

The Smith-Waterman and Needleman- Wunsch algorithms are both dynamic programming methods used for sequence alignment, but they differ in purpose: Smith-Waterman performs local alignment, while Needleman- Wunsch performs global alignment.



Needleman-Wunsch Algorithm (Global Alignment)

Purpose: Aligns two sequences from beginning to end, optimizing the overall match.

Steps:

1. Initialization:

- Create a scoring matrix with dimensions $(m+1) \times (n+1)$, where m and n are the lengths of the sequences.
- Initialize the first row and column with gap penalties.

2. Matrix Filling:

- Fill in the matrix using a recurrence relation:

$$F(i, j) = \max \left\{ \begin{array}{l} F(i-1, j-1) + \text{match/mismatch score} \\ F(i-1, j) + \text{gap penalty} \\ F(i, j-1) + \text{gap penalty} \end{array} \right.$$

3. Traceback:

- Start from the bottom-right cell and trace back to the top-left to find the optimal alignment path.

Use Case: Comparing full-length DNA or protein sequences.

Smith-Waterman Algorithm (Local Alignment)

Purpose: Finds the best matching subsequence between two sequences.

Steps:

1. Initialization:

- Similar matrix setup, but the first row and column are initialized to zero.

2. Matrix Filling:

- Use a modified recurrence relation:

$$F(i,j) = \max \begin{cases} 0 \\ F(i-1,j-1) + \text{match/mismatch score} \\ F(i-1,j) + \text{gap penalty} \\ F(i,j-1) + \text{gap penalty} \end{cases}$$

- The zero ensures that negative scores are reset, allowing local alignment.

3. Traceback:

- Start from the cell with the highest score and trace back until a cell with zero is reached.

Use Case: Identifying conserved regions or motifs within sequences.

Feature	Needleman -Wunsch	Smith- Waterman
Alignment Type	Global	Local
Initialization	Gap penalties	Zeros
Traceback Start	Bottom- right cell	Cell with highest score
Use Case	Full sequence comparison	Subsequence similarity

Reference:

https://en.wikipedia.org/wiki/Smith%E2%80%93Waterman_algorithm

<https://www.toolify.ai/de/ai-news-de/lokale-sequenzausrichtung-mit-smithwaterman-algorithmus-643293>