

Generalized Algebraic Dynamic Programming: ADP over General Data Structures

Bled 2015

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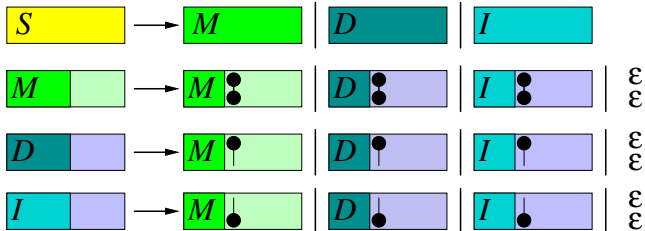
Bioinformatics Group, Dept. of Computer Science, University of Leipzig

Institute for Theoretical Chemistry, University of Vienna

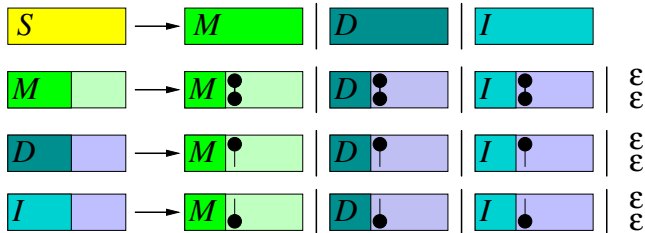
The Church of 

Feb 15, 2015 – Feb 22, 2015

Alignment with Affine Gap Costs (Gotoh)



Alignment with Affine Gap Costs (Gotoh)



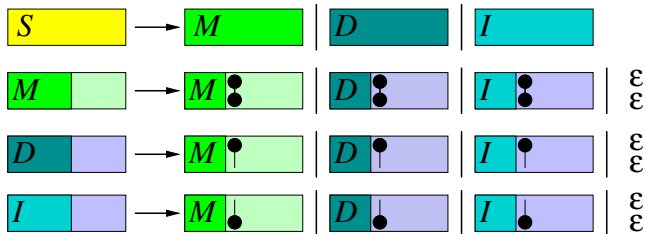
$$\begin{array}{l}
 S \rightarrow M \quad | \quad D \quad | \quad I \\
 M \rightarrow M(\overset{u}{\underset{v}{|}}) \quad | \quad D(\overset{u}{\underset{v}{|}}) \quad | \quad I(\overset{u}{\underset{v}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}}) \\
 D \rightarrow M(\overset{u}{\underset{-}{|}}) \quad | \quad D(\overset{u}{\underset{-}{|}}) \quad | \quad I(\overset{u}{\underset{-}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}}) \\
 I \rightarrow M(\overset{-}{\underset{v}{|}}) \quad | \quad D(\overset{-}{\underset{v}{|}}) \quad | \quad I(\overset{-}{\underset{v}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}})
 \end{array}$$

Alignment with Affine Gap Costs (Gotoh)

$$\begin{array}{l}
 S_{m,n} \rightarrow M_{m,n} \quad | \quad D_{m,n} \quad | \quad I_{m,n} \\
 M_{i,j} \rightarrow M_{i-1,j-1} \left(\begin{array}{c} u_i \\ v_j \end{array} \right) \quad | \quad D_{i-1,j-1} \left(\begin{array}{c} u_i \\ v_j \end{array} \right) \quad | \quad I_{i-1,j-1} \left(\begin{array}{c} u_i \\ v_j \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon_0 \\ \varepsilon_0 \end{pmatrix} \\
 D_{i,j} \rightarrow M_{i-1,j} \left(\begin{array}{c} u_i \\ - \end{array} \right) \quad | \quad D_{i-1,j} \left(\begin{array}{c} u_i \\ \cdot \end{array} \right) \quad | \quad I_{i-1,j} \left(\begin{array}{c} u_i \\ - \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon_0 \\ \varepsilon_0 \end{pmatrix} \\
 I_{i,j} \rightarrow M_{i,j-1} \left(\begin{array}{c} - \\ v_j \end{array} \right) \quad | \quad D_{i,j-1} \left(\begin{array}{c} - \\ v_j \end{array} \right) \quad | \quad I_{i,j-1} \left(\begin{array}{c} \cdot \\ v_j \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon_0 \\ \varepsilon_0 \end{pmatrix}
 \end{array}$$

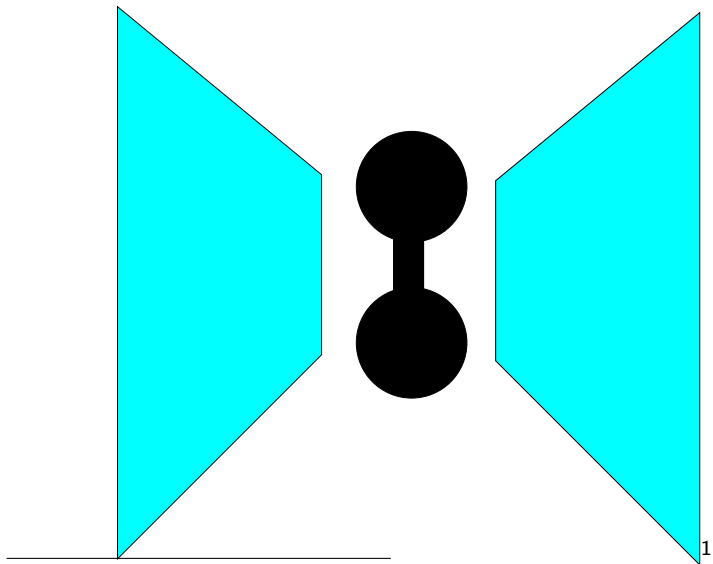
$$\begin{array}{l}
 S \rightarrow M \quad | \quad D \quad | \quad I \\
 M \rightarrow M \left(\begin{array}{c} u \\ v \end{array} \right) \quad | \quad D \left(\begin{array}{c} u \\ v \end{array} \right) \quad | \quad I \left(\begin{array}{c} u \\ v \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon \\ \varepsilon \end{pmatrix} \\
 D \rightarrow M \left(\begin{array}{c} u \\ - \end{array} \right) \quad | \quad D \left(\begin{array}{c} u \\ \cdot \end{array} \right) \quad | \quad I \left(\begin{array}{c} u \\ - \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon \\ \varepsilon \end{pmatrix} \\
 I \rightarrow M \left(\begin{array}{c} - \\ v \end{array} \right) \quad | \quad D \left(\begin{array}{c} - \\ v \end{array} \right) \quad | \quad I \left(\begin{array}{c} \cdot \\ v \end{array} \right) \quad | \quad \begin{pmatrix} \varepsilon \\ \varepsilon \end{pmatrix}
 \end{array}$$

Alignment with Affine Gap Costs (Gotoh)



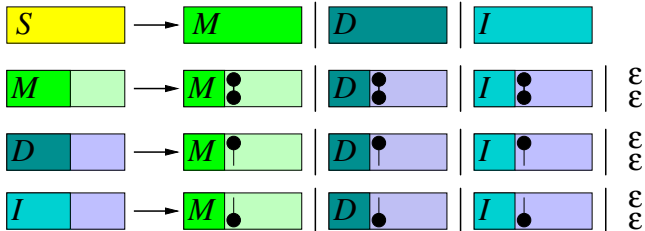
$$\begin{array}{l}
 S \rightarrow M \quad | \quad D \quad | \quad I \\
 M \rightarrow M(\overset{u}{\underset{v}{|}}) \quad | \quad D(\overset{u}{\underset{v}{|}}) \quad | \quad I(\overset{u}{\underset{v}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}}) \\
 D \rightarrow M(\overset{u}{\underset{-}{|}}) \quad | \quad D(\overset{u}{\underset{-}{|}}) \quad | \quad I(\overset{u}{\underset{-}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}}) \\
 I \rightarrow M(\overset{-}{\underset{v}{|}}) \quad | \quad D(\overset{-}{\underset{v}{|}}) \quad | \quad I(\overset{-}{\underset{v}{|}}) \quad | \quad (\overset{\varepsilon}{\underset{\varepsilon}{|}})
 \end{array}$$

Inside and Outside Combined

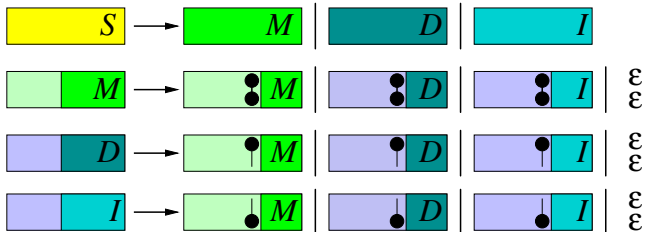
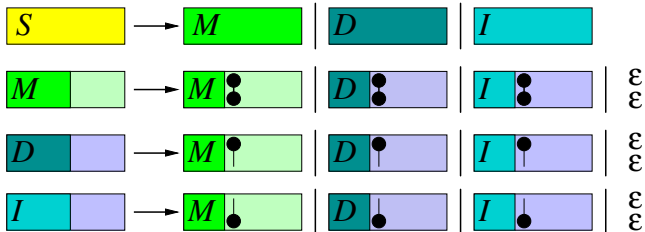


¹abstract art

Outside Gotoh: Just Mirror the Grammar?

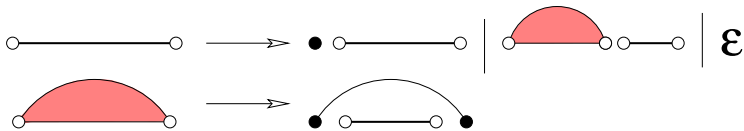


Outside Gotoh: Just Mirror the Grammar?



Unfortunately only a Special Case

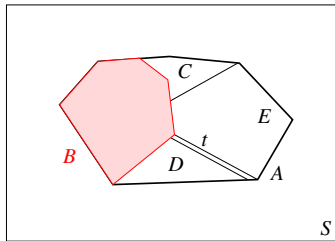
how would you mirror this RNA folding grammar?



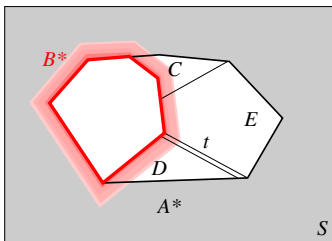
“mirroring” doesn’t generalize!

Inside to Outside Productions

Inside



Outside



$$A \cup A^* = S$$

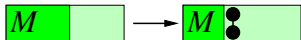
$$A \rightarrow BCDEt$$

$$B^* \rightarrow A^*CDEt$$

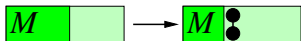
$$C^* \rightarrow BA^*DEt$$

\vdots

Outside Rules Step by Step

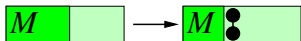


Outside Rules Step by Step

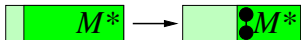


$$M_{i,j} \rightarrow M_{i-1,j-1} \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

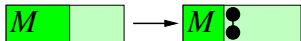
Outside Rules Step by Step



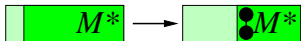
$$M_{i,j} \rightarrow M_{i-1,j-1} \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$



Outside Rules Step by Step

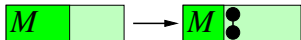


$$M_{i,j} \rightarrow M_{i-1,j-1} \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

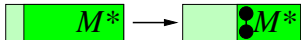


$$M_{i-1,j-1}^* \rightarrow M_{i,j}^* \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

Outside Rules Step by Step



$$M_{i,j} \rightarrow M_{i-1,j-1} \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

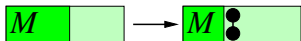


$$M_{i-1,j-1}^* \rightarrow M_{i,j}^* \begin{pmatrix} u_j \\ v_j \end{pmatrix}$$

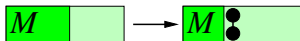
rewrite indices: +1/+1

$$M_{i,j}^* \rightarrow M_{i+1,j+1}^* \begin{pmatrix} u_{j+1} \\ v_{j+1} \end{pmatrix}$$

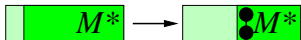
Outside Rules Step by Step



$$M_{i,j} \rightarrow M_{i-1,j-1} \begin{pmatrix} u_i \\ v_j \end{pmatrix}$$



$$M \rightarrow M \begin{pmatrix} u \\ v \end{pmatrix}$$

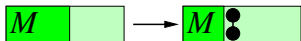


$$M_{i-1,j-1}^* \rightarrow M_{i,j}^* \begin{pmatrix} u_i \\ v_j \end{pmatrix}$$

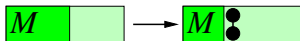
rewrite indices: +1/+1

$$M_{i,j}^* \rightarrow M_{i+1,j+1}^* \begin{pmatrix} u_{i+1} \\ v_{j+1} \end{pmatrix}$$

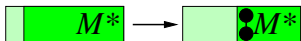
Outside Rules Step by Step



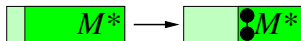
$$M_{i,j} \rightarrow M_{i-1,j-1} \left(\begin{array}{c} u_i \\ v_j \end{array} \right)$$



$$M \rightarrow M \left(\begin{array}{c} u \\ v \end{array} \right)$$



$$M_{i-1,j-1}^* \rightarrow M_{i,j}^* \left(\begin{array}{c} u_i \\ v_j \end{array} \right)$$



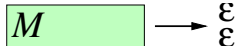
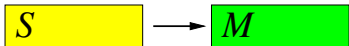
$$M^* \rightarrow M^* \left(\begin{array}{c} u \\ v \end{array} \right)$$

rewrite indices: +1/+1

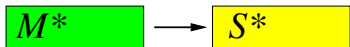
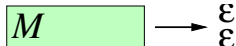
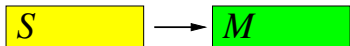
$$M_{i,j}^* \rightarrow M_{i+1,j+1}^* \left(\begin{array}{c} u_{i+1} \\ v_{j+1} \end{array} \right)$$

no rewrite necessary,
let ADPfusion figure it
out

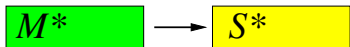
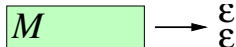
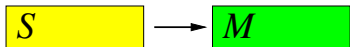
Start and End Symbols



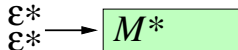
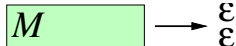
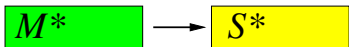
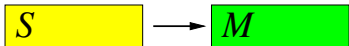
Start and End Symbols



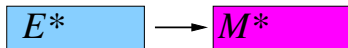
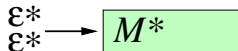
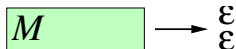
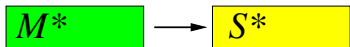
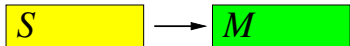
Start and End Symbols



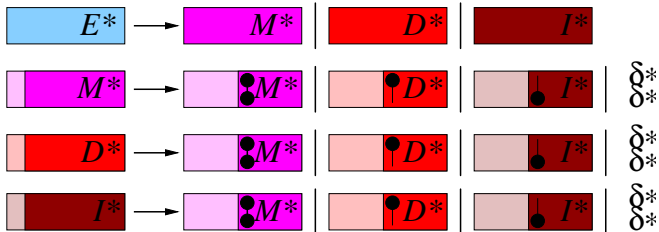
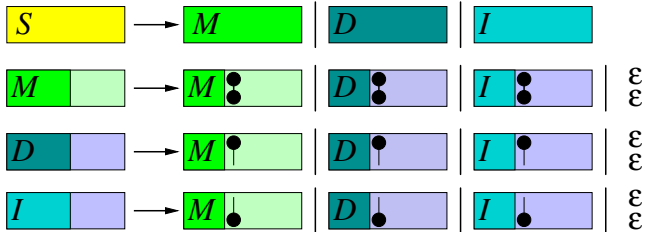
Start and End Symbols



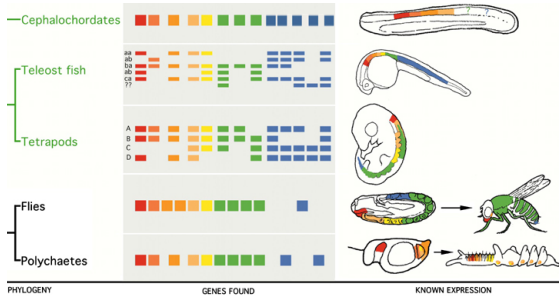
Start and End Symbols



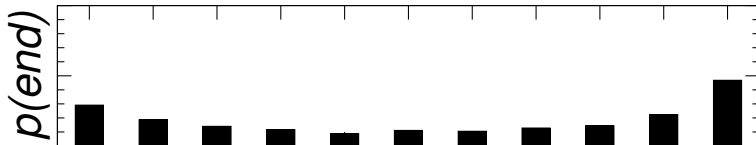
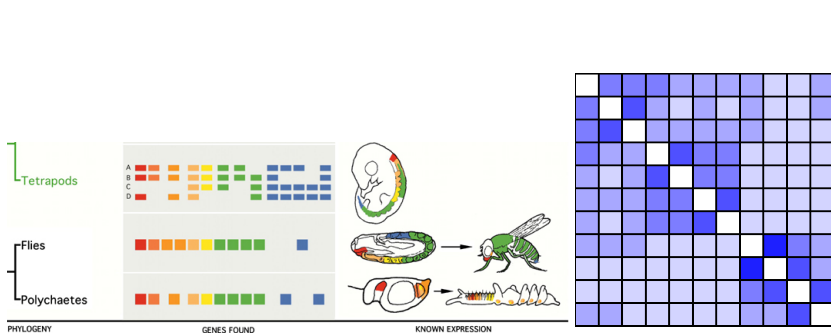
Inside & Outside Gotoh



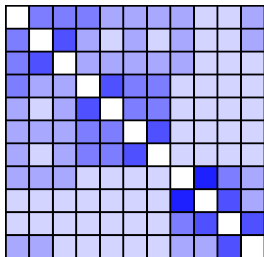
Hox Cluster History



Extracting Summary Information



Calculate Edge Probabilities



$$P(i \sim j) = \frac{1}{Z(S)} \sum_{p,q} \sum_{ACS} Z([p, A, i]) Z(\langle i, j \rangle) Z([j, S \setminus A, q]).$$

$$S_{p,q} \rightarrow A_{p,q}$$

$$A_{p,q} \rightarrow \varepsilon$$

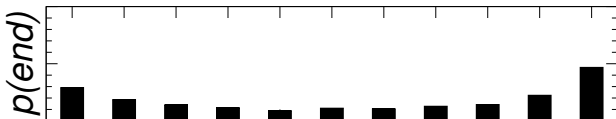
$$A_{p,q} \rightarrow A_{p,k}(k, q)$$

$$S \rightarrow A_{p,i}(i, j) A_{j,q}^*$$

$$A_{p,q} \text{ as left}$$

$$A_{p,q}^* \text{ mechanically derived}$$

Calculate End Probabilities



$$P(q \text{ is end}) = \frac{1}{Z(S)} \sum_{p, A \in S} Z([p, A, q]).$$

$$S_{p,q} \rightarrow A_{p,q}$$

$$A_{p,q} \rightarrow \varepsilon$$

$$A_{p,q} \rightarrow A_{p,k}(k, q)$$

$$S_i \rightarrow A_{p,i}$$

$$A_{p,q} \text{ as left}$$

Generalized ADP

Outside Grammars automatically derived from Inside grammars

Type-Rich DP index-type generic framework (with sequences and sets as examples)

- efficient algorithms as usual
- compatible with grammar products (grammars are objects)

Höner zu Siederdisen, Prohaska, Stadler. 2015

Algebraic Dynamic Programming over General Data Structures.

Hox figure: Building divergent body plans with similar genetic pathways; B J Swalla; Heredity