1: m}=b_{n+1: m} \mid X_{n}=a, Y_{n}=b_{n}\right) \\
& =\sum_{\bar{a}_{n+1: m} \in A^{m-n}} p\left(\left(a, b_{n}\right),\left(\bar{a}_{n+1}, b_{n+1}\right)\right) p\left(\left(\bar{a}_{n+1}, b_{n+1}\right),\left(\bar{a}_{n+2}, b_{n+2}\right)\right) \ldots \\
& \quad \ldots p\left(\left(\bar{a}_{m-1}, b_{m-1}\right),\left(\bar{a}_{m}, b_{m}\right)\right)
\end{aligned}
$$

## Algorithm for $\kappa$ [FJK problem 3.3.4]

Whenever $\mathbb{P}\left(X_{n}=a, Y_{n}=b_{n}\right)>0$

$$
\kappa_{n, m}^{a}\left(b_{n: m}\right):= \begin{cases}\mathbb{P}\left(Y_{n+1: m}=b_{n+1: m} \mid X_{n}=a, Y_{n}=b_{n}\right) & \text { if } n<m \\ 1 & \text { if } n=m\end{cases}
$$

solves the following backward recurrence equation

$$
\kappa_{n-1, m}^{a}\left(b_{n-1: m}\right)=\sum_{r \in A} \underbrace{p\left(\left(a, b_{n-1}\right),\left(r, b_{n}\right)\right)}_{q^{a r}\left(b_{n-1}, b_{n}\right)} \kappa_{n, m}^{r}\left(b_{n: m}\right), \quad n=1,2, \ldots, m .
$$

## Summary

We seek

$$
\mathbb{P}\left(X_{n}=a \mid Y_{0: m}=b_{0: m}\right)=\frac{\mathbb{P}\left(X_{n}=a, Y_{0: m}=b_{0: m}\right)}{\mathbb{P}\left(Y_{0: m}=b_{0: m}\right)}=\frac{\varphi_{n}^{a}\left(b_{0: m}\right)}{\sum_{r \in A} \varphi_{m}^{r}\left(b_{0: m}\right)}
$$

and by (9) and Algorithm for $\kappa$,

$$
\begin{equation*}
\varphi_{n}^{a}\left(b_{0: m}\right)=\kappa_{n, m}^{a}\left(b_{n: m}\right) \varphi_{n}^{a}\left(b_{0: n}\right) \tag{11}
\end{equation*}
$$

## Algorithm 3-smoothing/interpolation

1 Compute $\left\{\varphi_{n}^{r}\left(b_{0: n}\right)\right\}_{r}$ by Algorithm 1,
2 Compute $\kappa_{n, m}^{a}\left(b_{n: m}\right)$ by Algorithm for $\kappa, \phi_{n}^{a}\left(b_{0: m}\right)$ by (11) and the output (10).

## Next time

Continuous random variables, probability density functions, conditional densities ...

