Gotoh algorithm: Distance-based dynamic programming algorithm for global pairwise alignment where gap of length k is penalized $a+bk$ (a is gap–opening penalty, b is gap–continuation penalty).

Gotoh O (1982) An improved algorithm for matching biological sequences. J Mol Biol 162:705–708

Goal is to align sequences A and B.

Let $d^{AB}(A^i, B^j)$ be penalty (distance) associated with best alignment between A^i and B^j that ends by pairing A_i and B_j.

Let $d^{A-}(A^i, B^j)$ be penalty (distance) associated with best alignment between A^i and B^j that ends by pairing A_i with a gap character.

Let $d^{-B}(A^i, B^j)$ be penalty (distance) associated with best alignment between A^i and B^j that ends by pairing B_j with a gap character.

Initial Conditions: $d^{AB}(A^0, B^0) = 0, d^{A-}(A^0, B^0) = d^{-B}(A^0, B^0) = \infty$. There are other boundary conditions that will not be detailed ...

Let $w(i, j)$ be penalty for aligning type i with type j (neither i nor j can represent a gap character here).

$$\begin{aligned}
d^{AB}(A^i, B^j) &= \min(d^{AB}(A^{i-1}, B^{j-1}), d^{A-}(A^{i-1}, B^{j-1}), \\
&\quad d^{-B}(A^{i-1}, B^{j-1})) + w(A_i, B_j)
\end{aligned}$$

$$\begin{aligned}
d^{A-}(A^i, B^j) &= \min(d^{AB}(A^{i-1}, B^j) + a, d^{A-}(A^{i-1}, B^j), \\
&\quad d^{-B}(A^{i-1}, B^j) + a) + b
\end{aligned}$$

$$\begin{aligned}
d^{-B}(A^i, B^j) &= \min(d^{AB}(A^i, B^{j-1}) + a, d^{A-}(A^i, B^{j-1}) + a, \\
&\quad d^{-B}(A^i, B^{j-1})) + b
\end{aligned}$$

Score of best alignment is minimum of $d^{AB}(A, B)$, $d^{A-}(A, B)$, and $d^{-B}(A, B)$.

Traceback procedure is then employed to recover optimal alignment

Smith–Waterman algorithm is a similarity-based dynamic programming algorithm for local alignment with "affine" gap weights.

The algorithm that is usually termed "Smith-Waterman" is a combination of ideas from Gotoh (1982, see above) and ...

Smith, T.F. and Waterman, M.S. 1981. Identification of common molecular subsequences. J. Mol. Biol. 147:195–197.

The Smith–Waterman algorithm is quite similar to the Gotoh algorithm seen above.

Goal is to align sequences A and B.

Let $s^{AB}(A^i, B^j)$ be similarity score associated with the best local alignment between A^i and B^j that ends by pairing A_i and B_j. If this score would be negative, we set $s^{AB}(A^i, B^j)$ to 0.

Let $s^{A-}(A^i, B^j)$ be similarity score associated with best local alignment between A^i and B^j that ends by pairing A_i with a gap character.

Let $s^{-B}(A^i, B^j)$ be similarity score associated with best local alignment between A^i and B^j that ends by pairing B_j with a gap character.

Initial Conditions: $s^{AB}(A^i, B^j) = 0$ when i or j or both are 0, $s^{A-}(A^i, B^j) = s^{-B}(A^i, B^j) = -\infty$ when i or j or both are 0.

Let $w(i,j)$ be similarity score for aligning type i with type j (neither i nor j can represent a gap character here).

$$
\begin{aligned}
s^{AB}(A^i, B^j) \;=\; & \max(0, s^{AB}(A^{i-1}, B^{j-1}) + w(A_i, B_j), \\
& \quad s^{A-}(A^{i-1}, B^{j-1}) + w(A_i, B_j), s^{-B}(A^{i-1}, B^{j-1}) + w(A_i, B_j))
\end{aligned}
$$

$$
\begin{aligned}
s^{A-}(A^i, B^j) \;=\; & \max(s^{AB}(A^{i-1}, B^j) + a, s^{A-}(A^{i-1}, B^j), \\
& \quad s^{-B}(A^{i-1}, B^j) + a) + b
\end{aligned}
$$

$$
\begin{aligned}
s^{-B}(A^i, B^j) \;=\; & \max(s^{AB}(A^i, B^{j-1}) + a, s^{A-}(A^i, B^{j-1}) + a, \\
& \quad s^{-B}(A^i, B^{j-1})) + b
\end{aligned}
$$

Score of best alignment is maximum over all (A^i, B^j) of $s^{AB}(A^i, B^j)$, $s^{A-}(A^i, B^j)$, and $s^{-B}(A^i, B^j)$.

Traceback procedure is again used to recover best local alignment. However, the traceback begins at the position corresponding to the highest value among all values of $s^{AB}(A^i, B^j)$, $s^{A-}(A^i, B^j)$, $s^{-B}(A^i, B^j)$. The traceback ends either at the (A^0, B^0) entry or at the first entry on the traceback path that is equal to 0.

For this algorithm to return sensible alignments, a and b should be less than 0. Also, the expected score of two "random" sequences should be negative.