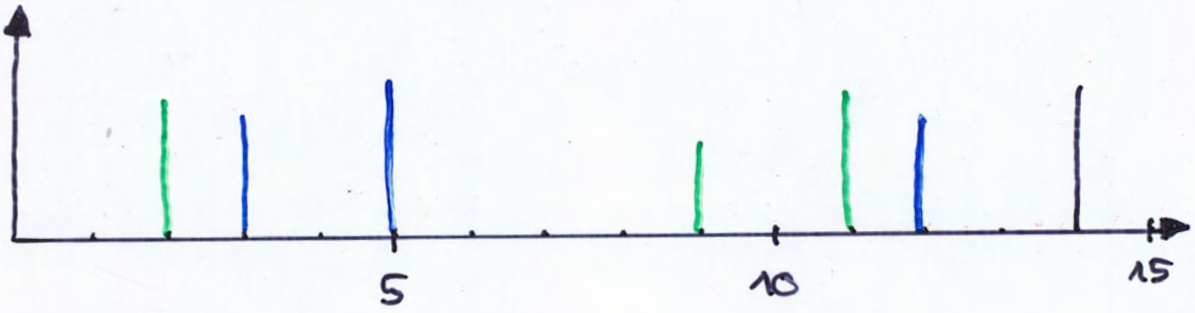
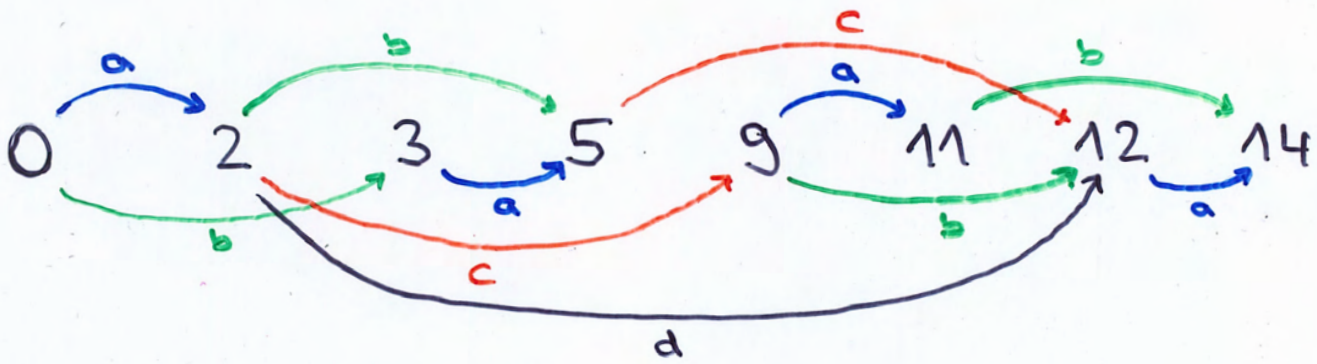
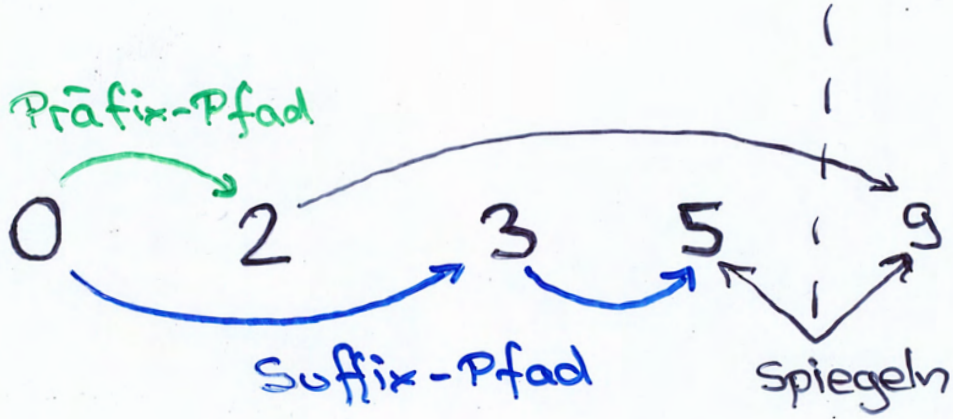
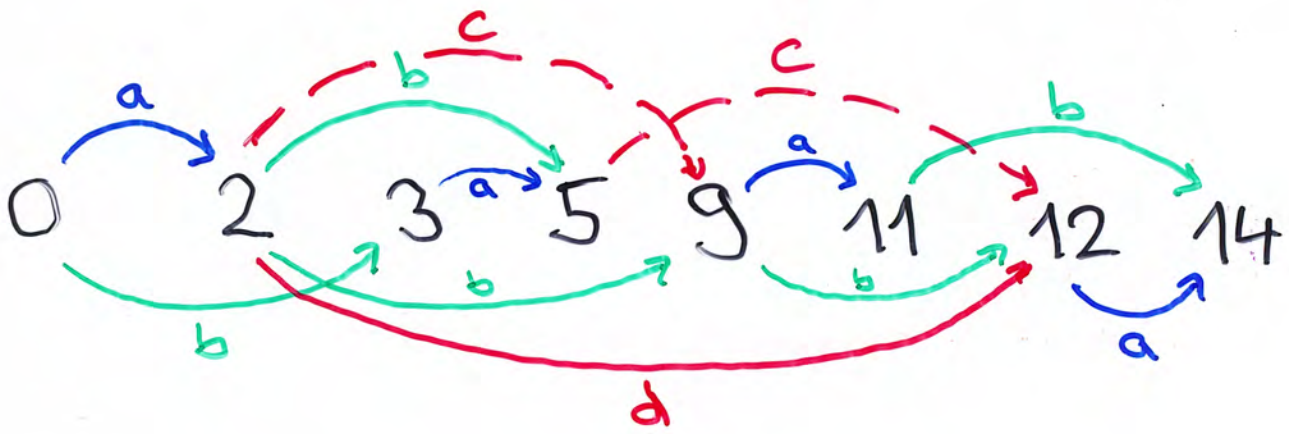
$$\mathcal{M} = \{0, 2, 3, 5, 9, 11, 12, 14\}$$





$x_0 = 0 \quad x_1 = 2 \quad x_2 = 3 \quad x_3 = 5 \quad | \quad y_3 = 9 \quad y_2 = 11 \quad y_1 = 12 \quad y_0 = 14$





	$x_0=0$	$x_1=2$	$x_2=3$	$x_3=5$	
$x_0=0$	0	1	1	2	
$x_1=2$	1	$-\infty$	2	3	Kante (x_3, y_1) ✓
$x_2=3$	1	2	$-\infty$	3	keine Kante (x_3, y_2) ✗
$x_3=5$	2	3	3	$-\infty$	

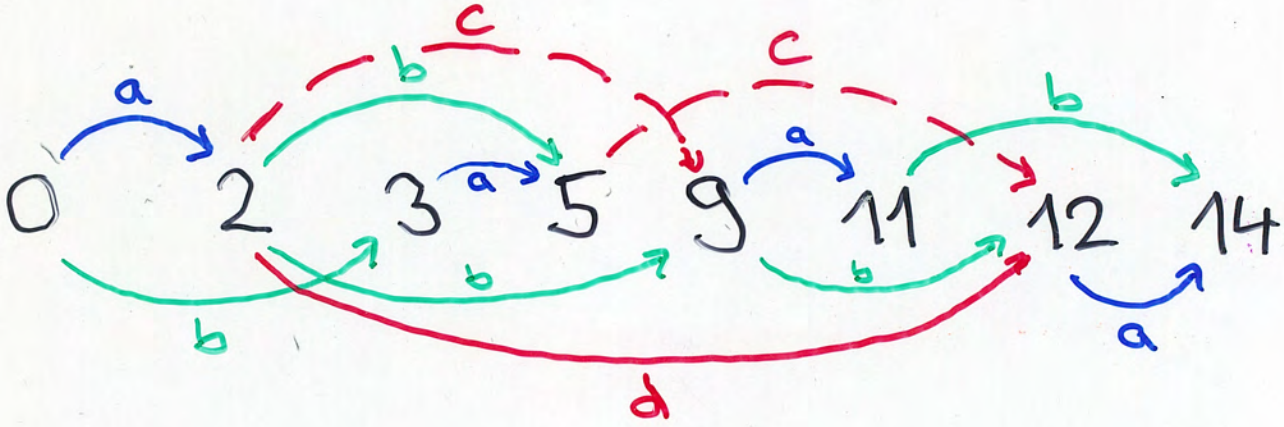
Symmetrie

Backtracing: 0 3 5 12 14

b a c a

↑ starte hier!

$D[3,1]=3$, $y_1 - x_3 = 7 = \mu(c)$



	$x_0=0$	$x_1=2$	$x_2=3$	$x_3=5$	
$x_0=0$	0	1	1	2	
$x_1=2$	1	$-\infty$	2	3	Kante (x_3, y_1) ✓
$x_2=3$	1	2	$-\infty$	3	keine Kante (x_3, y_2) ✗
$x_3=5$	2	3	3	$-\infty$	

Berechnung für Q symmetrisch

Symmetrie

Backtracing: 0 3 5 12 14

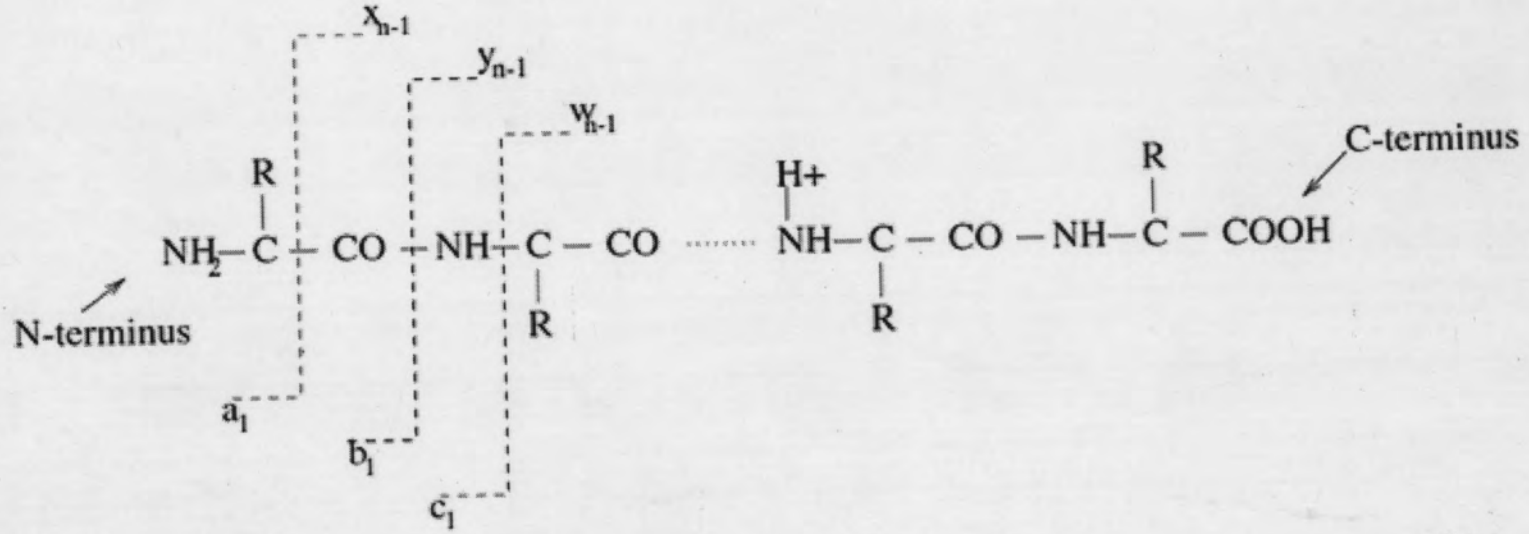
b a c a

↑ starte hier!

$D[3,1]=3$, $y_1 - x_3 = 7 = \mu(c)$

Collision-induced Fragmentation

- By collision with neutral gas molecules, fragmentation is induced by transfer of kinetic energy from the neutral gas molecules to the peptide.
- Commonly occurs at peptide bonds.
- Forms pairs of ions: b- and y-ions (most common), a- and z-ions, c- and x-ions.



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)

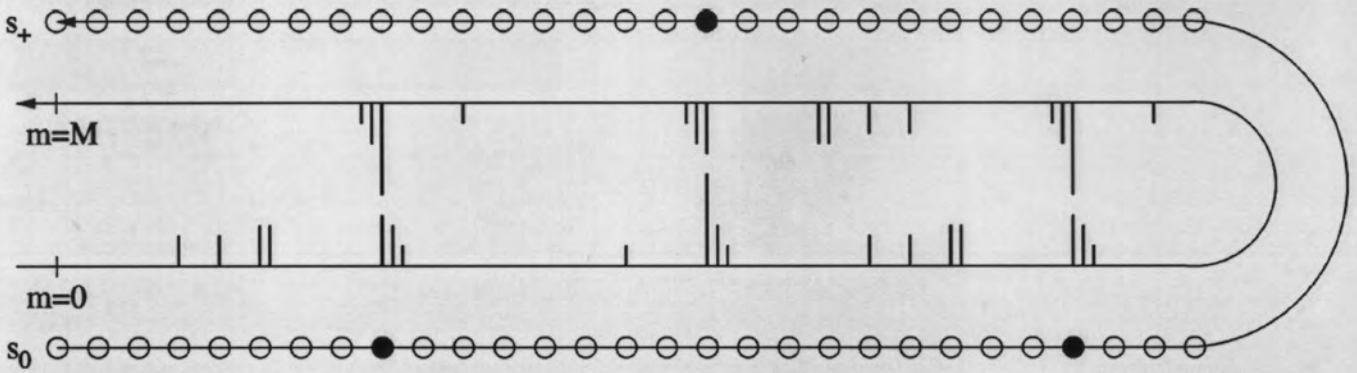


Figure 4. Folding the spectrum in the middle illustrates the internal mirror symmetry of the problem. The Markov chain models a sequence with four amino acids. The filled circles correspond to the amino acid boundaries. Around each amino acid boundary a peak pattern is generated, once for the N-terminal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

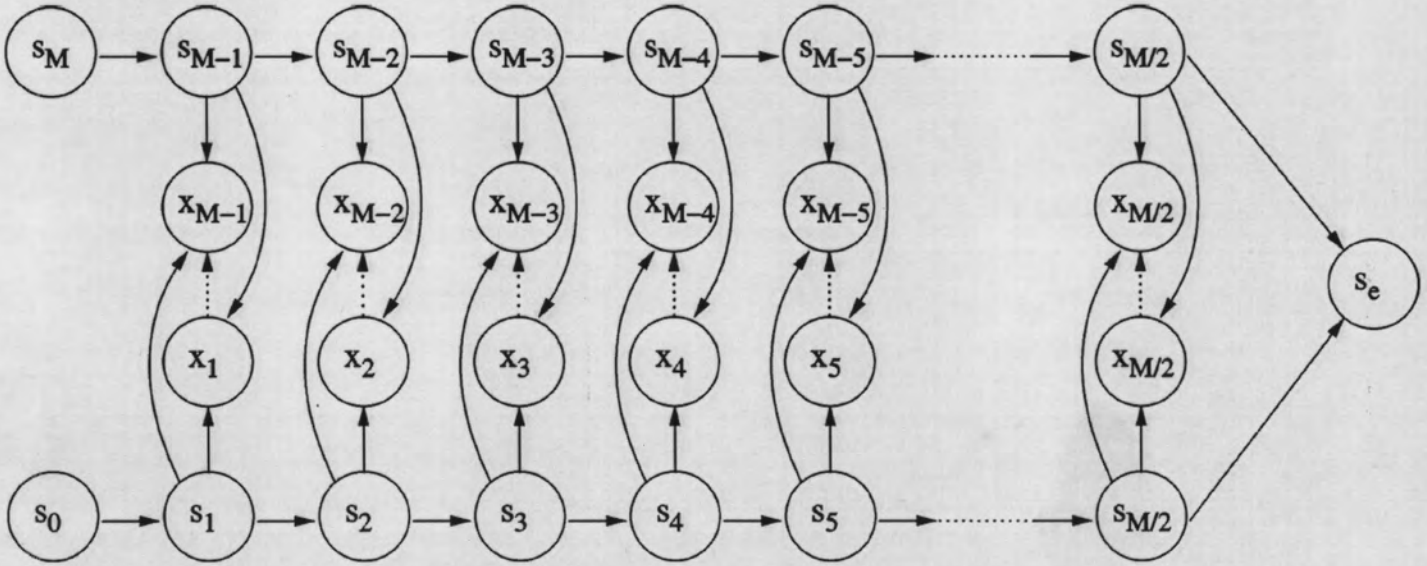
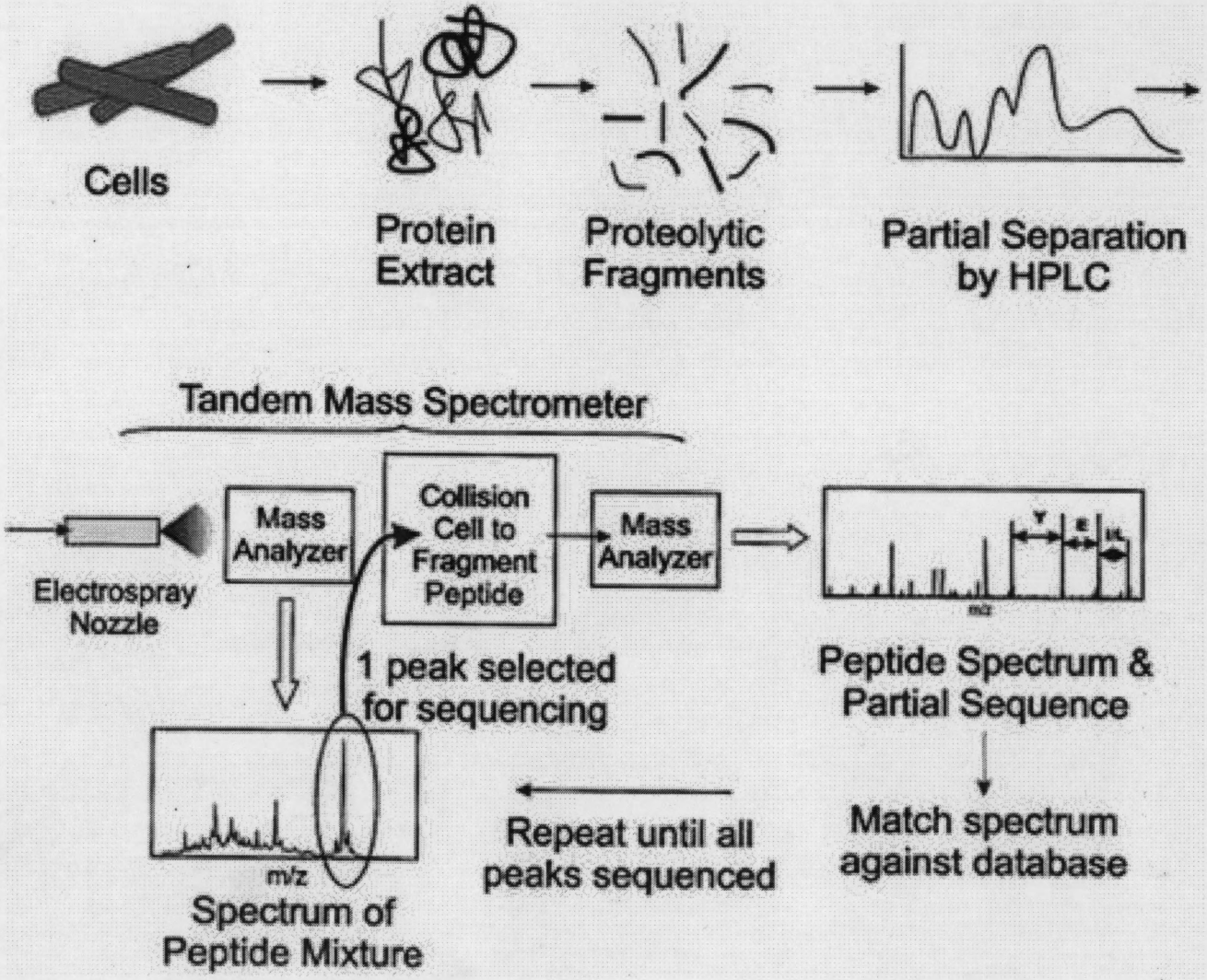


Figure 5. The dependency structure of the factorial hidden Markov model consists of two Markov chains, one for the first half of the peptide and one for the second half of the peptide. The emission variables depend on both Markov chains, thereby coupling them.

Analysis of a Peptide



Peptid denovo Seq.: Rekurrenz für ideale Daten

$$D[i,j] = \begin{cases} D[i-1,j] & \text{falls } i \geq j+2,\ (x_{i-1},x_i) \in E \quad \text{(nicht} \\ D[i,j-1] & \text{falls } j \geq i+2,\ (x_{j-1},x_j) \in E \quad \text{Nebendiag.)} \\ \max\{D[\ell,j] : (x_\ell, x_{j+1}) \in E,\ \ell = 0,\dots,j-1\} & \text{falls } i = j+1 \\ \max\{D[i,\ell] : (x_\ell, x_{i+1}) \in E,\ \ell = 0,\dots,i-1\} & \text{falls } j = i+1 \\ 1 & \text{falls } i=j=0 \quad \text{(Init)} \\ 0 & \text{sonst} \end{cases}$$

Fülle Matrix $i=0,\dots,n$ und $j=0,\dots,n$