Nussinov algorithm

- Algorithm to predict RNA structure
- also called RNA folding

- it maximise base pairs

Nussinov-Matrix

- Matrix N is used as a data structure
- Length of RNA sequence S: n
- Matrix dimensions: n * n

Nussinov-Matrix

- Matrix N
- N_{ij} = max(|P| | is non-crossing RNA ij-substructure of S)
- non-crossing:

Nussinov algorithm

- $N_{ii} = 0$; $N_{ii-1} = 0$

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max_{\substack{i \leq k < j \\ S_k, S_j complementary}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

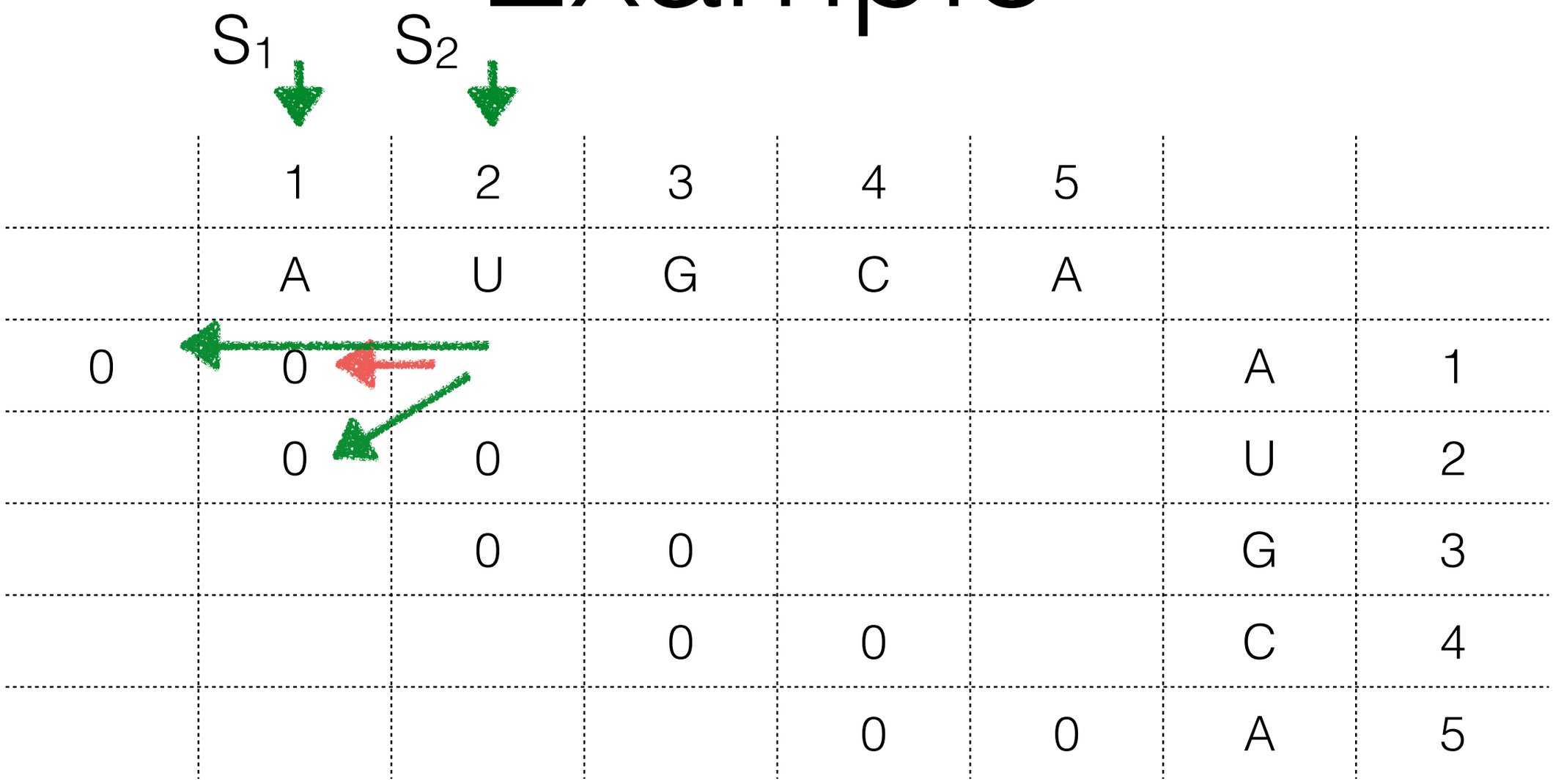
Example

	1	2	3	4	5		
	A	U	G	C	A		
0	0					A	1
	0	0				U	2
		0	0			G	3
			0	0		C	4
				0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \, complementary}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

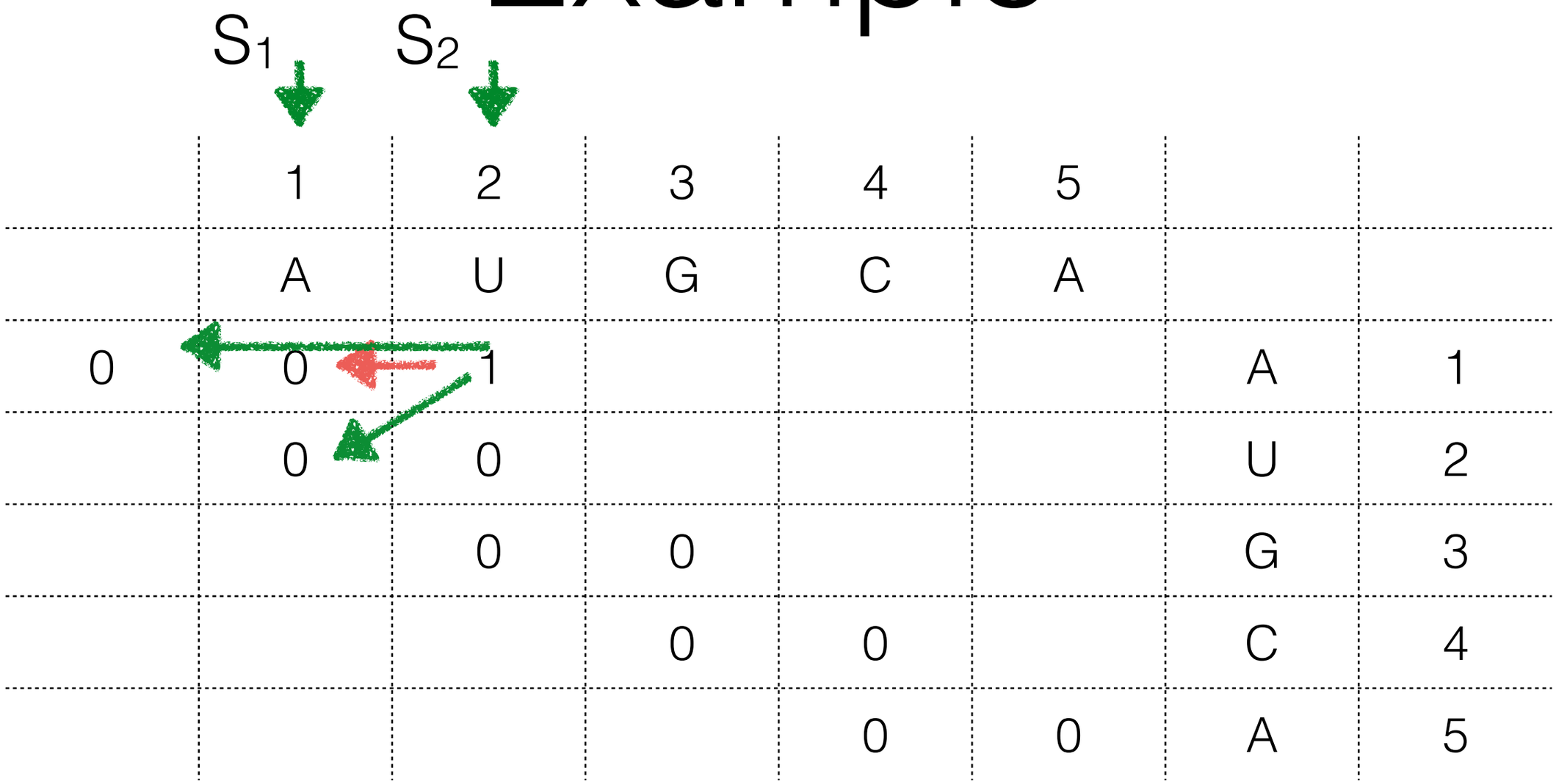
Example



$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example



$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_1 S_2

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1				A	1
	0	0	0			U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_3

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1				A	1
	0	0	0			U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

S_1

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_3

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1				A	1
	0	0	0			U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

S_2

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_4

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1			A	1
	0	0	0			U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

S_2

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_4

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1			A	1
	0	0	0			U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

S_3

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{S_k, S_j \text{complementary}} \; \max\limits_{i \le k < j} \; N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

S_4

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1			A	1
	0	0	0	1		U	2
		0	0	1		G	3
			0	0	0	C	4
				0	0	A	5

S_3

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \text{complementary}}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1			A	1
	0	0	0	1		U	2
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			0	0	0	C	4
				0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{S_k, S_j \text{complementary}} \; \max\limits_{i \le k < j} \; N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1	2		A	1
	0	0	0	1		U	2
		0	0	1	1	G	3
			0	0	0	C	4
				0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{S_k, S_j \text{complementary}} \; \max\limits_{i \le k < j} \; N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example

	1	2	3	4	5		
	A	U	G	C	A		
0	0	1	1	2	2	A	1
	0	0	0	1	1	U	2
		0	0	1	1	G	3
			0	0	0	C	4
				0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{\substack{i \le k < j \\ S_k, S_j \, complementary}} N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

Figure from [1]

Example - Traceback

		1	2	3	4	5		
		A	U	G	C	A		
0	0	0	1	1	2	2	A	1
	0	0	0	0	1	1	U	2
		0	0	0	1	1	G	3
			0	0	0	0	C	4
				0	0	0	A	5

$$N_{ij} = \max \begin{cases} N_{ij-1} \\ \max\limits_{S_k, S_j \text{complementary}} \; \max\limits_{i \le k < j} \; N_{ik-1} + N_{k+1j-1} + 1 \end{cases}$$

(3,4) and (1,2) are paired

Figure from [1]

List of references

- [1] Lecture “Part 1 - RNA Structure and RNA Structure Prediction” Bioinformatics II, Prof Backofen. Chair of Bioinformatics, Albert-Ludwig-Universität Freiburg. 2013

  URL: http://www.bioinf.uni-freiburg.de//Lehre/Courses/2013_SS/V_RNA/slides/nussinov.pdf, visited 14/11/2014