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Titre de la thèse : Modélisation de l'apparement évolutif entre les structures tridimensionnelles de protéines

L'essentiel de la machinerie biochimique du vivant repose sur les protéines et leur structure tri-dimensionnelle (3D). Or à ce jour la plupart des méthodes d'étude des relations évolutives entre individus ou espèces se basent sur l'analyse des séquences de nucléotides ou d'acides-aminés. L'objectif de cette thèse est de développer des modèles de génétique des populations prenant en compte l'évolution de structures 3D, de mettre en place des méthodes statistiques d'inférence ancestrale adaptées et d'exploiter des outils récents et efficaces de calcul de distances entre structures 3D (Ritchie, D.W., Ghoorah, A.W. Mavridis, L., Venkatraman, V. Bioinformatics, 2012) afin d'étudier les relations évolutives entre structures protéiques.

- Publications :

- Nicolas Champagnat, Benoît Henry ¹
Probabilités et statistiques - IECL - Institut Élie Cartan de Lorraine
TOSCA - TO Simulate and CALibrate stochastic models
CRISAM - Inria Sophia Antipolis - Méditerranée , IECL - Institut Élie Cartan de Lorraine : UMR7502
We consider a branching population where individuals live and reproduce independently. Their lifetimes are i.i.d. and they give birth at a constant rate b . The genealogical tree spanned by this process is called a splitting tree, and the population counting process is a homogeneous, binary Crump-Mode-Jagers process. We suppose that mutations affect individuals independently at a constant rate θ during their lifetimes, under the infinite-alleles assumption: each new mutation gives a new type, called allele, to his carrier. We study the allele frequency spectrum which is the numbers $A(k, t)$ of types represented by k alive individuals in the population at time t . Thanks to a new construction of the coalescent point process describing the genealogy of individuals in the splitting tree, we are able to compute recursively all joint factorial moments of $(A(k, t))$ $k \geq 1$. These moments allow us to give an elementary proof of the almost sure convergence of the frequency spectrum in a supercritical splitting tree.

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Probabilités et statistiques - IECL - Institut Élie Cartan de Lorraine

We consider a general branching population where the lifetimes of individuals are i.i.d. with arbitrary distribution and each individual gives birth to new individuals at Poisson times independently from each others. The population counting process is a Binary Homogeneous Crump-Jagers-Mode process. Moreover, we suppose that the individuals experience mutations at Poisson rate θ under the infinite-alleles assumption. These mutations lead to a partition of the population by type. In this paper, we obtain central limit theorems for the frequency spectrum when time goes to infinity. We also obtain CLT for the population counting process. To this end, we use classical renewal theory and recent works [18, 6, 5] on this model to obtain the moments of the error. Then, we can precisely study the asymptotic behaviour of these moments thanks to Lévy processes theory. These results in conjunction with a new decomposition of the splitting tree allow us to obtain the wanted Theorems.