

Supplemental material (File S2) for *Fixation dynamics of beneficial alleles in prokaryotic polyploid chromosomes and plasmids* (Santer et al., bioRxiv, 2021)

```
In[*]:= ClearAll["Global`*"]
$Assumptions = {_ ∈ Reals, n > 1}
Out[*]:= {_ ∈ ℝ, n > 1}
```

Solution of $x_{\text{mut}}(t)$

```
In[*]:= sol = DSolve[x'[t] == -s * x[t]^2 + x[t] (s + a * (b * Exp[b * t] / (a * Exp[b * t] + (b - a)))) && x[0] == f, x, t]
Out[*]:= {{x -> Function[{t],
    (e^(s t) (-a + b + a e^(b t)) f (b + s) / (b^2 + a b f - b^2 f - a b e^(s t) f + b^2 e^(s t) f + b s - b f s - a e^(s t) f s + b e^(s t) f s + a e^((b+s) t) f s) ]}}
```

(There is only a single solution (as expected).)

```
In[*]:= xmut[t_] = FullSimplify[x[t] /. sol[[1]]]
Out[*]:= (e^(s t) (b + a (-1 + e^(b t))) f (b + s) / (b (b + a f - b f + s - f s) + e^(s t) f (a e^(b t) s - (a - b) (b + s))))
```

Inserting a, b gives

```
In[*]:= ab = {a -> (1 + s) (ξ + κ - 1), b -> (1 + s) (ξ - 1)};
In[*]:= xmut[t_] = FullSimplify[xmut[t] /. ab]
Out[*]:= (e^(s t) f (-1 + ξ + s ξ) (κ - e^((1+s) t) (-1+ξ) (-1 + κ + ξ))) / ((-1 + e^(s t)) f κ (-1 + ξ) - (-1 + ξ) (-1 + ξ + s ξ) + f s (-1 + κ + ξ + (-1 + e^(s t)) κ ξ - e^t (-1+ξ+s ξ) (-1 + κ + ξ)))
```

Decay of wild-type carrying cells $x_0(t)$ and convergence of $\frac{x_{\text{wt}}(t)}{x_0(t)}$

Define x_{hf} . For large t , $\frac{1}{t} \log x_{\text{wt}}(t)$ converges to $(1+s) (-1+\xi)$

```

In[ ]:=  $\xi \kappa = \left\{ \xi \rightarrow \frac{2n-3}{2n-1}, \kappa \rightarrow \frac{1}{2n-1} \right\};$ 

xhf[t_] = FullSimplify[ $\frac{b * e^{(b * t)}}{a * e^{(b * t)} + b - a}$  /. ab]

xwt[t_] = FullSimplify[ $1 - xmut[t] * (1 - xhf[t])$ ]

Assuming[{s > 0, (1 + s)  $\xi$  > 1,  $\xi$  > 0,  $\xi$  < 1, f > 0, f < 1,  $\kappa$  < 1 -  $\xi$ ,  $\kappa$  > 0},
  Limit[ $\frac{1}{t} \text{Log}[xwt[t]]$ , t  $\rightarrow \infty$ ]]

Out[ ]:= 
$$\frac{e^{(1+s)t} (-1+\xi) (-1+\xi)}{-\kappa + e^{(1+s)t} (-1+\xi) (-1+\kappa+\xi)}$$


Out[ ]:= 
$$\left( (-1+\xi) \left( -1 - \left( -1 + e^{t(-1+\xi+s\xi)} \right) f(s(-1+\kappa) + \kappa) + \xi + s\xi \right) \right) / \left( (-1+\xi) (-1+\xi+s\xi) + \right.$$


$$\left. f \left( - \left( -1 + e^{st} \right) \kappa (-1+\xi) + e^{t(-1+\xi+s\xi)} s(-1+\kappa+\xi) - s(-1+\kappa+\xi + (-1 + e^{st}) \kappa \xi) \right) \right)$$


Out[ ]:= ConditionalExpression[(1 + s) (-1 +  $\xi$ ), 2 (1 + s)  $\xi$  > 2 + s]

```

The condition $2(1+s)\xi > 2+s$ must hold to obtain the analytical result (above) with MMA:

For large t , $\frac{x_{wt}(t)}{x_0(t)}$ converges to

```

In[ ]:= Assuming[{s > 0, (1 + s)  $\xi$  > 1,  $\xi$  > 0,  $\xi$  < 1, f > 0, f < 1,  $\kappa$  < 1 -  $\xi$ ,  $\kappa$  > 0},
  Limit[ $\frac{1 - xmut[t] * (1 - xhf[t])}{1 - xmut[t]}$ , t  $\rightarrow \infty$ ]]

Out[ ]:= 
$$\frac{s(-1+\kappa) + \kappa}{(1+s)(-1+\kappa+\xi)}$$


```

Convergence

The plot below shows an example for $n=32$ that $\text{Limit}\left[\frac{1}{t} \text{Log}[xwt[t]], t \rightarrow \infty\right]$ equals $(1+s)(-1+\xi)$ also if $(1+s)\xi > 1 \Leftrightarrow s > \frac{1}{n-3/2}$ (left vertical line) holds and $2(1+s)\xi > 2+s \Leftrightarrow s > \frac{2}{n-5/2}$ (right vertical line) is not fulfilled.

```

In[ ]:= nrul = {n -> 16};
slist = {0.01, 0.02, 0.03, 0.04, 0.05,
         0.06, 0.07, 0.08, 0.09, 0.1, 0.15, 0.2, 0.25, 0.3}

(1 + slist) *  $\xi$  /.  $\xi \rightarrow \frac{2n-3}{2n-1}$  /. nrul
2  $\frac{1+slist}{2+slist} \xi$  /.  $\xi \rightarrow \frac{2n-3}{2n-1}$  /. nrul

y1 = Table[Limit[
   $\frac{1}{t} \text{Log}[xwt[t]]$  /. { $\xi \rightarrow \frac{2n-3}{2n-1}$ ,  $\kappa \rightarrow \frac{1}{2n-1}$ ,  $f \rightarrow 0.01$ } /. nrul, t ->  $\infty$ ], {s, slist}]
y2 = Table[(1 + s) (-1 +  $\xi$ ) /.  $\xi \rightarrow \frac{2n-3}{2n-1}$  /. nrul, {s, slist}]
ListPlot[{Transpose[{slist, y1}], Transpose[{slist, y2}]},
  PlotMarkers -> "OpenMarkers",
  GridLines -> {{ $\frac{2}{n-5/2}$  /. nrul,  $\frac{1}{n-3/2}$  /. nrul}, {0, 0}},
  AxesLabel -> {s, "Limit[ $\frac{1}{t} \text{Log}[xwt[t]]$ , t ->  $\infty$ ]"}, PlotRange -> Full,
  PlotLegends -> {"Numerical solution", (1 + s) (-1 +  $\xi$ )}]

```

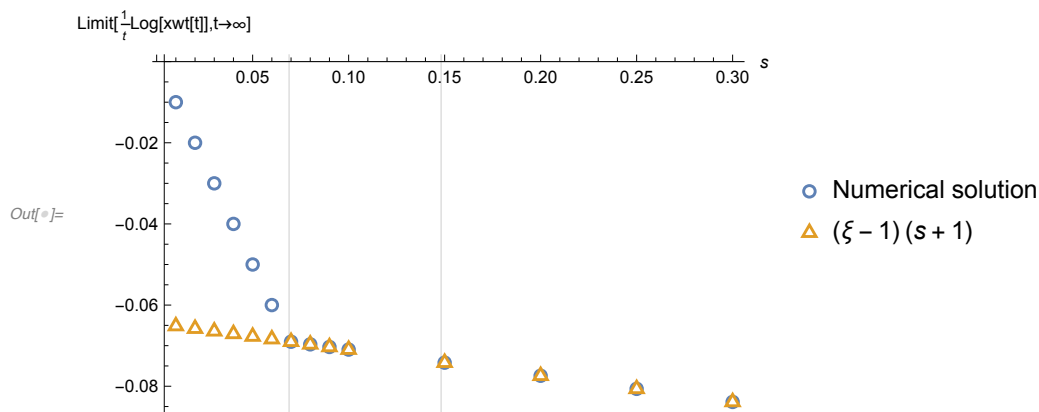
Out[]:= {0.01, 0.02, 0.03, 0.04, 0.05, 0.06, 0.07, 0.08, 0.09, 0.1, 0.15, 0.2, 0.25, 0.3}

Out[]:= {0.944839, 0.954194, 0.963548, 0.972903, 0.982258, 0.991613,
1.00097, 1.01032, 1.01968, 1.02903, 1.07581, 1.12258, 1.16935, 1.21613}

Out[]:= {0.940138, 0.944746, 0.949309, 0.953827, 0.958301, 0.962731, 0.967119,
0.971464, 0.975768, 0.980031, 1.00075, 1.02053, 1.03943, 1.0575}

Out[]:= {-0.01, -0.02, -0.03, -0.04, -0.05, -0.06, -0.0690323, -0.0696774,
-0.0703226, -0.0709677, -0.0741935, -0.0774194, -0.0806452, -0.083871}

Out[]:= {-0.0651613, -0.0658065, -0.0664516, -0.0670968,
-0.0677419, -0.0683871, -0.0690323, -0.0696774, -0.0703226,
-0.0709677, -0.0741935, -0.0774194, -0.0806452, -0.083871}



Computation of the heterozygosity window

In[*]:= `Hw[n_, s_] = Simplify[$\frac{-\text{Log}\left[\frac{s(-1+\kappa)+\kappa}{(1+s)(-1+\kappa+\xi)}\right]}{(1+s)(\xi-1)}$ /. $\xi \rightarrow \frac{2n-3}{2n-1}$ /. $\kappa \rightarrow \frac{1}{2n-1}$]`

Out[*]=
$$\frac{(-1+2n) \text{Log}\left[\frac{-1+2(-1+n)s}{1+s}\right]}{2(1+s)}$$

In[*]:= `Plot[Hw[n, 0.3], {n, 1, 100}]`

