Biostatistics 615/815 Lecture 22: Baum-Welch Algorithm Advanced Hidden Markov Models

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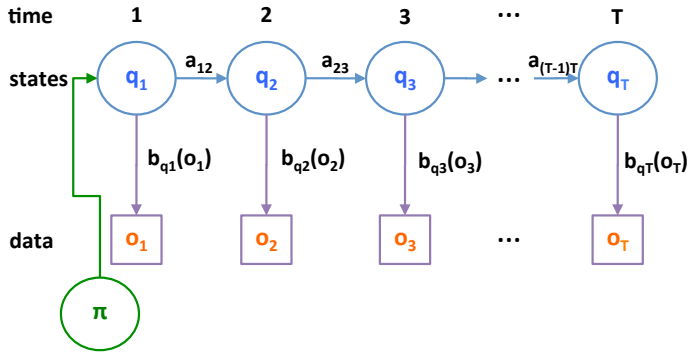
Revisiting Hidden Markov Model



Statistical analysis with HMM

HMM for a deterministic problem

- Given
  - Given parameters $\lambda = \{\pi, A, B\}$
  - and data $\mathbf{o} = (o_1, \cdots, o_T)$
- Forward-backward algorithm
  - Compute $\Pr(q_t|\mathbf{o}, \lambda)$
- Viterbi algorithm
  - Compute $\arg\max_{\mathbf{q}} \Pr(\mathbf{q}|\mathbf{o}, \lambda)$

HMM for a stochastic process / algorithm

- Generate random samples of $\mathbf{o}$ given λ

Deterministic Inference using HMM

- If we know the exact set of parameters, the inference is deterministic given data
  - No stochastic process involved in the inference procedure
  - Inference is deterministic just as estimation of sample mean is deterministic
- The computational complexity of the inference procedure is exponential using naive algorithms
- Using dynamic programming, the complexity can be reduced to $O(n^2 T)$.

Using Stochastic Process for HMM Inference

Using random process for the inference

- Randomly sampling **o** from $\Pr(\mathbf{o}|\lambda)$.
- Estimating $\arg\max_\lambda \Pr(\mathbf{o}|\lambda)$.
  - No analyitic algorithm available
  - Simplex, E-M algorithm, or Simulated Annealing is possible apply
- Estimating the distribution $\Pr(\lambda|\mathbf{o})$.
  - Gibbs Sampling

Recap : The E-M Algorithm

Expectation step (E-step)

- Given the current estimates of parameters $\theta^{(t)}$, calculate the conditional distribution of latent variable **z**.
- Then the expected log-likelihood of data given the conditional distribution of **z** can be obtained

$$Q(\theta|\theta^{(t)}) = \mathbf{E}_{\mathbf{z}|\mathbf{x},\theta^{(t)}}\left[\log p(\mathbf{x},\mathbf{z}|\theta)\right]$$

Maximization step (M-step)

- Find the parameter that maximize the expected log-likelihood

$$\theta^{(t+1)} = \arg\max_\theta Q(\theta|\theta^t)$$

Baum-Welch for estimating $\arg\max_\lambda \Pr(\mathbf{o}|\lambda)$

Assumptions

- Transition matrix is identical between states
  - $a_{ij} = \Pr(\mathbf{q}_{t+1} = j|\mathbf{q}_t = i) = \Pr(\mathbf{q}_t = j|\mathbf{q}_{t-1} = i)$
- Emission matrix is identical between states
  - $b_i(j) = \Pr(\mathbf{o}_t = j|\mathbf{q}_t = i) = \Pr(\mathbf{o}_{t=1} = j|\mathbf{q}_{t-1} = i)$
- This is NOT the only possible configurations of HMM
  - For example, a_{ij} can be parameterized as a function of t.
  - Multiple sets of **o** independently drawn from the same distribution can be provided.
  - Other assumptions will result in different formulation of E-M algorithm

E-step of the Baum-Welch Algorithm

1. Run the forward-backward algorithm given $\lambda^{(\tau)}$

$$\begin{aligned}
\alpha_t(i) &= \Pr(o_1,\cdots,o_t,q_t=i|\lambda^{(\tau)}) \\
\beta_t(i) &= \Pr(o_{t+1},\cdots,o_T|q_t=i,\lambda^{(\tau)}) \\
\gamma_t(i) &= \Pr(q_t=i|\mathbf{o},\lambda^{(\tau)}) = \frac{\alpha_t(i)\beta_t(i)}{\sum_k \alpha_t(k)\beta_t(k)}
\end{aligned}$$

2. Compute $\xi_t(i,j)$ using $\alpha_t(i)$ and $\beta_t(i)$

$$\begin{aligned}
\xi_t(i,j) &= \Pr(q_t=i,q_{t+1}=j|\mathbf{o},\lambda^{(\tau)}) \\
&= \frac{\alpha_t(i)a_{ij}b_j(o_{t+1})\beta_{t+1}(j)}{\Pr(\mathbf{o}|\lambda^{(\tau)})} \\
&= \frac{\alpha_t(i)a_{ij}b_j(o_{t+1})\beta_{t+1}(j)}{\sum_{(k,l)}\alpha_t(k)a_{kl}b_l(o_{t+1})\beta_{t+1}(l)}
\end{aligned}$$

E-step : $\xi_t(i,j)$

$$\xi_t(i,j) = \Pr(q_t = i, q_{t+1} = j | \mathbf{o}, \lambda^{(\tau)})$$

- Quantifies joint state probability between consecutive states
- Need to estimate transition probability
- Requires $O(n^2 T)$ memory to store entirely.
  - Only $O(n^2)$ is necessary for running Baum-Welch algorithm

M-step of the Baum-Welch Algorithm

Let $\lambda^{(\tau+1)} = (\pi^{(\tau+1)}, A^{(\tau+1)}, B^{(\tau+1)})$

$$\begin{aligned}
\pi^{(\tau+1)}(i) &= \frac{\sum_{t=1}^{T} \Pr(q_t = i | \mathbf{o}, \lambda^{(\tau)})}{T} = \frac{\sum_{t=1}^{T} \gamma_t(i)}{T} \\
a_{ij}^{(\tau+1)} &= \frac{\sum_{t=1}^{T-1} \Pr(q_t = i, q_{t+1} = j | \mathbf{o}, \lambda^{(\tau)})}{\sum_{t=1}^{T-1} \Pr(q_t = i | \mathbf{o}, \lambda^{(\tau)})} = \frac{\sum_{t=1}^{T-1} \xi_t(i,j)}{\sum_{t=1}^{T-1} \gamma_t(i)} \\
b_i(k)^{(\tau+1)} &= \frac{\sum_{t=1}^{T} \Pr(q_t = i, o_t = k | \mathbf{o}, \lambda^{(\tau)})}{\sum_{t=1}^{T} \Pr(q_t = i | \mathbf{o}, \lambda^{(\tau)})} = \frac{\sum_{t=1}^{T} \gamma_t(i) I(o_t = k)}{\sum_{t=1}^{T} \gamma_t(i)}
\end{aligned}$$

A detailed derivation can be found at

- Welch, "Hidden Markov Models and The Baum Welch Algorithm", IEEE Information Theory Society News Letter, Dec 2003

Additional function to `HMM615.h`

```
class HMM615 {
  ...
  // assign newVal to dst, after computing the relative differences between them
// note that dst is call-by-reference, and newVal is call-by-value
  static double update(double& dst, double newVal) {
    // calculate the relative differences
    double relDiff = fabs((dst-newVal)/(newVal+ZEPS));
    dst = newVal; // update the destination value
    return relDiff;
  }
  ...
};
```


Handling large number of states

```
class HMM615 {
  ...
  void normalize(std::vector<double>& v) { // additional function
    double sum = 0;
    for(int i=0; i < (int)v.size(); ++i) sum += v[i];
    for(int i=0; i < (int)v.size(); ++i) v[i] /= sum;
  }
  void forward() {
    for(int i=0; i < nStates; ++i)
      alphas.data[0][i] = pis[i] * emis.data[i][outs[0]];
    for(int t=1; t < nTimes; ++t) {
      for(int i=0; i < nStates; ++i) {
        alphas.data[t][i] = 0;
        for(int j=0; j < nStates; ++j) {
          alphas.data[t][i] += (alphas.data[t-1][j] * trans.data[j][i]
                                * emis.data[i][outs[t]]);
        }
      }
      normalize(alphas.data[t]); // **ADD THIS LINE**
    }
  }
  ...
};
```

Additional function to Matrix615.h

```
template <class T>
void Matrix615<T>::fill(T val) {
  int nr = rowNums();
  for(int i=0; i < nr; ++i) {
    std::fill(data[i].begin(),data[i].end(),val);
  }
}
```


Additional function to Matrix615.h

```
// print the content of matrix
template <class T>
void Matrix615<T>::print(std::ostream& o) {
  int nr = rowNums();
  int nc = colNums();

  for(int i=0; i < nr; ++i) {
    for(int j=0; j < nc; ++j) {
      if ( j > 0 ) o << "\t";
      o << data[i][j];
    }
    o << std::endl;
  }
}
```


Baum-Welch algorithm : initialization

```
// return a pair of (# iter, relative diff) given tolerance
std::pair<int,double> HMM615::baumWelch(double tol) {
  // temporary variables to use internally

  Matrix615<double> xis(nStates,nStates); // Pr(q_{t+1} = j | q_t = j)
  Matrix615<double> sumXis(nStates,nStates); // sum_t xis(i,j)
  Matrix615<double> sumObsGammas(nStates,nObs); // sum_t gammas(i)I(o_t=j)
  std::vector<double> sumGammas(nStates);  // sum_t gammas(i)
  double tmp, sum, relDiff = 1.;

  int iter;
  for(iter=0; (iter < MAX_ITERATION) && ( relDiff > tol ); ++iter) {
    relDiff = 0;

    // E-step : compute Pr(q|o,lambda)
    forwardBackward();
```


Baum-Welch algorithm : M-step

```
    // initialize temporary storage
    std::fill(sumGammas.begin(),sumGammas.end(),0);
    sumXis.fill(0); sumObsGammas.fill(0); xis.fill(0);

    // M-step : updates pis, trans, and emis
    for(int t=0; t < nTimes-2; ++t) {
      sum = 0;  // sum stores sum of xis
      for(int i=0; i < nStates; ++i)
        for(int j=0; j < nStates; ++j)
          sum += (xis.data[i][j] = alphas.data[t][i] * trans.data[i][j]
                  * betas.data[t+1][j] * emis.data[j][outs[t+1]]);
      // update sumGammas, sumObsGamms, sumXis
      for(int i=0; i < nStates; ++i) {
        sumGammas[i] += gammas.data[t][i];
        sumObsGammas.data[i][outs[t]] += gammas.data[t][i];
        for(int j=0; j < nStates; ++j)
          sumXis.data[i][j] += (xis.data[i][j] /= sum);
      }
    }
```

Baum-Welch algorithm : M-step

```
    for(int i=0; i < nStates; ++i) {
      relDiff += update( pis[i], sumGammas[i]/(nTimes-1) );
      for(int j=0; j < nStates; ++j) {
        relDiff += update(trans.data[i][j],
           sumXis.data[i][j] / (sumGammas[i] - gammas.data[nTimes-1][i] + ZEPS));
      }
      for(int j=0; j < nObs; ++j ) {
        relDiff += update(emis.data[i][j],
           sumObsGammas.data[i][j] / (sumGammas[i] + ZEPS) );
      }
    }
  }
  return std::pair<int,double>(iter,relDiff);
}
```


A working example : Biased dice example

- Observations : $O = \{1, 2, \cdots, 6\}$
- Hidden states : $S = \{FAIR, 1 - BIASED, \cdots, 6 - BIASED\}$
- Priors : $\pi = \{0.70, 0.05, 0.05, \cdots, 0.05\}$
- Transition matrix :

$$A = \begin{pmatrix} 0.94 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.94 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.94 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.94 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.94 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.94 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.94 \end{pmatrix}$$

- Emission matrix :

$$B = \begin{pmatrix} 1/6 & 1/6 & 1/6 & 1/6 & 1/6 & 1/6 \\ 0.95 & 0.01 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.95 & 0.01 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.95 & 0.01 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.95 & 0.01 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.95 & 0.01 \\ 0.01 & 0.01 & 0.01 & 0.01 & 0.01 & 0.95 \end{pmatrix}$$

Biased dice example : `main()` function

```
#include <iostream>
#include <iomanip>
#include "Matrix615.h"
#include "HMM615.h"
int main(int argc, char** argv) {
  if ( argc != 5 ) {
    std::cerr << "Usage: baumWelch [trans0] [emis0] [pis0] [obs]" << std::endl;
    return -1;
  }

  std::vector<int> obs;
  Matrix615<double> trans(argv[1]);
  int ns = trans.rowNums();
  if ( ns != trans.colNums() ) {
    std::cerr << "Transition matrix is not square" << std::endl;
    return -1;
  }

  Matrix615<double> emis(argv[2]);
```


Biased dice example : `main()` function (cont'd)

```
if ( ns != emis.rowNums() ) {
  std::cerr << "Emission and transition matrices do not match" << std::endl;
  return -1;
}
int no = emis.colNums();

readFromFile<int> (obs, argv[4]);
int nt = (int)obs.size();

HMM615 hmm(ns, no, nt);

readFromFile<double> (hmm.pis, argv[3]);
if ( ns != (int)hmm.pis.size() ) {
  std::cerr << "Transition and Prior matrices do not match" << std::endl;
  return -1;
}
hmm.trans = trans;
hmm.emis = emis;
hmm.outs = obs;
```

Biased dice example : main() function (cont'd)

```
  std::pair<int,double> result = hmm.baumWelch(1e-6);

  std::cout << "# ITERATIONS : " << result.first << "\t";
  std::cout << "SUM RELATIVE DIFF : " << result.second << std::endl;
  std::cout << std::fixed << std::setprecision(5);
  std::cout << "PIS:" << std::endl;
  for(int i=0; i < ns; ++i) {
    if ( i > 0 ) std::cout << "\t";
    std::cout << hmm.pis[i];
  }
  std::cout << std::endl;
  std::cout << "------------------------------------------------------------" << std::endl;
  std::cout << "TRANS:" << std::endl;
  hmm.trans.print(std::cout);
  std::cout << "------------------------------------------------------------" << std::endl;
  std::cout << "EMIS:" << std::endl;
  hmm.emis.print(std::cout);
  std::cout << "------------------------------------------------------------" << std::endl;
  return 0;
}
```


Biased dice example : Results with 20,000 samples

```
$ ./baumWelch trans.dice.txt emis.dice.txt pis.dice.txt outs.dice.txt
# ITERATIONS : 23       SUM RELATIVE DIFF : 9.80431e-07
PIS:
0.14951 0.13582 0.12723 0.16745 0.14518 0.13736 0.13739
------------------------------------------------------------
TRANS:
0.94159 0.00924 0.01111 0.01126 0.00741 0.01374 0.00569
0.01018 0.93318 0.00870 0.01134 0.00943 0.01317 0.01401
0.00604 0.01632 0.93780 0.00884 0.01215 0.01029 0.00855
0.01189 0.00874 0.00855 0.94798 0.00932 0.00724 0.00641
0.01172 0.00859 0.00735 0.00957 0.94645 0.00688 0.00944
0.00874 0.00969 0.01066 0.01206 0.00886 0.93777 0.01235
0.01215 0.01143 0.00803 0.01010 0.00774 0.00876 0.94180
------------------------------------------------------------
EMIS:
0.16357 0.16859 0.17141 0.16421 0.15995 0.17227
0.94908 0.01052 0.01026 0.01450 0.00669 0.00895
0.00624 0.95081 0.01055 0.01392 0.00936 0.00912
0.01113 0.01117 0.95023 0.00826 0.00948 0.00974
0.01012 0.00871 0.00989 0.95121 0.01051 0.00956
0.00877 0.00848 0.00983 0.00827 0.95513 0.00951
0.00956 0.00874 0.00722 0.00981 0.01338 0.95128
------------------------------------------------------------
```


Biased dice example : Starting with uniform parameters

```
$ ./baumWelch trans0.dice.txt emis0.dice.txt pis0.dice.txt outs.dice.txt
# ITERATIONS : 2        SUM RELATIVE DIFF : 0
PIS:
0.14285 0.14285 0.14285 0.14285 0.14285 0.14285 0.14285
------------------------------------------------------------
TRANS:
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
0.14286 0.14286 0.14286 0.14286 0.14286 0.14286 0.14286
------------------------------------------------------------
EMIS:
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
0.16002 0.15312 0.19127 0.17027 0.16217 0.16317
------------------------------------------------------------
```


Starting with incorrect emission matrix

```
$ cat emis1.dice.txt
0.16666667 0.16666667 0.16666667 0.16666667 0.16666667 0.16666667
0.5 0.1 0.1 0.1 0.1 0.1
0.1 0.5 0.1 0.1 0.1 0.1
0.1 0.1 0.5 0.1 0.1 0.1
0.1 0.1 0.1 0.5 0.1 0.1
0.1 0.1 0.1 0.1 0.5 0.1
0.1 0.1 0.1 0.1 0.1 0.5
```

Starting with incorrect emission matrix

```
$ ./baumWelch trans0.dice.txt emis1.dice.txt pis0.dice.txt outs.dice.txt
# ITERATIONS : 37       SUM RELATIVE DIFF : 7.50798e-07
PIS:
0.14951 0.13582 0.12723 0.16745 0.14518 0.13736 0.13739
------------------------------------------------------------
TRANS:
0.94159 0.00924 0.01111 0.01126 0.00741 0.01374 0.00569
0.01018 0.93318 0.00870 0.01134 0.00943 0.01317 0.01401
0.00604 0.01632 0.93780 0.00884 0.01215 0.01029 0.00855
0.01189 0.00874 0.00855 0.94798 0.00932 0.00724 0.00641
0.01172 0.00859 0.00735 0.00957 0.94645 0.00688 0.00944
0.00874 0.00969 0.01066 0.01206 0.00886 0.93777 0.01235
0.01215 0.01143 0.00803 0.01010 0.00774 0.00876 0.94180
------------------------------------------------------------
EMIS:
0.16357 0.16859 0.17141 0.16421 0.15995 0.17227
0.94908 0.01052 0.01026 0.01450 0.00669 0.00895
0.00624 0.95081 0.01055 0.01392 0.00936 0.00912
0.01113 0.01117 0.95023 0.00826 0.00948 0.00974
0.01012 0.00871 0.00989 0.95121 0.01051 0.00956
0.00877 0.00848 0.00983 0.00827 0.95513 0.00951
0.00956 0.00874 0.00722 0.00981 0.01338 0.95128
------------------------------------------------------------
```


Summary : Baum-Welch Algorithm

- E-M algorithm for estimating HMM parameters
- Assumes identical transition and emission probabilities across t
- The framework can be accomodated for differently contrained HMM
- Requires many observations to reach a reliable estimates

Rapid Inference with Uniform HMM

Uniform HMM

- Definition
  - $\pi_i = 1/n$
  - $a_{ij} = \begin{cases} \frac{\theta}{n} & i \neq j \\ 1 - \frac{n-1}{n}\theta & i = j \end{cases}$
  - $b_i(k)$ has no restriction.
- Independent transition between n states
- Useful model in genetics and speech recognition.

The Problem

- The time complexity of HMM inference is $O(n^2 T)$.
- For large n, this still can be a substantial computational burden.
- Can we reduce the time complexity by leveraging the simplicity?

Forward Algorithm with Uniform HMM

Original Forward Algorithm

$$\alpha_t(i) = \Pr(o_1, \cdots, o_t, q_t = i|\lambda) = \left[\sum_{j=1}^n \alpha_{t-1}(j) a_{ij}\right] b_i(o_t)$$

Rapid Forward Algorithm for Uniform HMM

$$\begin{aligned} \alpha_t(i) &= \left[\sum_{j=1}^n \alpha_{t-1}(j) a_{ij}\right] b_i(o_t) \\ &= \left[(1 - \tfrac{n-1}{n}\theta)\alpha_{t-1}(i) + \textstyle\sum_{j \neq i} \alpha_{t-1}(j) \frac{\theta}{n}\right] b_i(o_t) \\ &= \left[(1-\theta)\alpha_{t-1}(i) + \frac{\theta}{n}\right] b_i(o_t) \end{aligned}$$

- Assuming normalizaed $\sum_i \alpha_t(i) = 1$ for every t.
- The total time complexity is $O(nT)$.

Backward Algorithm with Uniform HMM

Original Forward Algorithm

$$\beta_t(i) = \Pr(o_{t+1}, \cdots, o_T | q_t = i, \lambda) = \sum_{j=1}^{n} \beta_{t+1}(j) a_{ji} b_j(o_{t+1})$$

Rapid Forward Algorithm for Uniform HMM

$$\begin{aligned}
\beta_t(i) &= \sum_{j=1}^{n} \beta_{t+1}(j) a_{ji} b_j(o_{t+1}) \\
&= (1 - \tfrac{n-1}{n}\theta)\beta_{t+1}(i) b_i(o_{t+1}) + \tfrac{\theta}{n} \textstyle\sum_{j \neq i} \beta_{t+1}(j) b_j(o_{t+1}) \\
&= (1-\theta)\beta_{t+1}(i) b_i(o_{t+1}) + \frac{\theta}{n}
\end{aligned}$$

Assuming $\sum_i \beta_t(i) b_i(o_t) = 1$ for every t.

Implementing Uniform HMM

```
#include <cmath>
#include "Matrix615.h"
class uHMM615 {
 public:
  int n; // number of states and observations
  int T; // number of time slots;
  double theta; // trans(i,j) = theta/n if ( i != j)
  Matrix615<double> emis;
  Matrix615<double> alphas;
  Matrix615<double> betas;
  Matrix615<double> gammas;
  std::vector<int> outs;
  uHMM615(int _n, int _T, int _o);
  // constructor : theta and emis has to be set separately
```


Implementing Uniform HMM

```
  void normalizeAlpha(std::vector<double>& v);       // normalize alphas
  void normalizeBeta(std::vector<double>& v, int o); // normalize betas
  double trans(int i, int j) {  // transition probability
    return ( i == j ) ? ( 1 - theta + theta / n ) : theta / n;
  }
  void forward();  // efficient forward algorithm
  void backward(); // efficient backward algorithm
  void forwardBackward(); // forward-backward algorithm
};
```


Example run from homework

```
....
990     27      0.000127432     0.000127432
991     68      0.999996        0.999996
992     68      0.999996        0.999996
993     63      0.000129007     0.000129007
994     68      0.999988        0.999988
995     1       0.000129009     0.000129009
996     68      0.999996        0.999996
997     68      0.999996        0.999996
998     85      0.000140803     0.000140803
999     68      0.999957        0.999957
1000    68      0.998875        0.998875
Uniform HMM: 0.09 seconds
Regular HMM: 4.88 seconds
```

Summary : Uniform HMM

- Rapid computation of forward-backward algorithm leveraging symmetric structure
- Rapid Baum-Welch algorithm is also possible in a similar manner
- It is important to understand the computational details of exisitng methods to further tweak the method when necessary.