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Reconstruction of mathematical frame models of bacterial transcription regulation based on transcriptional regulatory networks

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Motivation and Aim: In recent years, an enormous amount of full genome sequencing data has been accumulated, including bacterial data. However, the analysis of these data lags behind the rate of their accumulation, particularly in the context of transcription regulation. For example, for the most studied model organism *Escherichia coli*, the complete description of genetic regulation has not yet been completely solved [1]. Even less information is available for other bacteria. The use of mathematical modelling techniques makes it possible to assess the impact of transcription regulation processes on the behaviour of a model system in dynamics. For example, simulations can provide general answers to the following questions: how gene expression changes at the transcription level with or without the participation of selected transcription factors (TFs); what contribution a series of TFs have to the system behaviour when their mutual regulation is taken into account, etc. Only experiment can answer these questions more accurately.

Methods and Algorithms: The developed method makes it possible to derive fusion rate functions from the available structure of the operon promoter region, which specifies the interaction variants between TFs and their binding sites (TFBSs). The equations are constructed in terms of generalized Hill functions [2]. Resulting models of transcription processes and their regulation are described by differential equations. The program is implemented in the Java programming language.

Results: This work presents the development of a previously developed algorithm for reconstruction of frame models based on the structure of bacterial transcriptional regulatory networks (TRNs) [3]. The new iteration takes into account the structure of operon – TFs roles and possible locations of TFBSs on the promoter region. These parameters more accurately specify the effects of regulation. The output contains the operon regulation model equations in text format, i.e. one file – one model. This is done for the convenience of further analysis. The algorithm was tested on bacterial genome sequencing data from the database of the Kurchatov Genomic Center of the Institute of Cytology and Genetics, SB RAS.

Conclusion: The developed tool complements previously developed algorithms [3, 4] for genome analysis.

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