Notes on Sequence Modelling

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1 Random Sequence Processes

Consider a random process R that generates arbitrary-length sequences of the form $\vec{R}_N = (R_1, R_2, \ldots, R_N)$, where N is a random variable governing the length of a sequence, and R_t is a random variable governing the value at *stage* t of the sequence. This sequence process is graphically depicted in Figure 1.1.

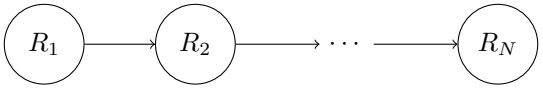

Figure 1.1: *A random process R for generating sequences of arbitrary length N. The arrows indicate transitions from one stage in the sequence to the next.*

We assume that each R_t randomly takes some discrete or continuous value $r_t \in \mathcal{R}$, and hence the probability (or probability density) of observing a particular sequence $\vec{r}$ of length $n = |\vec{r}|$ is given by

$$p(\vec{R}_N{=}\vec{r}) \quad = \quad p(N = n)\, p(R_1{=}r_1, \ldots, R_n{=}r_n \,|\, N = n)\,. \tag{1.1}$$

In practice, this definition presupposes that we know we have observed a *complete* sequence that started at stage 1 and ended at stage n. Suppose instead that the sequence $\vec{r}$ was observed one stage at a time. How do we know if the underlying process has actually terminated, or will instead continue to generate another observed value r_{n+1}? Similarly, how do we know that the first observed value r_1 was not in fact part of a longer, unobserved sequence of values? We assume that the random process R only ever produces complete sequences, independently of the observation process, which might provide partial or complete sequences of values. Furthermore, if the random process does not signal the start and end of generated sequences, then an observed sequence might actually comprise multiple, contiguously generated subsequences.

In order to handle such difficulties, we consider any arbitrary sequence $\vec{r}$ by default to be *incomplete*, and explicitly denote the corresponding, complete sequence by $\langle\vec{r}\rangle$. We can now introduce the notion of *partially complete* sequences. Thus, a *start sequence* is a generated sequence with an observed (or definite) start (at stage 1) but an unobserved (or indefinite) end, i.e. it might or might not terminate at stage n. This is denoted by $\langle\vec{r}$ if we are truly uncertain as to the termination, or by $\langle\vec{r}]$ if we actually know that the generated sequence does not terminate at stage n. Similarly, an *end sequence* is a generated sequence with an observed end (at stage n) but an unobserved start, i.e. it might or might not have initiated at the observed stage 1. This is denoted by $\vec{r}\rangle$ if we are truly uncertain as to sequence initiation, or by $[\vec{r}\rangle$ if we actually know that the generated sequence was not initiated at stage 1. Clearly, we may also specify the remaining incomplete sequences, namely $[\vec{r}]$, $\vec{r}]$ and $[\vec{r}$.

Under this augmented notation, knowledge about the start of a sequence can be encapsulated in a random indicator variable ι_{t-1}, which takes on the value 1 if some observed r_t is definitely the first stage in the generated sequence, or the value 0 if it is not. Similarly, the random indicator variable τ_{t+1} takes on the value 1 if r_t is definitely the last stage in the generated sequence, or the value 0 if it is not. In general, these indicators allow us to handle the observation of possibly concatenated, multiple, generated sequences. From now on, however, we shall assume (unless otherwise stated) that we are dealing with a single, contiguous sequence. Thus, notionally, the indicators ι_0 and τ_{n+1} can be thought to correspond to pseudo-stages 0 and $n{+}1$, such that an arbitrary generated sequence is initiated at stage 0 and terminated at some random stage $N + 1$. This augmented random process is depicted in Figure 1.2.

The probability of a given complete sequence $\langle\vec{r}\rangle$ is now defined as

$$p(\langle\vec{r}\rangle) \quad = \quad p(\iota_0{=}1, \tau_1{=}0, R_1 = r_1, \tau_2{=}0, \ldots, \tau_n{=}0, R_n = r_n, \tau_{n+1}{=}1)\,, \tag{1.2}$$

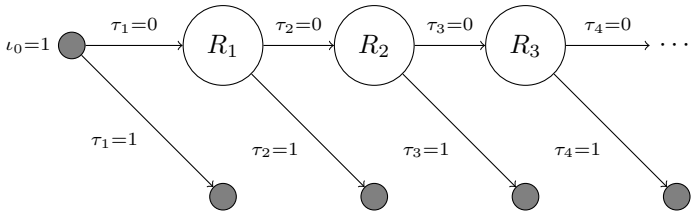

Figure 1.2: *A random process for generating complete sequences of arbitrary length, with explicit stages for sequence initiation and termination. Multiple arrows exiting from a node indicate different possible (mutually exclusive) stage transition pathways.*

such that

$$p(N{=}n) \quad = \quad p(\iota_0{=}1, \tau_1{=}0, \ldots, \tau_n{=}0, \tau_{n+1}{=}1)\,. \tag{1.3}$$

This has the form of a generalised Bernoulli sequence.

Note that when the context is clear, we may for convenience drop explicit mention of the random variable R_t. Similarly, we may denote $\iota_t = 1$ by ι_t^+, on the understanding that ι_t^- denotes the negation $\iota_t = 0$. Likewise, we may denote $\tau_t = 1$ by τ_t^+ and $\tau_t = 0$ by τ_t^-. Hence, it is plausible to simplify equation (1.2) as

$$p(\langle \vec{r} \rangle) \quad = \quad p(\iota_0^+, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \tau_{n+1}^+)\,. \tag{1.4}$$

Consequently, we may simplify the explicitly terminated process of Figure 1.2 to more resemble the implicitly terminatel process of Figure 1.1; the result is shown in Figure 1.3.

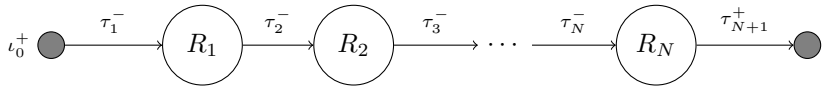

Figure 1.3: *A simplified represenation of a random process for generating complete sequences of random length N, with explicit stages for sequence initiation and termination, and explicit labelling of non-terminating transitions.*

In general, we may handle both complete and partial sequences by letting $\underline{\iota}$ denote the observed start-of-sequence symbol, and letting $\underline{\tau}$ denote the observed end-of-sequence symbol; hence

$$\begin{aligned} p(\underline{\iota}, \vec{r}, \underline{\tau}) \quad &= \quad p(\iota_0{=}\underline{\iota}, \tau_1{=}0, R_1{=}r_1, \ldots, \tau_n{=}0, R_n{=}r_n, \tau_{n+1}{=}\underline{\tau}) \\ &= \quad p(\underline{\iota}, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \underline{\tau})\,. \end{aligned} \tag{1.5}$$

1.1 Missing Values

The main difference between a complete, generated sequence $\vec{r} = (r_1, \ldots, r_n)$ and the observed sequence of values, say $\underline{\vec{r}} = (\underline{r}_1, \ldots, \underline{r}_n)$, is the possibility that some values were unobserved[1], i.e. *missing* or systematically *hidden*. For convenience, let $\underline{r}_t = *$ denote the case where the observed value of the t-th stage is missing. Likewise, let $\underline{\iota} = *$ if we do not know whether or not we observed the start of the generated sequence, and let $\underline{\tau} = *$ if we do not kow whether or not we observed the end of the generated sequence. The '*' symbol is just a representational device – its presence has no effect on the computed probabilities, other than to indicate that the true values of the variables ι_0 and/or τ_{n+1} should be marginalised out. Thus, for example:

$$p(\vec{r}) \quad = \quad p(*, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, *) \;=\; p(\tau_1^-, r_1, \ldots, \tau_n^-, r_n)\,. \tag{1.6}$$

In practice, we allow for both observed values and missing values by introducing an indicator function $\delta(\cdot)$, where $\delta(x{=}y) = 1$ if $x = y$ and $\delta(x{=}y) = 0$ if $x \neq y$; by definition, we take $\delta(x{=}*) = 1$. Hence, we obtain

$$p(\underline{\iota}, \vec{r}, \underline{\tau}) \quad = \quad \sum_{\iota_0=0}^{1} \delta(\iota_0{=}\underline{\iota}) \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1}{=}\underline{\tau})\; p(\iota_0, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \tau_{n+1})\,. \tag{1.7}$$

[1] We are ignoring the very real problem of aligning the observed values with the generated stages. This difficulty can be partially alleviated under the assumption of stationary distributions, such that each stage behaves like the previous one.

In general, if the domain $\mathcal{R}$ is discrete, then the likelihood of an observed sequence is given by

$$\begin{aligned} p(\underline{\iota}, \vec{\underline{r}}, \underline{\tau}) \quad &= \quad \sum_{\iota_0=0}^{1} \delta(\iota_0 = \underline{\iota}) \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1} = \underline{\tau}) \sum_{r_1 \in \mathcal{R}} \delta(r_1 = \underline{r}_1) \cdots \sum_{r_n \in \mathcal{R}} \delta(r_n = \underline{r}_n) \\ &\qquad p(\iota_0, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \tau_{n+1}) \,. \end{aligned} \tag{1.8}$$

Alternatively, if $\mathcal{R}$ is continuous, then the likelihood becomes

$$\begin{aligned} p(\underline{\iota}, \vec{\underline{r}}, \underline{\tau}) \quad &= \quad \sum_{\iota_0=0}^{1} \delta(\iota_0 = \underline{\iota}) \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1} = \underline{\tau}) \int_{\mathcal{R}} \delta(r_1 - \underline{r}_1) \cdots \int_{\mathcal{R}} \delta(r_n - \underline{r}_n) \\ &\qquad p(\iota_0, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \tau_{n+1}) \, dr_1 \, dr_2 \cdots dr_n \,, \end{aligned} \tag{1.9}$$

where $\delta(\cdot)$ is now the Dirac delta function, and where, by extension, we define $\delta(x - *) = 1$. On the understanding that $\sum$ and $\delta(x = y)$ must be swapped respectively for $\int$ and $\delta(x - y)$ as needed for a continuous or semi-continuous domain, we may, without loss of generality, henceforth simply utilise the discrete form (1.8).

1.2 Forward–Backward Algorithm

The likelihood (1.8) of an observed sequence $\vec{\underline{r}}$ has been written in a computationally inefficient form, but can in practice be efficiently evaluated by nesting the summations, using a modification of the *forward–backward algorithm* to include knowledge of sequence initiation and termination. The precise details of these calculations depend upon the chosen factorisation of the probability model, which is itself a function of the explicit dependencies between various stages in the sequence. Such dependency modelling is dealt with further in Section 2.

Despite not knowing these dependencies in advance, however, the basic form of the forward–backward algorithm can still be formulated. The first requirement is that the sequence process be *causal*, meaning that each stage of a sequence (including the termination stage but excluding the initiation stage) depends only on the preceding stages, and never on future stages. This causality allows us to split a generated sequence into two parts at some arbitrary *pivot* stage t, as shown in Figure 1.4. The second requirement is that the dependence on past stages can be limited in scope to some arbitrary *historical* stage s, as also shown.

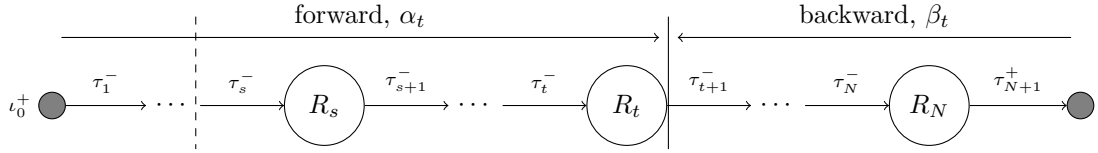

Figure 1.4: *Causality allows the sequence to be partitioned at some pivot stage t, thereby dividing the sequence into past and future stages. Further limitation of past dependencies to some historical stage s defines the active region for one step of the forward–backward algorithm.*

Let us now define the sub-sequence $\vec{r}_{s,t} = (r_s, r_{s+1}, \ldots, r_t)$; by definition, $\vec{r}_{s,t} = (\,)$ if $s > t$. Then observe, for a sufficiently long sequence, that

$$\begin{aligned} p(\underline{\iota}, \vec{\underline{r}}, \underline{\tau}) \quad &= \quad p(\underline{\iota}, \vec{\underline{r}}_{1,s-1}, \vec{\underline{r}}_{s,t}, \vec{\underline{r}}_{t+1,n}, \underline{\tau}) \\ &= \quad \sum_{r_s \in \mathcal{R}} \delta(r_s = \underline{r}_s) \cdots \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t) \, p(\underline{\iota}, \vec{\underline{r}}_{1,s-1}, \vec{r}_{s,t}, \vec{\underline{r}}_{t+1,n}, \underline{\tau}) \\ &= \quad \sum_{r_s \in \mathcal{R}} \delta(r_s = \underline{r}_s) \cdots \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t) \, p(\underline{\iota}, \vec{\underline{r}}_{1,s-1}, \vec{r}_{s,t}) \, p(\vec{\underline{r}}_{t+1,n}, \underline{\tau} \,|\, \underline{\iota}, \vec{\underline{r}}_{1,s-1}, \vec{r}_{s,t}) \\ &= \quad \sum_{r_s \in \mathcal{R}} \delta(r_s = \underline{r}_s) \cdots \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t) \, \alpha_t(\vec{r}_{s,t}) \, \beta_t(\vec{r}_{s,t}) \,, \end{aligned} \tag{1.10}$$

where

$$\alpha_t(\vec{r}_{s,t}) \quad = \quad p(\underline{\iota}, \tau_1^-, \underline{r}_1, \ldots, \tau_{s-1}^-, \underline{r}_{s-1}, \tau_s^-, r_s, \ldots, \tau_t^-, r_t) \tag{1.11}$$

is the foward factor and

$$\beta_t(\vec{r}_{s,t}) \quad = \quad p(\tau_{t+1}^-, \underline{r}_{t+1}, \ldots, \tau_n^-, \underline{r}_n, \underline{\tau} \,|\, \underline{\iota}, \tau_1^-, \underline{r}_1, \ldots, \tau_{s-1}^-, \underline{r}_{s-1}, \tau_s^-, r_s, \ldots, \tau_t^-, r_t) \tag{1.12}$$

is the backward factor. The entire forward pass of the forward–backward algorithm starts at the initiation stage with $\underline{\iota}$ and recursively computes α_t for each $t = 1, 2, \ldots, n$. Likewise, the backward pass starts at termination stage with $\underline{\tau}$, and recursively computes β_t for each $t = n, n-1, \ldots, 1$. The precise details of these recursive calculations rely upon the nature of the fine-grained dependencies, as disdcussed in the next section.

2 Markov Sequence Processes

In Section 1, we defined a causal random sequence process R, such that each stage of a sequence, including the termination stage, depends only on the preceding stages. This causal process, depicted in Figure 2.1, is simply the random process from Figure 1.3 with additional, explicit dependencies (in the form of dashed arrows). Hence, under the Markov assumption of conditional independence, the causal sequence process

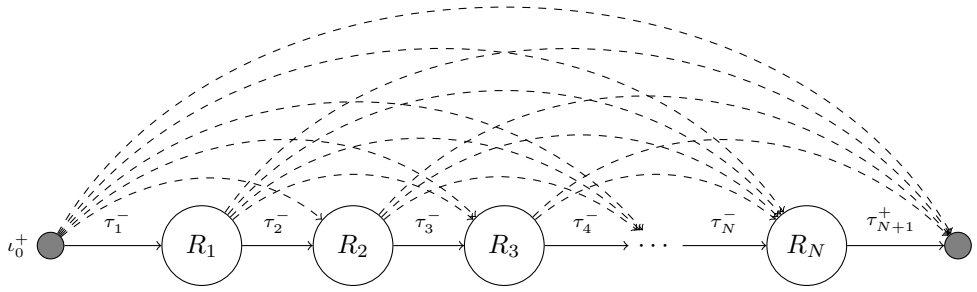

Figure 2.1: *A fully-dependent, causal process for generating complete, random sequences of random length N. Solid arrows indicate stage transitions. Both dashed arrows and solid arrows indicate parent–child dependencies, such that each stage is conditionally dependent on the preceding stages.*

leads to the fully-dependent conditional model

$$\begin{aligned} p(\iota_0, \vec{r}, \tau_{n+1}) \quad &= \quad p(\iota_0, \tau_1^-, r_1, \ldots, \tau_n^-, r_n, \tau_{n+1}) \\ &= \quad p(\iota_0)\, p(\tau_1^- \,|\, \iota_0)\, p(r_1 \,|\, \iota_0, \tau_1^-)\, p(\tau_2^- \,|\, \iota_0, \tau_1^-, r_1)\, p(r_2 \,|\, \iota_0, \tau_1^-, r_1, \tau_2^-) \\ &\quad \cdots p(\tau_n^- \,|\, \iota_0, \ldots, \tau_{n-1}^-, r_{n-1}) p(r_n \,|\, \iota_0, \ldots, \tau_n^-)\, p(\tau_{n+1} \,|\, \iota_0, \ldots, r_n) \\ &= \quad p(\iota_0) \left\{ \prod_{t=1}^{n} p(\tau_t^-, r_t \,|\, \iota_0, \vec{\tau}_{1,t-1}^-, \vec{r}_{1,t-1}) \right\} p(\tau_{n+1} \,|\, \iota_0, \vec{\tau}_{1,n}^-, \vec{r}_{1,n})\,. \end{aligned} \tag{2.1}$$

In practice, this full model is considerably simplified by dropping some or even most of the explicit (dashed) dependencies. For example, one might limit the conditionality on past stages to a maximum of m depenencies. This leads to the so-called *m-th order Markov model*, given by

$$\begin{aligned} p(\iota_0, \vec{r}, \tau_{n+1}) \quad &= \quad p(\iota_0) \left\{ \prod_{t=1}^{m} p(\tau_t^-, r_t \,|\, \iota_0, \vec{\tau}_{1,t-1}^-, \vec{r}_{1,t-1}) \right\} \left\{ \prod_{t=m+1}^{n} p(\tau_t^-, r_t \,|\, \vec{\tau}_{t-m,t-1}^-, \vec{r}_{t-m,t-1}) \right\} \\ &\quad \times p_m^*(\tau_{n+1} \,|\, \iota_0, \vec{\tau}_{1,n}^-, \vec{r}_{1,n})\,, \end{aligned} \tag{2.2}$$

where

$$p_m^*(\cdot \,|\, \iota_0, \vec{\tau}_{1,t}^-, \vec{r}_{1,t}) \quad = \quad \begin{cases} p(\cdot \,|\, \iota_0, \vec{\tau}_{1,t}^-, \vec{r}_{1,t})\,, & \text{for } t < m\,, \\ p(\cdot \,|\, \vec{\tau}_{t-m+1,t}^-, \vec{r}_{t-m+1,t})\,, & \text{for } t \geq m \end{cases}\,. \tag{2.3}$$

In the special case of $m = 1$, the first-order Markov model, depicted in Figure 1.3, takes on the especially-simple conditional form (assuming a non-empty sequence) of

$$p(\iota_0, \vec{r}, \tau_{n+1}) \quad = \quad p(\iota_0)\, p(\tau_1^-, r_1 \,|\, \iota_0) \left\{ \prod_{t=2}^{n} p(\tau_t^-, r_t \,|\, \tau_{t-1}^-, r_{t-1}) \right\} p(\tau_{n+1} \,|\, \tau_n^-, r_n)\,. \tag{2.4}$$

An example from the realm of natural language understanding is the lexicographical analysis of the character sequences of words using bigrams (pairs of adjacent characters, corresponding to $m = 1$), and trigrams (triples of adjacent characters, corresponding to $m = 2$), etc. The second-order Markov sequence process, for example, is depicted in Figure 2.2.

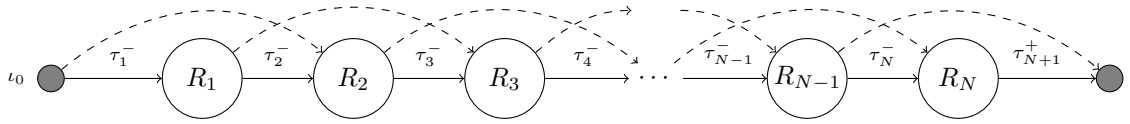

Figure 2.2: *A 2nd-order Markov process for generating complete, random sequences of random length N.*

2.1 Markov Forward–Backward Algorithm

The basic description of the forward–backward algorithm in Section 1.2 can now be refined under the restriction of the general, causal sequence process to an m-th order Markov process. Specifically, we take the limiting historical stage to be $s = \max(1, t - m + 1)$ for $t > 0$ (i.e. non-empty sequences). Then, for the initial stages $t < m$, for $m > 1$, the forward factor (1.11) becomes

$$\alpha_t(\vec{r}_{1,t}) \;=\; p(\iota_0, \tau_1^-, r_1, \ldots, \tau_t^-, r_t) \;=\; p(\iota_0) \prod_{i=1}^{t} p(\tau_i^-, r_i \,|\, \iota_0, \vec{\tau}_{1,i-1}^-, \vec{r}_{1,i-1}) \,. \tag{2.5}$$

Furthermore, if $t < m - 1$ then at stage $t + 1$ we have

$$\begin{aligned} \alpha_{t+1}(\vec{r}_{1,t+1}) \;&=\; p(\iota_0, \tau_1^-, r_1, \ldots, \tau_{t+1}^-, r_{t+1}) \;=\; p(\iota_0) \prod_{i=1}^{t+1} p(\tau_i^-, r_i \,|\, \iota_0, \vec{\tau}_{1,i-1}^-, \vec{r}_{1,i-1}) \\ &=\; \alpha_t(\vec{r}_{1,t})\, p(\tau_{t+1}^-, r_{t+1} \,|\, \iota_0, \vec{\tau}_{1,t}^-, \vec{r}_{1,t}) \,. \end{aligned} \tag{2.6}$$

Note that for $m > 1$ the forward pass commences from

$$\alpha_1(r_1) \;=\; p(\iota_0)\, p(\tau_1^-, r_1 \,|\, \iota_0) \,. \tag{2.7}$$

However, if the sequence is sufficiently long, then for later stages $t \geq m$ we obtain

$$\begin{aligned} \alpha_t(\vec{r}_{t-m+1,t}) \;&=\; p(\underline{\iota}, \tau_1^-, \underline{r}_1, \ldots, \tau_{t-m}^-, \underline{r}_{t-m}, \tau_{t-m+1}^-, r_{t-m+1}, \ldots, \tau_t^-, r_t) \\ &=\; \sum_{\iota_0=0}^{1} \delta(\iota_0 = \underline{\iota}) \sum_{r_1 \in \mathcal{R}} \delta(r_1 = \underline{r}_1) \cdots \sum_{r_{t-m} \in \mathcal{R}} \delta(r_{t-m} = \underline{r}_{t-m}) \\ &\qquad p(\iota_0) \left\{ \prod_{i=1}^{m} p(\tau_i^-, r_i \,|\, \iota_0, \vec{\tau}_{1,i-1}^-, \vec{r}_{1,i-1}) \right\} \left\{ \prod_{i=m+1}^{t} p(\tau_i^-, r_i \,|\, \vec{\tau}_{i-m,i-1}^-, \vec{r}_{i-m,i-1}) \right\} \end{aligned} \tag{2.8}$$

from equation (2.2). Moving to the next stage $t + 1$ then provides the recursive result that

$$\begin{aligned} \alpha_{t+1}(\vec{r}_{t-m+2,t+1}) \;&=\; p(\underline{\iota}, \tau_1^-, \underline{r}_1, \ldots, \tau_{t-m+1}^-, \underline{r}_{t-m+1}, \tau_{t-m+2}^-, r_{t-m+2}, \ldots, \tau_{t+1}^-, r_{t+1}) \\ &=\; \sum_{\iota_0=0}^{1} \delta(\iota_0 = \underline{\iota}) \sum_{r_1 \in \mathcal{R}} \delta(r_1 = \underline{r}_1) \cdots \sum_{r_{t-m+1} \in \mathcal{R}} \delta(r_{t-m+1} = \underline{r}_{t-m+1}) \\ &\qquad p(\iota_0) \left\{ \prod_{i=1}^{m} p(\tau_i^-, r_i \,|\, \iota_0, \vec{\tau}_{1,i-1}^-, \vec{r}_{1,i-1}) \right\} \left\{ \prod_{i=m+1}^{t+1} p(\tau_i^-, r_i \,|\, \vec{\tau}_{i-m,i-1}^-, \vec{r}_{i-m,i-1}) \right\} \\ &=\; \sum_{r_{t-m+1} \in \mathcal{R}} \delta(r_{t-m+1} = \underline{r}_{t-m+1})\, \alpha_t(\vec{r}_{t-m+1,t})\, p(\tau_{t+1}^-, r_{t+1} \,|\, \vec{\tau}_{t-m+1,t}^-, \vec{r}_{t-m+1,t}) \,. \end{aligned} \tag{2.9}$$

For the special case of $m = 1$, the forward pass reduces to

$$\begin{aligned} \alpha_1(r_1) \;&=\; \sum_{\iota_0=0}^{1} \delta(\iota_0 = \underline{\iota})\, p(\iota_0)\, p(\tau_1^-, r_1 \,|\, \iota_0) \,, \\ \alpha_{t+1}(r_{t+1}) \;&=\; \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t)\, \alpha_t(r_t)\, p(\tau_{t+1}^-, r_{t+1} \,|\, \tau_t^-, r_t) \,. \end{aligned} \tag{2.10}$$

Similarly, for stages $t \geq m$ the backward factor (1.12) becomes

$$\begin{aligned}
\beta_t(\vec{r}_{t-m+1,t}) &= p(\tau_{t+1}^-, \underline{r}_{t+1}, \ldots, \tau_n^-, \underline{r}_n, \underline{\tau} \,|\, \tau_{t-m+1}^-, r_{t-m+1}, \ldots, \tau_t^-, r_t) \\
&= \sum_{r_{t+1} \in \mathcal{R}} \delta(r_{t+1} = \underline{r}_{t+1}) \cdots \sum_{r_n \in \mathcal{R}} \delta(r_n = \underline{r}_n) \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1} = \underline{\tau}_{n+1}) \\
&\quad \left\{ \prod_{i=t+1}^{n} p(\tau_i^-, r_i \,|\, \vec{\tau}_{i-m,i-1}^-, \vec{r}_{i-m,i-1}) \right\} p(\tau_{n+1} \,|\, \vec{\tau}_{n-m+1,n}^-, \vec{r}_{n-m+1,n}) \,. \qquad (2.11)
\end{aligned}$$

Furthermore, if $t > m$ then we may move backward to stage $t-1$ to obtain the recursive relationship

$$\begin{aligned}
\beta_{t-1}(\vec{r}_{t-m,t-1}) &= p(\tau_t^-, \underline{r}_t, \ldots, \tau_n^-, \underline{r}_n, \underline{\tau} \,|\, \tau_{t-m}^-, r_{t-m}, \ldots, \tau_{t-1}^-, r_{t-1}) \\
&= \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t) \cdots \sum_{r_n \in \mathcal{R}} \delta(r_n = \underline{r}_n) \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1} = \underline{\tau}_{n+1}) \\
&\quad \left\{ \prod_{i=t}^{n} p(\tau_i^-, r_i \,|\, \vec{\tau}_{i-m,i-1}^-, \vec{r}_{i-m,i-1}) \right\} p(\tau_{n+1} \,|\, \vec{\tau}_{n-m+1,n}^-, \vec{r}_{n-m+1,n}) \\
&= \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t)\, p(\tau_t^-, r_t \,|\, \vec{\tau}_{t-m,t-1}^-, \vec{r}_{t-m,t-1})\, \beta_t(\vec{r}_{t-m+1,t}) \,. \qquad (2.12)
\end{aligned}$$

stages $t < m$

$$\beta_t(\vec{r}_{1,t}) = p(\tau_{t+1}^-, \underline{r}_{t+1}, \ldots, \tau_n^-, \underline{r}_n, \underline{\tau} \,|\, \iota_0, \tau_1^-, r_1, \ldots, \tau_t^-, r_t) \,, \qquad (2.13)$$

In general, the backward pass is defined via

$$\beta_{t-1}(\vec{r}_{t-m,t-1}) = \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t)\, p_m^*(\tau_t^-, r_t \,|\, \iota_0, \vec{\tau}_{1,t-1}^-, \vec{r}_{1,t-1})\, \beta_t(\vec{r}_{t-m+1,t}) \,. \qquad (2.14)$$

For the special case of $m = 1$, the backward pass reduces to

$$\begin{aligned}
\beta_n(r_n) &= \sum_{\tau_{n+1}=0}^{1} \delta(\tau_{n+1} = \underline{\tau})\, p(\tau_{n+1} \,|\, \tau_n^-, r_n) \,, \\
\beta_{t-1}(r_{t-1}) &= \sum_{r_t \in \mathcal{R}} \delta(r_t = \underline{r}_t)\, p(\tau_t^-, r_t \,|\, \tau_{t-1}^-, r_{t-1})\, \beta_t(r_t) \,. \qquad (2.15)
\end{aligned}$$

3 Stateful Markov Sequence Processes

Consider the first-order Markov process R depicted in Figure 1.3. Suppose now that the random variable R_t at stage t can be decomposed into the tuple $R_t = (S_t, X_t)$, where S_t is a random *state* variable taking values $s_t \in \mathcal{S}$, and X_t is a random *value* variable taking values $x_t \in \mathcal{X}$. As is usual, we presuppose that the stage transitions in the sequence generating process are primarily between states, e.g. from S_{t-1} to S_t. It follows that the value is generated after the state has been determined, i.e. X_t depends upon S_t. Keeping to the first-order Markov interpretation of stage-to-stage dependencies leads to the *stateful* process depicted in Figure 3.1, with full cross-dependencies between (S_t, X_t) and (S_{t+1}, X_{t+1}).

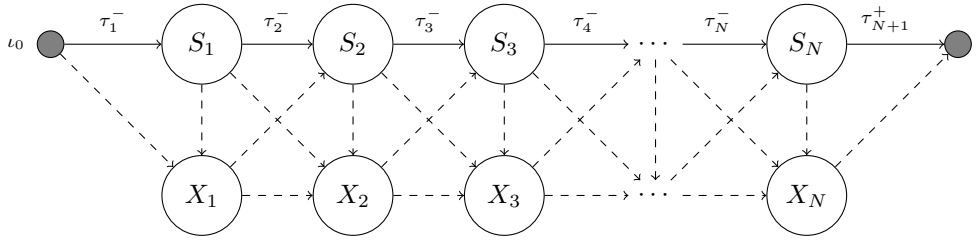

Figure 3.1: *A random process for generating complete state–value sequences of arbitrary length, with explicit cross-dependencies between adjacent stages.*

Hence, the fully-structured state–valuel model is now given by

$$
\begin{aligned}
p(\iota, \vec{s}, \vec{x}, \tau) \;=\;& p(\iota_0 = \iota)\, p(\tau_1 = 0 \mid \iota_0 = \iota)\, p(S_1 = s_1 \mid \iota_0 = \iota, \tau_1 = 0) \\
& \times\; p(X_1 = x_1 \mid S_1 = s_1, \iota_0 = \iota, \tau_1 = 0) \\
& \times \left\{ \prod_{t=2}^{n} p(\tau_t = 0 \mid S_{t-1} = s_{t-1}, X_{t-1} = x_{t-1}) \right. \\
& \qquad \times\; p(S_t = s_t \mid \tau_t = 0, S_{t-1} = s_{t-1}, X_{t-1} = x_{t-1}) \\
& \qquad \left. \times\; p(X_t = x_t \mid S_t = s_t, S_{t-1} = s_{t-1}, X_{t-1} = x_{t-1}) \right\} \\
& \times p(\tau_{n+1} = \tau \mid S_n = s_n, X_n = x_n) \\
=\;& p(\iota)\, p(\tau_1^- \mid \iota)\, p(s_1 \mid \iota, \tau_1^-)\, p(x_1 \mid s_1, \iota, \tau_1^-) \\
& \times \left\{ \prod_{t=2}^{n} p(\tau_t^- \mid s_{t-1}, x_{t-1})\, p(s_t \mid \tau_t^-, s_{t-1}, x_{t-1})\, p(x_t \mid s_t, s_{t-1}, x_{t-1}) \right\} \\
& \times p(\tau \mid s_n, x_n)\,. \qquad (3.1)
\end{aligned}
$$

Conditioning the state S_t on both the previous state S_{t-1} and its value X_{t-1} can be useful in some circumstances, e.g. in sequence classification problems. However, due to the increased complexity of such models, it is more usual to further restrict the stateful process by also imposing the first-order Markov assumption at the level of the state–value dependencies themselves. In terms of the process depicted in Figure 3.1, this means retaining only direct node-to-node dependencies, rather than stage-to-stage dependencies. This restricted process is depicted in Figure 3.2.

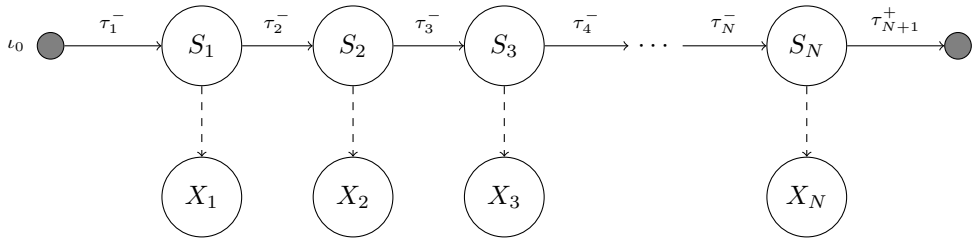

Figure 3.2: *A first-order Markov process for generating complete state–value sequences of arbitrary length.*

The corresponding sequence model is now given by

$$
\begin{aligned}
p(\iota, \vec{s}, \vec{x}, \tau) \;=\;& p(\iota_0 = \iota)\, p(\tau_1 = 0 \mid \iota_0 = \iota)\, p(S_1 = s_1 \mid \iota_0 = \iota, \tau_1 = 0)\, p(X_1 = x_1 \mid S_1 = s_1) \\
& \times \left\{ \prod_{t=2}^{n} p(\tau_t = 0 \mid S_{t-1} = s_{t-1})\, p(S_t = s_t \mid \tau_t = 0, S_{t-1} = s_{t-1}) \right. \\
& \qquad \left. \times\; p(X_t = x_t \mid S_t = s_t) \right\} p(\tau_{n+1} = \tau \mid S_n = s_n) \\
=\;& p(\iota)\, p(\tau_1^- \mid \iota)\, p(s_1 \mid \iota, \tau_1^-)\, p(x_1 \mid s_1) \\
& \times \left\{ \prod_{t=2}^{n} p(\tau_t^- \mid s_{t-1})\, p(s_t \mid \tau_t^-, s_{t-1})\, p(x_t \mid s_t) \right\} p(\tau \mid s_n)\,. \qquad (3.2)
\end{aligned}
$$

3.1 Hidden State Sequences

In the previous section, we considered the joint probability $p(\iota, \vec{s}, \vec{x}, \tau)$ of a stateful, first-order Markov process (Figure 3.2) under the assumption that the initiation and termination markers of the sequence were known in advance and that both the sequence $\vec{s}$ of states and the sequence $\vec{x}$ of values were fully observed. Let us now consider the implications of having unobserved (or *hidden* or *missing*) markers, states and/or values. Firstly, let us use an underline symbol, e.g. $\underline{\iota}$, to denote a variable with an observed value that might be either known or missing, and let the bare variable, e.g. ι, denote a known (but possibly arbitrary) value. As noted in Section 1, we use the '*' symbol to denote a missing value, e.g.

$\underline{\iota} = *$, on the understanding that its use in a probability expression implies the marginalisation of the expression over all possible values of the affected variable.

Thus, if the value of X_t of some stage t is unobserved, then we write $\underline{x}_t = *$ to denote marginalisation over all possible values of $x_t \in \mathcal{X}$. Since X_t depends only upon S_t, we may then define $p(X_t = * \,|\, S_t) = 1$ for all $t = 1, 2, \ldots, n$, and so $p(\underline{x}_t \,|\, s_t)$ is likewise well defined.

Similarly, if the termination marker τ_{n+1} is unobserved, then we write $\underline{\tau} = *$ to indicate maginalisation over $\tau_{n+1} \in \{0, 1\}$, with the consequence that $p(\tau_{n+1} = * \,|\, S_n) = 1$ and hence $p(\underline{\tau} \,|\, s_n)$ is well defined. However, if the initiation marker ι_0 is unobserved, i.e. $\underline{\iota} = *$ from above, then the marginalisation is more difficult because ι_0 also conditions S_1 via $p(S_1 \,|\, \iota_0, \tau_1)$. To allow for this, we note that

$$p(\iota, \tau_1^-, s_1) \;=\; p(\iota_0 = \iota)\, p(\tau_1 = 0 \,|\, \iota_0 = \iota)\, p(S_1 = s_1 \,|\, \iota_0 = \iota, \tau_1 = 0)\,, \tag{3.3}$$

and so define

$$p(\underline{\iota}, \tau_1^-, s_1) \;=\; \sum_{\iota=0}^{1} \delta(\iota = \underline{\iota})\, p(\iota, \tau_1^-, s_1)\,, \tag{3.4}$$

where $\delta(\cdot) = 1$ (or else 0) if its argument is true (or else false); by definition, we take $\delta(a = *) = 1$. Hence, we may write

$$p(\underline{\iota}, \vec{s}, \vec{\underline{x}}, \underline{\tau}) \;=\; p(\underline{\iota}, \tau_1^-, s_1)\, p(\underline{x}_1 \,|\, s_1) \left\{ \prod_{t=2}^{n} p(\tau_t^- \,|\, s_{t-1})\, p(s_t \,|\, \tau_t^-, s_{t-1})\, p(\underline{x}_t \,|\, s_t) \right\} p(\underline{\tau} \,|\, s_n)\,. \tag{3.5}$$

Finally, if state S_t is unobserved, then $\underline{s}_t = *$ denotes marginalisation over all $s_t \in \mathcal{S}$. Once again, this marginalisation is made difficult because S_t is involved in multiple dependencies, conditioning X_t, τ_{t+1} and possibly S_{t+1}. The possibility that multiple states might be unobserved complicates this marginalisation even further. Note that a process in which the observed state sequence $\vec{\underline{s}}$ is entirely unknown is called a *hidden Markov model* (or HMM). In order to deal with hidden states, it is convenient to assume that states take discrete[2] values, such that $\mathcal{S} = \{\sigma_1, \sigma_2, \ldots, \sigma_S\}$. Thus, let $\vec{s}$ represent some *completion* of $\vec{\underline{s}}$, i.e. an arbitrary sequence $\vec{s} = (\sigma_{i_1}, \sigma_{i_2}, \ldots, \sigma_{i_n})$ that is consistent with all observed states in $\vec{\underline{s}}$. Then we may define

$$p(\underline{\iota}, \vec{\underline{s}}, \vec{\underline{x}}, \underline{\tau}) \;=\; \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1) \cdots \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, p(\underline{\iota}, \vec{s}, \vec{\underline{x}}, \underline{\tau})\,. \tag{3.6}$$

This is just the marginalisation over every plausible completion $\vec{s}$ of the observed sequence $\vec{\underline{s}}$. Note that if S_t is a hidden state, then $\underline{s}_t = *$ and $\delta(s_t = *) = 1$ for all $s_t \in \mathcal{S}$; otherwise, the summation over s_t collapses to the observed value $\underline{s}_t$.

3.2 Modified Forward–Backward Algorithm

The observed sequence model (3.6) can be efficiently evaluated by marginalising over the state of each stage in turn, using a modification of the *forward–backward algorithm* to include knowledge of sequence initiation and termination. The forward pass involves first summing over all terms containing s_1, then over all remaining terms containing s_2, and so on up to s_n. This is equivalent to evaluating the reordered model

$$\begin{aligned} p(\underline{\iota}, \vec{\underline{s}}, \vec{\underline{x}}, \underline{\tau}) \;=\; & \left\{ \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n) \cdots \left\{ \sum_{s_2 \in \mathcal{S}} \delta(s_2 = \underline{s}_2) \right. \right. \\ & \left\{ \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, p(\underline{\iota}, \tau_1^-, s_1)\, p(\underline{x}_1 \,|\, s_1)\, p(\tau_2^- \,|\, s_1)\, p(s_2 \,|\, \tau_2^-, s_1) \right\} \\ & \left. \left. p(\underline{x}_2 \,|\, s_2)\, p(\tau_3^- \,|\, s_2)\, p(s_3 \,|\, \tau_3^-, s_2) \right\} \cdots\; p(\underline{x}_n \,|\, s_n)\, p(\underline{\tau} \,|\, s_n) \right\}. \end{aligned} \tag{3.7}$$

The forward pass commences with the first stage of the sequence, and includes the inner terms that are dependent on state s_1, namely

$$\begin{aligned} \alpha_1(s_1) \;&=\; p(\underline{\iota}, \tau_1^-, s_1)\, p(\underline{x}_1 \,|\, s_1) \\ &=\; p(\underline{\iota}, \tau_1^-, s_1, \underline{x}_1) \;\equiv\; p(\underline{\iota}, \vec{\underline{s}}_0 \circ s_1, \vec{\underline{x}}_1)\,, \end{aligned} \tag{3.8}$$

[2]For states with continuous values, we would need to replace the state summations by integrations, and the use of the Kronecker $\delta(a = b)$ by the Dirac $\delta(a - b)$.

where the operator '$\circ$' indicates the concatenation of either two elements, two sequences or an element and a sequence, to form a longer sequence. Recall that $\vec{s}_0$ is an empty sequence.

The next step of the forward pass now moves on to the second stage and includes terms dependent on state s_2 at that stage:

$$\begin{aligned}
\alpha_2(s_2) &= \left\{ \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, \alpha_1(s_1)\, p(\tau_2^- \mid s_1)\, p(s_2 \mid \tau_2^-, s_1) \right\} p(\underline{x}_2 \mid s_2) \\
&= \left\{ \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, p(\iota, \tau_1^-, s_1, \underline{x}_1)\, p(\tau_2^- \mid s_1)\, p(s_2 \mid \tau_2^-, s_1) \right\} p(\underline{x}_2 \mid s_2) \\
&= \left\{ \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, p(\iota, \tau_1^-, s_1, \underline{x}_1, \tau_2^-, s_2) \right\} p(\underline{x}_2 \mid s_2) \\
&= p(\iota, \tau_1^-, \underline{s}_1, \underline{x}_1, \tau_2^-, s_2)\, p(\underline{x}_2 \mid s_2) \\
&= p(\iota, \tau_1^-, \underline{s}_1, \underline{x}_1, \tau_2^-, s_2, \underline{x}_2) \;\equiv\; p(\iota, \vec{s}_1 \circ s_2, \vec{x}_2)\,. \qquad (3.9)
\end{aligned}$$

Recursively, the last step of the forward pass stops at the n-th stage, giving

$$\begin{aligned}
\alpha_n(s_n) &= \left\{ \sum_{s_{n-1} \in \mathcal{S}} \delta(s_{n-1} = \underline{s}_{n-1})\, \alpha_{n-1}(s_{n-1})\, p(\tau_n^- \mid s_{n-1})\, p(s_n \mid \tau_n^-, s_{n-1}) \right\} p(\underline{x}_n \mid s_n) \\
&\equiv\; p(\iota, \vec{s}_{n-1} \circ s_n, \vec{x}_{n-1})\, p(\underline{x}_n \mid s_n) \;=\; p(\iota, \vec{s}_{n-1} \circ s_n, \vec{x}_n)\,. \qquad (3.10)
\end{aligned}$$

The remaining terms then give the observed joint likelihood

$$p(\iota, \vec{s}, \vec{x}, \tau) = \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, \alpha_n(s_n)\, p(\tau \mid s_n)\,. \qquad (3.11)$$

Conversely, the backaward pass involves first summing over all terms containing s_n, then over all remaining terms containing s_{n-1}, and so on down s_1. This is equivalent to evaluating the reordered model

$$\begin{aligned}
p(\iota, \vec{s}, \vec{x}, \tau) = \Bigg\{ & \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, p(\iota, \tau_1^-, s_1)\, p(\underline{x}_1 \mid s_1)\, p(\tau_2^- \mid s_1) \cdots \\
& \left\{ \sum_{s_{n-1} \in \mathcal{S}} \delta(s_{n-1} = \underline{s}_{n-1})\, p(s_{n-1} \mid \tau_{n-1}^-, s_{n-2})\, p(\underline{x}_{n-1} \mid s_{n-1})\, p(\tau_n^- \mid s_{n-1}) \right. \\
& \left. \left\{ \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, p(s_n \mid \tau_n^-, s_{n-1})\, p(\underline{x}_n \mid s_n)\, p(\tau \mid s_n) \right\} \right\} \cdots \Bigg\}\,. \qquad (3.12)
\end{aligned}$$

The backward pass commences at the end of the sequence with the termination term that depends on state s_n, namely

$$\beta_n(s_n) = p(\tau \mid s_n)\,. \qquad (3.13)$$

The next step in the backward pass then moves backward to the n-th stage and incorporates the terms that depend on state s_{n-1}, including the non-terminating transition from s_{n-1} to s_n

$$\begin{aligned}
\beta_{n-1}(s_{n-1}) &= p(\tau_n^- \mid s_{n-1}) \left\{ \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, p(s_n \mid \tau_n^-, s_{n-1})\, p(\underline{x}_n \mid s_n)\, \beta_n(s_n) \right\} \\
&= p(\tau_n^- \mid s_{n-1}) \left\{ \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, p(s_n \mid \tau_n^-, s_{n-1})\, p(\underline{x}_n \mid s_n)\, p(\tau \mid s_n) \right\} \\
&= p(\tau_n^- \mid s_{n-1}) \left\{ \sum_{s_n \in \mathcal{S}} \delta(s_n = \underline{s}_n)\, p(s_n, \underline{x}_n, \tau \mid \tau_n^-, s_{n-1}) \right\} \\
&= p(\tau_n^- \mid s_{n-1})\, p(\underline{s}_n, \underline{x}_n, \tau \mid \tau_n^-, s_{n-1}) \\
&= p(\tau_n^-, \underline{s}_n, \underline{x}_n, \tau \mid s_{n-1}) \;\equiv\; p(\circ\overleftarrow{\underline{s}}_n, \overleftarrow{\underline{x}}_n, \tau \mid s_{n-1})\,. \qquad (3.14)
\end{aligned}$$

Observe that we have explicitly included the concatenation operator to indicate the presence of τ_n^-. Symbolically, we may write $p(\vec{r}) = p(\vec{r}_t \circ \overleftarrow{r}_{t+1}) = p(\vec{r}_t \circ) p(\overleftarrow{r}_{t+1}) = p(\vec{r}_t) p(\circ \overleftarrow{r}_{t+1})$.

Recursively, the last step of the backward pass reaches the first stage, giving

$$\begin{aligned} \beta_1(s_1) &= p(\tau_2^- \,|\, s_1) \sum_{s_2 \in \mathcal{S}} \delta(s_2 = \underline{s}_2)\, p(s_2 \,|\, \tau_2^-, s_1)\, p(\underline{x}_2 \,|\, s_2)\, \beta_2(s_2) \\ &= p(\tau_2^- \,|\, s_1)\, p(\underline{s}_2, \underline{x}_2, \tau_3^-, \ldots, \underline{s}_n, \underline{x}_n, \underline{\tau} \,|\, \tau_2^-, s_1) \\ &\equiv p(\circ \overleftarrow{\underline{s}}_2, \overleftarrow{\underline{x}}_2, \underline{\tau} \,|\, s_1)\,. \end{aligned} \tag{3.15}$$

The remaining terms then give the observed likelihood

$$p(\underline{\iota}, \vec{\underline{s}}, \vec{\underline{x}}, \underline{\tau}) = \sum_{s_1 \in \mathcal{S}} \delta(s_1 = \underline{s}_1)\, p(\underline{\iota}, \tau_1^-, s_1)\, \beta_1(s_1)\,. \tag{3.16}$$

In general, we obtain

$$\begin{aligned} p(\underline{\iota}, \vec{\underline{s}}, \vec{\underline{x}}, \underline{\tau}) &= \sum_{s_t \in \mathcal{S}} \delta(s_t = \underline{s}_t)\, p(\underline{\iota}, \vec{\underline{s}}_{t-1} \circ s_t \circ \overleftarrow{\underline{s}}_{t+1}, \vec{\underline{x}}_t \circ \overleftarrow{\underline{x}}_{t+1}, \underline{\tau}) \\ &= \sum_{s_t \in \mathcal{S}} \delta(s_t = \underline{s}_t)\, p(\underline{\iota}, \vec{\underline{s}}_{t-1} \circ s_t, \vec{\underline{x}}_t)\, p(\circ \overleftarrow{\underline{s}}_{t+1}, \overleftarrow{\underline{x}}_{t+1}, \underline{\tau} \,|\, s_t) \\ &= \sum_{s_t \in \mathcal{S}} \delta(s_t = \underline{s}_t)\, \alpha_t(s_t)\, \beta_t(s_t)\,, \end{aligned} \tag{3.17}$$

for all $t = 1, 2, \ldots, n$. The case for $t = n$ comes from equations (3.11) and (3.13); alternatively, recall that $\overleftarrow{r}_{n+1}$ is an empty sequence.

4 Discrete-state Sequence Models

Consider the stateful, first-order Markov process depicted by Figure 3.2. Let us now restrict our attention to the class of corresponding sequence models where the state S_t at any stage t may now only take *discrete* values in the set $\mathcal{S} = \{\sigma_1, \sigma_2, \ldots, \sigma_S\}$. Hence, the sequence of states may arbitrarily be specified as $\vec{s} = (\sigma_{i_1}, \sigma_{i_2}, \ldots, \sigma_{i_n})$, where each $i_t \in \{1, 2, \ldots, S\}$. In the event that a particular state S_t is unobserved, we say that the state is *missing* or *hidden*, and denote $i_t = *$ and $s_t = *$. In the situation where all values of $\vec{s}$ are unobserved, the sequence model (3.2) is known as a *hidden-state Markov model* (HMM).

The sequence model (3.2) may now be explicitly conditioned on a general parameter θ that governs the various discrete state distributions. Each term in the model depends directly on the stage index t and indirectly on the state index i_t. Furthermore, each term represents either the initial state, the terminal state, or the non-terminal transitions between states at adjacent stages. Hence, let $\theta = (\Pi, \Gamma, \Omega)$, such that the probability of an arbitrary, observed[3] sequence (with no hidden states) is given by

$$p(\underline{\iota}, \vec{\underline{s}}, \vec{\underline{x}}, \underline{\tau} \,|\, \theta) = \pi_{\underline{\iota},1,i_1}\, o_{1,i_1}(x_1) \left\{ \prod_{t=1}^{n-1} \omega_{0,t,i_t}\, \Gamma_{t,i_t,i_{t+1}}\, o_{t+1,i_{t+1}}(x_{t+1}) \right\} \omega_{\underline{\tau},n,i_n}\,. \tag{4.1}$$

The initial state S_1 of the sequence at stage $t = 1$ is governed by the parameter $\vec{\pi}$, where

$$\pi_{0,t,i} = p(\iota_{t-1} = 0 \,|\, \theta)\, p(\tau_t = 0 \,|\, \iota_{t-1} = 0, \theta)\, p(S_t = \sigma_i \,|\, \iota_{t-1} = 0, \tau_t = 0, \theta)\,, \tag{4.2}$$

$$\pi_{1,t,i} = p(\iota_{t-1} = 1 \,|\, \theta)\, p(\tau_t = 0 \,|\, \iota_{t-1} = 1, \theta)\, p(S_t = \sigma_i \,|\, \iota_{t-1} = 1, \tau_t = 0, \theta)\,, \tag{4.3}$$

and

$$\begin{aligned} \pi_{*,t,i} &= p(\iota_{t-1} = * \,|\, \theta)\, p(\tau_t = 0 \,|\, \iota_{t-1} = *, \theta)\, p(S_t = \sigma_i \,|\, \iota_{t-1} = *, \tau_t = 0, \theta) \\ &= p(\tau_t = 0, S_t = \sigma_i \,|\, \theta) \;=\; \pi_{0,t,i} + \pi_{1,t,i}\,. \end{aligned} \tag{4.4}$$

Observe that each state S_t for $t > 1$ is a non-initial state, governed by π_{0,t,i_t}. However, such terms do not explicitly appear in model (4.1), except if $\underline{\iota} \neq 1$, since they are already accounted for by the

[3] We assume that all observed sequences are non-zero in length, since zero-length sequences are typically unobservable unless the generating process explicitly signals the start and end of each sequence. The modelling of zero-length sequences will require an extra parameter.

state transitions. These implicit terms become important when it comes to parameter estimation (see Section 4.3).

The terminal state S_n at stage $t = n$ is likewise governed by the parameter $\vec{\omega}$, where

$$\omega_{0,t,i} \;=\; p(\tau_{t+1}{=}0 \,|\, S_t{=}\sigma_i, \theta)\,, \tag{4.5}$$
$$\omega_{1,t,i} \;=\; p(\tau_{t+1}{=}1 \,|\, S_t{=}\sigma_i, \theta)\,, \tag{4.6}$$

and

$$\omega_{*,t,i} \;=\; p(\tau_{t+1}{=}* \,|\, S_t{=}\sigma_i, \theta) \;=\; \omega_{0,t,i} + \omega_{1,t,i} \;=\; 1\,. \tag{4.7}$$

Observe that each state S_t for $t < n$ is a non-terminal state, and is explicitly modelled by the term ω_{0,t,i_t}.

Lastly, the permissible transitions between the states S_t and S_{t+1} of consecutive stages t and $t+1$ are governed by the parameter Γ, where

$$\Gamma_{t,i,j} \;=\; p(S_{t+1}{=}\sigma_j \,|\, S_t{=}\sigma_i, \tau_{t+1}{=}0, \theta)\,. \tag{4.8}$$

Note that the model also includes the likelihood of each observed value x_t at stage t, for $t = 1, 2, \ldots, n$. This so-called *data likelihood* is governed by the separate model

$$o_{t,i}(x) \;=\; p(X_t{=}x \,|\, S_t{=}\sigma_i, \theta) \qquad \forall x \in \mathcal{X}\,. \tag{4.9}$$

We do not, however, explicitly declare the parameterisation structure of this likelihood model (see Section **??** for a plausible model if X_t takes discrete values). It suffices for our calculations that each $o_{t,i_t}(x_t)$ is available when required.

Finally, note that in the situtation where any state in the observed state sequence $\vec{s}$ is hidden, we have to marginalise model (4.1) over each such missing state. Hence, in general, we may define

$$\begin{aligned} p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta) \;=\; & \sum_{i'_1=1}^{S} \delta(i'_1{=}i_1) \sum_{i'_2=1}^{S} \delta(i'_2{=}i_2) \cdots \sum_{i'_n=1}^{S} \delta(i'_n{=}i_n) \\ & \pi_{\underline{\iota},1,i'_1}\, o_{1,i'_1}(x_1) \left\{ \prod_{t=1}^{n-1} \omega_{0,t,i'_t}\, \Gamma_{t,i'_t,i'_{t+1}}\, o_{t+1,i'_{t+1}}(x_{t+1}) \right\} \omega_{\underline{\tau},n,i'_n}\,, \end{aligned} \tag{4.10}$$

where $\delta(\cdot)$ is an indicator function taking the value 1 (or 0) if its argument is true (or false). Note that if S_t is a hidden state, then $i_t = *$ and $\delta(i'_t{=}*) = 1$ for all $i'_t \in \{1, 2, \ldots, S\}$; otherwise, the summation over i'_t collapses to the observed value i_t. The observation likelihood given by model (4.10) can be efficiently computed by an extension of the forward–backward algorithm, described in the next section.

4.1 Modified Forward–Backward Algorithm

The sequence model (4.10) can be efficiently evaluated by marginalising over the state of each stage in turn, using a modification of the *forward–backward algorithm* to include knowledge of sequence initiation and termination. The forward pass involves first summing over all terms containing i'_1, then over all remaining terms containing i'_2, and so on up to summing over i'_n. This is equivalent to evaluating the reordered model

$$\begin{aligned} p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta) \;=\; & \left\{ \sum_{i'_n=1}^{S} \delta(i'_n{=}i_n) \cdots \left\{ \sum_{i'_2=1}^{S} \delta(i'_2{=}i_2) \right. \right. \\ & \left. \times \left\{ \sum_{i'_1=1}^{S} \delta(i'_1{=}i_1)\, \pi_{\underline{\iota},1,i'_1}\, o_{1,i'_1}(x_1)\, \omega_{0,1,i'_1}\, \Gamma_{1,i'_1,i'_2} \right\} \right. \\ & \left. o_{2,i'_2}(x_2) \omega_{0,2,i'_2}\, \Gamma_{2,i'_2,i'_3} \right\} \cdots\; o_{n,i'_n}(x_n)\, \omega_{\underline{\tau},n,i'_n} \Bigg\}\,. \end{aligned} \tag{4.11}$$

Conversely, the backaward pass reverses the order of evaluation, first summing over all terms containing i'_n, and then over all remaining terms containing i'_{n-1}, and so on down to summing over i'_1. This is

equivalent to evaluating the reordered model

$$\begin{aligned} p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta) &= \left\{ \sum_{i'_1=1}^{S} \delta(i'_1 = i_1)\, \pi_{\underline{\iota},1,i'_1}\, o_{1,i'_1}(x_1)\, \omega_{0,1,i'_1} \cdots \right. \\ &\quad \times \left\{ \sum_{i'_{n-1}=1}^{S} \delta(i'_{n-1} = i_{n-1})\, \Gamma_{n-2,i'_{n-2},i'_{n-1}}\, o_{n-1,i'_{n-1}}(x_{n-1})\, \omega_{0,n-1,i'_{n-1}} \right. \\ &\quad\quad \left. \left. \times \left\{ \sum_{i'_n=1}^{S} \delta(i'_n = i_n)\, \Gamma_{n-1,i'_{n-1},i'_n}\, o_{n,i'_n}(x_n)\, \omega_{\underline{\tau},n,i'_n} \right\} \right\} \cdots \right\}. \end{aligned} \tag{4.12}$$

A more efficient mechanism for evaluation comes from making use of the first-order Markov dependencies. Notionally, from the process depicted in Figure 3.2, we may arbitrarily consider the transition from some stage t to stage $t+1$, and partition the sequence into: (i) past values from the initial node up to and including S_t and X_t; and (ii) future values from S_{t+1} and X_{t+1} up to and including the terminal node. Note that the termination or non-termination of stage t is governed by τ_{t+1}, which is therefore a future value. The Markov dependency then implies that the future values are conditioned only on state S_t via τ_{t+1} and S_{t+1}. Hence, remembering that notionally $s_t = \sigma_{i_t}$, model (4.10) reduces to

$$\begin{aligned} p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta) &= \sum_{i=1}^{S} p(S_t = \sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta) \\ &= \sum_{i=1}^{S} \delta(i = i_t)\, p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i \circ \overleftarrow{s}_{t+1}, \vec{x}, \underline{\tau} \,|\, \theta) \\ &= \sum_{i=1}^{S} \delta(i = i_t)\, p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_t \,|\, \theta)\, p(\downarrow\!\overleftarrow{s}_{t+1}, \overleftarrow{x}_{t+1}, \underline{\tau} \,|\, S_t = \sigma_i, \theta) \\ &= \sum_{i=1}^{S} \delta(i = i_t)\, \alpha_{t,i}\, \beta_{t,i}\,, \end{aligned} \tag{4.13}$$

where $\circ$ represents sequence concatenation. The forward step $\alpha_{t,i}$ is defined as

$$\begin{aligned} \alpha_{t,i} &= p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_t \,|\, \theta) \\ &= p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_{t-1} \,|\, \theta)\, p(X_t = x_t \,|\, S_t = \sigma_{i_t}, \theta) \\ &= \bar{\alpha}_{t,i}\, o_{t,i}(x_t)\,, \end{aligned} \tag{4.14}$$

where $\bar{\alpha}_{t,i}$ is recursively defined as

$$\begin{aligned} \bar{\alpha}_{t,i} &= p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_{t-1} \,|\, \theta) \\ &= \sum_{j=1}^{S} p(S_{t-1} = \sigma_j, \underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_{t-1} \,|\, \theta) \\ &= \sum_{j=1}^{S} \delta(j = i_{t-1})\, p(\underline{\iota}, \vec{s}_{t-2} \circ \sigma_j \circ \sigma_i, \vec{x}_{t-1} \,|\, \theta) \\ &= \sum_{j=1}^{S} \delta(j = i_{t-1})\, p(\underline{\iota}, \vec{s}_{t-2} \circ \sigma_j, \vec{x}_{t-1} \,|\, \theta)\, p(\tau_t = 0 \,|\, S_{t-1} = \sigma_j, \theta) \\ &\qquad \times p(S_t = \sigma_i \,|\, \tau_t = 0, S_{t-1} = \sigma_j, \theta) \\ &= \sum_{j=1}^{S} \delta(j = i_{t-1})\, \alpha_{t-1,j}\, \omega_{0,t-1,j}\, \Gamma_{t-1,j,i}\,, \end{aligned} \tag{4.15}$$

for $t = 2, 3, \ldots, n$. The forward pass commences with the first step

$$\begin{aligned} \alpha_{1,i} &= p(\underline{\iota}, S_1 = \sigma_i, X_1 = x_1 \,|\, \theta) \\ &= p(\iota_0 = \underline{\iota})\, p(\tau_1 = 0 \,|\, \iota = \underline{\iota}, \theta)\, p(S_1 = \sigma_i \,|\, \iota_0 = \underline{\iota}, \tau_1 = 0, \theta)\, p(X_1 = x_1 \,|\, S_1 = \sigma_i, \theta) \\ &= \pi_{\underline{\iota},1,i}\, o_{1,i}(x_1)\,. \end{aligned} \tag{4.16}$$

Hence, observe that α_{2,i'_2}, is just the entire summation over i'_1 from the forward model (4.11). Also note that the standard forward pass derivation commences with the equivalent of $\pi_{*,1,i}$ and does not include the $\delta(\cdot)$ or ω terms.

Conversely to the forward pass, the backward step $\beta_{t,i}$ is defined as

$$\begin{aligned}
\beta_{t,i} &= p(\downarrow\overleftarrow{s}_{t+1}, \overleftarrow{x}_{t+1}, \underline{\tau} \,|\, S_t{=}\sigma_i, \theta) \\
&= p(\tau_{t+1}{=}0 \,|\, S_t{=}\sigma_i, \theta)\, p(\overleftarrow{s}_{t+1}, \overleftarrow{x}_{t+1}, \underline{\tau} \,|\, \tau_{t+1}{=}0, S_t{=}\sigma_i, \theta) \\
&= \omega_{0,t,i}\, \bar{\beta}_{t,i}\,,
\end{aligned} \tag{4.17}$$

where

$$\begin{aligned}
\bar{\beta}_{t,i} &= p(\overleftarrow{s}_{t+1}, \overleftarrow{x}_{t+1}, \underline{\tau} \,|\, \tau_{t+1}{=}0, S_t{=}\sigma_i, \theta) \\
&= \sum_{j=1}^{S} p(S_{t+1}{=}\sigma_j, \overleftarrow{s}_{t+1}, \overleftarrow{x}_{t+1}, \underline{\tau} \,|\, \tau_{t+1}{=}0, S_t{=}\sigma_i, \theta) \\
&= \sum_{j=1}^{S} \delta(j{=}i_{t+1})\, p(\sigma_j \circ \overleftarrow{s}_{t+2}, x_{t+1} \circ \overleftarrow{x}_{t+2}, \underline{\tau} \,|\, \tau_{t+1}{=}0, S_t{=}\sigma_i, \theta) \\
&= \sum_{j=1}^{S} \delta(j{=}i_{t+1})\, p(S_{t+1}{=}\sigma_j \,|\, \tau_{t+1}{=}0, S_t{=}\sigma_i, \theta)\, p(X_{t+1} = x_{t+1} \,|\, S_{t+1}{=}\sigma_j, \theta) \\
&\qquad \times p(\downarrow\overleftarrow{s}_{t+2}, \overleftarrow{x}_{t+2}, \underline{\tau} \,|\, S_{t+1}{=}\sigma_j, \theta) \\
&= \sum_{j=1}^{S} \delta(j{=}i_{t+1})\, \Gamma_{t,i,j}\, o_{t+1,j}(x_{t+1})\, \beta_{t+1,j}\,,
\end{aligned} \tag{4.18}$$

for $t = n-1, n-2, \ldots, 1$. The backward pass commences with the first step

$$\beta_{n,i} \;=\; p(\tau_{n+1}{=}\underline{\tau} \,|\, S_n{=}\sigma_i, \theta) \;=\; \omega_{\underline{\tau},n,i}\,. \tag{4.19}$$

Observe that $\bar{\beta}_{n-1,i'_{n-1}}$ is just the entire summation over i'_n from the backward model (4.12). Also note that the standard backward pass derivation commences with the equivalent of $\omega_{*,n,i} = 1$, and does not include the $\delta(\cdot)$ or ω terms.

4.2 Posterior Prediction

Given an observed sequence with one or more missing values, it is useful to be able to predict the probable values of the missing variables. For stateful Markov sequences, this typically means predicting the state S_t at some (or each) stage t. Alternatively, one might wish to predict a future value of S_{t+1} or X_{t+1} given a partially observed sequence. The foward–backward algorithm of Section 4.1 enables all of these calculations.

For instance, from equation (4.13), the posterior probabilities of state S_t given an observed sequence are computed as

$$\begin{aligned}
\gamma_{t,i} &= p(S_t{=}\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \\
&= \frac{p(S_t{=}\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\
&= \frac{\delta(i = i_t)\, \alpha_{t,i}\, \beta_{t,i}}{\sum_{i'=1}^{S} \delta(i' = i_t)\, \alpha_{t,i'}\, \beta_{t,i'}}\,.
\end{aligned} \tag{4.20}$$

Observe that $\gamma_{t,i}$ reduces to $\delta(i = i_t)$ in the special case where $s_t = \sigma_{i_t}$ is known.

Similarly, we may predict the next state S_{n+1} in a given observed sequence of length $n = |\vec{x}|$ via

$$\begin{aligned}
p(\downarrow\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) &= p(\tau_{n+1}{=}0, S_{n+1}{=}\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \\
&= \frac{p(\tau_{n+1}{=}0, S_{n+1}{=}\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\
&= \delta(\underline{\tau}{=}0)\, \frac{p(\underline{\iota}, \vec{s} \circ \sigma_i, \vec{x} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\
&= \delta(\underline{\tau}{=}0)\, \frac{\bar{\alpha}_{n+1,i}}{\sum_{i'=1}^{S} \delta(i'{=}i_n)\, \alpha_{n,i'}\, \beta_{n,i'}}\,,
\end{aligned} \tag{4.21}$$

from equation (4.15). Consequently, we may also predict the future value of X_{t+1} via

$$\begin{aligned} p(\downarrow x \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) &= \sum_{i=1}^{S} p(\downarrow \sigma_i, x \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \\ &= \sum_{i=1}^{S} p(\downarrow \sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta)\, p(X_{n+1}{=}x \,|\, S_{n+1}{=}\sigma_i, \theta) \\ &= \delta(\underline{\tau}{=}0)\, \frac{\sum_{i=1}^{S} \bar{\alpha}_{n+1,i}\, o_{n+1,i}(x)}{\sum_{i'=1}^{S} \delta(i'{=}i_n)\, \alpha_{n,i'}\, \beta_{n,i'}} \,. \end{aligned} \tag{4.22}$$

Proceding to predicting stage transitions, the forward–backward calculations also enable us to compute the posterior probabilities of the joint states of stages t and $t+1$ via

$$\begin{aligned} \xi_{t,i,j} &= p(S_t{=}\sigma_i, S_{t+1}{=}\sigma_j \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \\ &= \frac{p(S_t{=}\sigma_i, S_{t+1}{=}\sigma_j, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(i = i_t)\delta(j = i_{t+1})\, \frac{p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i \circ \sigma_j \circ \overleftarrow{s}_{t+2}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(i = i_t)\delta(j = i_{t+1})\, \frac{\alpha_{t,i}\, \omega_{0,t,i}\, \Gamma_{t,i,j}\, o_{t+1,j}(x_{t+1})\, \beta_{t+1,j}}{\sum_{i'=1}^{S} \delta(i'{=}i_t)\, \alpha_{t,i'}\, \beta_{t,i'}} \,, \end{aligned} \tag{4.23}$$

since

$$\begin{aligned} p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i \circ \sigma_j \circ \overleftarrow{s}_{t+2}, \vec{x}, \underline{\tau} \,|\, \theta) &= p(\underline{\iota}, \vec{s}_{t-1} \circ \sigma_i, \vec{x}_t \,|\, \theta)\, p(\downarrow \sigma_j, x_{t+1} \,|\, S_t{=}\sigma_i, \theta) \\ &\quad \times p(\downarrow \overleftarrow{s}_{t+2}, \overleftarrow{x}_{t+2}, \underline{\tau} \,|\, S_{t+1}{=}\sigma_j, \theta) \\ &= \alpha_{t,i}\, \omega_{0,t,i}\, \Gamma_{t,i,j}\, o_{t+1,j}(x_{t+1})\, \beta_{t+1,j} \,, \end{aligned} \tag{4.24}$$

from the forward pass (4.14) and the backward pass (4.17). Observe that

$$\begin{aligned} \gamma_{t,i} &= p(S_t{=}\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \\ &= \sum_{j=1}^{S} p(S_t{=}\sigma_i, S_{t+1}{=}\sigma_j \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \sum_{j=1}^{S} \xi_{t,i,j} \,, \end{aligned} \tag{4.25}$$

from equations (4.20) and (4.23).

Finally, the modified forward–backward algorithm also allows us to predict the start and/or end of partially observed sequences. For instance, at the start of a sequence we can predict

$$\begin{aligned} p(\iota_0{=}\underline{\iota}', S_1{=}\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) &= \frac{p(\iota_0{=}\underline{\iota}', S_1{=}\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(\underline{\iota}'{=}\underline{\iota})\, \delta(i{=}i_1)\, \frac{p(\underline{\iota}', \sigma_i \circ \vec{s}_2, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(\underline{\iota}'{=}\underline{\iota})\, \delta(i{=}i_1)\, \frac{\pi_{\underline{\iota}',1,i}\, o_{1,i}(x_1)\, \beta_{1,i}}{\sum_{i'=1}^{S} \delta(i'{=}i_1)\, \alpha_{1,i'}\, \beta_{1,i'}} \\ &= \delta(\underline{\iota}'{=}\underline{\iota})\, \gamma_{1,i}\, \frac{\pi_{\underline{\iota}',1,i}}{\bar{\alpha}_{1,i}} \;=\; \gamma_{1,i}\, \kappa_{\underline{\iota}',1,i} \,, \end{aligned} \tag{4.26}$$

where

$$\kappa_{\underline{\iota}',1,i} \;=\; p(\iota_0{=}\underline{\iota}' \,|\, S_1{=}\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \begin{cases} \delta(\underline{\iota}'{=}\underline{\iota}) & \text{if } \underline{\iota} = 0 \text{ or } 1 \\ \frac{\pi_{\underline{\iota}',1,i}}{\pi_{0,1,i} + \pi_{1,1,i}} & \text{if } \underline{\iota} = * \end{cases} \,, \tag{4.27}$$

from equations (4.13), (4.16) and (4.4). It then follows that

$$p(\iota_0{=}\underline{\iota}' \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \sum_{i=1}^{S} p(\iota_0{=}\underline{\iota}', S_1{=}\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \sum_{i=1}^{S} \gamma_{1,i}\, \kappa_{\underline{\iota}',1,i} \,. \tag{4.28}$$

Likewise, at the end of a sequence we can predict

$$\begin{aligned} p(\tau_{n+1}=\underline{\tau}', S_n=\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) &= \frac{p(\tau_{n+1}=\underline{\tau}', S_n=\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(\underline{\tau}'=\underline{\tau})\,\delta(i=i_n)\,\frac{p(\underline{\iota}, \vec{s}_{n-1}\circ\sigma_i, \vec{x}, \underline{\tau}' \,|\, \theta)}{p(\underline{\iota}, \vec{s}, \vec{x}, \underline{\tau} \,|\, \theta)} \\ &= \delta(\underline{\tau}'=\underline{\tau})\,\delta(i=i_n)\,\frac{\alpha_{n,i}\,\omega_{\underline{\tau}',n,i}}{\sum_{i'=1}^{S}\delta(i'=i_n)\,\alpha_{n,i'}\,\beta_{n,i'}} \\ &= \delta(\underline{\tau}'=\underline{\tau})\,\gamma_{n,i}\frac{\omega_{\underline{\tau}',n,i}}{\beta_{n,i}} \;=\; \gamma_{n,i}\,\zeta_{\underline{\tau}',n,i}\,, \end{aligned} \tag{4.29}$$

where

$$\zeta_{\underline{\tau}',n,i} \;=\; p(\tau_{n+1}=\underline{\tau}' \,|\, S_n=\sigma_i, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \begin{cases} \delta(\underline{\tau}'=\underline{\tau}) & \text{if } \underline{\tau}=0 \text{ or } 1 \\ \omega_{\underline{\tau}',n,i} & \text{if } \underline{\tau}=* \end{cases}\,, \tag{4.30}$$

from equations (4.13) and (4.19). It then follows that

$$p(\tau_{n+1}=\underline{\tau}' \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \sum_{i=1}^{S} p(\tau_{n+1}=\underline{\tau}', S_n=\sigma_i \,|\, \underline{\iota}, \vec{s}, \vec{x}, \underline{\tau}, \theta) \;=\; \sum_{i=1}^{S}\gamma_{n,i}\,\zeta_{\underline{\tau}',n,i}\,. \tag{4.31}$$

An example of the use of these posterior predictions is given in Section 4.4, when estimating the model parameters from observations with missing data.

4.3 Posterior Parameter Estimation with Known Data

We desire to estimate the model parameter $\theta = (\Pi, \Gamma, \Omega)$ given an ordered set $\mathbb{V} = \{\vec{v}^{(d)}\}_{d=1}^{D}$ of observed state and value sequences, where each observation takes the form of $\vec{v}^{(d)} = (\underline{\iota}^{(d)}, \vec{s}^{(d)}, \vec{x}^{(d)}, \underline{\tau}^{(d)})$. As before, we assume that $\vec{x}^{(d)}$ is a contiguous sequence of observed values with no missing values, whereas each 'observed' state s_t might either be known, i.e. $s_t = \sigma_{i_t}$, or missing, i.e. $s_t = *$ and $i_t = *$. Similarly, the sequence initiation and termination markers, $\underline{\iota}^{(d)}$ and $\underline{\tau}^{(d)}$ respectively, might also be known or unknown. In this section, let us suppose that each $\vec{v}^{(d)}$ is entirely known. The case of hidden data is analysed in the next section.

Due to the typical shortage of observed data, let us additionally assume that the distributions for the sub-parameters are stationary in time; that is, $\Gamma_{t,i,j} \equiv \Gamma_{i,j}$ for any stage t, and likewise $\pi_{\underline{\iota},t,i} \equiv \omega_{\underline{\iota},i}$, $\omega_{\underline{\tau},t,i} \equiv \omega_{\underline{\tau},i}$ and $o_{t,i}(x) \equiv o_i(x)$. Then, from equation (4.1), we obtain the likelihood of the d-th observed sequence as

$$p(v^{(d)} \,|\, \theta) \;=\; \pi_{\underline{\iota}^{(d)},i_1^{(d)}}\,o_{i_1^{(d)}}(x_1^{(d)})\left\{\prod_{t=1}^{n^{(d)}-1}\omega_{0,i_t^{(d)}}\,\Gamma_{i_t^{(d)},i_{t+1}^{(d)}}\,o_{i_{t+1}^{(d)}}(x_{t+1}^{(d)})\right\}\omega_{\underline{\tau}^{(d)},i_{n^{(d)}}^{(d)}}\,, \tag{4.32}$$

where $n^{(d)} = |\vec{x}^{(d)}|$, and the log-likelihood as

$$\ell(v^{(d)} \,|\, \theta) \;=\; \log\pi_{\underline{\iota}^{(d)},i_1^{(d)}} + \sum_{t=1}^{n^{(d)}-1}\log\omega_{0,i_t^{(d)}}\Gamma_{i_t^{(d)},i_{t+1}^{(d)}} + \sum_{t=1}^{n^{(d)}}\log o_{i_t^{(d)}}(x_{i_t^{(d)}}) + \log\omega_{\underline{\tau}^{(d)},i_{n^{(d)}}^{(d)}}\,. \tag{4.33}$$

Now, under the assumption that the observed sequences are independent, the log-likelihood of the observed data is given by

$$L(\theta) \;=\; \log p(\mathbb{V} \,|\, \theta) \;=\; \log\prod_{d=1}^{D}p(v^{(d)} \,|\, \theta) \;=\; \sum_{d=1}^{D}\ell(v^{(d)}, \theta)\,. \tag{4.34}$$

Hence, to estimate θ we maximise the log-likelihood subject to the necessary (Lagrangian) constraints

on the sub-parameters. Starting with the state transitions, we maximise

$$\begin{aligned} F_\Gamma(\theta) &= \sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1} \log \Gamma_{i_t^{(d)},i_{t+1}^{(d)}} - \sum_{i=1}^{S}\lambda_i\left(\sum_{j=1}^{S}\Gamma_{i,j}-1\right) \qquad (4.35)\\ \Rightarrow \frac{\partial F_\Gamma(\theta)}{\partial \Gamma_{i,j}} &= \sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1} \delta(i=i_t^{(d)})\,\delta(j=i_{t+1}^{(d)})\,\frac{1}{\Gamma_{i,j}} - \lambda_i \;=\; 0 \text{ when } \theta=\hat{\theta}\\ \Rightarrow \hat{\lambda}_i &= \sum_{j=1}^{S}\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1} \delta(i=i_t^{(d)})\,\delta(j=i_{t+1}^{(d)}) \;=\; \sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1}\delta(i=i_t^{(d)})\\ \Rightarrow \hat{\Gamma}_{i,j} &= \frac{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1}\delta(i=i_t^{(d)})\,\delta(j=i_{t+1}^{(d)})}{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}-1}\delta(i=i_t^{(d)})}\,. \qquad (4.36)\end{aligned}$$

Observe that this estimate corresponds to counting all the transitions from state i to state j across all the data, and then normalising these counts by the sum over j.

Similarly, for sequence termination or non-termination, we maximise

$$\begin{aligned} F_\Omega(\theta) &= \sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\log\omega_{0,i_t^{(d)}} + \log\omega_{\underline{\tau}^{(d)},i_{n^{(d)}}^{(d)}}\right\} - \sum_{i=1}^{S}\lambda_i\left(\omega_{0,i}+\omega_{1,i}-1\right) \qquad (4.37)\\ \Rightarrow \frac{\partial F_\Omega(\theta)}{\partial\omega_{0,i}} &= \sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\frac{\delta(i=i_t^{(d)})}{\omega_{0,i}} + \frac{\delta(\underline{\tau}^{(d)}=0)\,\delta(i=i_{n^{(d)}}^{(d)})}{\omega_{0,i}}\right\} - \lambda_i\,,\\ \frac{\partial F_\Omega(\theta)}{\partial\omega_{1,i}} &= \sum_{d=1}^{D}\left\{\frac{\delta(\underline{\tau}^{(d)}=1)\,\delta(i=i_{n^{(d)}}^{(d)})}{\omega_{1,i}}\right\} - \lambda_i\,. \qquad (4.38)\end{aligned}$$

Hence, by multiplying the two derivatives by $\omega_{0,i}$ and $\omega_{1,i}$, respectively, adding the terms and setting the result to zero, we obtain

$$\begin{aligned} \hat{\lambda}_i &= \sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\delta(i=i_t^{(d)})\\ \Rightarrow \hat{\omega}_{0,i} &= \frac{\sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\delta(i=i_t^{(d)}) + \delta(\underline{\tau}^{(d)}=0)\,\delta(i=i_{n^{(d)}}^{(d)})\right\}}{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\delta(i=i_t^{(d)})}\,,\\ \hat{\omega}_{1,i} &= \frac{\sum_{d=1}^{D}\delta(\underline{\tau}^{(d)}=1)\,\delta(i=i_{n^{(d)}}^{(d)})}{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\delta(i=i_t^{(d)})}\,. \qquad (4.39)\end{aligned}$$

Observe that this latter estimate corresponds to counting the various terminal states over all observed sequences, and then normalising these counts by the overall count of each state. Also note that we have assumed that $\underline{\tau}^{(d)}$ is known; unfortunately, these estimates will be inaccurate if $\underline{\tau}^{(d)}$ is unknown, since they ascribe equal weight to $\underline{\tau}^{(d)}=0$ and $\underline{\tau}^{(d)}=1$ regardless of $v^{(d)}$. The correct estimates in the case of missing data will be analysed in the next section.

Finally, for sequence initiation or non-initiation, we recall the comment made in Section 4 that each stage transition is both explicitly a non-terminal transition and implicitly a non-initial transtion; that is, each state transition $\Gamma_{t,i,j}$ also implies a sequence non-initiation $\pi_{0,t+1,j}$. Hence, from equation (4.33), we maximise the function

$$\begin{aligned} F_\Pi(\theta) &= \sum_{d=1}^{D}\left\{\log\pi_{\underline{\iota}^{(d)},i_1^{(d)}} + \sum_{t=2}^{n^{(d)}}\log\pi_{0,i_t^{(d)}}\right\} - \lambda\left(\sum_{i=1}^{S}\{\pi_{0,i}+\pi_{1,i}\}-1\right) \qquad (4.40)\\ \Rightarrow \frac{\partial F_\Pi(\theta)}{\partial\pi_{0,i}} &= \sum_{d=1}^{D}\left\{\frac{\delta(\underline{\iota}^{(d)}=0)\,\delta(i_1^{(d)}=i)}{\pi_{0,i}} + \sum_{t=2}^{n^{(d)}}\frac{\delta(i_t^{(d)}=i)}{\pi_{0,i}}\right\} - \lambda\,,\\ \frac{\partial F_\Pi(\theta)}{\partial\pi_{1,i}} &= \sum_{d=1}^{D}\left\{\frac{\delta(\underline{\iota}^{(d)}=1)\,\delta(i_1^{(d)}=i)}{\pi_{1,i}}\right\} - \lambda\,. \qquad (4.41)\end{aligned}$$

Thus, by multiplying the two derivatives by $\pi_{0,i}$ and $\pi_{1,i}$, respectively, adding and summing the terms over i, and setting the result to zero, we obtain

$$\begin{aligned}
\hat{\lambda} &= \sum_{i=1}^{S}\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\delta(i_t^{(d)}=i) \;=\; \sum_{d=1}^{D} n^{(d)} \\
\Rightarrow \hat{\pi}_{0,i} &= \frac{\sum_{d=1}^{D}\left\{\delta(\underline{\iota}^{(d)}=0)\,\delta(i_1^{(d)}=i)+\sum_{t=2}^{n^{(d)}}\delta(i_t^{(d)}=i)\right\}}{\sum_{d=1}^{D} n^{(d)}}\,, \\
\hat{\pi}_{1,i} &= \frac{\sum_{d=1}^{D}\delta(\underline{\iota}^{(d)}=1)\,\delta(i_1^{(d)}=i)}{\sum_{d=1}^{D} n^{(d)}}\,.
\end{aligned} \tag{4.42}$$

Observe that this latter estimate corresponds to counting the various initial states over all observed sequences, and then normalising these counts by the overall count of all states. Also note that these estimates are inaccurate if $\underline{\iota}$ is unknown; the correct estimates are derived in the next section.

4.4 Posterior Parameter Estimation with Missing Data

In contrast to Section 4.3, suppose now that any or all values of $\underline{\iota}^{(d)}$, $\underline{\tau}^{(d)}$ and $\vec{s}^{(d)}$ may be unknown when observing the d-th sequence $v^{(d)}$. The basic procedure is then to first estimate these missing values from the observed data $\mathbb{V}$, and then to estimate the most likely model parameter value $\hat{\theta}$ given $\mathbb{V}$ and the missing values. This is the principle of the *expectation–maximisation* (EM) algorithm, which underlies the modified *Baum–Welch* parameter estimation algorithm derived here.

Suppose we let $\mathbb{Z} = \{z^{(d)}\}_{d=1}^{D}$ denote the ordered set of missing values corresponding to the observed values $\mathbb{V} = \{v^{(d)}\}_{d=1}^{D}$, where $z^{(d)} = (\underline{\iota}^{(d)}, \vec{s}^{(d)}, \underline{\tau}^{(d)})$; that is, notionally $\mathbb{Z}$ contains the true (but still unknown) values missing from $\mathbb{V}$. Hence, we take an expectation of the log-likelihood over all possible values of $\mathbb{Z}$, namely[4]

$$\begin{aligned}
Q(\theta) &= E_{\mathbb{Z}\,|\,\mathbb{V},\theta}\left[\log p(\mathbb{Z},\mathbb{V}\,|\,\theta)\right] \\
&= E_{\mathbb{Z}\,|\,\mathbb{V},\theta}\left[\sum_{d=1}^{D}\log p(z^{(d)},v^{(d)}\,|\,\theta)\right] \\
&= \sum_{d=1}^{D} E_{\mathbb{Z}\,|\,\mathbb{V},\theta}\left[\ell(\overline{\underline{\iota}^{(d)}},\overline{\vec{s}^{(d)}},\vec{x}^{(d)},\overline{\underline{\tau}^{(d)}};\theta)\right] \\
&= \sum_{d=1}^{D}\sum_{\underline{\iota}=0}^{1}\sum_{\overline{i_1}=1}^{S}\cdots\sum_{\overline{i_{n^{(d)}}}}^{S}\sum_{\overline{\tau}=0}^{1} p(\underline{\iota},\overline{\vec{s}},\overline{\tau}\,|\,\underline{\iota}^{(d)},\vec{s}^{(d)},\vec{x}^{(d)},\underline{\tau}^{(d)},\theta)\,\ell(\underline{\iota},\overline{\vec{s}},\vec{x}^{(d)},\overline{\tau};\theta) \\
&= \sum_{d=1}^{D}\sum_{\underline{\iota}=0}^{1}\sum_{\overline{i_1}=1}^{S}\cdots\sum_{\overline{i_{n^{(d)}}}}^{S}\sum_{\overline{\tau}=0}^{1} p(z\,|\,v^{(d)},\theta)\,\ell(\overline{v^{(d)}};\theta)\,,
\end{aligned} \tag{4.43}$$

where $z = (\underline{\iota},\overline{\vec{s}},\overline{\tau})$ and $\overline{v^{(d)}} = (\underline{\iota},\overline{\vec{s}},\vec{x}^{(d)},\overline{\tau})$. In principle, the optimal parameter value $\hat{\theta}$ is estimated by maximising this expected log-likelihood subject to parameter constraints.

In practice, it is difficult to optimise this nonlinear expression analytically. A feasible alternative is to iteratively apply the EM algorithm:

1. *Expectation step:* Compute the expected log-likelihood conditioned on a known parameter estimate $\hat{\theta}_k$, namely

$$\begin{aligned}
Q(\theta,\hat{\theta}_k) &= E_{\mathbb{Z}\,|\,\mathbb{V},\hat{\theta}_k}\left[\log p(\mathbb{Z},\mathbb{V}\,|\,\theta)\right] \\
&= \sum_{d=1}^{D}\sum_{\underline{\iota}=0}^{1}\sum_{\overline{i_1}=1}^{S}\cdots\sum_{\overline{i_{n^{(d)}}}}^{S}\sum_{\overline{\tau}=0}^{1} p(z\,|\,v^{(d)},\hat{\theta}_k)\,\ell(\overline{v^{(d)}};\theta)\,.
\end{aligned} \tag{4.44}$$

[4] Other expectations are possible, e.g. over the joint distribution $\mathbb{Z},\mathbb{V}\,|\,\theta$. This latter produces macro-averaged parameter estimates of the form $\sum_{d=1}^{D}\phi^{(d)}/\sum_{d=1}^{D}\psi^{(d)}$, whereas the discriminative distribution $\mathbb{Z}\,|\,\mathbb{V},\theta$ often leads to micro-averaged estimates of the form $\sum_{d=1}^{D}[\phi^{(d)}/\psi^{(d)}]/D$.

2. *Maximisation step:* Obtain the optimal parameter estimate $\hat{\theta}_{k+1}$ that maximises the conditional expected log-likehood, namely

$$\hat{\theta}_{k+1} \;=\; \arg\max_{\theta} Q(\theta, \hat{\theta}_k)\,. \tag{4.45}$$

These two steps are iterated until $\hat{\theta}_k$ has converged to a value $\hat{\theta}^*$ that maximises $Q(\hat{\theta}^*) = Q(\hat{\theta}^*, \hat{\theta}^*)$.

Following the methodology of Section 4.3, we now break the optimisation of $Q(\theta, \hat{\theta})$ down into separate maximisation problems over each sub-parameter. For instance, we iteratively estimate the state transitions Γ by optimising

$$\begin{aligned}
Q_\Gamma(\theta, \hat{\theta}) &= \sum_{d=1}^{D} \sum_{\underline{\iota}=0}^{1} \sum_{\overline{\imath_1}=1}^{S} \cdots \sum_{\overline{\imath_{n^{(d)}}}=1}^{S} \sum_{\overline{\tau}=0}^{1} \sum_{t=1}^{n^{(d)}-1} p(z \,|\, v^{(d)}, \hat{\theta}) \, \log \Gamma_{\overline{\imath_t}, \overline{\imath_{t+1}}} \\
&= \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \sum_{i=1}^{S} \sum_{j=1}^{S} p(S_t = \sigma_i, S_{t+1} = \sigma_j \,|\, v^{(d)}, \hat{\theta}) \, \log \Gamma_{i,j} \\
&= \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \sum_{i=1}^{S} \sum_{j=1}^{S} \hat{\xi}_{t,i,j}^{(d)} \, \log \Gamma_{i,j}\,,
\end{aligned} \tag{4.46}$$

subject to the appropriate contraints. Note that use has been made of equation (4.23). Hence, borrowing the Lagrangian constraints from equation (4.35), we estimate the value $\hat{\Gamma}'$ that maximises

$$\begin{aligned}
F_\Gamma(\theta, \hat{\theta}) &= \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \sum_{i=1}^{S} \sum_{j=1}^{S} \hat{\xi}_{t,i,j}^{(d)} \, \log \Gamma_{i,j} - \sum_{i=1}^{S} \lambda_i \left(\sum_{j=1}^{S} \Gamma_{i,j} - 1 \right) \qquad (4.47) \\
\Rightarrow \frac{\partial F_\Gamma(\theta, \hat{\theta})}{\partial \Gamma_{i,j}} &= \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \frac{\hat{\xi}_{t,i,j}^{(d)}}{\Gamma_{i,j}} - \lambda_i \;=\; 0 \text{ when } \theta = \hat{\theta}' \\
\Rightarrow \hat{\lambda}_i' &= \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \sum_{j=1}^{S} \hat{\xi}_{t,i,j} \;=\; \sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \hat{\gamma}_{t,i} \\
\Rightarrow \hat{\Gamma}_{i,j}' &= \frac{\sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \hat{\xi}_{t,i,j}^{(d)}}{\sum_{d=1}^{D} \sum_{t=1}^{n^{(d)}-1} \hat{\gamma}_{t,i}^{(d)}} \qquad (4.48)
\end{aligned}$$

from equation (4.25).

Similarly, we iteratively estimate the sequence initiation distributions $\pi_{0,i}$ and $\pi_{1,i}$ by optimising

$$\begin{aligned}
Q_\Pi(\theta, \hat{\theta}) &= \sum_{d=1}^{D} \sum_{\underline{\iota}=0}^{1} \sum_{\overline{\imath_1}=1}^{S} \cdots \sum_{\overline{\imath_{n^{(d)}}}=1}^{S} \sum_{\overline{\tau}=0}^{1} p(z \,|\, v^{(d)}, \hat{\theta}) \left\{ \log \pi_{\underline{\iota}, \overline{\imath_1}} + \sum_{t=2}^{n^{(d)}} \log \pi_{0, \overline{\imath_t}} \right\} \\
&= \sum_{d=1}^{D} \left\{ \sum_{\underline{\iota}=0}^{1} \sum_{\overline{\imath_1}=1}^{S} p(\iota_0 = \underline{\iota}, S_1 = \sigma_{\overline{\imath_1}} \,|\, v^{(d)}, \hat{\theta}) \, \log \pi_{\underline{\iota}, \overline{\imath_1}} \right. \\
&\qquad \left. + \sum_{t=2}^{n^{(d)}} \sum_{\overline{\imath_t}=1}^{S} p(S_t = \sigma_{\overline{\imath_t}} \,|\, v^{(d)}, \hat{\theta}) \, \log \pi_{0, \overline{\imath_t}} \right\} \\
&= \sum_{d=1}^{D} \sum_{i=1}^{S} \left\{ \sum_{\underline{\iota}'=0}^{1} \hat{\gamma}_{1,i}^{(d)} \, \hat{\kappa}_{\underline{\iota}',1,i}^{(d)} \log \pi_{\underline{\iota}',i} + \sum_{t=2}^{n^{(d)}} \hat{\gamma}_{t,i}^{(d)} \log \pi_{0,i} \right\}
\end{aligned} \tag{4.49}$$

subject to the appropriate contraints. Note that we have utilised equations (4.23) and (4.26). Hence,

borrowing the Lagrangian constraint of equation (4.40), we maximise

$$\begin{aligned} F_\Pi(\theta,\hat{\theta}) &= \sum_{d=1}^{D}\sum_{i=1}^{S}\left\{\sum_{\underline{t}'=0}^{1}\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{\underline{t}',1,i}^{(d)}\log\pi_{\underline{t}',i}+\sum_{t=2}^{n^{(d)}}\hat{\gamma}_{t,i}\,\log\pi_{0,i}\right\} \\ &\quad -\lambda\left(\sum_{i=1}^{S}\{\pi_{0,i}+\pi_{1,i}\}-1\right) \qquad (4.50) \\ \Rightarrow \frac{\partial F_\Pi(\theta,\hat{\theta})}{\partial\pi_{0,i}} &= \sum_{d=1}^{D}\left\{\frac{\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{0,1,i}^{(d)}}{\pi_{0,i}}+\sum_{t=2}^{n^{(d)}}\frac{\hat{\gamma}_{t,i}}{\pi_{0,i}}\right\}-\lambda \;=\; 0 \text{ when } \theta=\hat{\theta}', \\ \frac{\partial F_\Pi(\theta,\hat{\theta})}{\partial\pi_{1,i}} &= \sum_{d=1}^{D}\frac{\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{1,1,i}^{(d)}}{\pi_{1,i}}-\lambda \;=\; 0 \text{ when } \theta=\hat{\theta}' \\ \Rightarrow \hat{\lambda}' &= \sum_{d=1}^{D}\sum_{i=1}^{S}\left\{\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{0,1,i}^{(d)}+\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{1,1,i}^{(d)}+\sum_{t=2}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)}\right\} \;=\; \sum_{d=1}^{D}\sum_{i=1}^{S}\sum_{t=1}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)} \;=\; \sum_{d=1}^{D}n^{(d)} \qquad (4.51) \end{aligned}$$

which leads to

$$\begin{aligned} \hat{\pi}'_{0,i} &= \frac{\sum_{d=1}^{D}\left\{\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{0,1,i}^{(d)}+\sum_{t=2}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)}\right\}}{\sum_{d=1}^{D}n^{(d)}}, \\ \hat{\pi}'_{1,i} &= \frac{\sum_{d=1}^{D}\hat{\gamma}_{1,i}^{(d)}\,\hat{\kappa}_{1,1,i}^{(d)}}{\sum_{d=1}^{D}n^{(d)}}. \qquad (4.52) \end{aligned}$$

Finally, we iteratively estimate the sequence termination distributions $\omega_{0,i}$ and $\omega_{1,i}$ by optimising

$$\begin{aligned} Q_\Omega(\theta,\hat{\theta}) &= \sum_{d=1}^{D}\sum_{\underline{t}=0}^{1}\sum_{\overline{i_1}=1}^{S}\cdots\sum_{\overline{i_{n^{(d)}}}=1}^{S}\sum_{\overline{\tau}=0}^{1}p(z\,|\,v^{(d)},\hat{\theta})\left\{\sum_{t=1}^{n^{(d)}-1}\log\omega_{0,\overline{i_t}}+\log\omega_{\overline{\tau},\overline{i_{n^{(d)}}}}\right\} \\ &= \sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\sum_{\overline{i_t}=1}^{S}p(S_t=\sigma_{\overline{i_t}}\,|\,v^{(d)},\hat{\theta})\,\log\omega_{0,\overline{i_t}}\right. \\ &\qquad \left.+\sum_{\overline{i_n^{(d)}}=1}^{S}\sum_{\overline{\tau}=0}^{1}p(\tau_{n^{(d)}+1}=\overline{\tau},S_{n^{(d)}}=\sigma_{\overline{i_{n^{(d)}}}}\,|\,v^{(d)},\hat{\theta})\,\log\omega_{\overline{\tau},\overline{i_{n^{(d)}}}}\right\} \\ &= \sum_{d=1}^{D}\sum_{i=1}^{S}\left\{\sum_{t=1}^{n^{(d)}-1}\hat{\gamma}_{t,i}^{(d)}\log\omega_{0,i}+\sum_{\underline{\tau}'=0}^{1}\hat{\gamma}_{n^{(d)},i}^{(d)}\,\hat{\zeta}_{\underline{\tau}',n^{(d)},i}^{(d)}\log\omega_{\underline{\tau}',i}\right\} \qquad (4.53) \end{aligned}$$

subject to the appropriate contraints. Note that we have utilised equations (4.23) and (4.29). Hence,

borrowing the Lagrangian constraint of equation (4.37), we maximise

$$\begin{aligned}
F_\Omega(\theta,\hat{\theta}) &= \sum_{d=1}^{D}\sum_{i=1}^{S}\left\{\sum_{t=1}^{n^{(d)}-1}\hat{\gamma}_{t,i}^{(d)}\log\omega_{0,i}+\sum_{\underline{\tau}'=0}^{1}\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{\underline{\tau}',n^{(d)},i}^{(d)}\log\omega_{\underline{\tau}',i}\right\} \\
&\quad -\sum_{i=1}^{S}\lambda_i\left(\omega_{0,i}+\omega_{1,i}-1\right) \qquad (4.54)\\
\Rightarrow \frac{\partial F_\Omega(\theta,\hat{\theta})}{\partial\omega_{0,i}} &= \sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\frac{\hat{\gamma}_{t,i}^{(d)}}{\omega_{0,i}}+\frac{\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{0,n^{(d)},i}^{(d)}}{\omega_{0,i}}\right\}-\lambda_i \;=\; 0 \text{ when } \theta=\hat{\theta}',\\
\frac{\partial F_\Omega(\theta,\hat{\theta})}{\partial\omega_{1,i}} &= \sum_{d=1}^{D}\left\{\frac{\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{1,n^{(d)},i}^{(d)}}{\omega_{1,i}}\right\}-\lambda_i \;=\; 0 \text{ when } \theta=\hat{\theta}'\\
\Rightarrow \hat{\lambda}_i' &= \sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\hat{\gamma}_{t,i}^{(d)}+\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{0,n^{(d)},i}^{(d)}+\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{1,n^{(d)},i}^{(d)}\right\} \;=\; \sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)}\\
\Rightarrow \hat{\omega}_{0,i}' &= \frac{\sum_{d=1}^{D}\left\{\sum_{t=1}^{n^{(d)}-1}\hat{\gamma}_{t,i}^{(d)}+\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{0,n^{(d)},i}^{(d)}\right\}}{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)}},\\
\hat{\omega}_{1,i}' &= \frac{\sum_{d=1}^{D}\hat{\gamma}_{n^{(d)},i}^{(d)}\hat{\zeta}_{1,n^{(d)},i}^{(d)}}{\sum_{d=1}^{D}\sum_{t=1}^{n^{(d)}}\hat{\gamma}_{t,i}^{(d)}} \;=\; 1-\hat{\omega}_{0,i}'. \qquad (4.55)
\end{aligned}$$

Observe in comparison to equation (4.39) for known data that each certainty, represented by a $\delta(\cdot)$ term, has now been replaced by a corresponding posterior probability.