

Hidden 1-Counter Markov Models and How to Learn Them

Mehmet Kurucan¹ and Mete Özbaltan² and Sven Schewe³ and Dominik Wojtczak³

¹Ardahan University, Ardahan, Turkey

²Erzurum Technical University, Erzurum, Turkey

³University of Liverpool, Liverpool, UK

mehmetkurucan@ardahan.edu.tr, mete.ozbaltan@erzurum.edu.tr,
sven.schewe@liverpool.ac.uk, d.wojtczak@liverpool.ac.uk

Abstract

We introduce hidden 1-counter Markov models (H1MMs) as an attractive sweet spot between standard hidden Markov models (HMMs) and probabilistic context-free grammars (PCFGs). Both HMMs and PCFGs have a variety of applications, e.g., speech recognition, anomaly detection, and bioinformatics. PCFGs are more expressive than HMMs, e.g., they are more suited for studying protein folding or natural language processing. However, they suffer from slow parameter fitting, which is cubic in the observation sequence length. The same process for HMMs is just linear using the well-known forward-backward algorithm. We argue that by adding to each state of an HMM an integer counter, e.g., representing the number of clients waiting in a queue, brings its expressivity closer to PCFGs. At the same time, we show that parameter fitting for such a model is computationally inexpensive: it is bi-linear in the length of the observation sequence and the maximal counter value, which grows slower than the observation length. The resulting model of H1MMs allows us to combine the best of both worlds: more expressivity with faster parameter fitting.

1 Introduction

One of the major challenges in modelling sequential data are long-term dependencies with a nested hierarchical structure. These are common in many domains such as natural language, music, or queuing systems. The two most widely used probabilistic models for sequential data are Hidden Markov Models (HMMs) and probabilistic context-free grammars (PCFGs). While HMMs are simple and fast to learn, PCFGs are much slower to learn, but can model such long-term dependencies easily. We argue here that there is a middle ground. There is a natural model that allows us to trade expressivity for computational complexity, namely, hidden one-counter Markov model (H1MM) that we define in this paper.

Probabilistic models that incorporate a non-negative integer counter are natural models for queuing systems [Etessami *et al.*, 2010] or epidemics [Bahi-Jaber and Pontier, 2003],

where the counter keeps track of the number of clients waiting or the number of people infected, respectively. Probabilistic counter models are also commonly used in the analysis of software [Braverman, 2006; Ben-Amram and Genaim, 2013].

Counter systems are often abstractions, where the counter value is bounded in principle, e.g., by the number of people in the world or by the number of atoms in the universe. Such bounds are, however, so vast that studying the infinite-state model with its concise representation instead is not only appropriate but also more efficient. Moreover, correctness proofs that do not rely on a bound of the counter are more robust.

One counter automata recognize one counter languages and can be used for, e.g., parsing bracketed arithmetic expressions [Fischer *et al.*, 1968], validation of XML documents [Chitic and Rosu, 2004] or checking whether or not a given sentence has the same number of noun and verb phrases. Such checks cannot be done by finite automata that can only recognize regular languages, which one counter languages are a superset of. On the other hand, one counter languages are a subclass of the context-free languages, which can be recognized by pushdown automata.

Checking whether or not a given input string of length n is a member of a context-free language takes cubic time using, e.g., the CYK algorithm. If we, instead, opt for simpler one counter languages (which can be viewed as pushdown automata with a single stack symbol) we can obtain a substantial acceleration.

Probabilistic one counter automata (P1CAs) [Etessami *et al.*, 2010; Wojtczak, 2009] sit between Markov chains (MCs) and probabilistic pushdown automata (PPDAs) [Mayr *et al.*, 2006; Etessami and Yannakakis, 2009]: they can be viewed as special probabilistic pushdown automata with just a single stack symbol [Etessami *et al.*, 2010], while MCs can be viewed as P1CAs that never increase the counter value.

While learning a PCFG from observations, the reestimation of its parameters can be performed in cubic time in the size of the input sequence by the Inside-Outside algorithm [Eisner, 2016]. With the same computational complexity we can compute the probability of a PCFG generating a given output [Chappelier *et al.*, 1998].

On the other end of the spectrum, Markov chains allow for faster linear time parsing and analysis [Rabiner, 1990], but lack expressivity compared to one counter automata: they are

finite state models, and, different to context free systems, they cannot count.

Markov models are either manually designed as an abstraction of a system, or they are learned from observations. We study the latter problem: based on a series of observations, we want to *learn* adequate Markov models. Those models can then, after they have been learned, be used for analysis.

When learning models from observations, there is no access to the models themselves during learning; only the observations are available. That is, the probabilistic structures we want to learn are *hidden* from view during learning, though there are assumptions made about their size. While we cannot observe how the models evolve, we can make *observations* from a finite alphabet, where (in an automata model) the likelihood of making a particular observation depends on the automaton state. (For counter and pushdown models, this means that the observation is independent of the counter value and stack content, respectively.) For example, it could hold for a state q that we make observation a with a 40% chance, and observation b with a 60% chance.

Thus, when learning a PICA model from observation, we refer to them as a *hidden* one counter Markov model (H1MM), and when learning an MC from observations to a *hidden* Markov Model (HMM), etc.

For H1MM, we show that, while they are pushdown systems that generate stochastic languages that can be non-regular (when read as nondeterministic languages), they can be learned using algorithms that generalize those used in HMM learning. This results in a complexity of learning quadratic in the length of the input, though the growth can be truncated in many cases. E.g., when the counter system represents grammatical structures, those sentences with a nesting depth beyond a "human limit", while grammatically correct, can be considered incomprehensible and could be discarded.

We have adapted three fundamental algorithms, Forward, Backward and Baum-Welch, that are standard in the analysis of HMM. This has allowed us to reduce the computational complexity of estimating the parameters compared to stack-based models PPDAs, PCFGs, and their sub-classes. The adapted versions of these algorithms for H1MM analysis have quadratic time complexity, which is a huge step forward from the cubic running time known for the full pushdown models.

1.1 Related Work

Hidden Markov Models were created in a series of papers by Baum and his co-authors in 1960s [Baum and Petrie, 1966; Baum *et al.*, 1970]. HMMs has found numerous applications since then, but are not well-suited to handle natural language processing (NLP). To deal with NLP, Probabilistic Context Free Grammars (PCFGs) were constructed in [Baker, 1979]. Many extensions of HMMs were proposed over the years that give them a bit more "structure". These include Lexicon tree-HMMs [Lee and Ng, 2005] and Dynamically Weighted HMMs [Lee *et al.*, 2007] that were applied to spam deobfuscation, hierarchical hidden Markov models (HHMMs) [Fine *et al.*, 1998] that were later applied to information extraction [Skounakis *et al.*, 2003], and the special case of HHMMs, Structured HMMs [Galassi *et al.*, 2007] that are well-suited for user profiling purposes. None of these models are ca-

pable of simulating H1MMs as all these models are still essentially finite-state. An adaptation of the Viterbi algorithm for stochastic one-counter automata, which are similar to (but slightly less concise than) H1MMs, was studied in [Sakharov and Sakharov, 2018].

1.2 Structure of the Paper

The rest of this paper is organized as follows. In Section 2, we formally define the Hidden one-counter Markov model (H1MM). In Section 3, we show how to adapt the three fundamental algorithms that are used to solve the learning problem for HMMs. In Section 4, we examine the performance of our model against HMMs. Due to space constraints all the proofs can only be found in the full version of this paper.

2 Model and Problem Definitions

Let \mathbb{N}_0 be the set of non-negative integers.

A hidden one counter Markov model (H1MM) is a tuple $\mathcal{H} = (Q, \Sigma, A^0, A^+, B, q_0, q_F)$, consisting of

- a finite set Q of *states*,
- a finite set Σ of *observations*,
- *transition functions* $A^0 : Q \times \Delta_0 \times Q \rightarrow [0, 1]$ and $A^+ : Q \times \Delta_+ \times Q \rightarrow [0, 1]$,
- *an emission function* $B : Q \times \Sigma \rightarrow [0, 1]$, and
- a designated *initial and final states* $q_0 \in Q$ and $q_F \in Q$, respectively.

$\Delta_0 = \{0, 1\}$ and $\Delta_+ = \{-1, 0, 1\}$ are the possible changes for the counter value when the current counter value is 0 and the value is positive, respectively. We also require that A^+, A^0 , and B define for every state $q \in Q$ a probability distributions, i.e., $\sum_{\Delta \in \Delta_0, q' \in Q} A^0(q, \Delta, q') = \sum_{\Delta \in \Delta_+, q' \in Q} A^+(q, \Delta, q') = \sum_{o \in \Sigma} B(q, o) = 1$ holds.

A *configuration* of a H1MM is a pair (q, c) , consisting of a state $q \in Q$ and a counter value $c \in \mathbb{N}_0$. The unique initial configuration of a H1MM is $(q_0, 0)$.

A^0 and A^+ describe the dynamics of how the configuration of a model evolves, while B describes the dynamics of observing the evolution of the underlying model. Specifically, matrices A^0 and A^+ specify the probability of transition from any one state to another while changing the counter by a given constant when the counter value is 0 and when the counter is positive, respectively. For example $A^+(q, -1, q') = 0.3$ means that, when the model is in state q with a positive counter value, then there is a chance of 30% that the model moves to state q' while decrementing the counter value by 1. Matrix B specifies for each state the probability of making a particular observation when at that state. (Note that we assume this probability does not depend on the counter value, but only on the state.) For instance, $B(q, \sigma) = 0.25$ means that when the system is in state (q, c) for arbitrary counter value $c \geq 0$ there is a chance of 25% that σ is observed.

When we discuss the dynamics of a H1MM, we emphasize that the configurations at position t of a run are probabilistic variables by denoting them by S_t . If the counter is 0, the transition matrix A^0 determines the dynamics:

$$Pr(S_{t+1} = (q', \Delta) \mid S_t = (q, 0)) = A^0(q, \Delta, q')$$

where q is the state of the system at step t , q' is the state at step $t + 1$, and $\Delta \in \Delta_0$ is the difference in the counter value between these two steps. (The probability of this transition for counter values $\Delta \notin \Delta_0$ is 0.)

If the current value of the counter c is positive, then the transition matrix A^+ is used instead:

$$Pr(S_{t+1} = (q', c + \Delta) \mid S_t = (q, c)) = A^+(q, \Delta, q')$$

When the previous counter value is positive, the counter value can only be decremented by 1, stay the same, or be incremented by 1, i.e., $\Delta \in \Delta_+ = \{-1, 0, 1\}$.

A *run* of length T of a H1MM \mathcal{H} is a finite trace $\rho = (q_0, c_0)(q_1, c_1)(q_2, c_2) \dots (q_T, c_T)$ of configurations with $c_0 = 0$, such that, for all integers t with $1 \leq t \leq T$ $Pr(S_t = q_t, C_t = c_t \mid S_{t-1} = q_{t-1}, C_{t-1} = c_{t-1}) > 0$. A run is *accepting* if $(q_T, c_T) = (q_F, 0)$ (i.e. if it ends in the final state with counter value 0).

The states and counter values are not directly observable. Instead, a hidden state q_t produces an output symbol o_t with the probability defined by the emission matrix B . Denoting by O_t the random variable of observation made at step t , we have

$$Pr(O_t = o \mid S_t = q) = B(q, o).$$

For the run above, one would see an *observation sequence* $\omega = o_0 o_1 o_2 \dots o_T$ with probability $\prod_{t=0}^T Pr(O_t = o_t \mid S_t = q_t)$.

If O , S , and C denote the sequence of random variables of observations, states, and counter values along a run, then

$$\begin{aligned} Pr(O = \omega, S = \rho) &= Pr(O = \omega \mid S = \rho) \cdot Pr(S = \rho) \\ &= \prod_{t=0}^T Pr(o_t \mid q_t) \times \prod_{t=1}^T Pr(q_t, c_t \mid q_{t-1}, c_{t-1}) \quad (1) \end{aligned}$$

The first factor in the third line of Equation 1 is the emission probability (for the given run), and the second factor is the probability that a given run is generated.

A *random multiset of runs* of predefined length T and size s for a H1MM \mathcal{H} , denoted $\mathcal{R}(\mathcal{H}, T, s)$, is produced by taking s independent samples from S , (i.e., by producing s randomly created runs.) In each of them we simply randomly select the next configuration according to the probabilities A^+ and A^0 .

A *random multiset of accepting runs* of predefined length T and size s for a H1MM \mathcal{H} , denoted $\mathcal{A}(\mathcal{H}, T, s)$, is produced by taking s independent samples from S , and then store the sampled run if it is accepting, and otherwise discard it; and repeat this until s examples have been added.

A *random multiset of observation sequences* of predefined length T and size s for a H1MM \mathcal{H} , denoted $\mathcal{O}(\mathcal{H}, T, s)$, is produced by first producing $\mathcal{A}(\mathcal{H}, T, s)$, and then sampling an observation sequence for each run in \mathcal{A} .

The **main problem** we study is, given a random multiset of observation sequences $\mathcal{O}(\mathcal{H}, T, s)$, find a H1MM \mathcal{H}' with a given number $|Q'|$ of states that is most likely to produce \mathcal{O} .

We note that a naive way of calculating the probability of seeing a given observation sequence ω can be very slow: if A

denotes all the accepting runs of \mathcal{H} of the same length as ω , then this probability is

$$Pr(O = \omega) = \frac{\sum_{\rho \in A} Pr(O = \omega \mid S = \rho) \cdot Pr(S = \rho)}{\sum_{\rho \in A} Pr(S = \rho)}$$

To calculate this value one would need to iterate over potentially exponentially many accepting runs in A . In the next section, we are going to show a dynamic programming solution to this problem that runs in polynomial time instead.

3 Adaptation of Algorithms

We adapt here the standard Forward, Backward and Baum-Welch algorithms, which are used for learning tasks in HMMs, to our model H1MM by factoring in the configuration the counter value.

The adapted Forward and Backward algorithms will consist of two phases which we call: *preliminary* and *normalization*. The first phase of both algorithms looks very similar to the original algorithms for HMMs, but with the value of the counter tracked. In the second phase, considering the specified initial configuration and terminal configuration, unnecessary paths are discarded from the trellis diagram and the probability of all the paths connecting these two configurations to each other is normalized.

The adapted version of Baum-Welch algorithm is used to update the parameters of the H1MM taking the evolution of the counter value into consideration. This algorithm consists of two different computational parts represented by functions ξ and γ defined as for HMMs [Bilmes, 2000]. These functions calculate, respectively, the probability of a given configuration at a given step t conditioned on the observation sequence and the probability of a particular pair of consecutive configurations conditioned on the observation sequence.

3.1 The Adapted Forward Algorithm

Let $o_{i:j} = o_i \dots o_j$ be the part of the observation sequence between steps i and j . The adapted Forward algorithm computes the probability of a given observation sequence $(o_{1:T})$ by summing over all possible runs that can generate the given observation sequence.

First Phase: Preliminary Forward Calculation

In this phase, we calculate the joint probability distribution of a given observation sequence $o_{1:t}$ and the hidden state-counter pair at step t being $S_t = (q, c)$ conditioned on the initial configuration being $S_0 = (q_0, 0)$, which we will denote by $\hat{\alpha}$. Formally:

$$\hat{\alpha}_t(q, c) = Pr(o_{1:t}, S_t \mid S_0)$$

Our algorithm calculates this value by summing over all paths that reach S_t as shown in Figure 1. The calculation starts at the base step at time $t = 0$. At this step, we know that we are at the initial configuration, i.e., at the starting state S_0 . So the base step value of $\hat{\alpha}$ is as follows:

- *Base Step:*

$$\hat{\alpha}_0(q, c) = \begin{cases} 1 & \text{if } q = q_0 \text{ and } c = 0 \\ 0 & \text{otherwise} \end{cases}$$

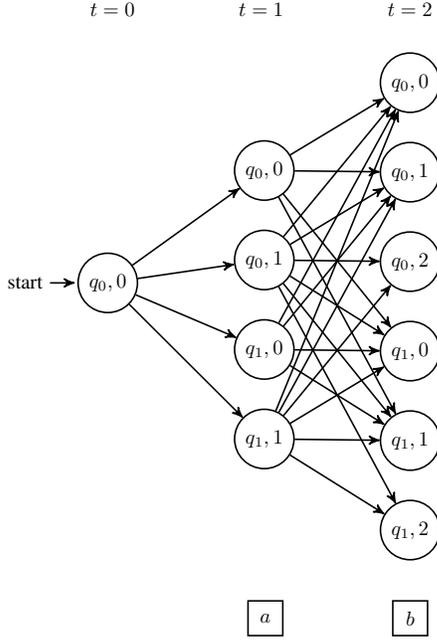


Figure 1: The trellis of the preliminary forward flow

For any other step we calculate the value of $\hat{\alpha}$ recursively:

- *Recursion Step:*

if $c - \Delta = 0$:

$$\hat{\alpha}_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=0}^1 \hat{\alpha}_{t-1}(q', c - \Delta) A^0(q', \Delta, q) B(q, o_t)$$

if $c - \Delta > 0$:

$$\hat{\alpha}_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=-1}^1 \hat{\alpha}_{t-1}(q', c - \Delta) A^+(q', \Delta, q) B(q, o_t)$$

Theorem 1. $\hat{\alpha}_t(q, c)$ calculates $Pr(o_{1:t}, S_t | S_0)$ correctly.

Second Phase: Normalized Forward

The second phase of the algorithm calculates $\alpha_t(q, c)$: the joint probability distribution of the observation sequence $o_{1:t}$ and the hidden state-counter pair at step t being $S_t = (q, c)$ under the condition that the initial configuration is $S_0 = (q_0, 0)$ and the terminal configuration has to be $S_T = (q_F, 0)$. Formally we write this as:

$$\alpha_t(q, c) = Pr(o_{1:t}, S_t | S_0, S_T)$$

The way to compute this is to remove all paths from the trellis diagram from which $S_T = (q_F, 0)$ cannot be reached in step T . Naturally, without normalization, the probabilities to take any of these paths is now $Pr(S_T | S_0)$, and no longer 1, and we need to normalize the probabilities accordingly.

- *Base Step:*

$$\alpha_T(q, c) = \begin{cases} \frac{\hat{\alpha}_T(q, c)}{Pr(S_T | S_0)} & : \text{if } q = q_F \text{ and } c = 0 \\ 0 & : \text{otherwise} \end{cases}$$

- *Recursion Step:*

if $c = 0$:

$$\alpha_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=0}^1 \frac{\alpha_{t+1}(q', c + \Delta) A^0(q, \Delta, q') \hat{\alpha}_t(q, c)}{\hat{\alpha}_{t+1}(q', c + \Delta)}$$

if $c > 0$:

$$\alpha_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=-1}^1 \frac{\alpha_{t+1}(q', c + \Delta) A^+(q, \Delta, q') \hat{\alpha}_t(q, c)}{\hat{\alpha}_{t+1}(q', c + \Delta)}$$

At the base step $t = T$, the calculation of normalization starts in the final state with zero counter $S_T = (q_F, 0)$. The rest of the hidden state-counter pairs are discarded because our model only accepts a run that ends at such final configuration at $t = T$ as shown in Figure 2. The accepting state is q_1 with zero counter value in this example. The normalized probability of $(q_1, 0)$, according to the equation of the base step, is found by dividing the preliminary probability of the forward flow of $(q_1, 0)$ with the total probability of reaching the final configuration from the initial configuration.

There are three important points regarding the calculation of the normalized probability of valid paths. First is that the calculation starts from the final state with a zero counter value. Second is that the time step is decremented by one in each iteration. Therefore, in this phase, the normalization calculation at a particular time step t will be used when calculating the normalized probability as the time step $t - 1$. The last point is that we need all the preliminary probability values of the forward flow that we calculated in the first phase.

Theorem 2. $\alpha_t(q, c)$ computes correctly the joint probability $Pr(o_{1:t}, S_t = (q, c) | S_0, S_T)$.

3.2 Adaptation of Backward Algorithm

The adapted Backward algorithm computes the probability of the future observation $o_{t+1:T}$ conditioned on the value of S_t .

First Phase: Preliminary Backward Calculation

We calculate here, $\hat{\beta}_t(q, c)$, the probability of reaching the terminal configuration at the final step T from a given configuration (q, c) at step t (given that we started at the initial configuration). Formally:

$$\hat{\beta}_t(q, c) = Pr(S_T = (q_F, 0) | S_t = (q, c), S_0)$$

The computation starts at the designated final configuration $S_T = (q_F, 0)$ at time $t = T$ as shown in Figure 2 but the base and recursion steps are different from the normalization of adapted Forward calculation. For instance, we do not look at the emitted observations in this phase.

- *Base Step:*

$$\hat{\beta}_T(q, c) = \begin{cases} 1 & : \text{if } q = q_F \text{ and } c = 0 \\ 0 & : \text{otherwise} \end{cases}$$

- *Recursion Step:*

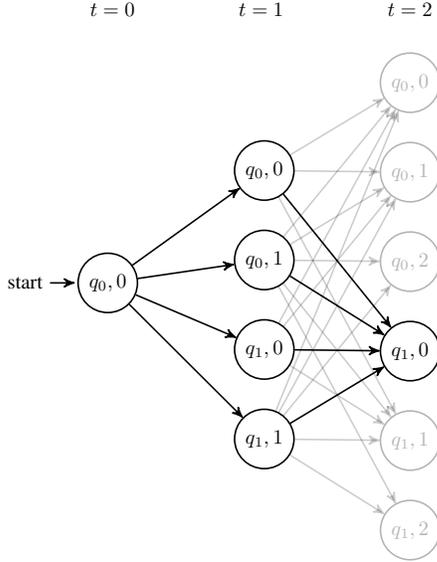


Figure 2: normalization calculation of adapted Forward algorithm

if $c = 0$:

$$\hat{\beta}_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=0}^1 \hat{\beta}_{t+1}(q', c + \Delta) A^0(q, \Delta, q')$$

if $c > 0$:

$$\hat{\beta}_t(q, c) = \sum_{q' \in Q} \sum_{\Delta=-1}^1 \hat{\beta}_{t+1}(q', c + \Delta) A^+(q, \Delta, q')$$

Theorem 3. $\hat{\beta}_t(q, c)$ calculates $Pr(S_T | S_t = (q, c), S_0)$ correctly.

Second Phase: Normalization Backward Flow

In this phase the probability of emitting the future observation sequence $o_{t+1:T}$ is calculated conditioned on the current configuration and that the terminal configuration is reached. Formally,

$$\beta_t(q, c) = Pr(o_{t+1:T} | S_t = (q, c), S_0, S_T)$$

The calculation of the normalization of the backward flow is started at the last time step T . The preliminary probability of the backward flow is needed here.

- *Base Step:*

$$\beta_T(q, c) = \begin{cases} 1 & q = q_F \text{ and } c = 0 \\ 0 & \text{otherwise} \end{cases}$$

- *Recursion Step:*

if $c = 0$:

$$\beta_t(q, c) =$$

$$\sum_{q' \in Q} \sum_{\Delta=0}^1 \frac{\beta_{t+1}(q', \Delta) A^0(q, \Delta, q') B(q', o_{t+1}) \hat{\beta}_{t+1}(q', \Delta)}{\hat{\beta}_t(q, c)}$$

if $c > 0$:

$$\beta_t(q, c) =$$

$$\sum_{q' \in Q} \sum_{\Delta=-1}^1 \frac{\beta_{t+1}(q', c + \Delta) A^+(q, \Delta, q') B(q', o_{t+1}) \hat{\beta}_{t+1}(q', c + \Delta)}{\hat{\beta}_t(q, c)}$$

Theorem 4. $\beta_t(q, c)$ calculates correctly the probabilities $Pr(o_{t+1:T} | S_t = (q, c), S_0, S_T)$.

3.3 Adaptation of Baum-Welch Algorithm

It is worth to point out that the original Baum-Welch algorithm is a special case of the Expectation Maximization (EM) algorithm [Bilmes, 2000] therefore the same aspect is considered on the adapted version when the counter variable is taken into account. The adapted algorithm runs a procedure that finds a set of parameters that get closer and closer to the optimal model. It is repeating the following steps:

E-Step

In this step, there are two calculations where each takes into account the counter value.

Theorem 5. $\gamma_t(q, c) = Pr(S_t | O, S_0, S_T)$ is the calculation of the marginal posterior distribution of a hidden variable $S_t = (q, c)$ where

$$\gamma_t(q, c) = \frac{\hat{\alpha}_t(q, c) \beta_t(q, c) \hat{\beta}_t(q, c)}{\hat{\alpha}_t(q_F, 0)}$$

Theorem 6. $\xi_t((q', c'), (q, c)) = Pr(S_{t-1}, S_t | O, S_0, S_T)$ calculates the joint posterior distribution of two successive hidden variables of the model where

$$\xi_t((q', c'), (q, c)) = \frac{\hat{\alpha}_{t-1}(q', c') A^{\delta(c')} (q', \Delta, q) B(q, o_t) \hat{\beta}_t(q, c) \beta_t(q, c)}{\hat{\alpha}_T(q_F, 0)}$$

and

$$\delta(c') = \begin{cases} 0 & : c' = 0 \\ + & : c' > 0 \end{cases}$$

M-Step

In the M-step, we use the posterior parameters (i.e., θ) to find new parameters (i.e., θ') of the model that maximize the expected likelihood as estimated in the E-step. We can write the joint probability distribution over hidden, counter and observation variables as follows:

$$Pr(S, C, \mathcal{O} | \theta) = \prod_{d=1}^D \prod_{t=1}^T B(o_t^{(d)}, S_t^{(d)}) A^{\delta(C_t^{(d)})} (S_t^{(d)}, C_{t+1}^{(d)} - C_t^{(d)}, S_{t+1}^{(d)})$$

where

$$\delta(C_t^{(d)}) = \begin{cases} 0, & C_t^{(d)} = 0 \\ +, & C_t^{(d)} > 0 \end{cases}$$

We consider multiple observation sequences to learn an optimal model. Here, D represents the number of observation sequences. We use Lagrange multipliers to obtain optimized

values for the model parameters. The updated formula for the emission matrix is

$$\hat{B}(q, o) = \frac{\sum_{d=1}^D \sum_{t=1}^T \gamma_t^{(d)}(S_t^{(d)}) \mathcal{I}(o_t^{(d)} = o)}{\sum_{d=1}^D \sum_{t=1}^T \gamma_t^{(d)}(S_t^{(d)})}$$

where $\mathcal{I}(o)$ denotes an indicator function which is 1 if $o_t = o$ is true, and 0 otherwise. The updated formulas for state transition matrices \hat{A}^0 and \hat{A}^+ , respectively, are

$$\hat{A}^0(q, \Delta, q') = \frac{\sum_{d=1}^D \sum_{\{t|C_t^{(d)}=0\}} \xi_t^{(d)}(S_t^{(d)}, S_{t+1}^{(d)})}{\sum_{S_{t+1}^{(d)}} \sum_{d=1}^D \sum_{\{t|C_t^{(d)}=0\}} \xi_t^{(d)}(S_t^{(d)}, S_{t+1}^{(d)})}$$

$$\hat{A}^+(q, \Delta, q') = \frac{\sum_{d=1}^D \sum_{\{t|C_t^{(d)}>0\}} \xi_t^{(d)}(S_t^{(d)}, S_{t+1}^{(d)})}{\sum_{S_{t+1}^{(d)}} \sum_{d=1}^D \sum_{\{t|C_t^{(d)}>0\}} \xi_t^{(d)}(S_t^{(d)}, S_{t+1}^{(d)})}$$

4 Experiments

All algorithms here were implemented in Python and evaluated on Intel i7 3.3 GHz CPU with 16 GB RAM. We also implemented the standard algorithms (forward, backward, Baum-Welch) for HMMs ourselves for a fair comparison. The full source-code and the inputs used will be made freely available online.

We tested the algorithm on the following input. We first created 6 different models $\mathcal{H}_i = (Q_i, \Sigma_i, A_i^0, A_i^+, B_i, q_0, q_F)$, where $i = 1, 2, \dots, 6$. Model \mathcal{H}_i has $i + 1$ states and Figure 2 shows \mathcal{H}_i where the probability values are omitted. Each model has a structure similar to this example, which was picked in order to exhibit an interesting counting behavior from the model. The probabilities of transitions and observations A_i^0 , A_i^+ , and B_i were then randomly selected.

Then using each \mathcal{H}_i , we created a random multi-set of observation sequences $\mathcal{O}_i(\mathcal{H}_i, T, 20000)$ that contain 20000 observation sequences with a fixed length $T = 16$.

To simplify the comparison, we let the number of states of HMM to have 2.24 times more states (exactly $\sqrt{5}$ more) than the H1MM model that it is compared with. This is because to describe the transition matrix of H1MM with n states one needs $5n^2$ values, while HMM utilises only n^2 values. This way we only compare models with the same total number of parameters and thus avoid the need to penalize the model with more parameters as one would do when using, e.g., Akaike or Bayesian information criteria for measuring the quality of models.

We noticed that both HMM and H1MM algorithm tend to get stuck in local minima very often. In order to avoid this, we followed the following procedure to train our models. We started with 100 different initial completely random (i.e., fully connected with probabilities picked uniformly at random) H1MM models (or HMM models). After each learning step, we discarded the bottom 25% of these models as measured by the value of their likelihood. Eventually we only had one model left that we trained until the learning process converged.

The running time of the learning process for HMMs $\mathcal{H}_i, i = 1, \dots, 6$ took: 10 minutes, 30 minutes, 1 hour, 4

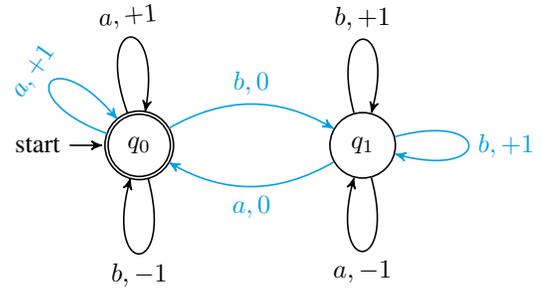


Figure 3: An example pICA model. Blue arrows are enabled when the counter value is zero, and the other arrows are enabled when the counter value is positive.

hours, 6 hours, 10 hours, respectively. The same task for the H1MM took: 1 hour, 6 hours, 22 hours, 79 hours, 218 hours, - (initialization was done by hand), respectively.

At the training step, the parameters of the model were reestimated using the adapted Baum-Welch algorithm discussed in the previous section. The learning algorithms has nested loops over the length T of the observation sequence, feasible maximum counter values $M \leq \frac{1}{2}T$, and goes twice over the number of hidden states $n = |Q|$ at each iteration step. Therefore, the complexity of the adapted Baum-Welch algorithm is $\mathcal{O}(n^2TM)$, where the counter value cannot exceed the remaining length of the observation sequence; in particular $M \leq \frac{1}{2}T$.

The learnt HMM and H1MM models were then compared with the original model. We chose as the performance metric the likelihood of a set of test observations, which were different from the observation sequences used in the learning process. We calculated the similarity score using the Kullback-Leibler (KL) divergence.

$$KL(P||Q) = P(x) \log \left(\frac{P(x)}{Q(x)} \right)$$

Here, $P(x)$ addresses the original likelihood distribution and $Q(x)$ shows the likelihood distribution of the model to be analyzed for every variable x . This estimates the difference between two likelihood distributions. Only if two distributions match perfectly, the KL score is zero otherwise and the closer to 0 it is the better. As we can see in Table 1, our H1MM algorithms learnt almost perfectly the original model, while HMMs struggle to get any close. The price we pay for that is obviously the longer running time, but we are still much faster compared to using PCFGs instead. In fact, based on the running time of our learning algorithms for HMM and H1MM, we can extrapolate that, if we were to implement the standard cubic inside-outside learning algorithm for PCFGs, it would timeout already for \mathcal{H}_3 .

Model	\mathcal{H}_1	\mathcal{H}_2	\mathcal{H}_3	\mathcal{H}_4	\mathcal{H}_5	\mathcal{H}_6
H1MM	0.008	0.0022	0.11	0.0027	0.0045	0.0064
HMM	4.94	5.44	5.24	5.26	6.799	5.11

Table 1: KL scores of all 6 individual models.

Acknowledgements

 This project has received funding from the European Union’s Horizon 2020 research and innovation programme under grant agreement No 956123. It has been supported by the EPSRC through the Programme Grant EP/V026887/1 (Digital navigation of chemical space for function).

References

- [Bahi-Jaber and Pontier, 2003] Narges Bahi-Jaber and Dominique Pontier. Modeling transmission of directly transmitted infectious diseases using colored stochastic petri nets. *Mathematical biosciences*, 185(1):1–13, 2003.
- [Baker, 1979] James K Baker. Trainable grammars for speech recognition. *The Journal of the Acoustical Society of America*, 65(S1):S132–S132, 1979.
- [Baum and Petrie, 1966] Leonard E Baum and Ted Petrie. Statistical inference for probabilistic functions of finite state markov chains. *The annals of mathematical statistics*, 37(6):1554–1563, 1966.
- [Baum *et al.*, 1970] Leonard E Baum, Ted Petrie, George Soules, and Norman Weiss. A maximization technique occurring in the statistical analysis of probabilistic functions of markov chains. *The annals of mathematical statistics*, 41(1):164–171, 1970.
- [Ben-Amram and Genaim, 2013] Amir M Ben-Amram and Samir Genaim. On the linear ranking problem for integer linear-constraint loops. In *Proceedings of the 40th Annual ACM Symposium on Principles of programming languages (POPL)*, pages 51–62, 2013.
- [Bilmes, 2000] Jeff Bilmes. A gentle tutorial of the em algorithm and its application to parameter estimation for gaussian mixture and hidden markov models. *Technical Report ICSI-TR-97-021, University of Berkeley*, 4, 06 2000.
- [Braverman, 2006] Mark Braverman. Termination of integer linear programs. In *International conference on computer aided verification*, pages 372–385. Springer, 2006.
- [Chappelier *et al.*, 1998] J.-C. Chappelier, M. Rajman, and Ch-Lausanne. A generalized cyk algorithm for parsing stochastic cfg, 1998.
- [Chitic and Rosu, 2004] Cristiana Chitic and Daniela Rosu. On validation of xml streams using finite state machines. In *Proceedings of the 7th International Workshop on the Web and Databases: colocated with ACM SIGMOD/PODS 2004*, pages 85–90, 2004.
- [Eisner, 2016] Jason Eisner. Inside-outside and forward-backward algorithms are just backprop (tutorial paper). In *Proceedings of the Workshop on Structured Prediction for NLP*, pages 1–17, Austin, TX, November 2016. Association for Computational Linguistics.
- [Etessami and Yannakakis, 2009] Kousha Etessami and Mihalis Yannakakis. Recursive markov chains, stochastic grammars, and monotone systems of nonlinear equations. *Journal of the ACM (JACM)*, 56(1):1–66, 2009.
- [Etessami *et al.*, 2010] Kousha Etessami, Dominik Wojtczak, and Mihalis Yannakakis. Quasi-birth-death processes, tree-like qbds, probabilistic 1-counter automata, and pushdown systems. *Perform. Eval.*, 67(9):837–857, September 2010.
- [Fine *et al.*, 1998] Shai Fine, Yoram Singer, and Naftali Tishby. The hierarchical hidden markov model: Analysis and applications. *Machine learning*, 32(1):41–62, 1998.
- [Fischer *et al.*, 1968] Patrick C Fischer, Albert R Meyer, and Arnold L Rosenberg. Counter machines and counter languages. *Mathematical systems theory*, 2(3):265–283, 1968.
- [Galassi *et al.*, 2007] Ugo Galassi, Attilio Giordana, and Lorenza Saitta. Incremental construction of structured hidden markov models. In *IJCAI*, pages 798–803, 2007.
- [Lee and Ng, 2005] Honglak Lee and Andrew Y Ng. Spam deobfuscation using a hidden markov model. In *CEAS*, 2005.
- [Lee *et al.*, 2007] Seunghak Lee, Iryoung Jeong, and Seungjin Choi. Dynamically weighted hidden markov model for spam deobfuscation. In *IJCAI*, volume 7, pages 2523–2529, 2007.
- [Mayr *et al.*, 2006] Richard Mayr, Antonín Kucera, and Javier Esparza. Model checking probabilistic pushdown automata. *Logical Methods in Computer Science*, 2, 2006.
- [Rabiner, 1990] Lawrence R. Rabiner. A tutorial on hidden markov models and selected applications in speech recognition. In Alex Waibel and Kai-Fu Lee, editors, *Readings in Speech Recognition*, pages 267–296. Morgan Kaufmann Publishers Inc., San Francisco, CA, USA, 1990.
- [Sakharov and Sakharov, 2018] Alexander Sakharov and Timothy Sakharov. The viterbi algorithm for subsets of stochastic context-free languages. *Information Processing Letters*, 135:68 – 72, 2018.
- [Skounakis *et al.*, 2003] Marios Skounakis, Mark Craven, and Soumya Ray. Hierarchical hidden markov models for information extraction. In *IJCAI*, pages 427–433, 2003.
- [Wojtczak, 2009] Dominik Wojtczak. *Recursive Probabilistic Models: efficient analysis and implementation*. PhD thesis, University of Edinburgh, UK, 2009.