Receptor recharge time drastically reduces the number of captured particles

Gregory Handy, Sean D. Lawley, Alla Borisyuk

Supporting Information (S1 Text)

This file contains the proof to Lemma \[ \text{Lemma 2} \] justification for calling \( \tau_e = (D\lambda_1)^{-1} \) the escape time, and additional details about the Lambert W Function.

Proof of Lemma \[ \text{Lemma 2} \]

Let \( X(t) \in \overline{\Omega} \) denote the position at time \( t \geq 0 \) of a particle diffusing in \( \overline{\Omega} \) with reflecting boundary conditions on \( \partial \Omega \) and diffusivity \( D > 0 \). Let \( g(x, t) \) denote the probability that the particle has not reached \( \partial \Omega_E \) by time \( t \geq 0 \) given that it starting at \( x \in \overline{\Omega} \). Precisely, define the stopping time

\[
 t_e := \inf\{t > 0 : X(t) \in \partial \Omega_E\},
\]

and let

\[
 g(x, t) := P(t_e > t | X(0) = x).
\]

It is known that \( g(x, t) \) satisfies the Kolmogorov backward equation

\[
 \frac{\partial}{\partial t} g = D \Delta g, \quad x \in \Omega, t > 0, \tag{18}
\]

\[
 g = 0, \quad x \in \partial \Omega_E, t > 0, \tag{19}
\]

\[
 \frac{\partial}{\partial \sigma} g = 0, \quad x \in \partial \Omega \setminus \partial \Omega_E, t > 0, \tag{20}
\]

\[
 g = 1, \quad x \in \Omega, t = 0. \tag{21}
\]

By \[ \text{[2]} \], there exists a set of eigenvalues and eigenfunctions as in the statement of the lemma. It is then easy to check that

\[
 g(x, t) = \sum_{k=1}^{\infty} (\phi_k, 1) e^{-D\lambda_k t} \phi_k(x)
\]

satisfies Eqs. \[ \text{[18-21]} \] If \( X(0) \) is distributed according to \( p(x) \), then

\[
 S(t) = \int_{\Omega} g(x, t)p(x) \, dx,
\]

and Eq \[ \text{[10]} \] follows.

Escape time.

To see why we refer to \( \tau_e = (D\lambda_1)^{-1} \) as the escape time, define \( t_e \) as in Eq \[ \text{[17]} \] It is known that the expected value of \( t_e \) (the so-called mean first passage time)

\[
 s_e(x) := E[t_e | X(0) = x],
\]

satisfies the elliptic problem

\[
 -1 = D \Delta s_e, \quad x \in \Omega,
\]

\[
 s_e = 0, \quad x \in \partial \Omega_E.
\]
\[
\frac{\partial}{\partial \sigma} s_e = 0, \quad x \in \partial \Omega \setminus \partial \Omega_E.
\]

If the \( X(0) \) is distributed according to its quasi-stationary distribution, \( \phi_1(x)/(\phi_1, 1) \geq 0 \) \([3]\), then the mean of \( t_e \) is

\[
\int_{\Omega} s_e(x)\phi_1(x)/(\phi_1, 1) \, dx.
\]

Now, using the PDEs and boundary conditions that \( \phi_1 \) and \( s_e \) satisfy and integrating by parts yields

\[
\int_{\Omega} s_e(x)\phi_1(x)/(\phi_1, 1) \, dx = -\frac{1}{\lambda_1} \int_{\Omega} s_e(x)\Delta \phi_1(x)/(\phi_1, 1) \, dx
\]

\[
= -\frac{1}{\lambda_1} \int_{\Omega} \Delta s_e(x)\phi_1(x)/(\phi_1, 1) \, dx
\]

\[
= \frac{1}{D\lambda_1} \int_{\Omega} \phi_1(x)/(\phi_1, 1) \, dx = \tau_e,
\]

as desired. We note that the boundary terms that appear from integrating by parts vanish since either \( s_e \) or the normal derivative of \( s_e \) is zero on the boundary.

**Note on Lambert W Function**

While \( W_{-1}(z) \) is a fairly standard function that is included in most modern computational software, we can use recent results to obtain a more tractable description of \( n_c \). It was recently proven \([4]\) that \( W_{-1}(z) \) satisfies

\[
-W_{-1}(-e^{-u-1}) < 1 + \sqrt{2u} + u,
\]

if \( u > 0 \). Therefore, combining this bound with Eq \([16]\) shows that if the ratio of particles to capture regions, \( n/m \), satisfies

\[
\frac{n}{m} \geq \frac{1}{T\bar{h}} \left(1 + \sqrt{2(T + \log(C/h))} + T + \log(C/h)\right),
\]

(22)

then \( n > n_c \) and the logarithmic bound in Theorem \([2]\) is tighter than the linear bound. Hence, if Eq \([22]\) is satisfied, then the recharge time significantly affects \( E[N] \).

**Supporting References**


