Subset seed extension to protein BLAST

Anna Gambin Sławomir Lasota Laurent Noé Michał Startek,
Maciej Sykulski and Gregory Kucherov

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Appendix

Evolution of seed alphabets and seeds

The fitness functions considered in the paper are as follows:

$$\mathrm{fitness}_1(M) = \frac{sens^F(M)}{sens^B(M)}. \tag{1}$$

$$\mathrm{fitness}_2(M) = \begin{cases} 0 & \text{if} \quad sens^B(M) > c \\ sens^F(M) & \text{otherwise} \end{cases}$$

$$\mathrm{fitness}_3(M) = \begin{cases} sens^F(M) & \text{if} \quad sens^F(M) < c \\ \frac{sens^F(M)}{sens^B(M)} & \text{otherwise} \end{cases}$$

$$\mathrm{fitness}_4(M) = \frac{sens^F(M)}{sens^B(M) + c}$$

It turned out that $\mathrm{fitness}_1(M)$ yields unsatisfactory results – the evolution just results in a smallest multiple seed possible, with minuscule foreground and background sensitivity (see Figure 1).

Fitness functions $\mathrm{fitness}_2(M)$, $\mathrm{fitness}_3(M)$ and $\mathrm{fitness}_4(M)$ reflect the trade-off between foreground sensitivity and background sensitivity. The resulting path of evolution for $\mathrm{fitness}_2(M)$ is shown on Figure 2, in this case for $c = 0,002195$. Figure 3 presents the path of evolution for $\mathrm{fitness}_3(M)$ with $c = 0.2$ and Figure 4 for $\mathrm{fitness}_4(M)$ and $c = 0.001$.

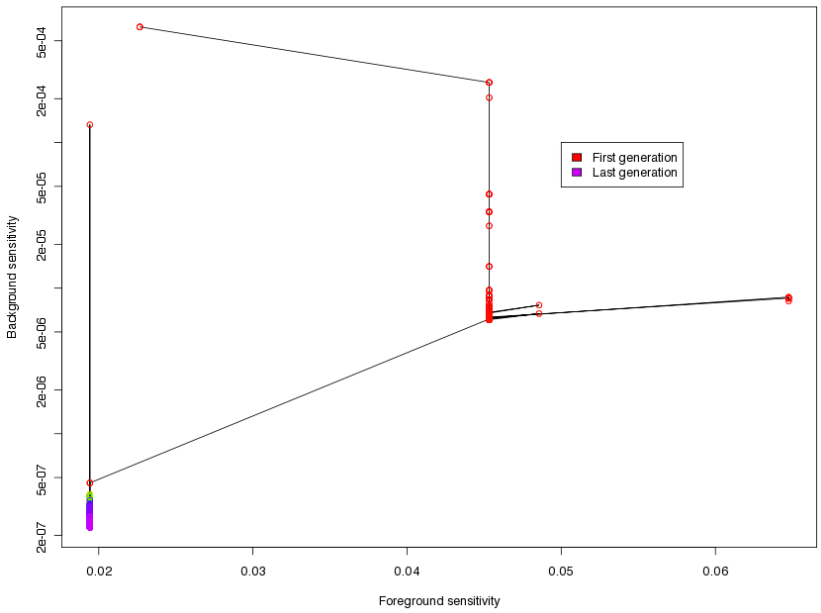


Figure 1: Path of evolution for fitness function $\texttt{fitness}_1$.

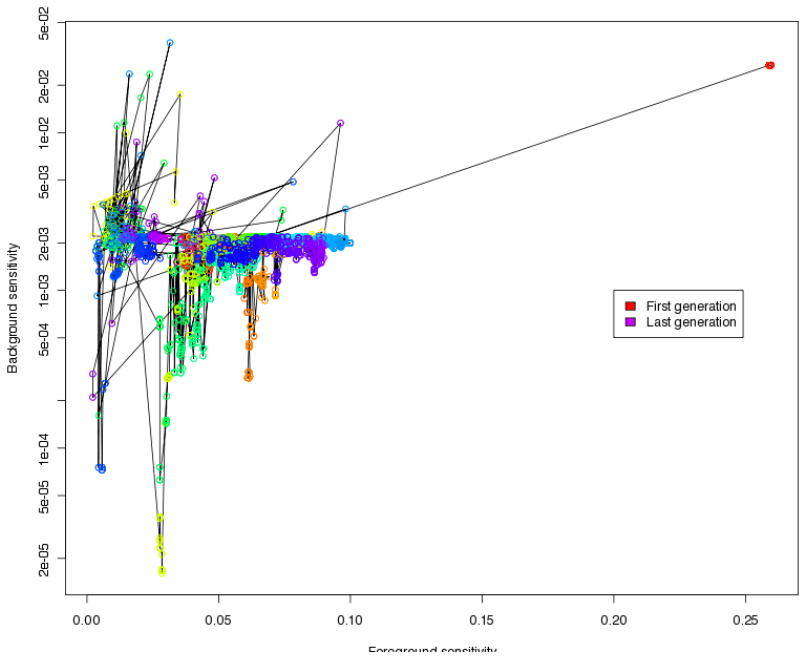


Figure 2: Path of evolution for fitness function $\mathtt{fitness}_2$.

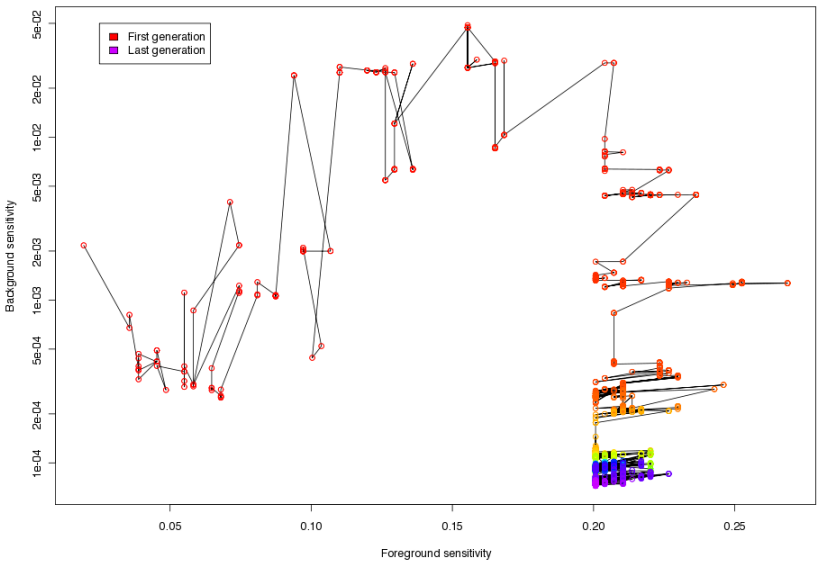


Figure 3: Path of evolution for fitness function $\mathtt{fitness}_3$.

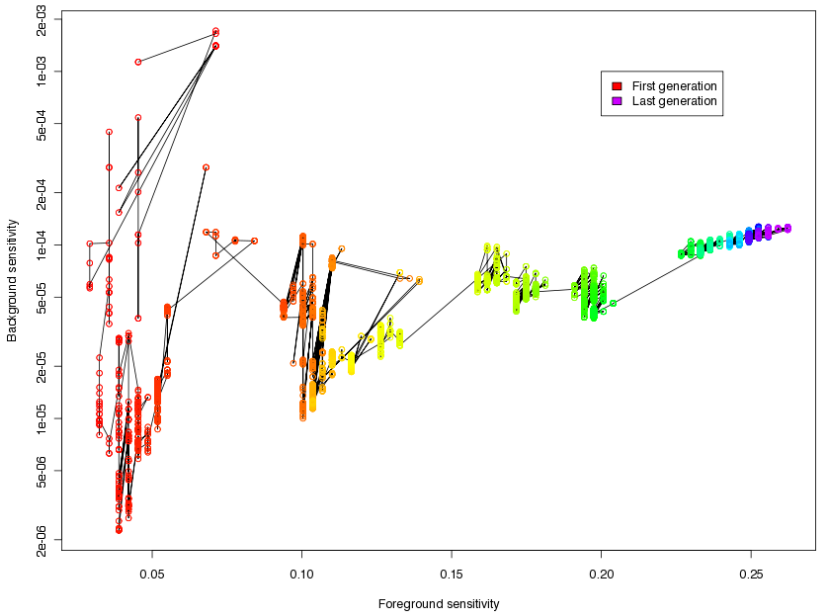
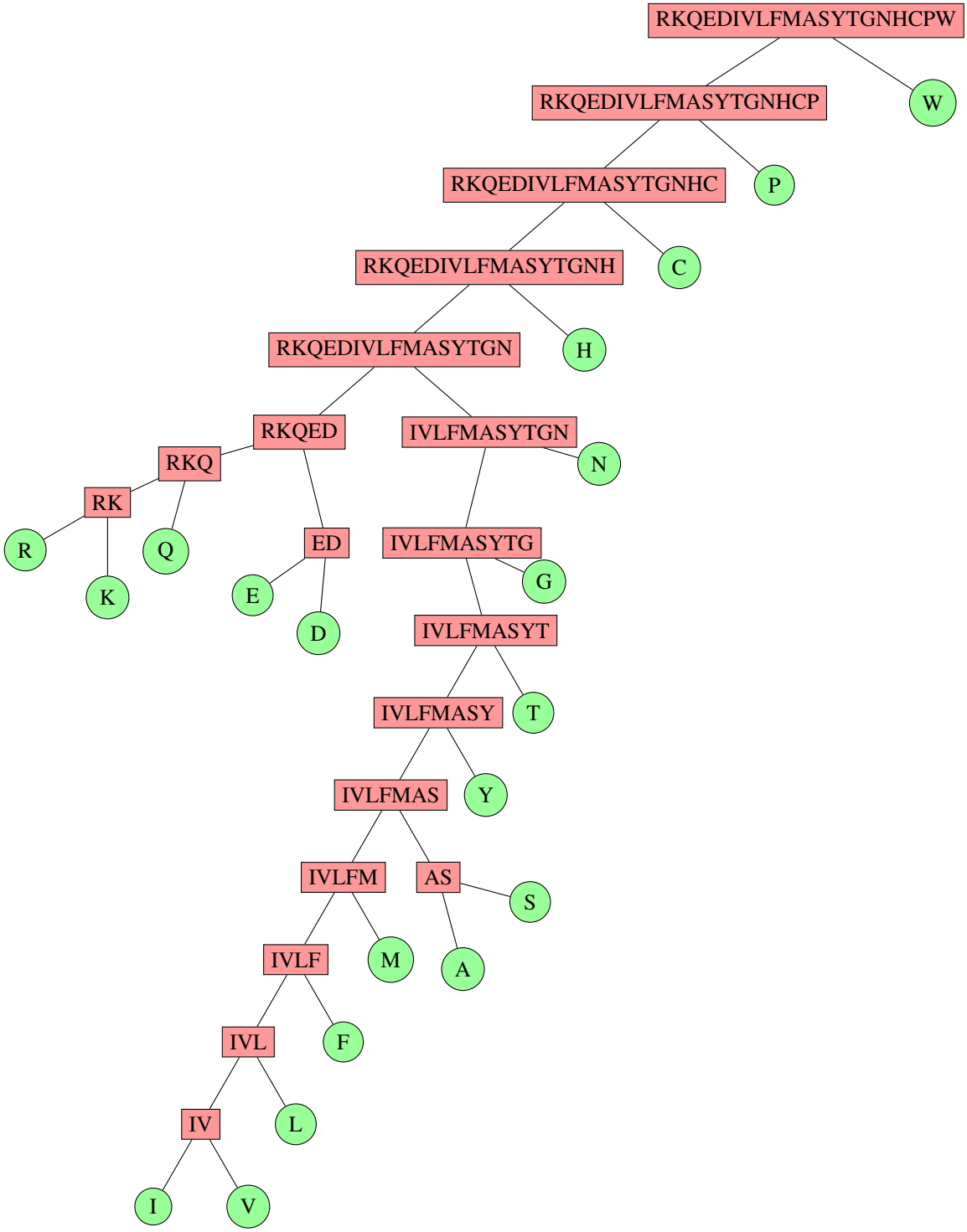


Figure 4: Path of evolution for fitness function $\mathtt{fitness}_4$.

Alphabet of the multiple seed used for experiments

The alphabet contains 8 letters. We provide its representation as a hierarchy of nested equivalence relations over amino acid alphabets. The hierarchical grouping of amino acids is also presented.

$$
\begin{aligned}
\_ &: \{\mathsf{CFYWMLIVGPATSNHQEDRK}\} \\
1 &: \{\mathsf{RKQED}, \mathsf{IVLFM}, A, S, Y, T, G, N, H, C, P, W\} \\
2 &: \{\mathsf{RKQED}, \mathsf{IVL}, F, M, A, S, Y, T, G, N, H, C, P, W\} \\
3 &: \{\mathsf{RKQ}, \mathsf{ED}, \mathsf{IVL}, F, M, A, S, Y, T, G, N, H, C, P, W\} \\
4 &: \{\mathsf{RK}, Q, \mathsf{ED}, \mathsf{IVL}, F, M, A, S, Y, T, G, N, H, C, P, W\} \\
5 &: \{\mathsf{RK}, Q, E, D, \mathsf{IV}, L, F, M, A, S, Y, T, G, N, H, C, P, W\} \\
6 &: \{R, K, Q, E, D, \mathsf{IV}, L, F, M, A, S, Y, T, G, N, H, C, P, W\} \\
\# &: \{R, K, Q, E, D, I, V, L, F, M, A, S, Y, T, G, N, H, C, P, W\}
\end{aligned}
\tag{2}
$$


RKQEDIVLFMASYTGNHCPW
RKQEDIVLFMASYTGNHCP
W
RKQEDIVLFMASYTGNHC
P
RKQEDIVLFMASYTGNH
C
RKQEDIVLFMASYTGN
H
RKQED
IVLFMASYTGN
RKQ
N
RK
R
Q
ED
IVLFMASYTG
K
E
G
D
IVLFMASYT
IVLFMASY
T
IVLFMAS
Y
IVLFM
AS
S
IVLF
M
A
IVL
F
IV
L
I
V