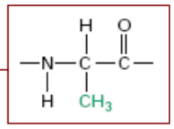
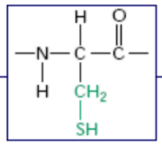
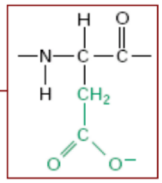
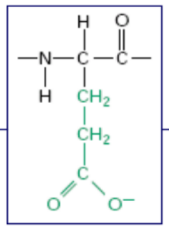
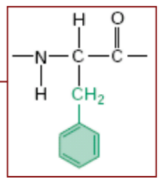
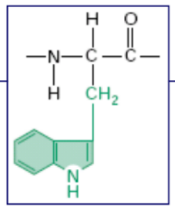
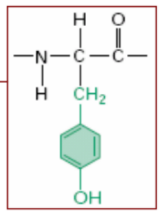
Peptid de novo Sequenzierung

Aminosäure-Reste

A:	Alanin	(Ala)		$C_3H_5N_1O_1$	71.037
C:	Cystein	(Cys)		$C_3H_5N_1O_1S_1$	103.009
D:	Asparaginsäure	(Asp)		$C_4H_5N_1O_3$	115.026
E:	Glutaminsäure	(Glu)		$C_5H_7N_1O_3$	129.042
F:	Phenylalanin	(Phe)		$C_9H_9N_1O_1$	147.068
...	...	...		...	...
W:	Tryptophan	(Trp)		$C_{11}H_{10}N_2O_1$	186.079
Y:	Tyrosin	(Tyr)		$C_9H_9N_1O_2$	163.063

Rekurrenz von Bafna & Edwards (2003)

THEOREM 2.:

$$
S[0][v][w] = \begin{cases} 0 & \text{if } \mathrm{RM}[v] \le \mathrm{RM}[w], \\ & \quad \mathrm{RM}[v] \in \mathcal{V}_M, \\ & \quad \mathrm{RM}[w] - \mathrm{RM}[v] \in \mathcal{V}_M, \\ & \quad M - \mathrm{RM}[w] \in \mathcal{V}_M; \\ -\infty & \text{otherwise.} \end{cases}
$$

$$
S[i][v][w] = \max \begin{cases} S[i-1][v][w] + \delta(i, \phi); \\ S[i-1][u][w] + \delta(i, \iota), \\ \quad \forall\ u\ s.t.\ \mathrm{RM}[u] = r_i(\iota) \in R_i^L, \\ \qquad \mathrm{RM}[u] \ge \mathrm{RM}[v], \\ \qquad \mathrm{RM}[u] - \mathrm{RM}[v] \in \mathcal{V}_M, \\ \qquad \mathrm{RM}[w] - \mathrm{RM}[u] \in \mathcal{V}_M; \\ S[i-1][v][u] + \delta(i, \iota), \\ \quad \forall\ u\ s.t.\ \mathrm{RM}[u] = r_i(\iota) \in R_i^R, \\ \qquad \mathrm{RM}[u] \le \mathrm{RM}[w], \\ \qquad \mathrm{RM}[u] - \mathrm{RM}[v] \in \mathcal{V}_M, \\ \qquad \mathrm{RM}[w] - \mathrm{RM}[u] \in \mathcal{V}_M. \end{cases}
$$

Fischer et al, NovoHMM (2005)

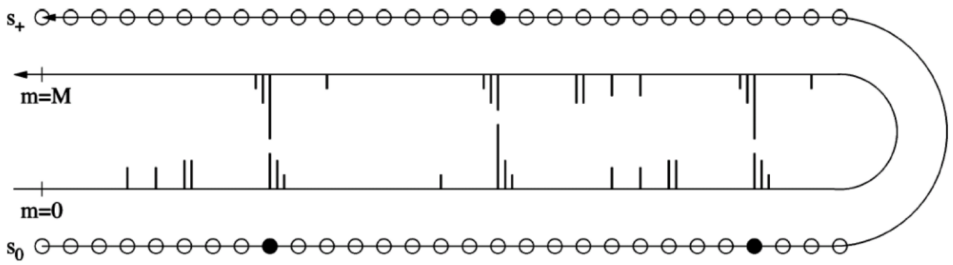


Figure 4. Folding the spectrum in the middle illustrates the internal mirror symmetry of the problem. The Markov chain models a sequence with four amino acids. The filled circles correspond to the amino acid boundaries. Around each amino acid boundary a peak pattern is generated, once for the N-terminal fragments and once for the C-terminal fragments.

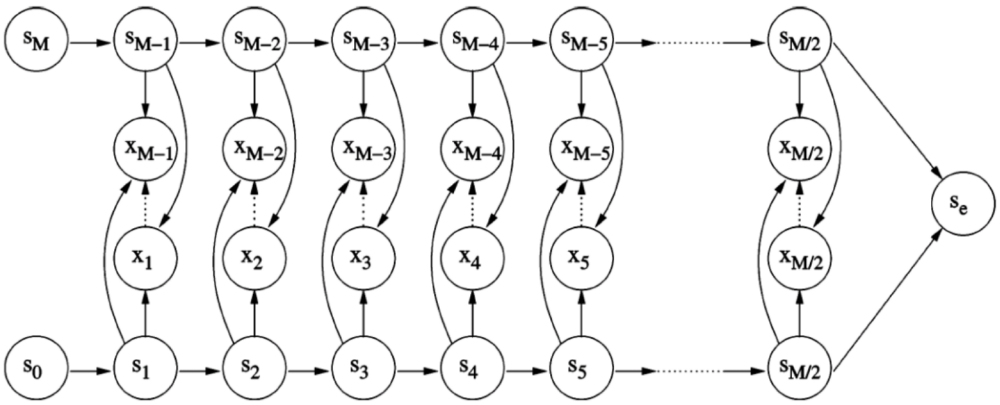


Figure 5. The dependency structure of the factorial hidden Markov model consists of two Markov chains, one for the first half of the peptide and one for the second half of the peptide. The emission variables depend on both Markov chains, thereby coupling them.