Graphical comparison of sequences using “Dotplots”.

Basic Principles.

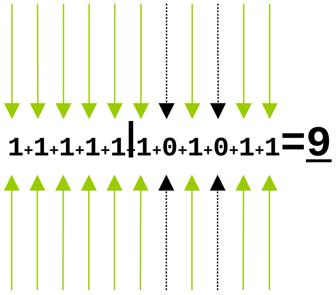
A “word size” (11 say)

A “Scoring scheme”
(1 for a match,
0 for a mismatch, say)

	A	T	G	C
A	1	0	0	0
T	0	1	0	0
G	0	0	1	0
C	0	0	0	1

A “Cut-off score” (8 say)

Diagonal runs of dots indicate similar regions



1+1+1+1+1+1+0+1+0+1+1=9

ACCTGCCCTGTCCAGCTTACATGCATGCTTATAGGGCATTTTACAT

ACCTGCCGATTCCATATTACGCATGCTTCTGGGTTACCGTTCAGGGCATTTTACATGTGCTG

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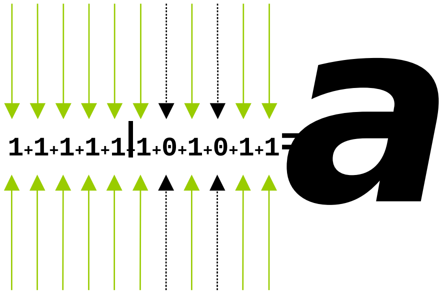

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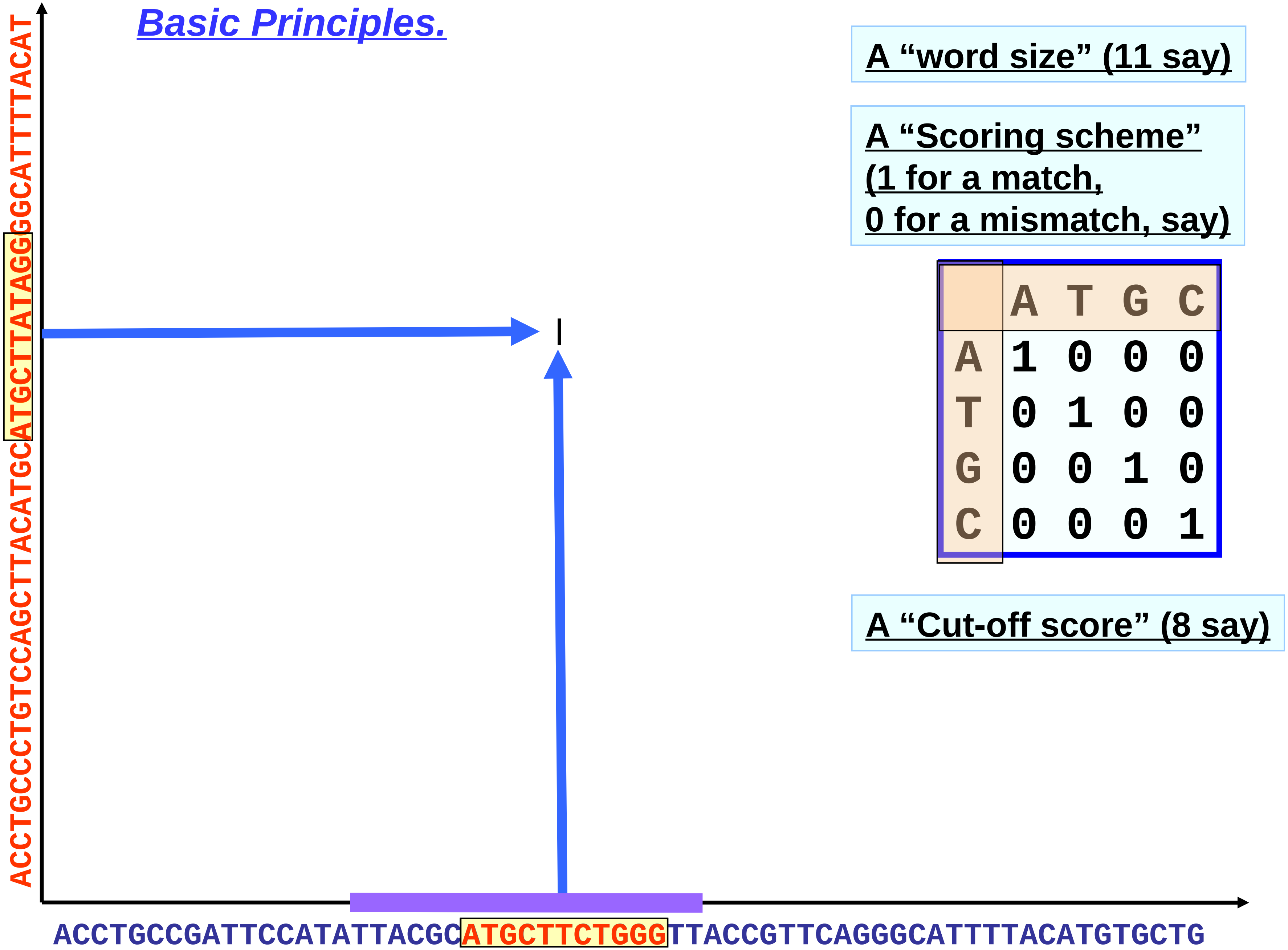

ACCTGCCCTGTCCAGCTTACATGCATGCTTATAGGGGCATTTTACAT

ACCTGCCGATTCCATATTACGCATGCTTCTGGGTTACCGTTCAGGGCATTTTACATGTGCTG

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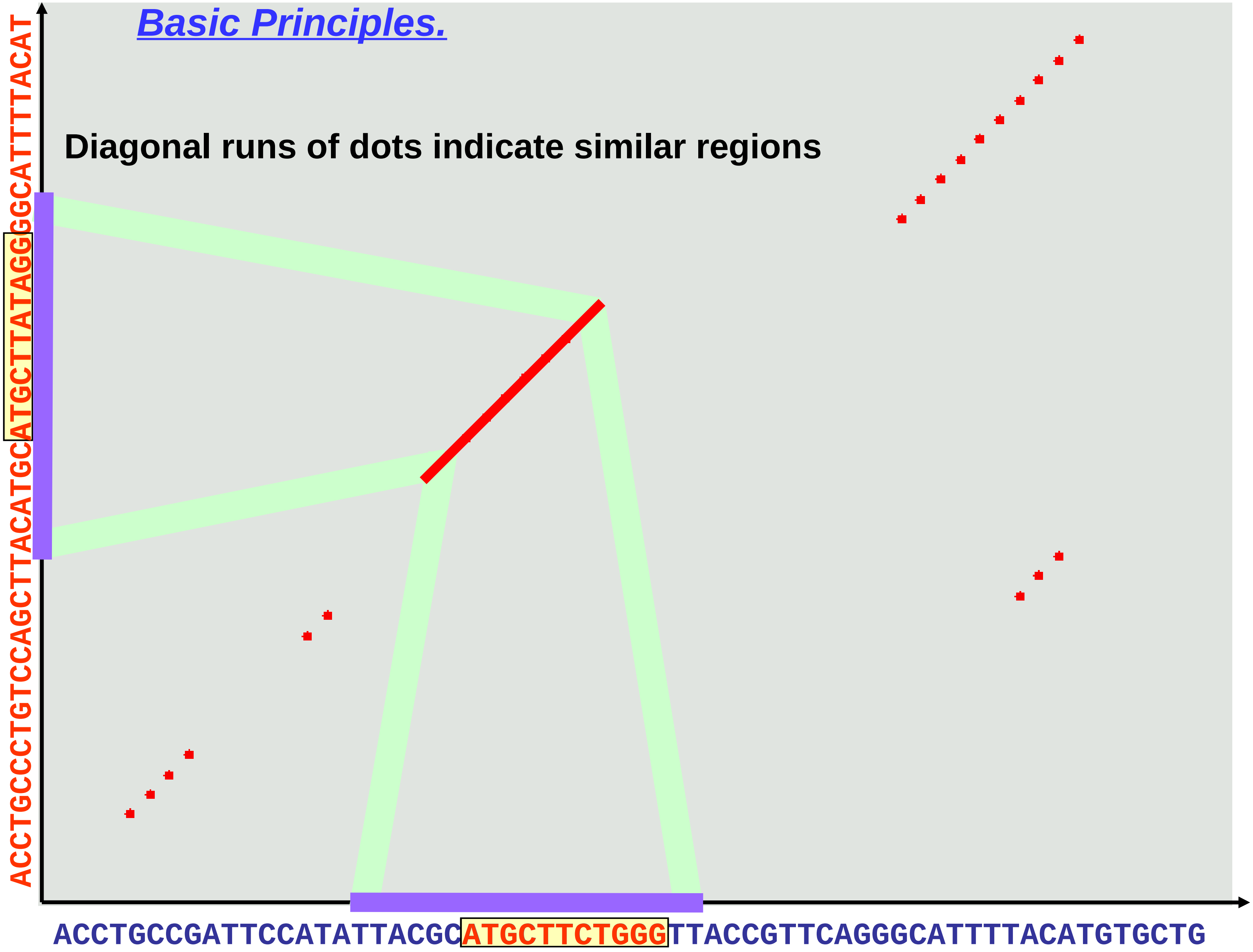

Diagonal runs of dots indicate similar regions

ACCTGCCCTGTCCAGCTTACATGCATGCTTATAGGGGCATTTTACAT
ACCTGCCGATTCCATATTACGCATGCTTCTGGGTTACCGTTCAGGGCATTTTACATGTGCTG

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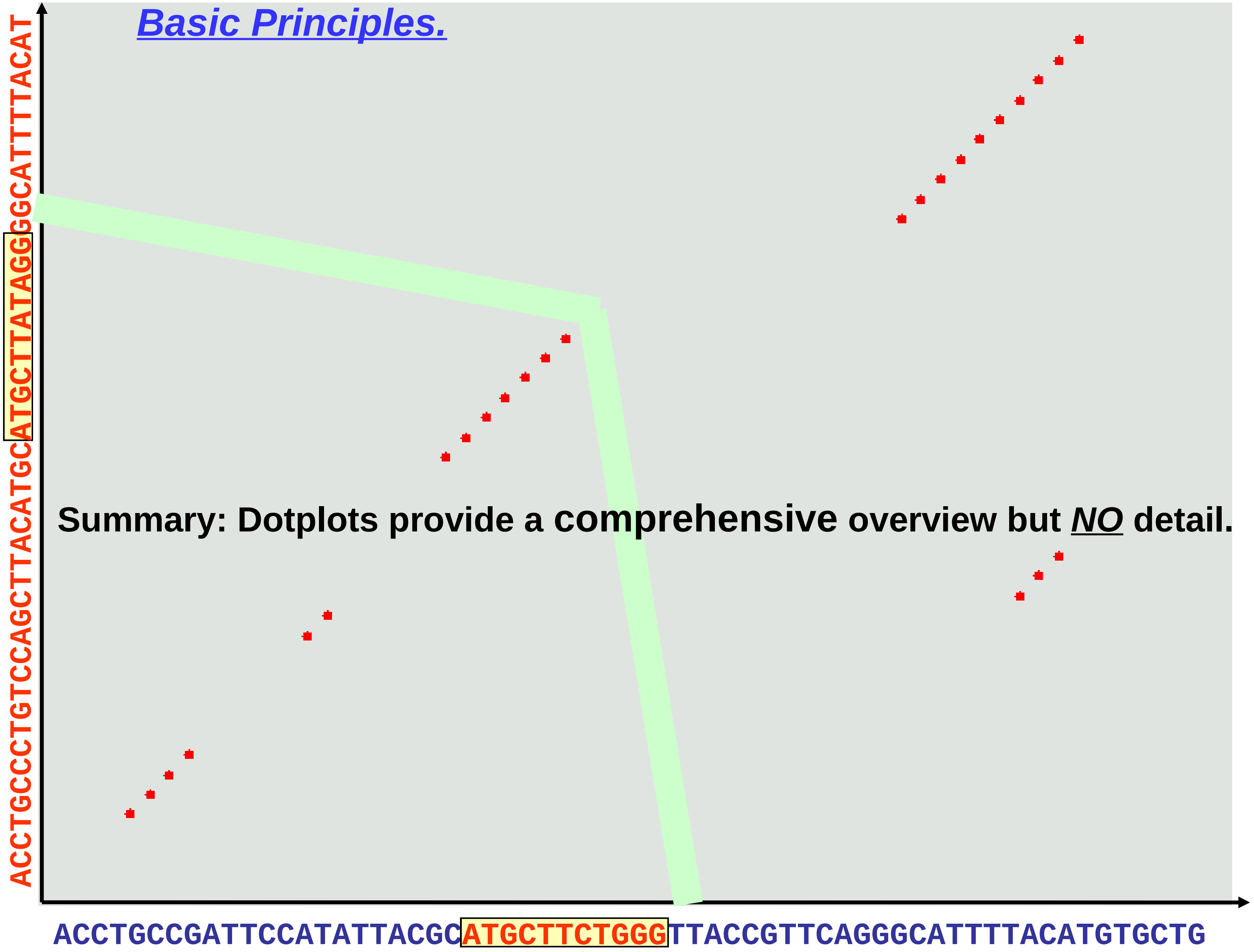

ACCTGCCCTGTCCAGCTTACATGCATGCTTATAGGGGCATTTTACAT
ACCTGCCGATTCCATATTACGCATGCTTCTGGGTTACCGTTCAGGGCATTTTACATGTGCTG

Summary: Dotplots provide a comprehensive overview but ***NO*** detail.

Graphical comparison of sequences using “Dotplots”.

Scoring Schemes.

DNA: Simplest Scheme is the Identity Matrix.

	A	T	G	C
A	1	0	0	0
T	0	1	0	0
G	0	0	1	0
C	0	0	0	1

More complex matrices can be used.
For example, the default EMBOSS DNA scoring matrix is:

	A	T	G	C
A	5	-4	-4	-4
T	-4	5	-4	-4
G	-4	-4	5	-4
C	-4	-4	-4	5

The use of negative numbers is only pertinent when these matrices are use for computing textual alignments.

Using a wider spread of scores eases the Expansion of the scoring matrix to sensibly include ambiguity codes.

Graphical comparison of sequences using “Dotplots”.

Scoring Schemes.

	A	C	G	T	S	W	R	Y	K	M	B	V	H	D	N	U
A	5	-4	-4	-4	-4	1	1	-4	-4	1	-4	-1	-1	-1	-2	-4
C	-4	5	-4	-4	-4	1	-4	1	1	-4	-1	-4	-1	-1	-2	-4
G	-4	-4	5	-4	1	-4	1	-4	1	-4	-1	-1	-4	-1	-2	-4
T	-4	-4	-4	5	1	-4	-4	1	-4	1	-1	-1	-1	-4	-2	5
S	-4	-4	1	1	-1	-4	-2	-2	-2	-2	-1	-1	-3	-3	-1	-4
W	1	1	-4	-4	-4	-1	-2	-2	-2	-2	-3	-3	-1	-1	-1	1
R	1	-4	1	-4	-2	-2	-1	-4	-2	-2	-3	-1	-3	-1	-1	-4
Y	-4	-1	-4	1	-2	-2	-4	-1	-2	-2	-1	-3	-1	-3	-1	1
K	-4	1	1	-4	-2	-2	-2	-2	-1	-4	-1	-3	-3	-1	-1	1
M	1	-4	-4	1	-2	-2	-2	-2	-4	-1	-3	-1	-1	-3	-1	-4
B	-4	-1	-1	-1	-1	-3	-3	-1	-1	-3	-1	-2	-2	-2	-1	-1
V	-1	-4	-1	-1	-1	-3	-1	-3	-3	-1	-2	-1	-2	-2	-1	-4
H	-1	-1	-4	-1	-3	-1	-3	-1	-3	-1	-2	-2	-1	-2	-1	-1
D	-1	-1	-1	-4	-3	-1	-1	-3	-1	-3	-2	-2	-2	-1	-1	-1
N	-2	-2	-2	-2	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-1	-2
U	-4	-4	-4	5	-4	1	-4	1	1	-4	-1	-4	-1	-1	-2	5

IUB DNA Alphabet

Code		Meaning
A		
C		
G		
T/U		
M	\`aMino\`	A|C
R	\`puRine\`	A|G
W	\`Weak\`	A|T
S	\`Strong\`	C|G
Y	\`pYrimidine\`	C|T
K	\`Keto\`	G|T
V	\`not T\`	A|C|G
H	\`not G\`	A|C|T
D	\`not C\`	A|G|T
B	\`not A\`	C|G|T
N	\`aNy\`	A|C|G|T

Using a wider spread of scores eases the expansion of the scoring matrix to sensibly include ambiguity codes.

Graphical comparison of sequences using “Dotplots”.

Scoring Schemes.

	A	B	C	D	E	F	G	H	I	K	L	M	N	P	Q	R	S	T	V	W	Y	Z
A	**2**	0	-2	0	0	-4	1	-1	-1	-1	-2	-1	0	1	0	-2	1	1	0	-6	-3	0
B	0	**2**	-4	3	2	-5	0	1	-2	1	-3	-2	2	-1	1	-1	0	0	-2	-5	-3	2
C	-2	-4	**12**	-5	-5	-4	-3	-3	-2	-5	-6	-5	-4	-3	-5	-4	0	-2	-2	-8	0	-5
D	0	3	-5	**4**	3	-6	1	1	-2	0	-4	-3	2	-1	2	-1	0	0	-2	-7	-4	3
E	0	2	-5	3	**4**	-5	0	1	-2	0	-3	-2	1	-1	2	-1	0	0	-2	-7	-4	3
F	-4	-5	-4	-6	-5	**9**	-5	-2	1	-5	2	0	-4	-5	-5	-4	-3	-3	-1	0	7	-5
G	1	0	-3	1	0	-5	**5**	-2	-3	-2	-4	-3	0	-1	-1	-3	1	0	-1	-7	-6	-1
H	-1	1	-3	1	1	-2	-2	**6**	-2	0	-2	-2	2	0	3	2	-1	-1	-2	-3	0	2
I	-1	-2	-2	-2	-2	1	-3	-2	**5**	-2	2	2	-2	-2	-2	-2	-1	0	4	-5	-1	-2
K	-1	1	-5	0	0	-5	-2	0	-2	**5**	-3	0	1	-1	1	3	0	0	-2	-3	-4	0
L	-2	-3	-6	-4	-3	2	-4	-2	2	-3	**6**	4	-3	-3	-2	-3	-3	-2	2	-2	-1	-3
M	-1	-2	-5	-3	-2	0	-3	-2	2	0	4	**6**	-2	-2	-1	0	-2	-1	2	-4	-2	-2
N	0	2	-4	2	1	-4	0	2	-2	1	-3	-2	**2**	-1	1	0	1	0	-2	-4	-2	1
P	1	-1	-3	-1	-1	-5	-1	0	-2	-1	-3	-2	-1	**6**	0	0	1	0	-1	-6	-5	0
Q	0	1	-5	2	2	-5	-1	3	-2	1	-2	-1	1	0	**4**	1	-1	-1	-2	-5	-4	3
R	-2	-1	-4	-1	-1	-4	-3	2	-2	3	-3	0	0	0	1	**6**	0	-1	-2	2	-4	0
S	1	0	0	0	0	-3	1	-1	-1	0	-3	-2	1	1	-1	0	**2**	1	-1	-2	-3	0
T	1	0	-2	0	0	-3	0	-1	0	0	-2	-1	0	0	-1	-1	1	**3**	0	-5	-3	-1
V	0	-2	-2	-2	-2	-1	-1	-2	4	-2	2	2	-2	-1	-2	-2	-1	0	**4**	-6	-2	-2
W	-6	-5	-8	-7	-7	0	-7	-3	-5	-3	-2	-4	-4	-6	-5	2	-2	-5	-6	**17**	0	-6
Y	-3	-3	0	-4	-4	7	-5	0	-1	-4	-1	-2	-2	-5	-4	-4	-3	-3	-2	0	**10**	-4
Z	0	2	-5	3	3	-5	-1	2	-2	0	-3	-2	1	0	3	0	0	-1	-2	-6	-4	**3**

For Protein sequence dotplots more complex scoring schemes are required. Scores must reflect far more than alphabetic identity.

Graphical comparison of sequences using “Dotplots”.

Faster plots for perfect matches.

To detect perfectly matching words, a dotplot program has a choice of strategies

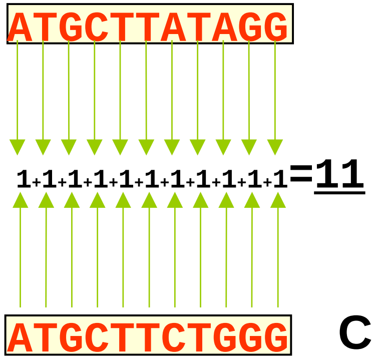
1) Select a scoring scheme

	A	T	G	C
A	1	0	0	0
T	0	1	0	0
G	0	0	1	0
C	0	0	0	1

and a word size (11, say)

For every pair of words, compute a word match score in the normal way

Only if the maximum possible cut-off score (11) is achieved



a

Celebrate with a dot

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To detect perfectly matching words, a dotplot program has a choice of strategies

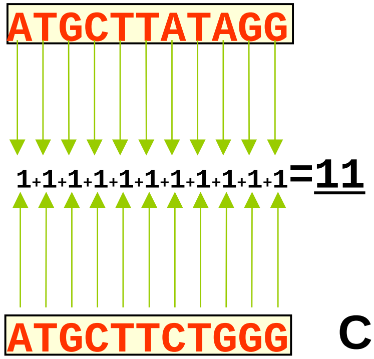
1) Select a scoring scheme

	A	T	G	C
A	1	0	0	0
T	0	1	0	0
G	0	0	1	0
C	0	0	0	1

and a word size (11, say)

For every pair of words, compute a word match score in the normal way

If the maximum possible cut-off score (still 11) is not achieved



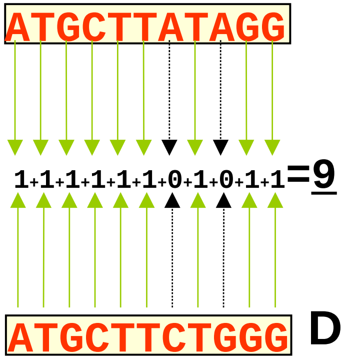
ATGCTTATAGG

1+1+1+1+1+1+1+1+1+1+1=11

ATGCTTCTGGG

a |

Celebrate with a dot



ATGCTTATAGG

1+1+1+1+1+1+0+1+0+1+1=9

ATGCTTCTGGG

r □

Do not celebrate with a dot

Graphical comparison of sequences using "Dotplots".

Faster plots for perfect matches.

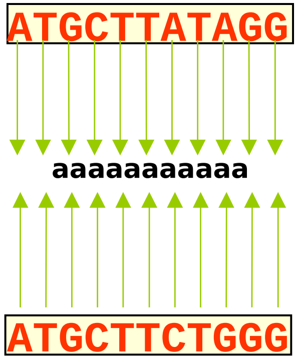
To detect perfectly matching words, a dotplot program has a choice of strategies

OR

2) For every pair of words, ……… see if the letters are exactly the same

If they are not

|



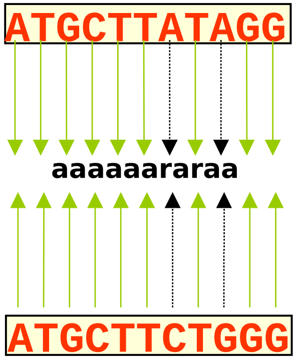
ATGCTTATAGG

aaaaaaaaaaa

ATGCTTCTGGG

a

Celebrate with a dot



ATGCTTATAGG

aaaaaararaa

ATGCTTCTGGG

r □

Do not celebrate with a dot

To detect *exactly* matching words, *fast* character string matching can replace *laborious* computation of match scores to be compared with a cut-off score

Many packages include a dotplot option specifically for detecting exactly matching words.

Particular advantage when seeking strong matches in long DNA sequences.

Graphical comparison of sequences using “Dotplots”.

Dotplot parameters.

There are three *parameters* to consider for a dotplot:

1) The scoring scheme.

2) The cut-off score.

3) The word size.

The End.