

Konrad-Zuse-Zentrum
für Informationstechnik Berlin

Takustraße 7
D-14195 Berlin-Dahlem
Germany

MARCUS WEBER

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Konrad-Zuse-Zentrum für Informationstechnik Berlin
Takustraße 7
D-14195 Berlin-Dahlem

Telefon: 030-84185-0
Telefax: 030-84185-125

e-mail: bibliothek@zib.de
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The funnel trap paradox

Marcus Weber, Zuse Institute Berlin (ZIB), Takustraße 7, 14195 Berlin, Germany, weber@zib.de

Abstract. In this article, an illustrative example is given for the coarse-graining of a Markov process which leads to a shift in the statistical weights of a two-states-system. The example is based on a 2D-funnel trap. The funnel trap is constructed in such a way, that the area inside and outside of the trap is identical. However, observing the flight of the insect as a Markov process, the probability for being “in the trap” is higher. This example can be transferred to several kinds of processes (like receptor-ligand-binding processes in chemistry) and describes the influence of “re-entering events”.

Keywords: Markov process, Robust Perron Cluster Analysis, Conformation Dynamics

MSC Classification: 60J25, 62H30, 82B30

Introduction

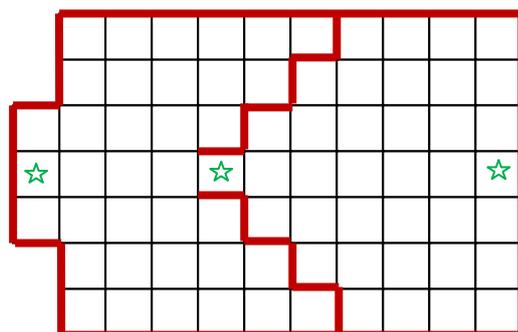


Fig. 1. Scheme of a funnel trap

A funnel trap (red line) is shown in Fig. 1. Its area is divided into 73 equally sized squares (black lines). The three squares which are marked with a green star will be important in the following sections. With this trap we will try to “catch an insect”. Note that 36 squares belong to the left (“in”) part and 36 squares belong to the right (“out”) part of the funnel trap. One marked square in the center of the funnel is neither “in” nor “out”. This is called the *transition square*. The first step is to model the flight of an insect inside this trap as a time-continuous Markov jump process between the given 73 boxes. This jump process will be constructed in such a way that there are good reasons to expect that the insect is “in” or “out” of the trap with almost the same probability (at the limit of an infinite observation time) because of the equivalence of the areas. However, there are also good reasons to expect that the insect stays “in the trap” for a longer period of time than “out of the trap” because of the funnel shape of the transition area. We will see that both points of view are correct. This is the paradox. The solution to this paradox is the following idea: The red line in Fig. 1 splits the trap into two rooms with equal areas and it also generates two states of the insect which are called “in-the-trap”-state and “out-of-the-trap”-state. These two kinds of separation need not be the same. An insect that has just left the “in”-room will re-enter it with a significant

probability, such that the insect has passed the transition square but is still in its “in-the-trap”-state with a certain degree. Note, that for practical reasons it is not necessary for a funnel trap to be like a one-way-street (I have already seen flies escaping from my funnel trap). It is sufficient that the trap separates the two *metastable states of the insect*. Once the insect is in its “in-the-trap”-state the catcher should have enough time to react, i.e., kill the insect or take it to another place.

Constructing the Markov Jump Process

The flight of the insect will be modeled with a continuous-time Markov jump process. The instantaneous jumps between the 73 squares are given by transition rates. These rates are organized as a 73x73-rate-matrix Q . Let us first reconsider the following known properties of transition rate matrices [1]. The diagonal elements of Q are negative and the off-diagonal elements are non-negative. For a given $t > 0$, the expression $\exp(Q(i, i) \cdot t)$ denotes the *holding probability* of square $i \in \{1, \dots, 73\}$. This is the probability that the flight time of the insect inside square i (without leaving it meanwhile) exceeds t . Instantaneous transitions only exist between two squares which are next to each other and share a common (black line) edge. All further entries of Q are zero. The non-negative ratio $-Q(i, j)/Q(i, i)$ denotes the conditional probability of the insect to enter square j in the moment it leaves its starting square i . Each row of Q has the row-sum zero, which means that the sum of the conditional probabilities (per starting square i) is “1” and that there is zero probability that the insect leaves the funnel trap (outer red line) or enters it from outside. Furthermore, the row-sum condition means that Q is negative-semidefinite. We will construct Q in such a way, that the dominant eigenvalue “0” is simple. The corresponding (adequately normalized) left eigenvector of Q is denoted as w . The i -th element $w(i)$ of w is the probability for the insect to be in square i (at the limit of an infinite observation time). A simple method for constructing a corresponding *rate matrix* Q which leads to the same observation probability (identical entries $w(i)$) for each square is given by the following procedure: Enter the transition rate $Q(i, j) = 1$ whenever instantaneous transitions between square i and square j are possible. Afterwards, insert the diagonal elements of Q such that the row-sums are zero. We aim at a two-states-separation of the insect (in the next section). From a naïve point of view, the marked transition square of Fig. 1 has to be assigned to the “in”-state or to the “out”-state of the insect. Thus, one of the two states is expected to have the probability (at infinite observation time) of 50.68% (=37/73), the other state has a probability of 49.32% (=36/73). We will call these numbers *the statistical weights of the states*. There is a simple possibility to manipulate the rates in Q in such a way, that the difference between these statistical weights is decreased. By multiplying a row i of Q with a positive real number $a > 0$, the relative probability of the insect to be in the corresponding square i is reduced by the factor $1/a$. Thus, we will multiply the row of Q corresponding to the transition square with factor 10. Furthermore, we will put a “lure” on the left *and* on the right side of the trap. The rows of Q corresponding to the left and the right marked square in Fig. 1 are multiplied with the factor 1/7. By these manipulations, we expect the difference between the statistical weights of the “in” and the “out” states to be 50.06% (=42.1/84.1) vs. 49.94% (=42/84.1). Which one of the states has the higher probability is expected to depend on the assignment of the transition square. This is the point of view when considering the splitting of the trap into two rooms.

Constructing the Two-States-Separation

Let us now consider the insect's point of view and take a more sophisticated look at the rate matrix Q . If one wants to compute the probability for finding the insect in a certain square after time-span t when the insect has started (let's say) in square $i = 1$, then this information can be computed in the following way: We have to evaluate the 73×73 -transition probability matrix $P_t = \text{expm}(Q \cdot t)$, where "expm" is the matrix exponential. The entry $P_t(i, j)$ denotes the conditional probability that an insect starting in square i will be in square j after time t . Thus, the entry $P_t(1, j)$ is the answer to the given question. Taking the matrix exponential is like a time-discretization from the time-continuous Markov jump process to a time-discrete Markov chain [1]. However, we do not aim at a time-discretization. We aim at a spatial discretization ("in" and "out"), i.e. we want to project the 73×73 -transition rate matrix Q to a 2×2 -transition matrix \tilde{Q} . In order to preserve the correct kinetics of the system, the spatial discretization has to commute with the time-discretization. This means that the time-discretized matrix $\tilde{P}_t = \text{expm}(\tilde{Q} \cdot t)$ should be equal to the spatial discretization of P_t . For a two state system, this is possible only if $\tilde{Q} = (\chi^T W \chi)^{-1} (\chi^T W Q \chi)$, where W is the diagonal matrix of the vector components of w , and χ is a 73×2 -matrix consisting of two column vectors χ_{in} and χ_{out} with entries between 0 and 1, see [2]. The vector element $\chi_{in}(i)$ denotes how much the square i counts for the "in-the-trap"-state of the insect. The vector element $\chi_{out}(i)$ denotes how much the square i counts for the "out-of-the-trap"-state of the insect. The two column vectors are visualized in Fig. 2.

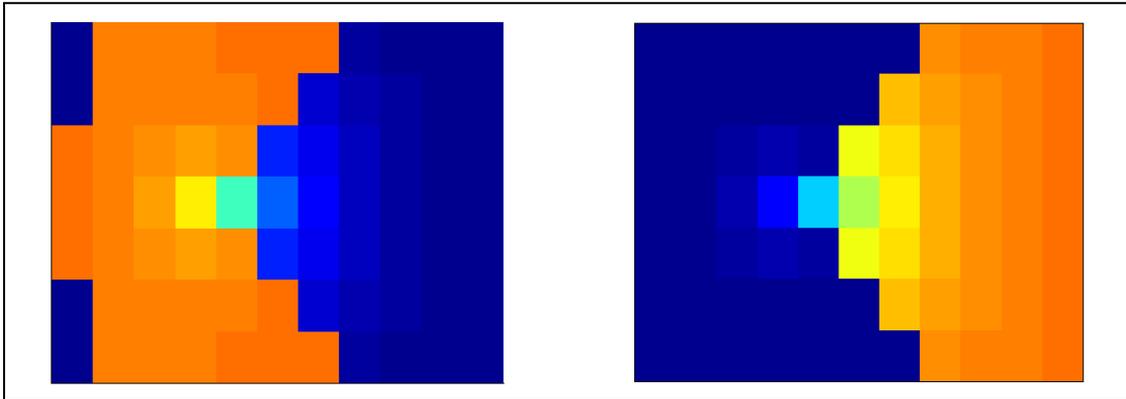


Figure. 2. In this scheme one can see the state of the insect when it is in a certain square of the funnel trap. The insect always partially attains both of the states ("in-the-trap" and "out-of-the-trap") with a certain degree. The squares in this figure are colored according to this degree. On the left side the "in-the-trap"-state is shown, on the right side it is the "out-of-the-trap"-state.

For a valid commutation of the discretizations, the column vectors χ_{in} and χ_{out} have to be linear combinations of the two dominant eigenvectors e_1 and e_2 of Q , where e_1 is a constant vector $e_1(i) \equiv 1$. The PCCA+ algorithm [3] determines these vectors to be

$$\chi_{in} = \frac{e_2 - \min(e_2) \cdot e_1}{\max(e_2) - \min(e_2)}, \quad \chi_{out} = \frac{\max(e_2) \cdot e_1 - e_2}{\max(e_2) - \min(e_2)}.$$

In order to compute the statistical weights of the two metastable states of the insect, we have to multiply the elements $w(i)$ of the dominant left eigenvector w of Q with the corresponding entry in the vector $\chi_{in}(i)$ or $\chi_{out}(i)$, respectively. Taking the sum over these products leads to

the following statistical weights: The insect is in its “in-the-trap”-state with a probability of 51.63% and in its “out-of-the trap”-state with a probability of 48.37%. As one can see in Fig. 2, there are more “yellow squares” in χ_{out} (right side) than in χ_{in} (left side), which means that the insect has a higher tendency to *re-enter* the left side than the right side after passing the transition square. Thus, there is a shift in the statistical weights towards the “in-the-trap”-state, because we expected the probabilities to be 50.06% and 49.94%.

Conclusion

The basic idea of this article is the following: **The funnel trap does not divide the area into two “rooms”, it rather generates two metastable states of the insect.**

With the presented mathematical tools, “re-entering events” could be interpreted in other fields of application, too. One example is a ligand-receptor-binding process. The receptor does not divide the space of the ligand into an unbound and a bound part, it rather generates two states of the ligand -- the ligand is in a “bound” or in an “unbound” state. There need not be a 1-to-1-correspondence between “decomposition of the space into two sets” and “two states of the ligand”.

References

- [1] **M. Kijima**. *Markov Processes for Stochastic Modeling*. Stochastic Modeling Series. Chapman and Hall, 1997.
- [2] **S. Kube and M. Weber**. A coarse graining method for the identification of transition rates between molecular conformations. *J. Chem. Phys.*, 126:024103–024113, 2007.
- [3] **P. Deufilhard and M. Weber**. Robust Perron Cluster Analysis in Conformation Dynamics. In M. Dellnitz, S. Kirkland, M. Neumann, and C. Schütte, editors, *Lin. Alg. App. – Special Issue on Matrices and Mathematical Biology*, volume 398C, pages 161–184. Elsevier, 2005.