Figures for "Supplementary Materials, Part 3, for the Blueprint of the "Alignment Neighborhood Explorer" (ANEX) (tentatively named)"

By Kiyoshi Ezawa

(Finished on December 10th, 2018;
added CC4 statement on August 14th, 2020)

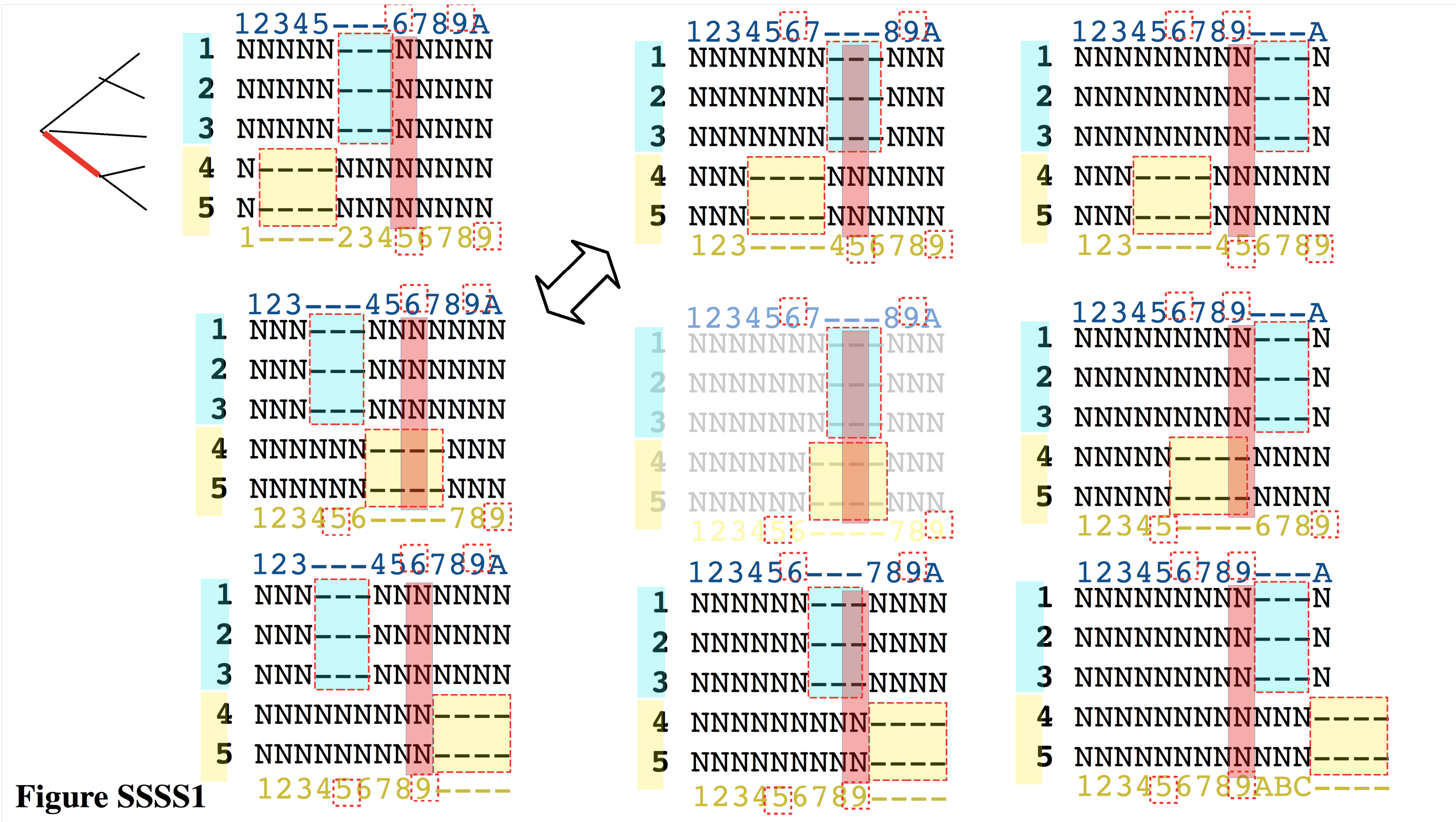


Figure SSSS1. Possible residue configurations of each column caused by simultaneous shifts of two vertically complementary gap-blocks.

The configurations are enumerated in a basically similar manner as shown in Figure 15 of "figures&legends1_ANEX.draft3+.pdf".

The main differences are:

(i) the complementary blocks are not allowed to horizontally overlap each other (e.g., the middle alignment drawn in light grey);

(ii) the horizontal swapping of the complementary blocks results in equivalent alignments that appear different (e.g., the two alignments mediated by the double-headed arrow), and thus such alignments consists of the identical set of columns (with different orders).

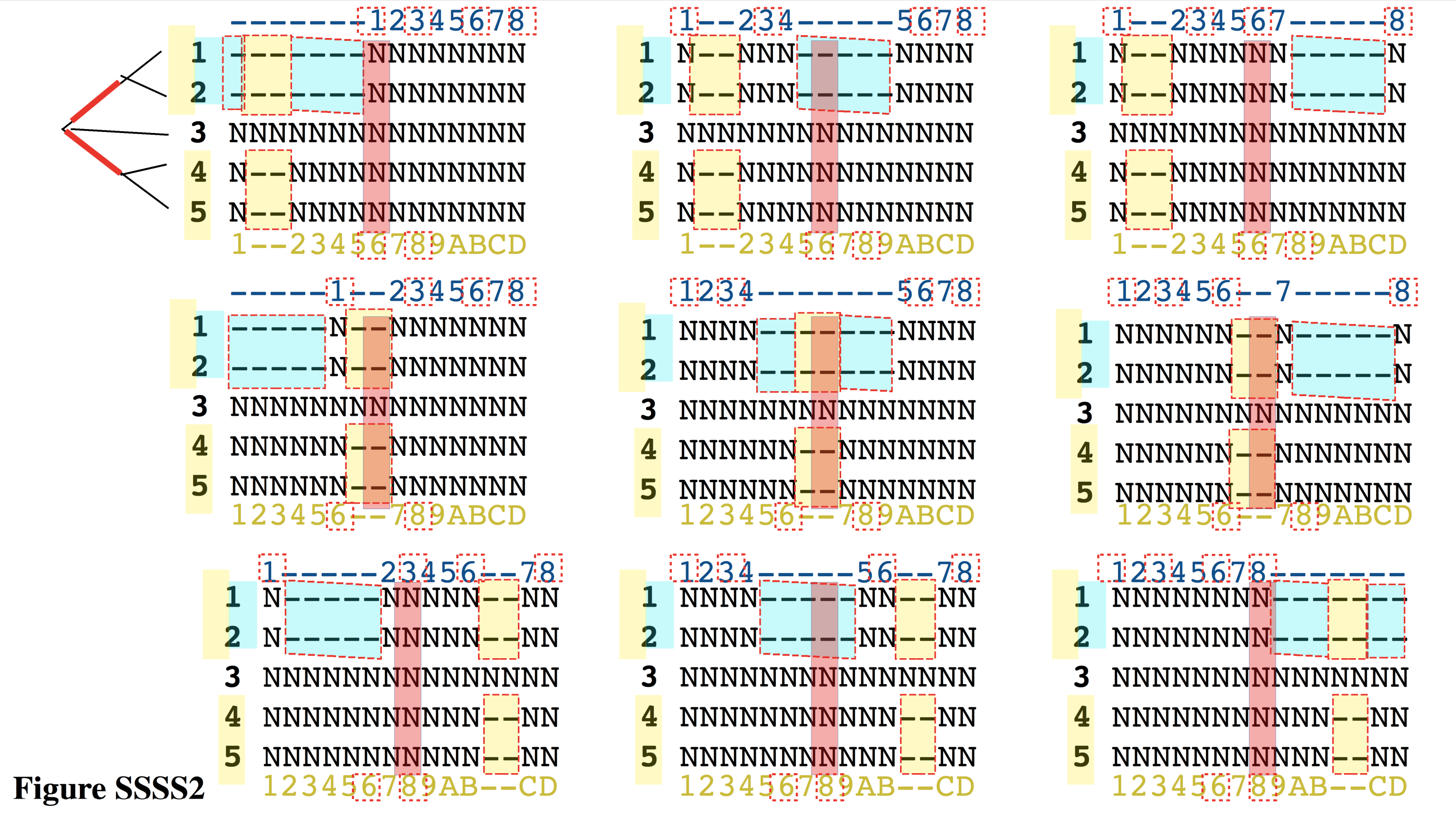


Figure SSSS2

Figure SSSS2. Possible residue configurations of each column caused by simultaneous shifts of two vertically nested gap-blocks.

Again, the configurations are enumerated in a basically similar manner as shown in Figure 15 of "figures&legends1_ANEX.draft3+.pdf".

Differently from the non-interfering case,

four sites (labelled 1, 3, 6, 8) from the upper semi-alignment can be used for the column highlighted in red. It should be noted, however, only 1 and 6 from the upper can be associated with 6 from the lower, and only 3 and 8 from the upper can be associated with 8 from the lower. This is because the vertically larger block involves sites from both of the semi-alignments.

It should also be noted that the residue configuration is identical if the vertically larger gap-block encompasses the column in question.

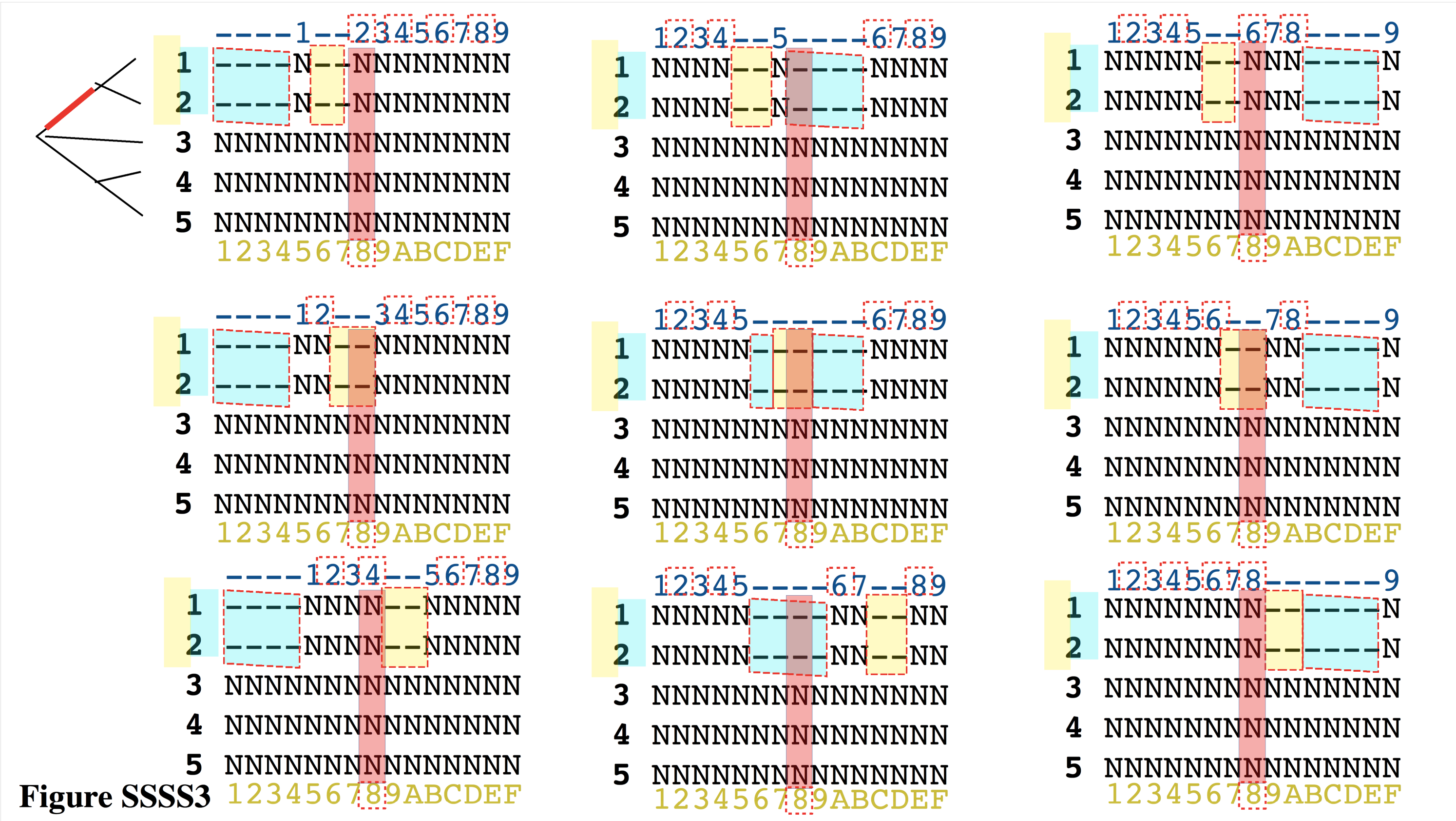


Figure SSSS3. Possible residue configurations of each column caused by simultaneous shifts of two vertically identical gap-blocks.

Again, the configurations are enumerated in a basically similar manner as shown in Figure 15 of “figures&legends1_ANEX.draft3+.pdf”.

Differently from the non-interfering case, four sites (labelled 2, 4, 6, 8) from the upper semi-alignment can be used for the column highlighted in red. They can be associated only with 8 in the lower semi-alignment.

It should also be noted that the residue configuration is identical if either of the two gap-blocks encompasses the column in question.

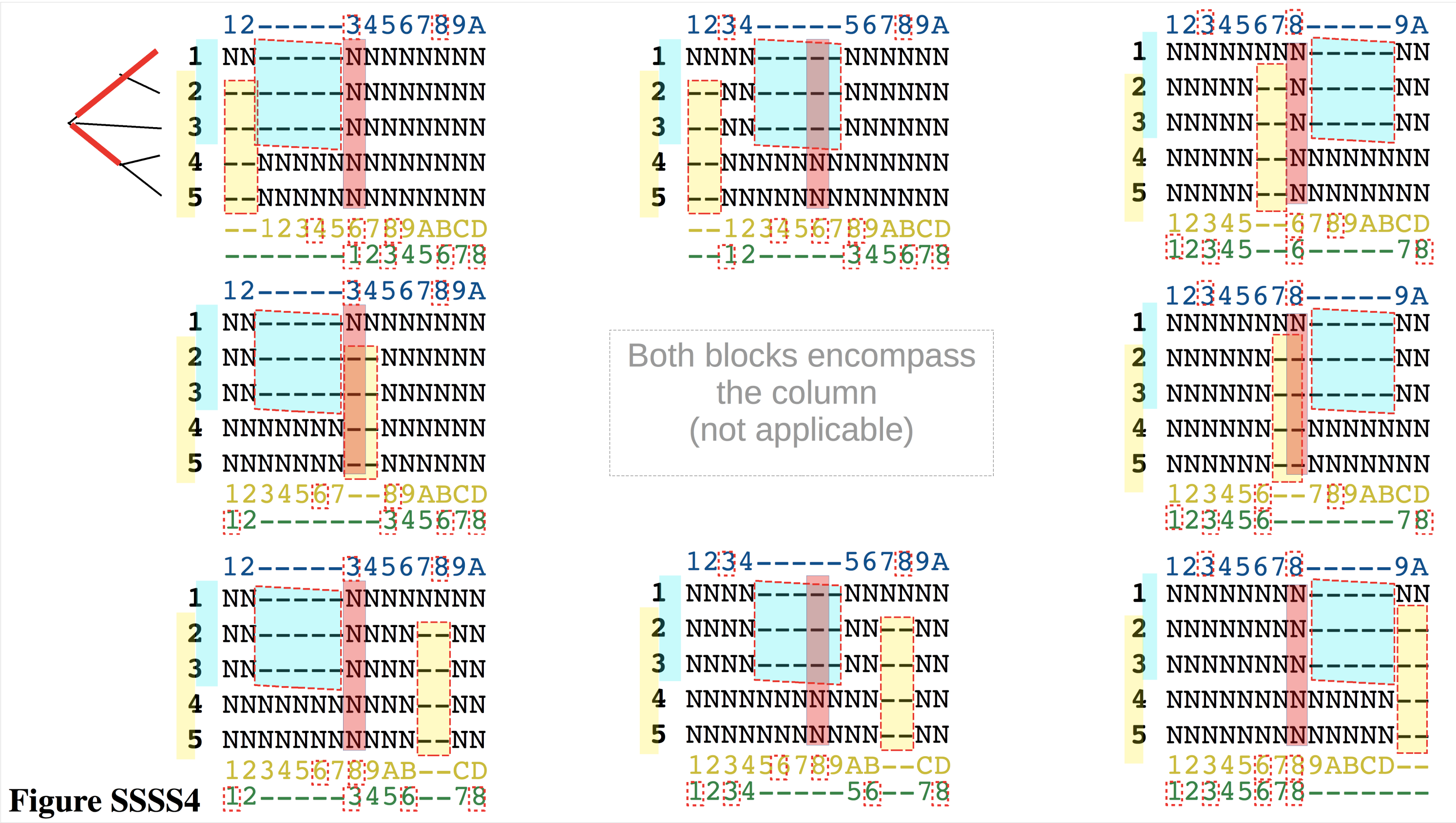


Figure SSSS4. Possible residue configurations of each column caused by simultaneous shifts of two vertically complementary gap-blocks.

The configurations are enumerated in a basically similar manner as shown in Figure SSSS1.

Differently from Figure SSSS1,

this case cannot allow the horizontal overlap of the two blocks *even in principle*, because they overlap *vertically*.

In this case, the sequences accommodating both gap-blocks contributes four sites (labelled 1, 3, 6, 8), but each site corresponds to a unique combination of the site from the sequences accommodating only the blue gaps (labelled 3, 8) and the site from the sequences accommodating only the yellow gaps (labelled 6, 8).

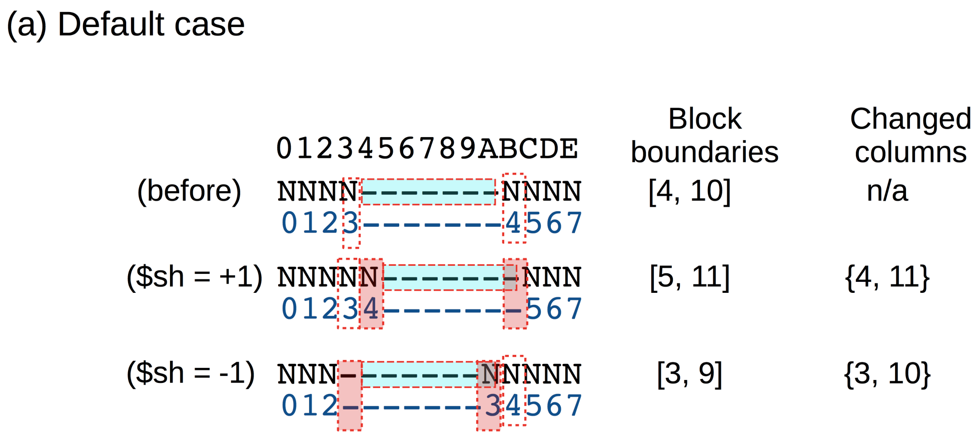


Figure SSSS5

Figure SSSS5. Columns changed by typical moves of gap-blocks.

The following notation is applicable to each panel:

The relevant gap-block is represented as a red dashed rectangular box shaded in transparent blue;

In the alignment before the move, relevant columns (or sites) are enclosed by open red dashed boxes;

In the alignments after the moves ($sh = +1/-1), the columns modified are enclosed by red dashed boxes shaded in transparent red.

The boundaries are written in a (0-based) full-closed notation.

(a) The default case, where the gap-blocks are not overlapping with one another, and thus can be moved freely.

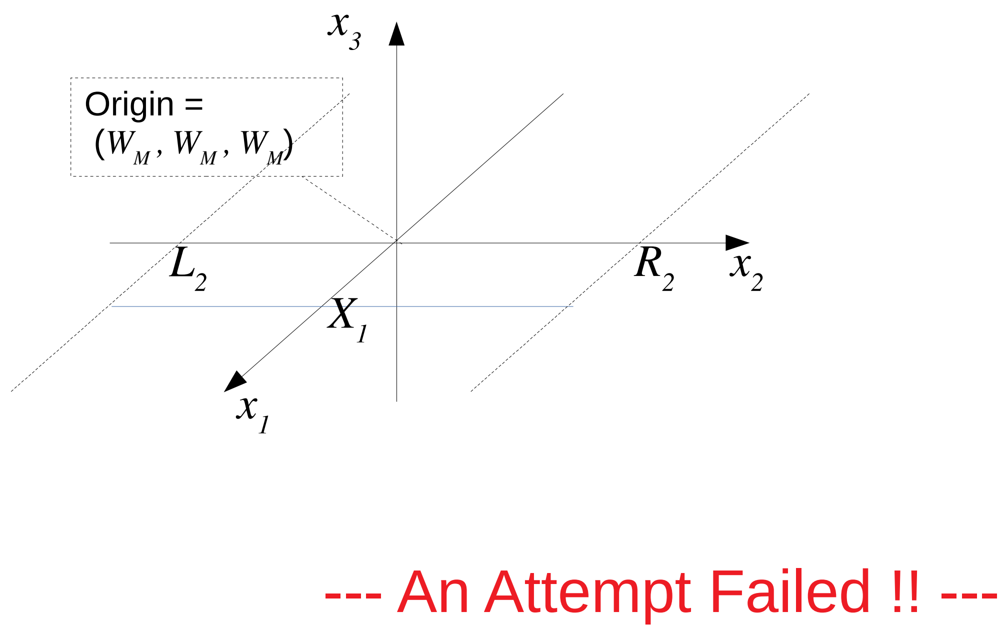


Figure SSSS6

Figure SSSS6. Moves within the coordinate space for exhaustively computing the probability increments due to simultaneous shifts of the gap-blocks.

For maximum clarity, the simplest non-trivial case of three blocks ($B = 3) is illustrated.

Also for clarity, we set the origin to be (W_M , W_M , W_M).

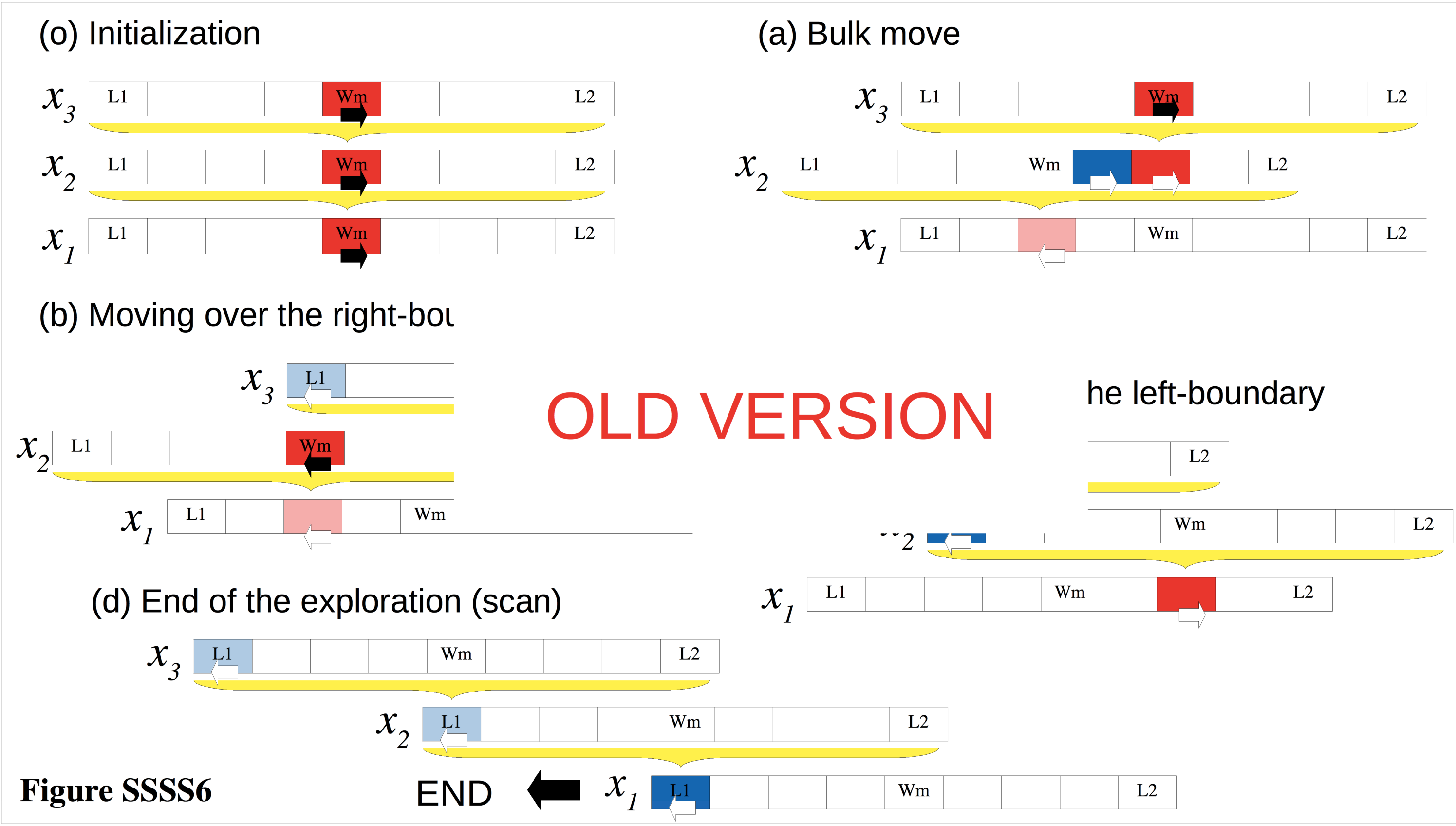
The notation of the coordinates conforms to Figure 3 of "simultaneous_moves_of_multiple_blocks_METH_xxx.odp".

The (x_1, x_2, x_3) here (or there) correspond to the (k_1, k_2, …, k_B(=3))

and also to

the ($bl_coords→[0], $bl_coords→[1], …, $bl_coords→[$B-1 (=2)]),

both in "suppl3_blueprint1_ANEX.draft8.odt".



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The notation of the coordinates conforms to Figure 3 of "simultaneous_moves_of_multiple_blocks_METH_xxx.odp".

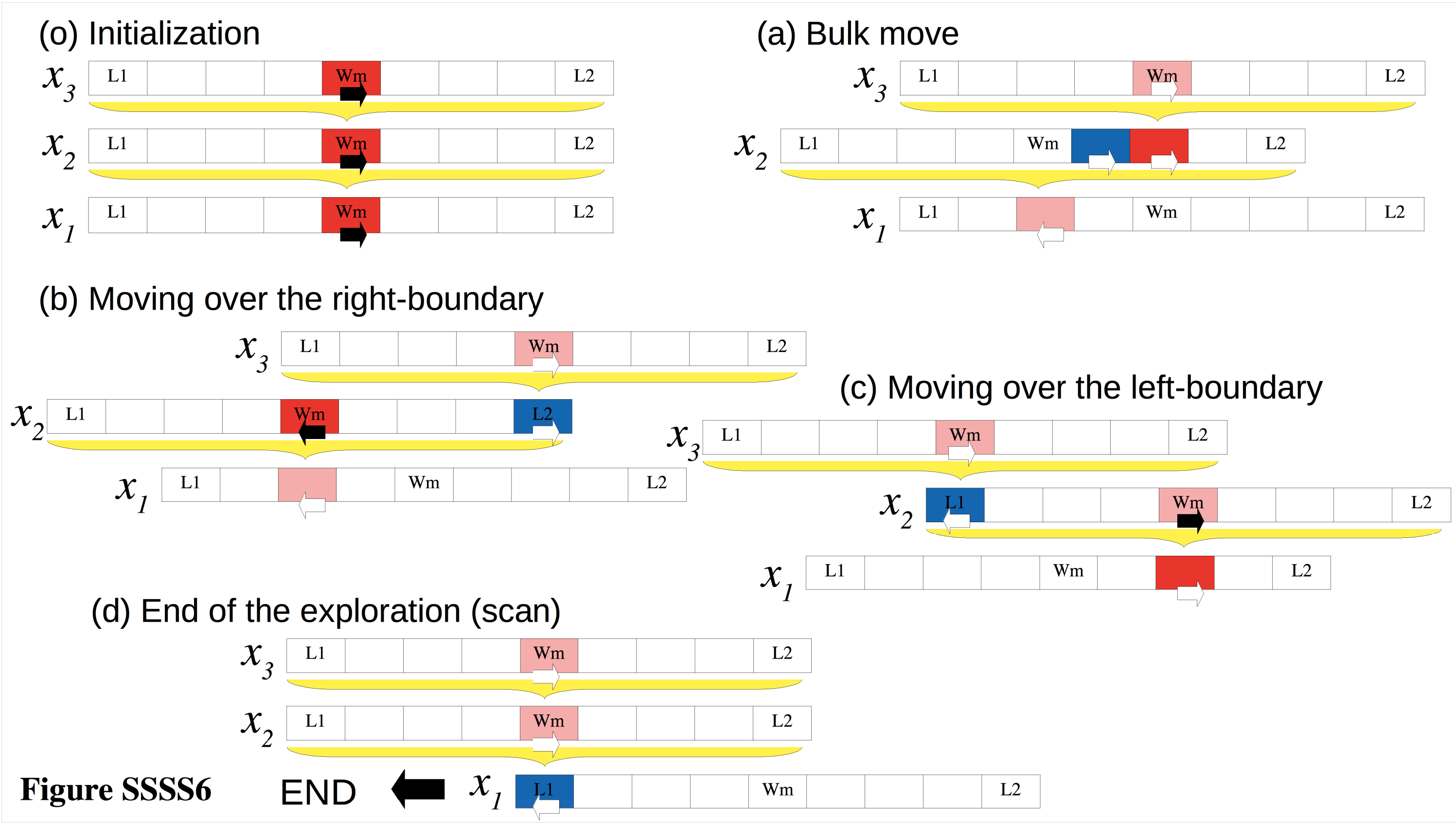
The (x_1, x_2, x_3) here (or there) correspond to the (k_1, k_2, …, k_B(=3)) = ($bl_coords→[0], $bl_coords→[1], …, $bl_coords→[$B-1 (=2)]), in "suppl3_blueprint1_ANEX.draft8.odt".

Each horizontal run of boxes represents an array (with the left/right boundaries (Lb/Rb) and the origin (Wm) shown).

Each downward brace indicates that the array above it is essentially the pointed element of the array below it.

The red and blue boxes, respectively, indicate the coordinates before and after the move. The arrows represents the directions of the shifts.

Especially, the un-transparent colors indicate the block coordinates "currently" handled, and the solid array indicates the shift "currently" updated. (NOTE: Panel a shows the configuration after the move, whereas panels b, c, and d show the configurations before the move.)



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The notation of the coordinates conforms to Figure 3 of "simultaneous_moves_of_multiple_blocks_METH_xxx.odp".

The (x_1, x_2, x_3) here (or there) correspond to the (k_1, k_2, …, k_B(=3)) = ($bl_coords→[0], $bl_coords→[1], …, $bl_coords→[$B-1 (=2)]), in "suppl3_blueprint1_ANEX.draft8.odt".

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Each downward brace indicates that the array above it is essentially the pointed element of the array below it.

The red and blue boxes, respectively, indicate the coordinates before and after the move. The arrows represents the directions of the shifts.

Especially, the un-transparent colors indicate the block coordinates "currently" handled, and the solid array indicates the shift "currently" updated. (NOTE: Panel a shows the configuration after the move, whereas panels b, c, and d show the configurations before the move.)

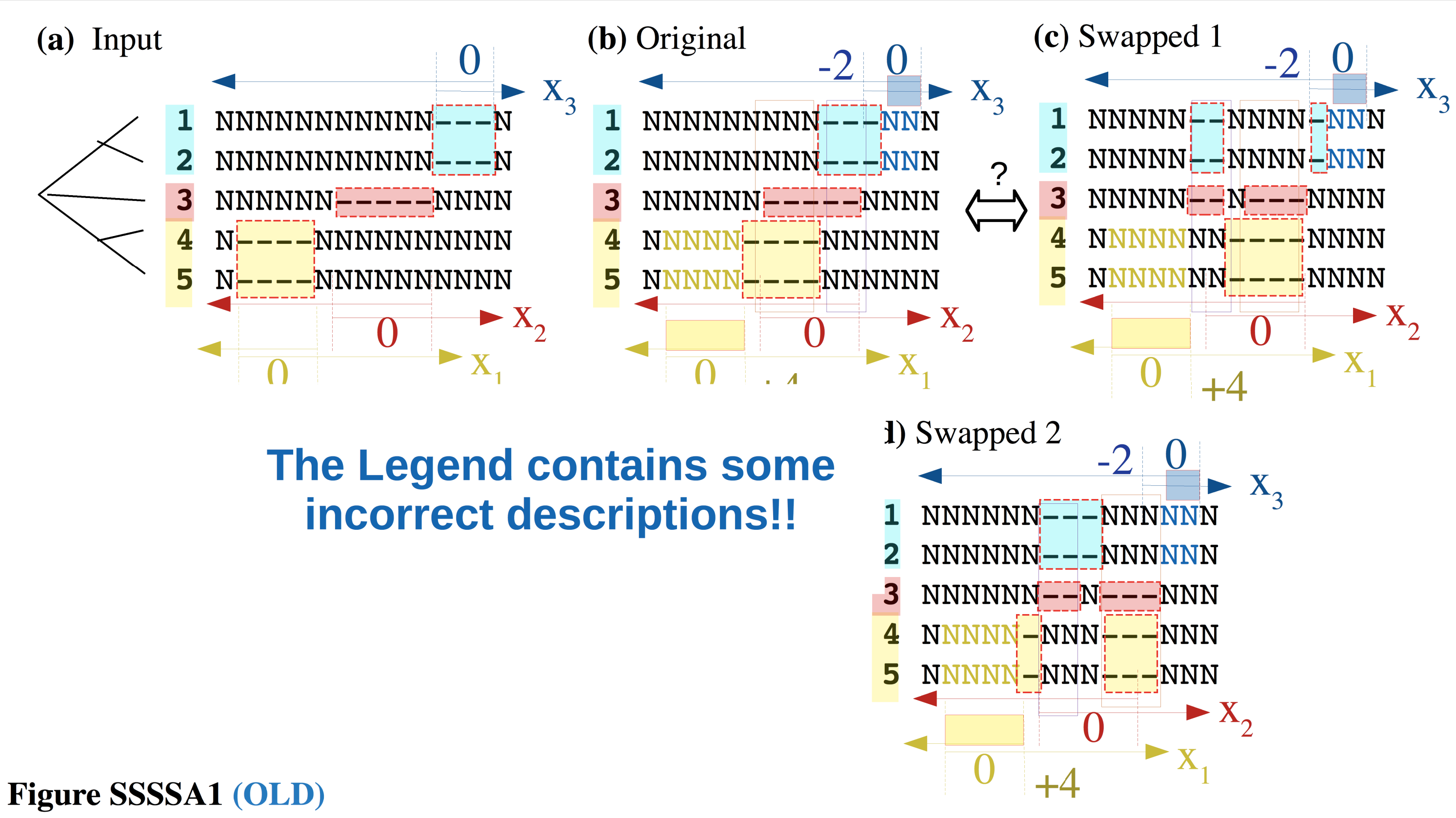


Figure SSSSA1 (OLD)

Figure SSSSA1. Examining the effect of column swapping when a combination of two gap-blocks is “complementary” to yet another gap-block. (Part 1)

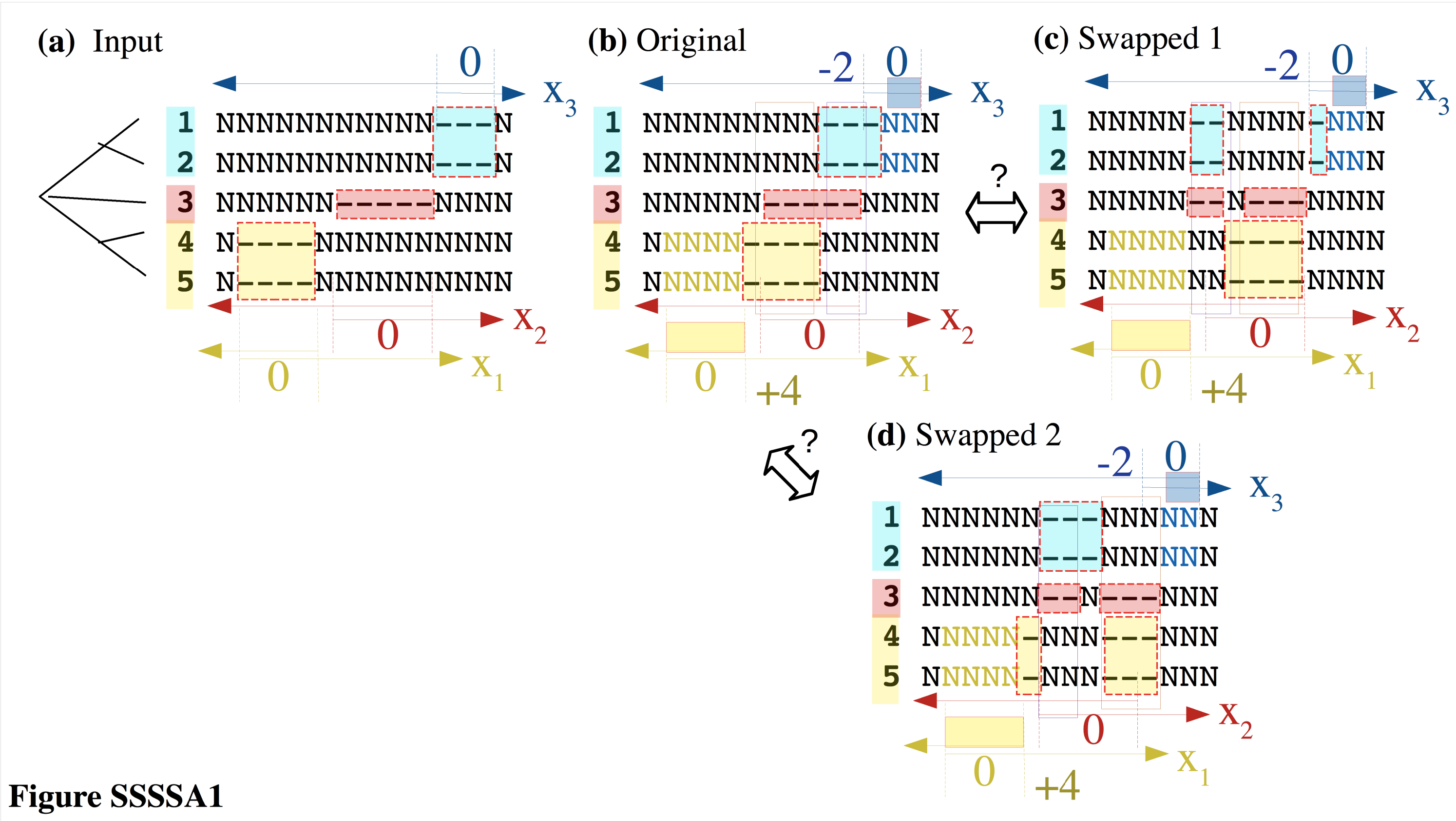
(a) Initial (or input) alignment.

(b) After the 1st block moves 4 sites to the right and the 3rd block moves 2 sites to the left, a pair of “complementary” blocks have no mediating columns in between.

(c) Swapping the 1st gap-block with its “complementary”, which arose by the horizontal overlap of the 2nd and 3rd gap-blocks.

(d) Swapping the 3rd gap-block with its “complementary”, which arose by the horizontal overlap of the 1st and 3rd gap-blocks.

~~Clearly, both swappings increased the minimal number of indels by 1. Thus,~~ **~~neither the alignment (c) nor (d) is equivalent to the alignment (b)~~.**



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(d) Swapping the 3rd gap-block with its "complementary", which arose by the horizontal overlap of the 1st and 3rd gap-blocks.

Each of the alignments (c) and (d) is equivalent to the alignment (b) (in terms of homology structures), because the order between the swapped blocks is NOT anchored by any column.

However, it is certain that (c) and (d) look more complicated than (b). Thus, **it would be better NOT to perform the swapping to (c) or (d) in cases like this.**

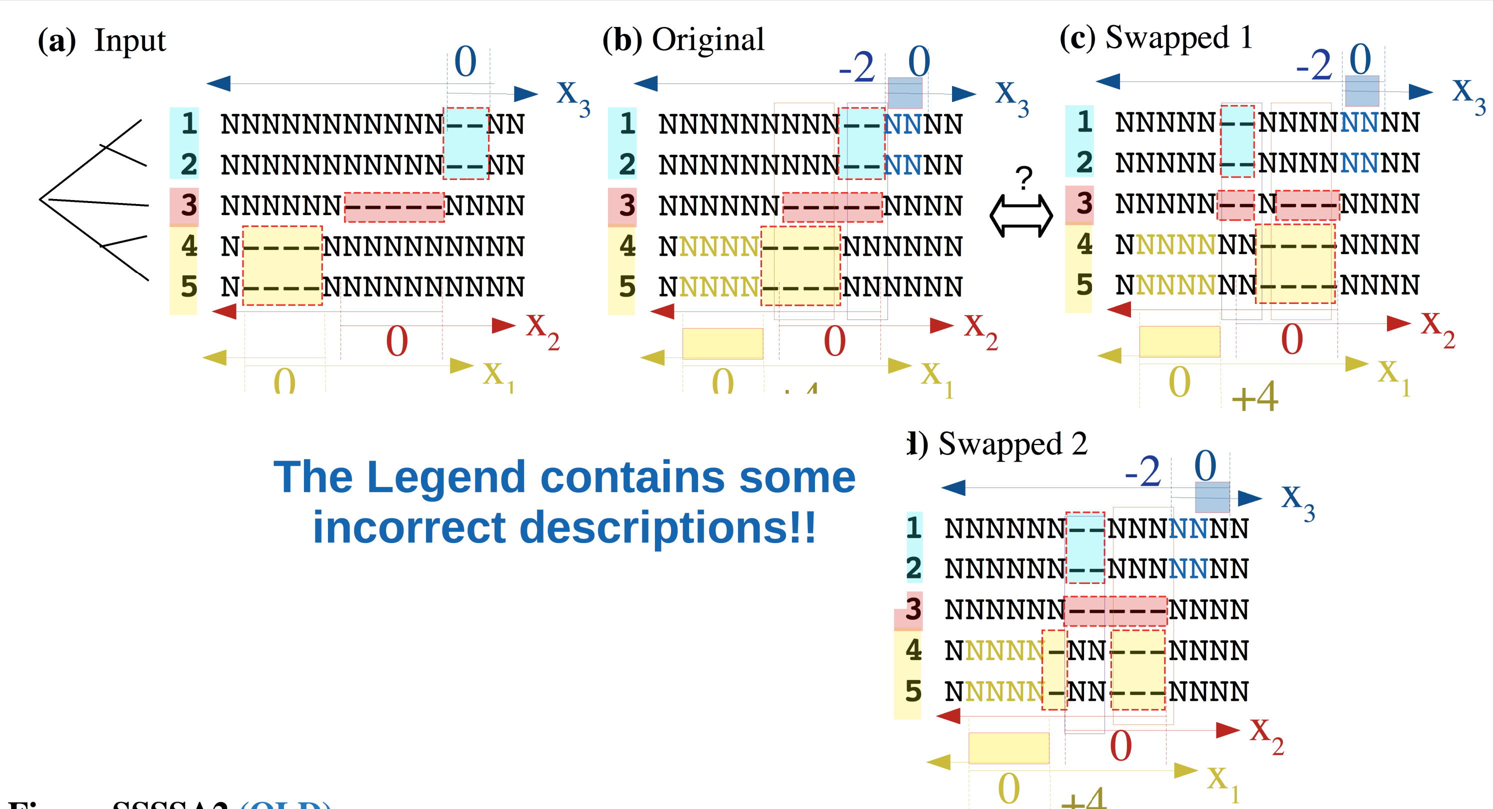

Figure SSSSA2 (OLD)

Figure SSSSA2. Examining the effect of column swapping when a combination of two gap-blocks is "complementary" to yet another gap-block. (Part 2)

Panels (a) – (d) are as in Figure SSSSA1.

The situation is mostly the same as in Part 1 (Figure SSSSA1); the only difference is that, in the original alignment (b), the 3rd block is horizontally included in the 2nd block.

~~As a result, the alignments after swapping (c and d) could result from 3 indels, as the original (b) can.~~

~~However, the causative (parsimonious) indel histories differ; whereas (b) can be caused by 3 histories, (c) and (d) can be caused only by 2 histories each.~~

~~This means that neither (c) nor (d) is equivalent to (b).~~

Another problem is that (b) is topologically different from (a). Thus, whether to consider them in a single coordinate space or not could change things significantly.

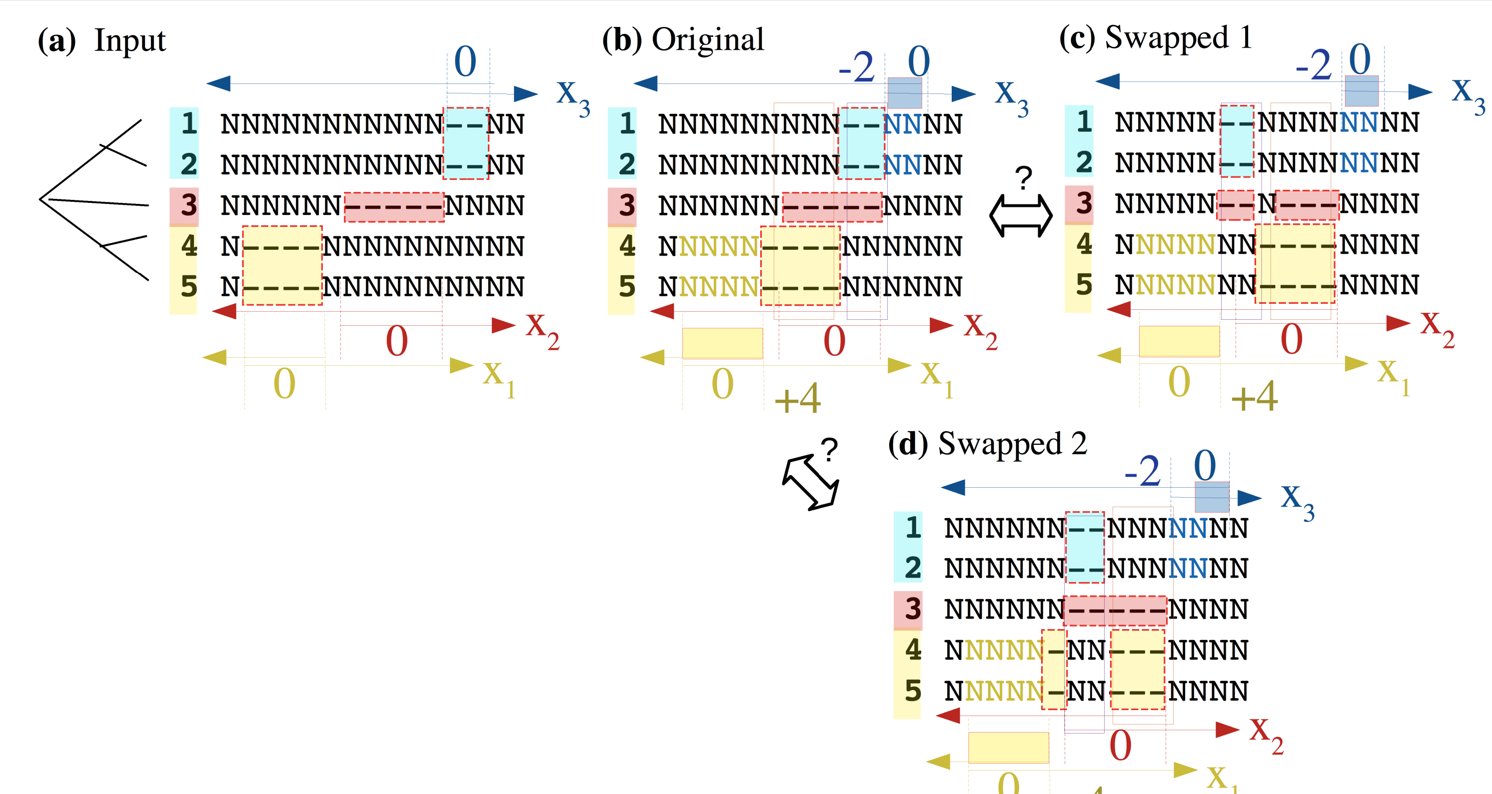

Figure SSSSA2

Figure SSSSA2. Examining the effect of column swapping when a combination of two gap-blocks is "complementary" to yet another gap-block. (Part 2)

Panels (a) – (d) are as in Figure SSSSA1.

The situation is mostly the same as in Part 1 (Figure SSSSA1); the only difference is that, in the original alignment (b), the 3rd block is horizontally included in the 2nd block.

As in Fig. SSSSA1, each of the alignments (c) and (d) is equivalent to the alignment (b) (in terms of <u>homology structures</u>), because the order among the swapped blocks is NOT anchored by any column.

However, it is certain that (c) and (d) look somewhat different from (b). Thus, **it would be better NOT to perform the swapping to (c) or (d) in cases like this.**

Another problem is that (b) is topologically different from (a). Thus, whether to consider them in a single coordinate space or not could change things significantly.

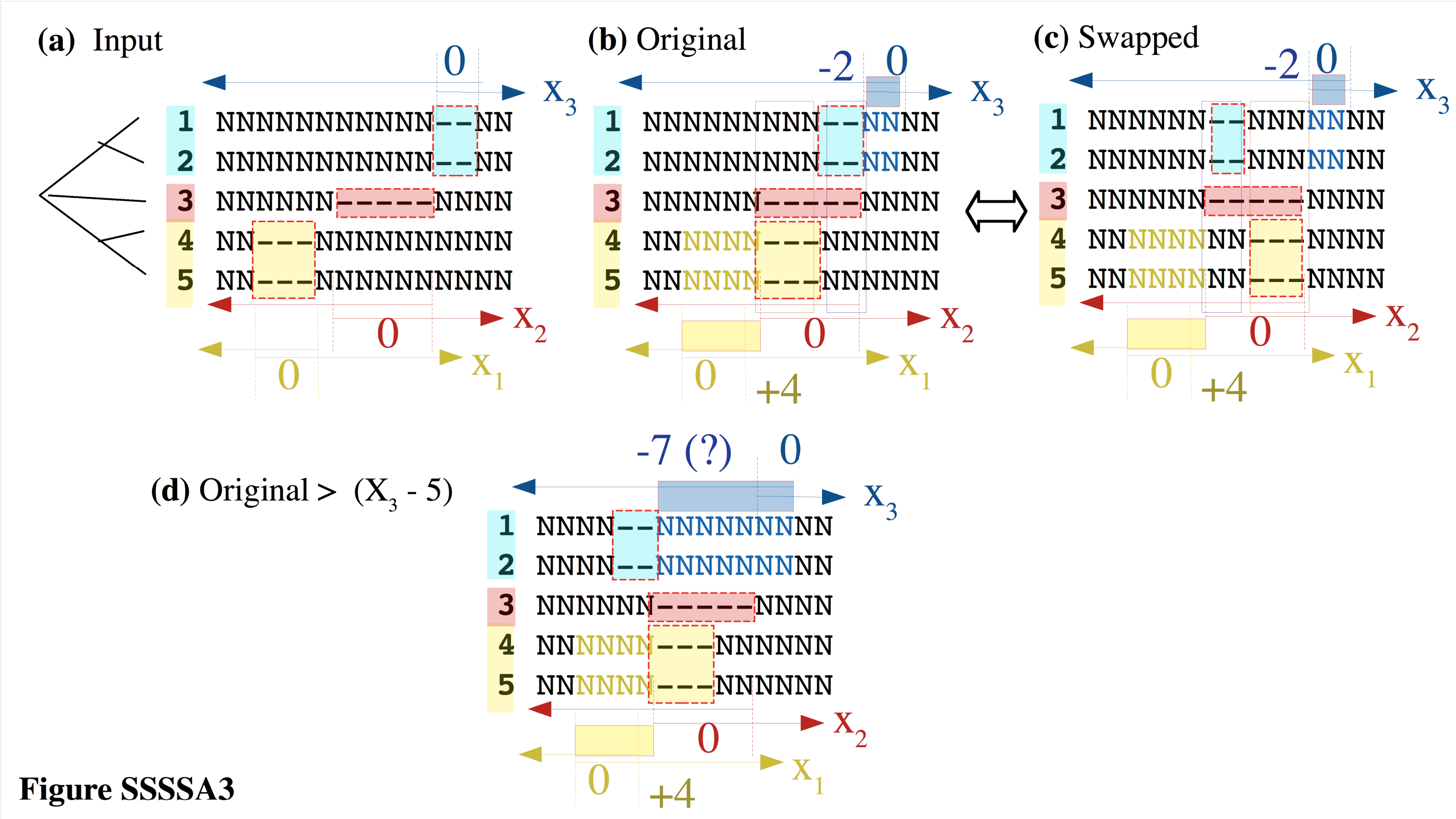

Figure SSSSA3. Examining the effect of column swapping when a combination of two gap-blocks is "complementary" to yet another gap-block. (Part 3)

Panels (a) – (c) are as in Figure SSSSA1.

The situation is mostly the same as in Part 1 (Figure SSSSA1); the only difference is that, in the original alignment (b), the 1st and 3rd blocks are horizontally included in the 2nd block.

As a result, the alignments after swapping (c) could be regarded as equivalent to the original (b)(, at least in terms of homology structures).

However, if the swapping like (b) > (c) is obligatory, we can NEVER examine some alignments such as in (d).

Another problem is that (b) is topologically different from (a). Thus, whether to consider them in a single coordinate space or not could change things significantly.

Therefore, **it may be better to respect the indel state of the input alignment throughout the exploration of each coordinate space, and to separately consider the issues of topology, redundancy (or degeneracy) and null columns.**

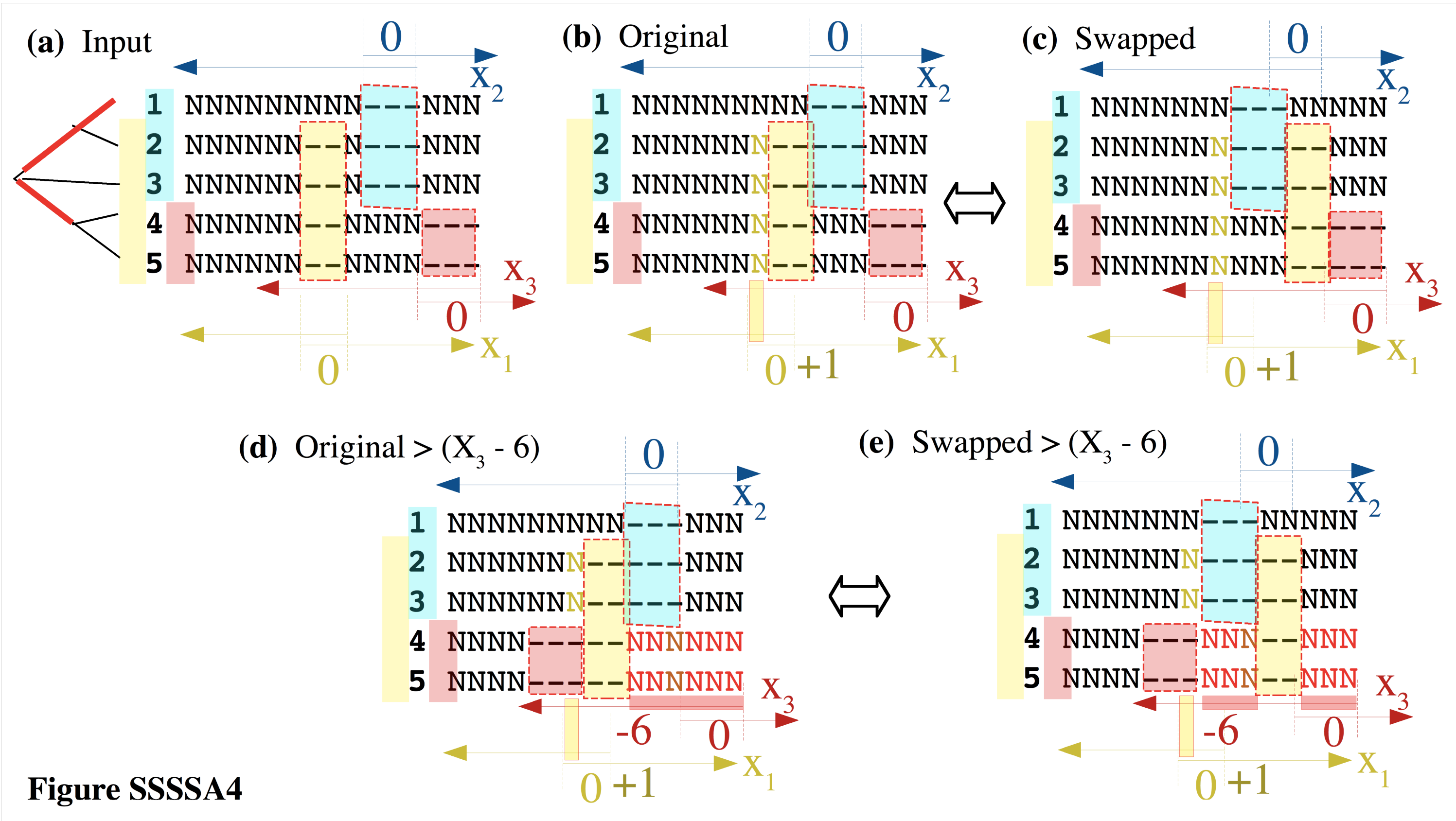

Figure SSSSA4. Examining the effect of column swapping when two gap-blocks vertically overlap but are non-nested, and another gap-block is complementary to one of the aforementioned two.

(a) Initial (or input) alignment. The 1st and 2nd blocks overlap vertically, and the 2nd and 3rd blocks are (vertically) complementary to each other.

(b) After the 1st block moves 1 site to the right, a pair of vertically overlapping blocks (1st and 2nd) have no mediating columns in between.

(c) Swapping the 1st gap-block with the 2nd one.

(d) From (b), shifting the 3rd block by 6 residues to the left.

(e) From (c), shifting the 3rd block by 6 residues to the left.

The alignments (b) and (c) are equivalent, at least in terms of homology structures; the equivalence applies also to alignments (d) and (e). (I'm not sure, though, whether my current algorithm can correctly handle alignments (c) and (d).)

Besides, (e) can also result from swapping 1st and 2nd blocks in (d). All these indicate that **the swapping is completely consistent with other moves**, at least for this combination of blocks.

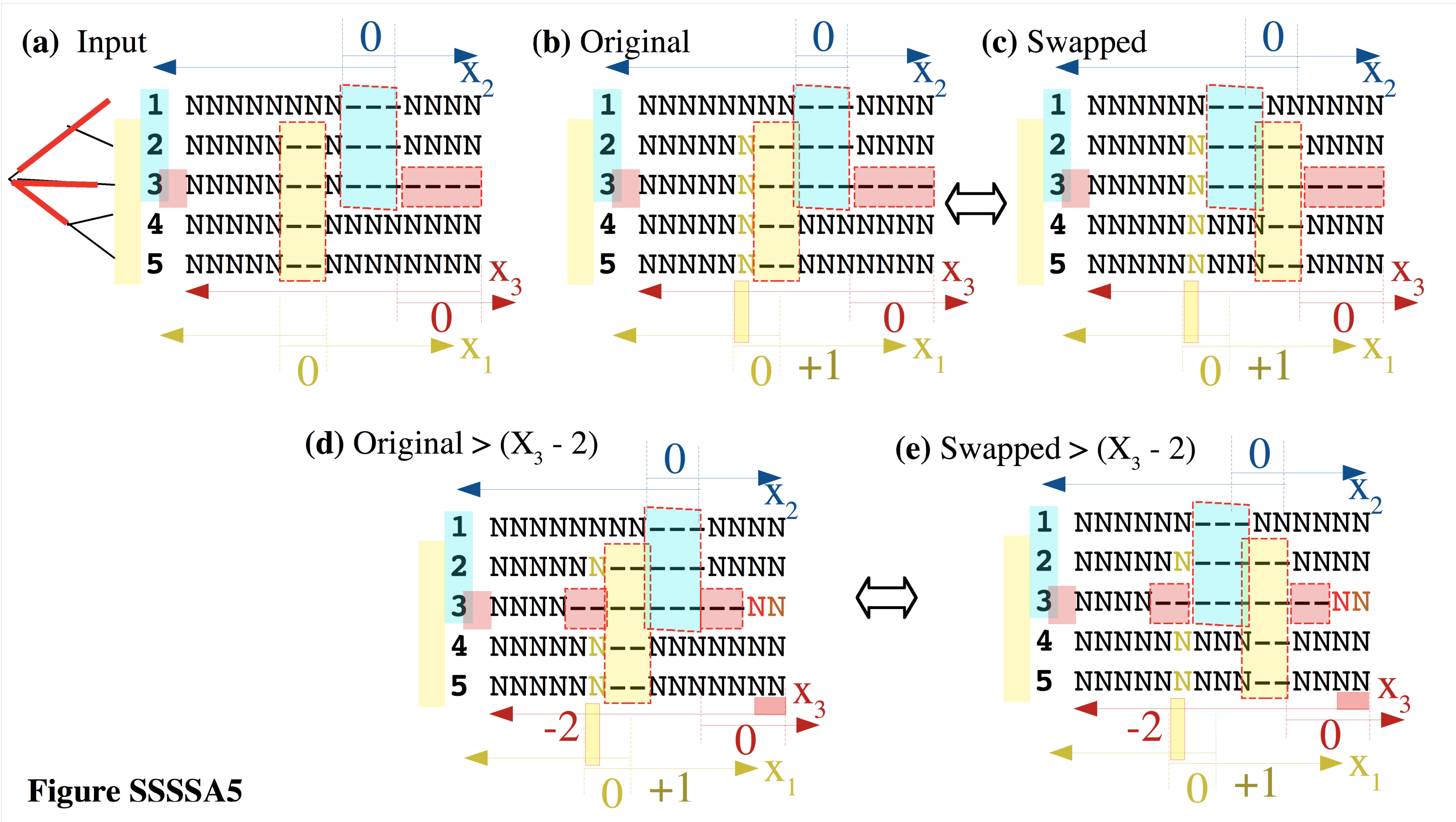

Figure SSSSA5. Examining the effect of column swapping when two gap-blocks vertically overlap but are non-nested, and another gap-block is vertically included in both of the aforementioned two.

(a) Initial (or input) alignment. The 1st and 2nd blocks overlap vertically, and the 3rd block is (vertically) included in the 1st and 2nd; especially, the 3rd block is a monophyletic child group of the 2nd.

(b) After the 1st block moves 1 site to the right, a pair of vertically overlapping blocks (1st and 2nd) have no mediating columns in between.

(c) Swapping the 1st gap-block with the 2nd one.

(d) From (b), shifting the 3rd block by 2 residues to the left.

(e) From (c), shifting the 3rd block by 2 residues to the left.

The alignments (b) and (c) are equivalent, at least in terms of homology structures; the equivalence applies also to alignments (d) and (e). (I'm not sure, though, whether my current algorithm can correctly handle alignment (c).)

Besides, (e) can also result from swapping 1st and 2nd blocks in (d). All these indicate that **the swapping is completely consistent with other moves**, at least for this combination of blocks.

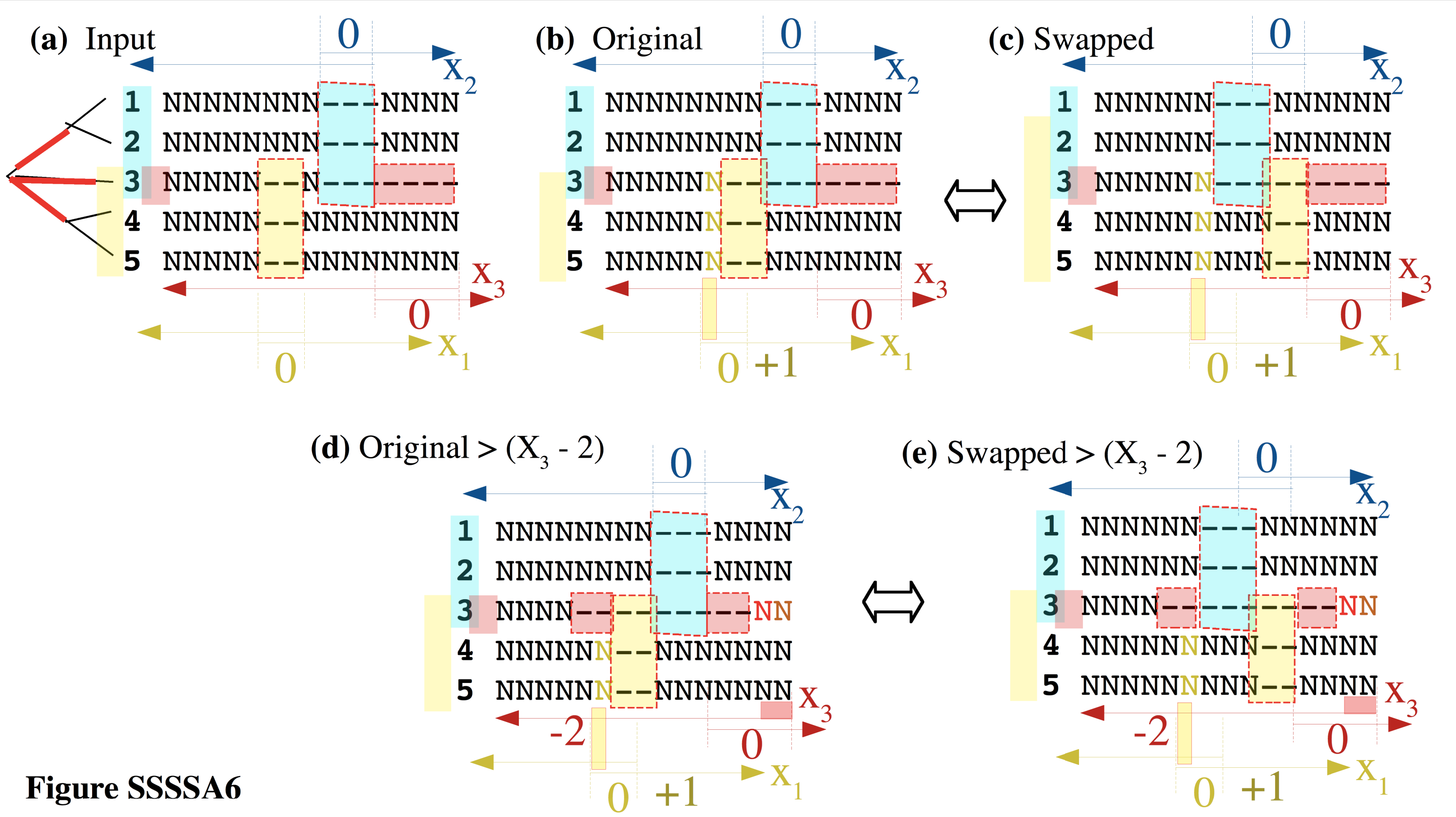

Figure SSSSA6. Examining the effect of column swapping when two gap-blocks vertically overlap but are non-nested, and another gap-block is vertically included in, actually a child monophyletic group of, both of the aforementioned two.

The situation in this figure is almost the same as that in Figure SSSSA5; the only difference is that the 3rd block in this figure affects a monophyletic group that is a child of both the monophyletic groups for the 1st and 2nd blocks, because the 1st block here is smaller than that in Fig. SSSSA5 by one sequence (no. 2).

Panels (a) – (e) are nearly identical to those in Fig. SSSSA5, except the difference in the 1st block.

The same conclusions as in Fig. SSSSA5 apply, regarding the equivalence and the consistency.

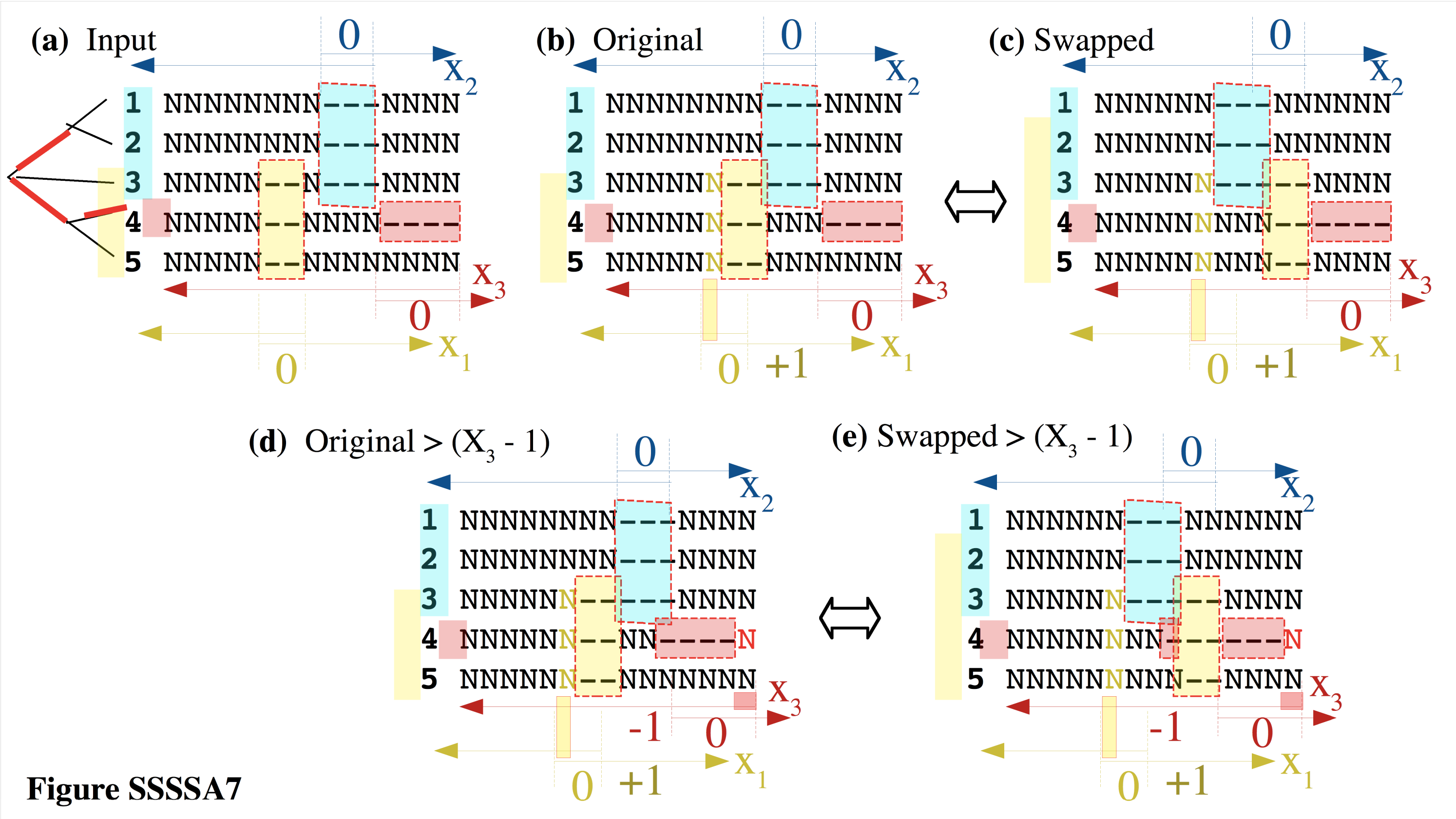

Figure SSSSA7. Examining the effect of column swapping when two gap-blocks vertically overlap but are non-nested, and another gap-block is vertically included in one of the aforementioned two, and also is a "sister" monophyletic group of the other.

The situation in this figure is almost the same as that in Figure SSSSA6; the only difference is that the 3rd block in this figure affects a monophyletic group that is a "sister" of the monophyletic group for the 2nd block, and that the 3rd block is vertically included in the 1st block..

Panels (a) – (c) are nearly identical to those in Fig. SSSSA6, except the difference in the 3rd block. Alignments (b) and (c) are equivalent, as far as homology structures are concerned.

(d) From (b), shifting the 3rd block by 1 residue to the left.

(e) From (c), shifting the 3rd block by 1 residue to the left.

Alignments (d) and (e) are equivalent, as far as homology structures are concerned.

NOTE that panel (e) can result also from swapping the two sets of columns in panel (d), as long as the sets of columns are defined by the horizontal span of the 1st and 2nd gap-blocks.

Thus, **at this point, the swapping is consistent with the shift of the 3rd block, conditioned on the caveat in the above NOTE.**

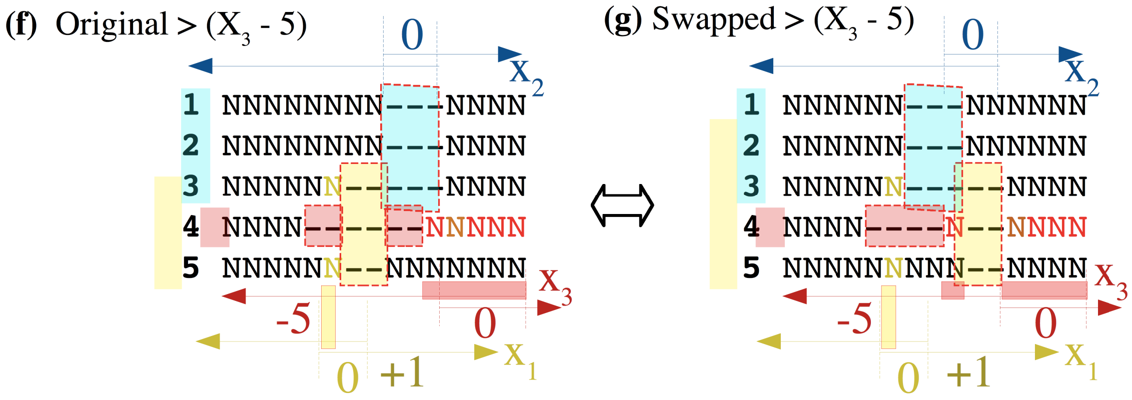

Figure SSSSA7 (sequel)

Figure SSSSA7 (sequel).

(f) From (b), shifting the 3rd block by 5 residues to the left.
(g) From (c), shifting the 3rd block by 5 residues to the left.
Alignments (f) and (g) are equivalent, as far as homology structures are concerned.
Besides, alignment (g) can result also from swapping the sets of columns in (f), as long as the sets are defined as horizontally spanning the 1st and 2nd gap-blocks.
Thus, with the above caveat (underlined), **swapping of the 1st and 2nd gap-blocks is consistent with the shifts of the 3rd block.**

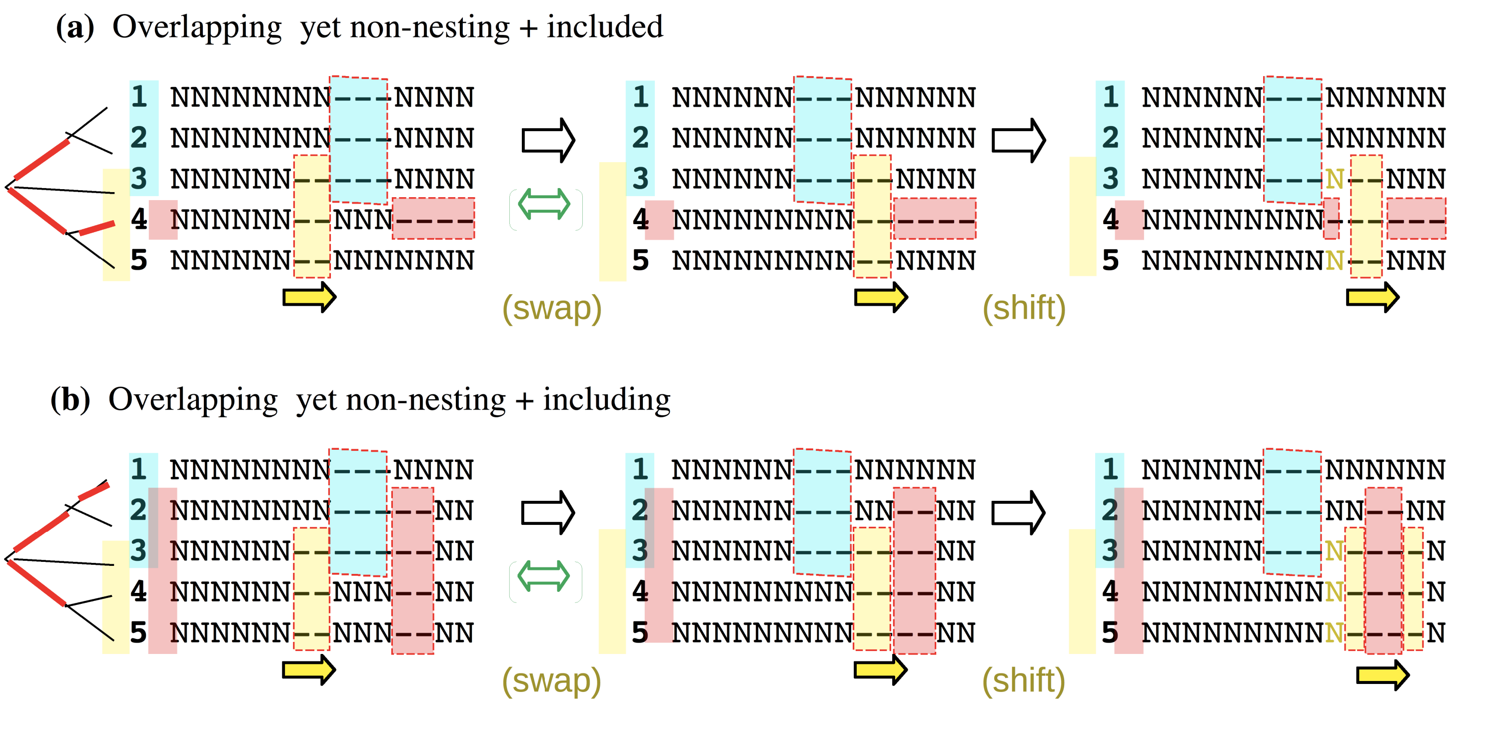

Figure SSSSA8 (1)

Figure SSSSA8. Summary of the actual effects of a "shift" of a gap-block, esp. on blocks "ahead". (1)

(a) When a block "shifts" beyond another block vertically overlapping yet non-nesting it, the two blocks are **swapped** before the shift. And when the block "shifts" further beyond the boundary with a yet another block vertically included in it, **the latter straddles the former**. (The ***shift*** of the yellow block after the swap could be regarded as the ***swapping*** of its left-most sub-column and its right-flanking sub-column.)

(b) The same **swapping** as in (a) for the shift beyond a vertically overlapping yet non-nesting block. Then, when the block "shifts" further beyond the boundary with a yet another block vertically including it, **the former straddles the former**.

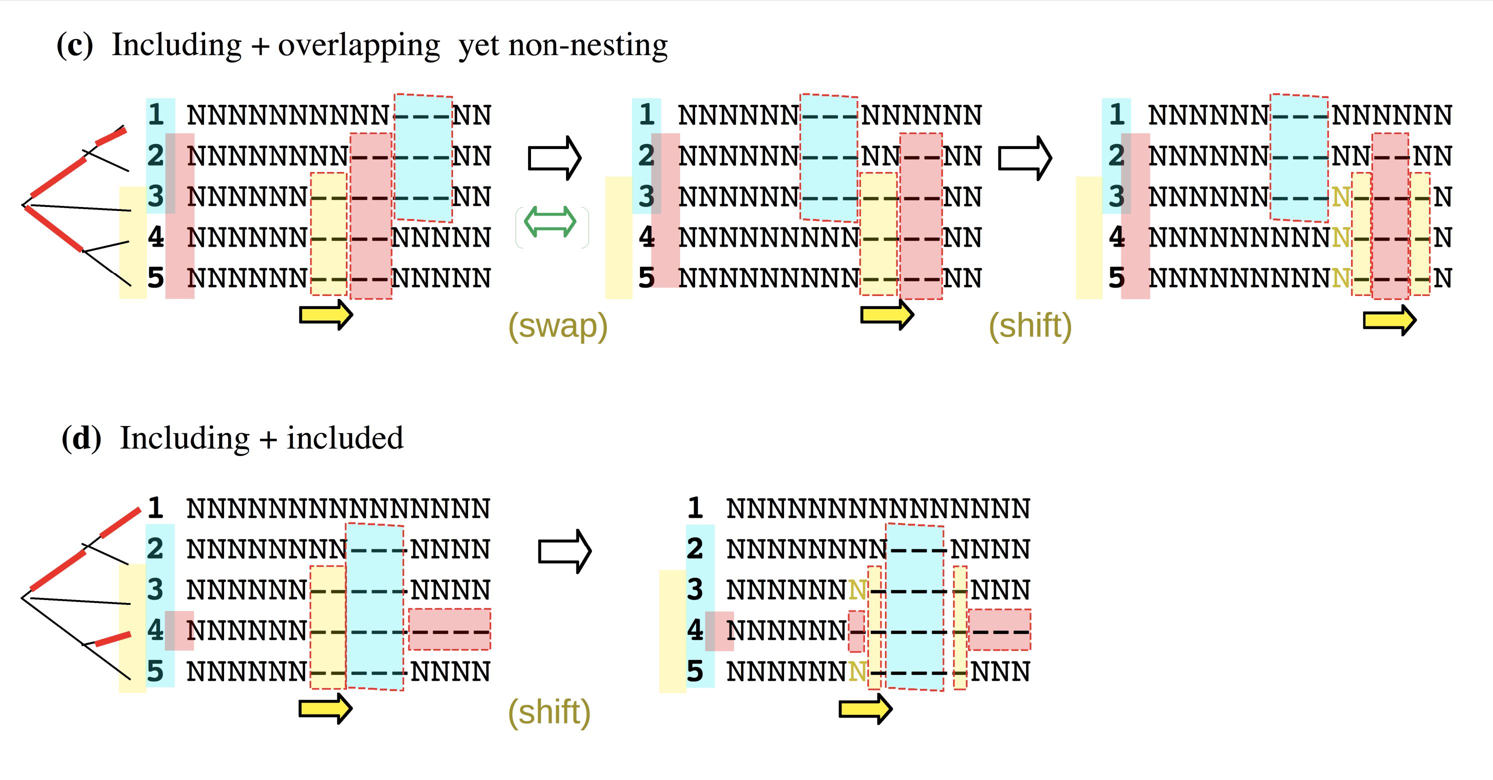

Figure SSSSA8 (2)

Figure SSSSA8. Summary of the actual effects of a "shift" of a gap-block, esp. on blocks "ahead". (2)

(c) When a (yellow) block "shifts" beyond the boundary with a second (red) block vertically including it, and beyond a third (blue) block vertically overlapping yet non-nesting it, the first and second blocks are **swapped** with the third one before the shift. Then, , **the first one "shifts" while straddling the second one**. (The ***shift*** of the first block after the swap could be regarded as the ***swapping*** of its left-most sub-column and its right-flanking sub-column.)

(d) When a block (yellow) is immediately adjacent to a second block (blue) vertically including it, which in turn is immediately adjacent to a third block (red) vertically included in the first one, the ***shift*** of the first block results in its **straddling** the second one and the ***swapping*** of its left-most sub-column with its right-flanking sub-column.

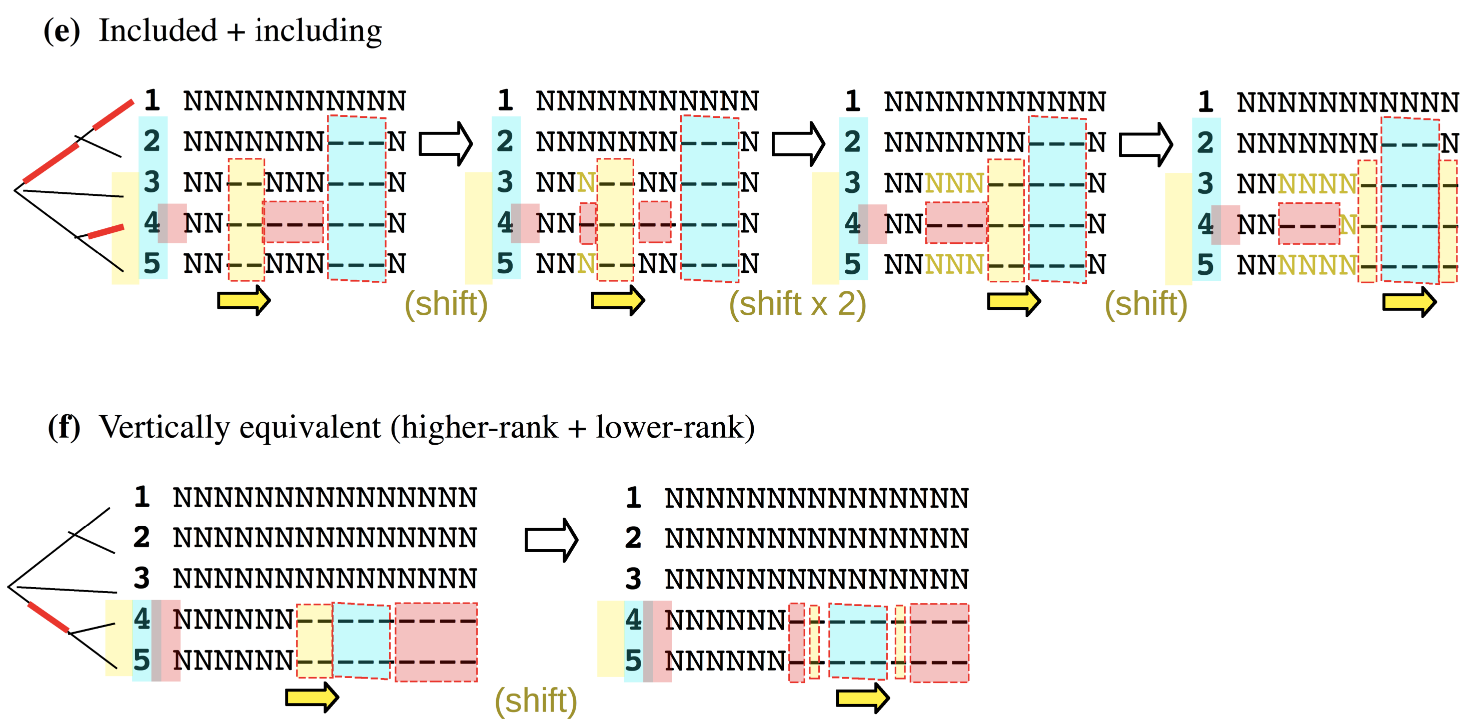

Figure SSSSA8 (3)

Figure SSSSA8. Summary of the actual effects of a "shift" of a gap-block, esp. on blocks "ahead". (3)

(e) When a block (yellow) is immediately adjacent to a second block (red) <u>vertically included</u> in it, which in turn is immediately adjacent to a third block (blue) <u>vertically including</u> in the first one, the ***shifts*** of the first block results first in the second one's ***straddling*** it, until the first block moves completely across the second one; then, a further ***shift*** of the first block results in its ***straddling*** the third one(, which could also be interpreted as the *swapping* of its left-most sub-column with its right-flanking sub-column).

(f) When a block (yellow) is immediately adjacent to a vertically <u>equivalent and higher-rank</u> second block (blue), which in tern is immediately adjacent to a <u>vertically equivalent and lower-rank</u> third one (red). The **shift** of the first block results in the pattern of moves practically identical to that in panel **(d)**.

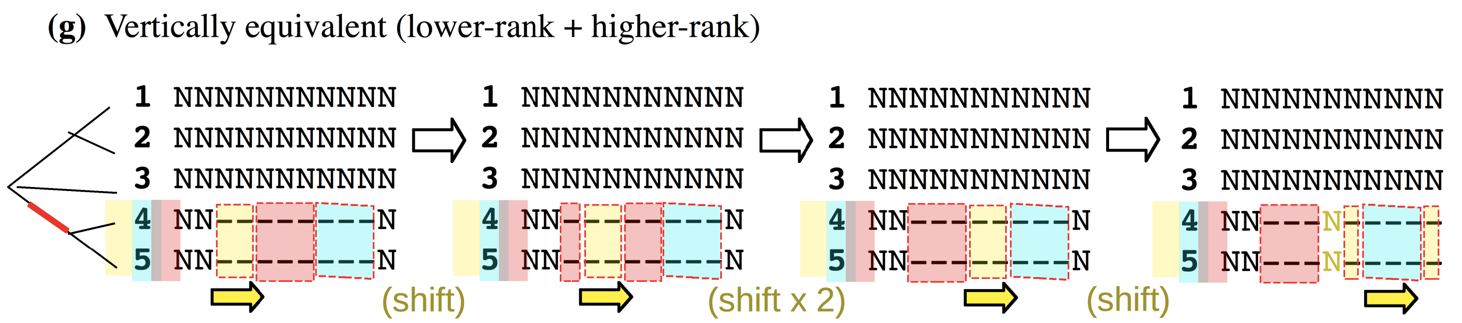

Figure SSSSA8 (4)

Figure SSSSA8. Summary of the actual effects of a “shift” of a gap-block, esp. on blocks “ahead”. (4)

(g) When a block (yellow) is immediately adjacent to a vertically <u>equivalent and lower-rank</u> second block (blue), which in tern is immediately adjacent to a <u>vertically equivalent and higher-rank</u> third one (red). The **shift** of the first block results in the pattern of moves practically identical to that in panel **(e)**.

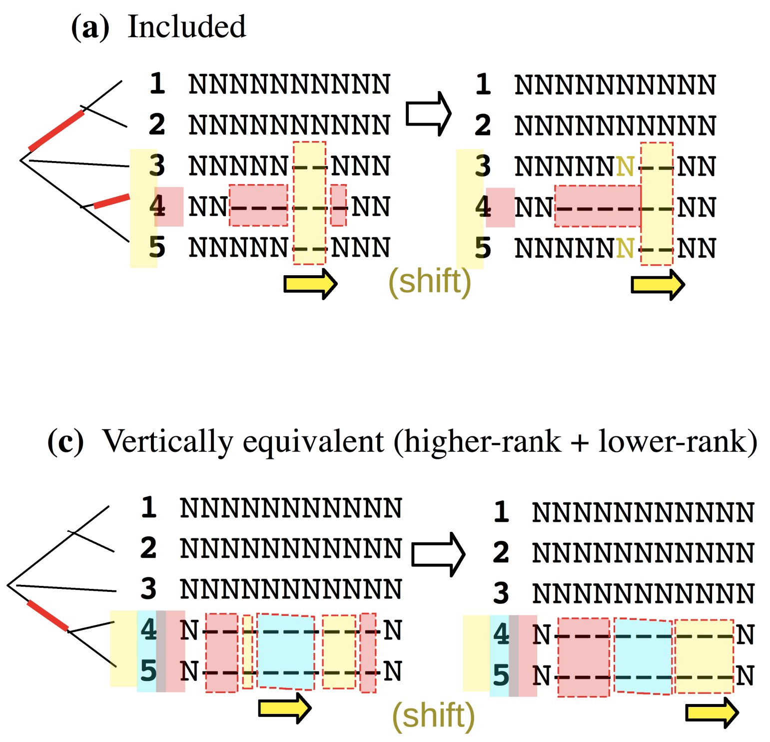

Figure SSSSA9 (1)

Figure SSSSA9. Summary of the actual effects of a "shift" of a gap-block, esp. on blocks "behind". (1)

(a) When a block (yellow) "***shift***"ing through another block (red) vertically included in it, and the former reaches the "frond end" of the latter, the "front end" of the latter moves to immediately behind the former.

(b) A block (yellow) ***straddles*** another block (red), which vertically includes the former. When the former ***"shift"***s and in consequence its "rear end" reaches the "rear end" of the latter, the "rear end" of the former moves to immediately ahead of the latter.

(c) A block (yellow) ***straddles*** a second block (blue), which is vertically equivalent to and ranks higher than the first one, and ***is straddled*** by a third one (red), which is vertically equivalent to and ranks lower than the first one. When the first one ***"shift"***s and in consequence its "rear end" reaches the "rear end" of the second one, and its "front end" reaches the "front end" of the third one, its "rear end" moves to immediately ahead of the second one, and the "front end" of the third one moves to immediately behind the second one.

(d) Vertically equivalent (lower-rank + higher-rank)

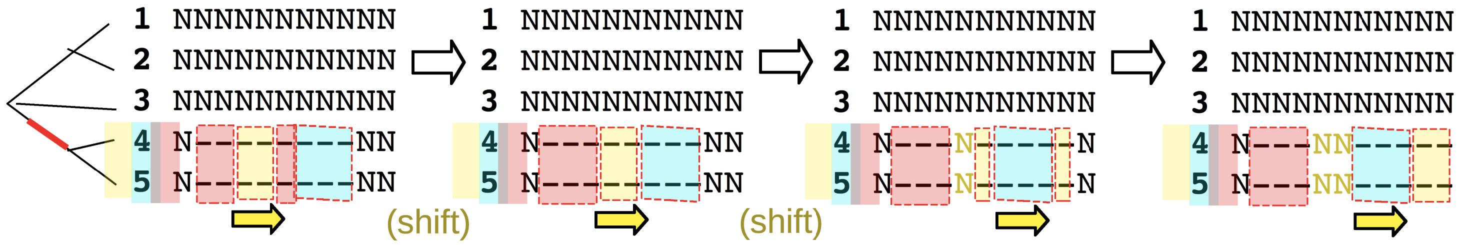

Figure SSSSA9 (2)

Figure SSSSA9. Summary of the actual effects of a "shift" of a gap-block, esp. on blocks "behind". (2)

(d) Consider that a block (yellow) is "shift"ing through a second, vertically equivalent and lower-rank,block (red) and then through a third, vertically equivalent and higher-rank, block (blue). When the first one "***shift***"s and in consequence its front-end reaches the front-end of the second one, the front-end of the second one moves to immediately behind the first one. And when the first one ***"shifts" further*** and in consequence its "rear end" reaches the "rear end" of the third one, its "rear end" moves to immediately ahead of the third one.

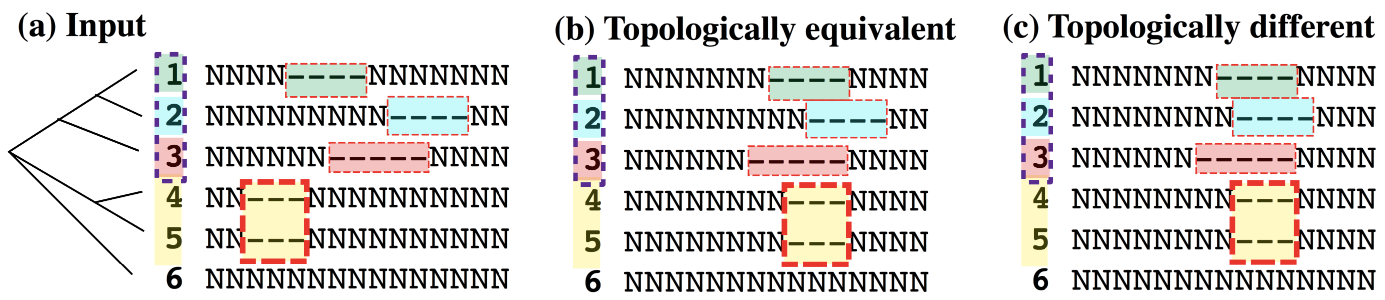

Figure SSSSA10 (1)

Figure SSSSA10. When topology changes for alignment with block and its "sibling" block-set.

(a) An example input alignment. In this case, an alignment block (enclosed by the red thick dashed box filled with yellow) has a "sibling" block-set (gap-blocks in sequences 1-3, whose projections onto sequence (node) IDs are enclosed by the purple dashed box).

(b) The result of shifts which is still regarded as **topologically equivalent with the input**, because the parsimonious indel histories are equivalent (up to the position-shifts of the indels). (Because of the residue in sequence 2 aligning the gaps in seqs 1, 3-5, a different indel history involving seq 6 *cannot* be parsimonious.)

(c) In this case, the resulting alignment has a second parsimonious indel history (involving an insertion into sequence 6), in addition to the history equivalent to that for the input (up to the position-shifts of the indels). Thus, this alignment is regarded as **topologically different from the input.**

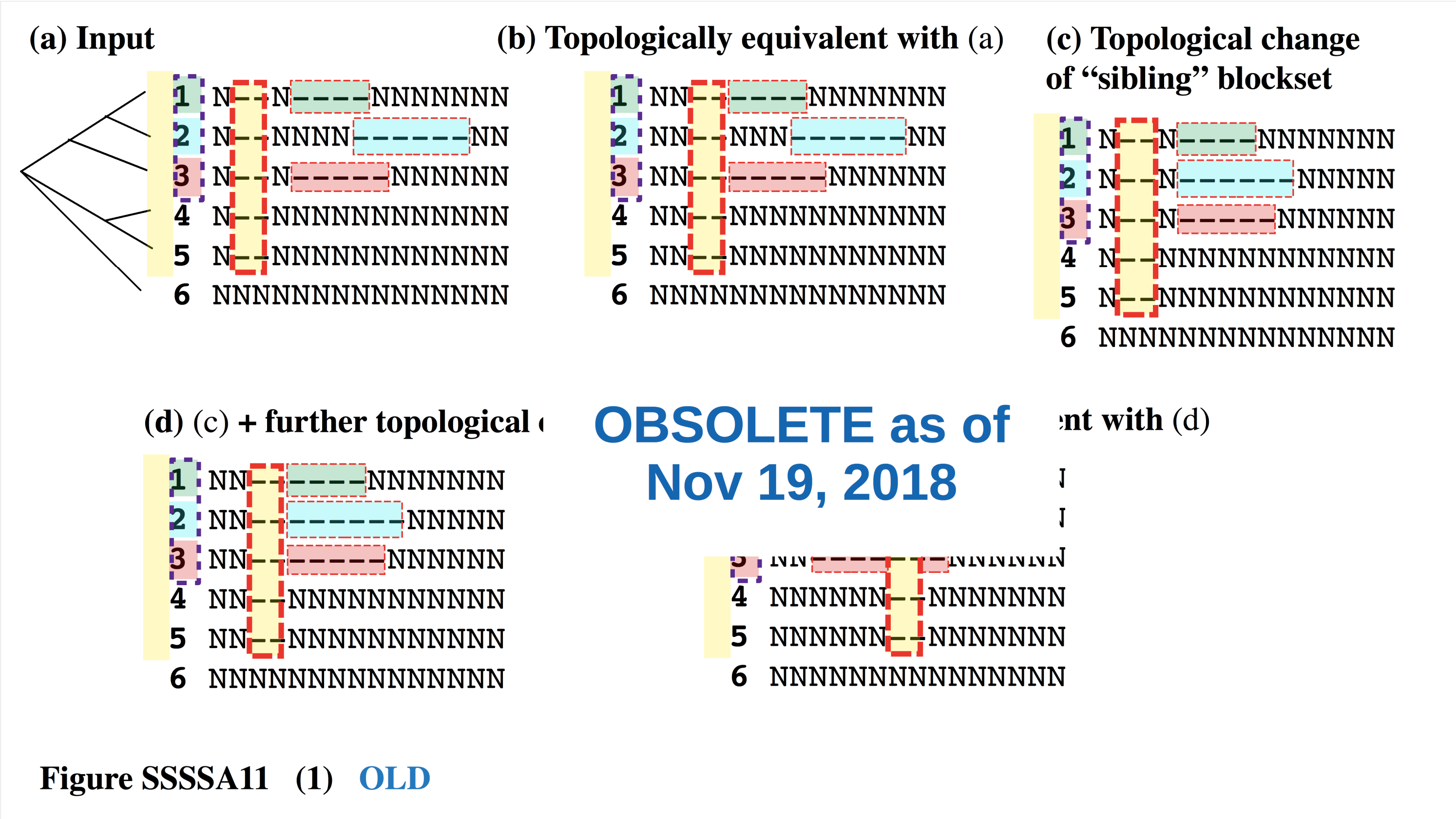

Figure SSSSA11. When topology changes for alignment with block and its "child" block-set.

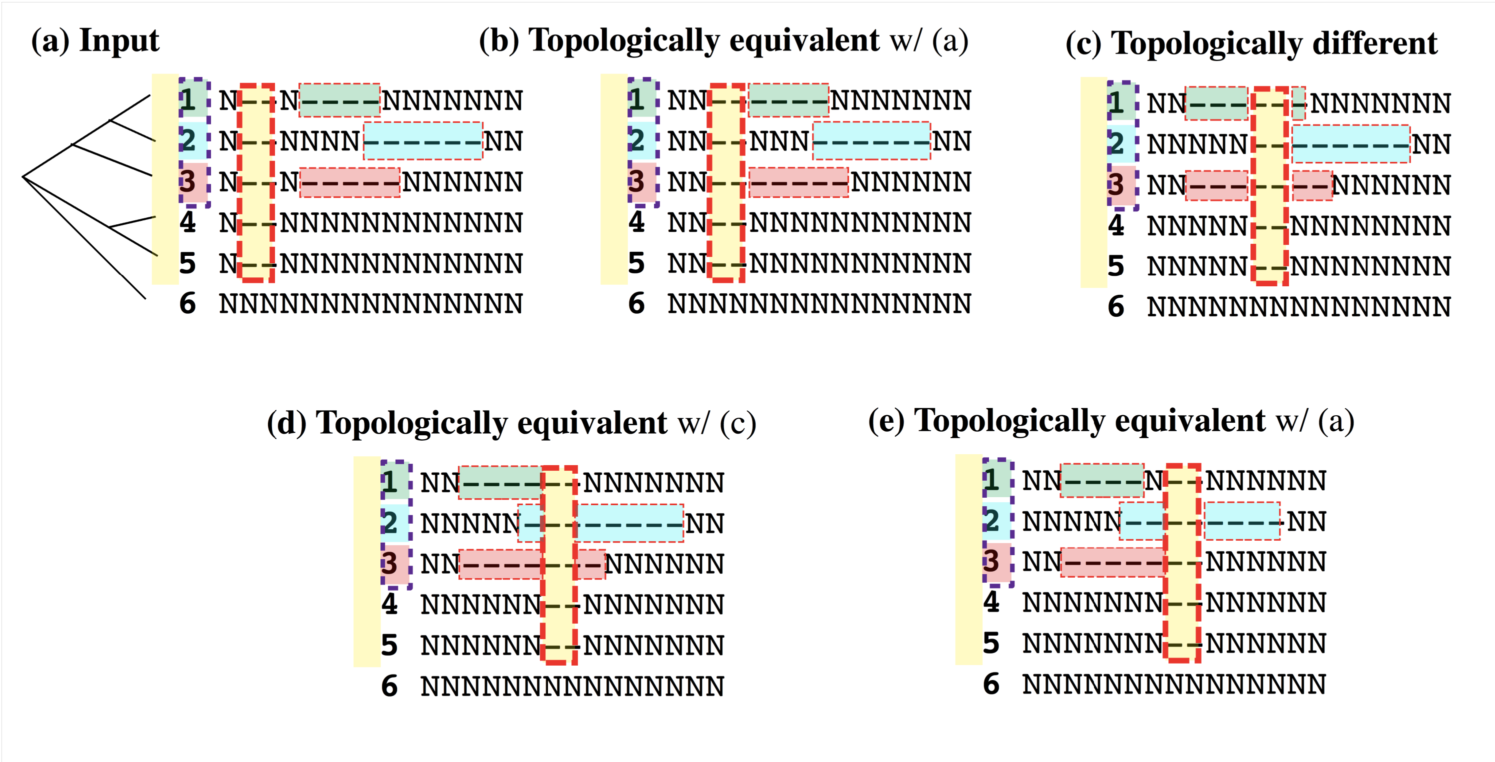

Figure SSSSA11 (1) NEW

Figure SSSSA11. When topology changes for alignment with block and its "child" block-set.

(a) An example input alignment. In this case, an alignment block (enclosed by the red thick dashed box filled with yellow) has a "child" block-set (gap-blocks in sequences 1-3, whose projections onto sequence (node) IDs are enclosed by the purple dashed box).

(b) The result of shifts which is still regarded as **topologically equivalent with the input**, because the parsimonious indel histories are equivalent (up to the position-shifts of the indels). (Because of the residue in sequence 2 aligning the gaps in seqs 1& 3, a different indel history involving seqs 4&5 *cannot* be parsimonious.)

(c) In this case, the resulting alignment has a second parsimonious indel history (involving a deletion from sequences 4&5), in addition to the history equivalent to that for the input (up to the position-shifts of the indels). Thus, this alignment is regarded as **topologically different from the input.**

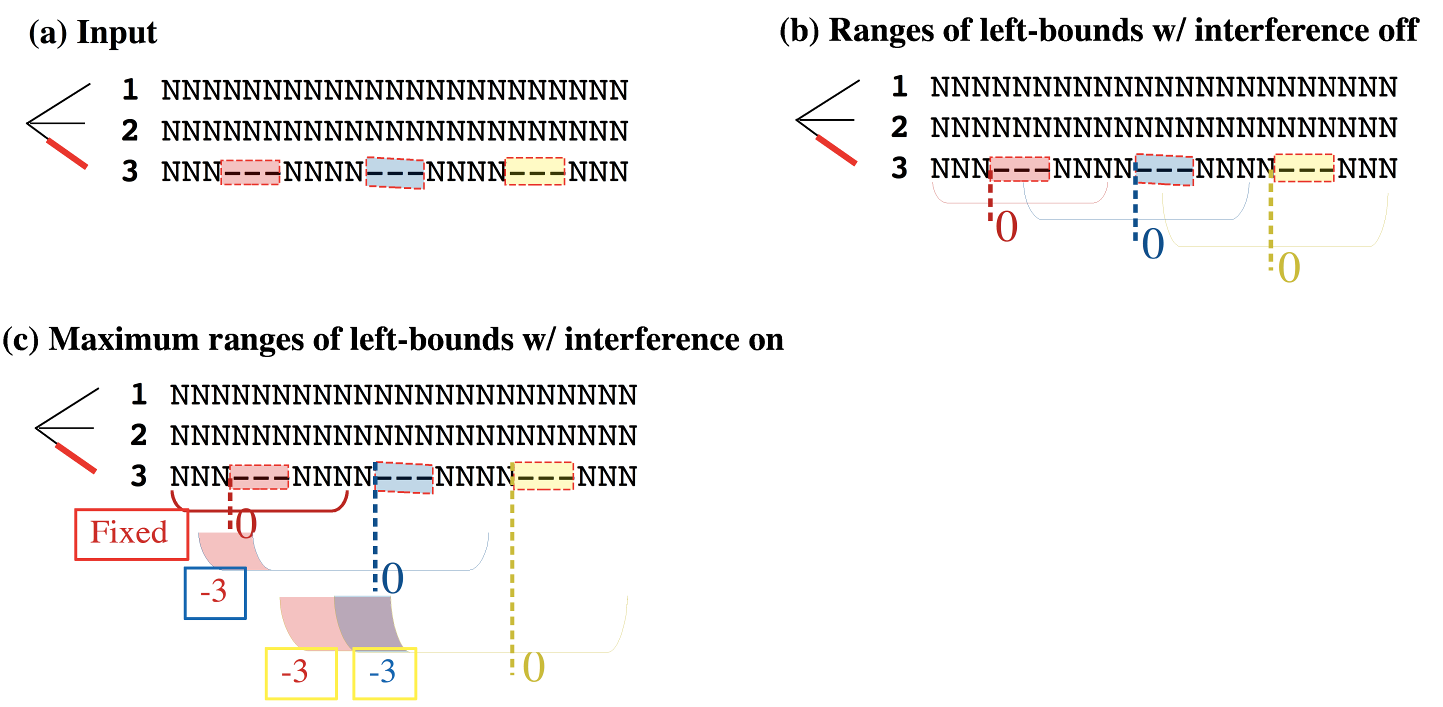

Figure SSSSA12 (1)

Figure SSSSA12. Ranges of coordinates of swappable gap-blocks that yield different degrees of degeneracy. Part 1: When no non-swappable blocks are in between swappable blocks.

(a) An input alignment, which contains three swappable gap-blocks (the dashed boxes colored in semi-transparent red, blue, and yellow). Here, they have an equal size of three.

(b) Ranges of (<u>the positions of)</u> the left-bounds of the swappable blocks (the downward convex parenthesis colored similarly (but in a bit dark manner) to the corresponding blocks), when their mutual interferences are switched off.

(c) The ranges for the same objects as in (b), but maximally extended by considering interferences among the blocks. The extended effects are colored according to the blocks swapped; their annotations are enclosed by rectangular frames with the same colors as the ranges.

According to the current coordinate convention, the range of the left-most block (red) is fixed (the "Fixed"); that of the middle block (blue) is extended to the left by the block-size (the "-3") when swapped with the red one; that of the right-most block (yellow) is extended to the left by the block-size when swapped with the blue one (the blue "-3"), and further by the block-size when swapped with the red one (the red "-3").

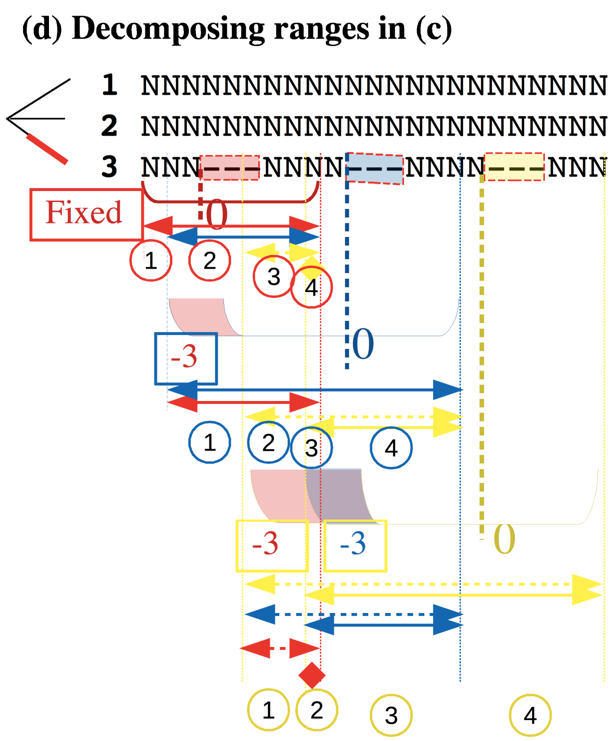

Figure SSSSA12 (2)

Figure SSSSA12. Ranges of coordinates of swappable gap-blocks that yield different degrees of degeneracy. Part 1.

(d) Decomposing the ranges of the positions of the left-bounds determined in (c). Each range is decomposed according to which blocks the subject block is swappable with.

The colored both-headed arrows below the range of each block (the colored downward convex parenthesis) show the ranges in which the latter block is swappable with the blocks with the corresponding colors. The numbers in the colored open circles are assigned to the segments of the range with the same color, each of which can accommodate a particular set of swappable blocks.

The dashed both-headed arrows indicates the swappable ranges *only* when the yellow block is swapped with both the red and blue blocks.

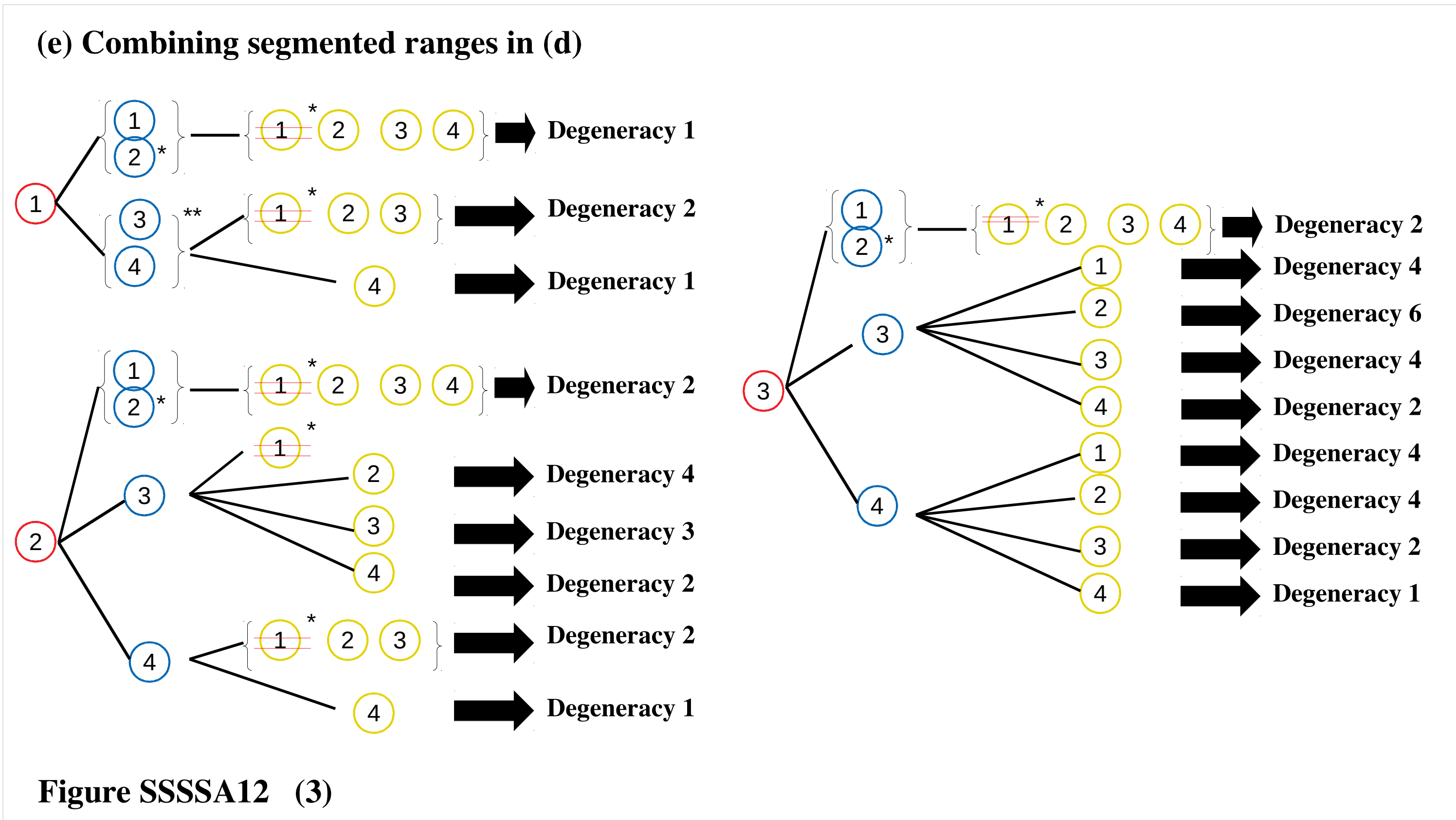

Figure SSSSA12. Ranges of coordinates of swappable gap-blocks that yield different degrees of degeneracy. Part 1.

(e) Combining the ranges segmented in (d), and assigning the degeneracy to each combination.

* Because the red block is out of the range of the yellow block, the yellow segment 1 cannot be realized, and thus the blue segments 1 and 2 need NOT be distinguished.

** Because the red block cannot be swapped with any other block, there is no need to distinguish the blue segments 3 and 4.

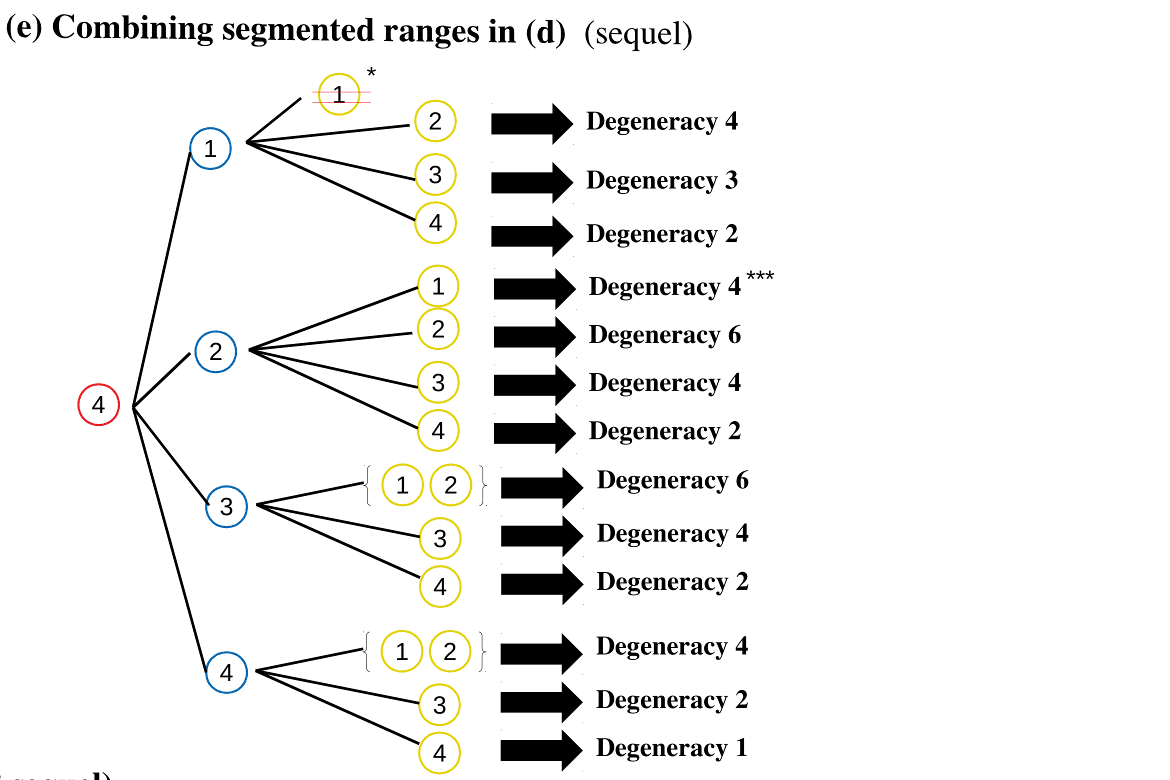

Figure SSSSA12 (3 sequel)

Figure SSSSA12. Ranges of coordinates of swappable gap-blocks that yield different degrees of degeneracy. Part 1.

(e) (sequel)

*** The degeneracy is 4, because the red 4 can never be occupied by the yellow block if the blue 2 and the yellow 1 are occupied by the blue and red blocks (regardless of which is occupied by which).

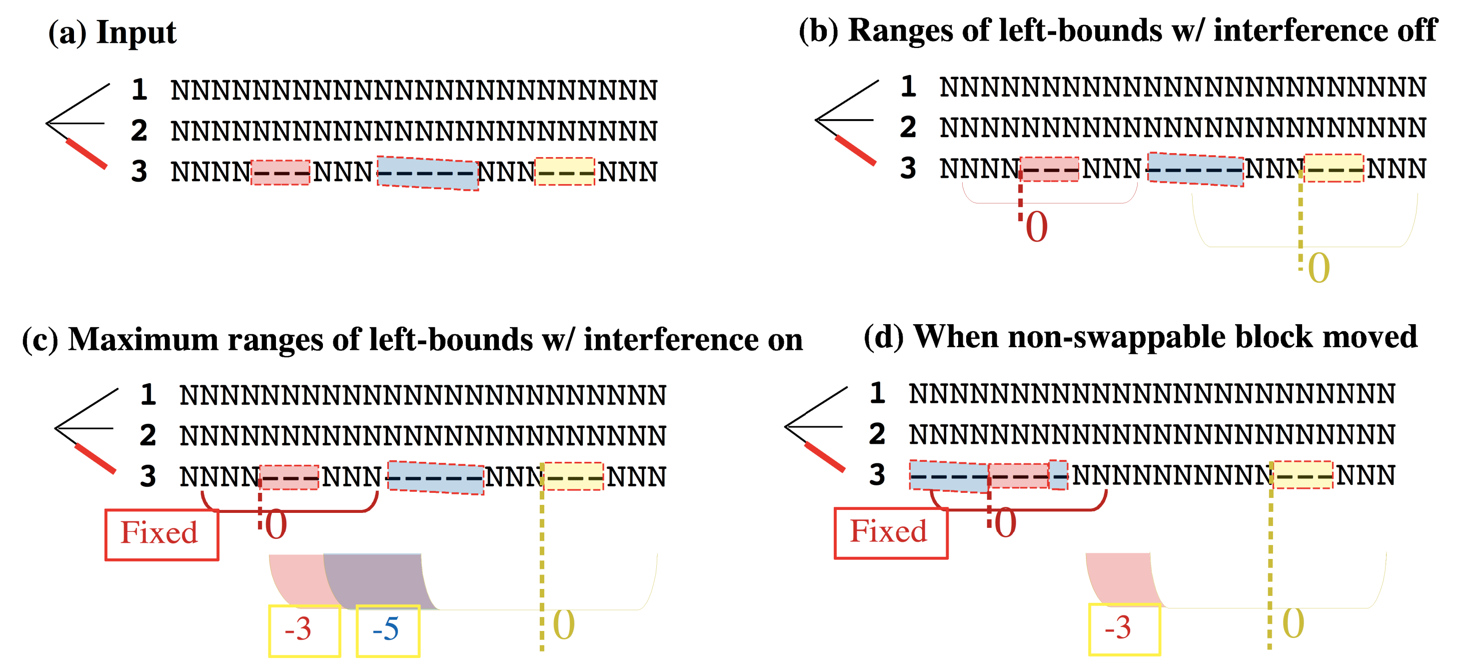

Figure SSSSA13 (1)

Figure SSSSA13. Ranges of coordinates of swappable gap-blocks that yield different degrees of degeneracy. Part 2: When some non-swappable blocks are in between swappable blocks.

(a), (b), (c) These panels follow almost the same notation as that for Figure SSSSA12 (a)-(c). The only difference is that the middle block has size of 5, i.e., longer than (and thus non-swappable with) the other two (red and yellow), and that the range of the yellow block has been omitted.

(d) When the non-swappable block (blue) moves sufficiently to the left, the swappable block on its right (yellow) cannot overlap it. This suppresses the extension of the range of the yellow block. (Note that the yellow range lacks the blue-shaded part.)

This figure indicates that the ranges of the swappable blocks can vary depending on the positions of the non-swappable blocks.