

SECTOR 1.1

Sector of Computer Logic in Information Processes

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DIRECTIONS OF ACTIVITY:

- Construction of algorithms of reasonable complexity (quadratic, cubic) for analysis of regulation on the DNA and RNA levels. Search for regulatory signals and given patterns in genomic sequences, identification of conserved and alternative RNA structures, and, in particular, analysis of attenuation-based regulation. Analysis of complex interacting regulatory systems in a cell.
- Construction of acceptable-complexity (quadratic, cubic) algorithms for reconciliation of protein phylogenetic trees. Application of these algorithms to construction of species trees and analysis of evolutionary events such as horizontal transfer.
- Development of the concept of information interaction and effective description of objects based on combining the theories: model completeness, descriptive set theory, stochastic games with discrete time, modal logic, information transformers categories, algorithmic complexity and randomness.

MAIN RESULTS

A new algorithm for identification of horizontally transferred genes was suggested and implemented. The algorithm computes the dissimilarity between gene and species trees and identifies the most offending gene in the tree. The algorithm was applied to clusters of orthologous genes (COGs).

The previously suggested algorithm for tree reconciliation was improved using normalization of branch lengths and introduction of a weighting scheme for duplications and losses. A new species tree for forty microorganisms represented in COGs was constructed.

The algorithm for identification of conserved RNA structures based on alignment of half-stems was improved by accounting for conservation of sequence boxes. A procedure searching for such boxes by multiple alignment of given sequences was suggested. The new algorithm takes into account energy parameters, pseudoknots and other biological details. The identified structures are merged into a consensus structure using the technique of identification of dense subgraphs. The algorithm was successfully tested on tRNA, RFN, T-box and S-box sequences, as well as simulated sequence fragments.

A new algorithm was developed for identification of weakly conserved signals with the cloverleaf topology.

The algorithms were applied to the number of problems of comparative genomics (joint work with Integrated Genomics, Inc.). This included description of structural properties of protein-DNA recognition, analysis of evolution of regulons in bacterial genomes, as well as studies of regulatory systems such as bacteriocin production, SOS-response, purine biosynthesis, biosynthesis of vitamins such as riboflavin, thiamin, and biotin.

It was shown that biosynthesis of riboflavin and thiamin is regulated by formation of alternative RNA secondary structures, and the same structural mechanism acts on different functional levels, attenuation (premature termination) of transcription and inhibition of translation initiation. This prediction was subsequently confirmed by independent experimental data. The THI-box pattern known to be involved in regulation of thiamin-related genes was extended and applied to identification of new thiamin regulon members such as thiamin transporters in the *Bacillus/Clostridium* group.

61 RFN elements were described in 49 bacterial genomes (in all taxonomic groups excluding spirochaetes, mycoplasmas and rickettsiae); all of them occur upstream of riboflavin biosynthesis and transport genes. Analysis of the topology and sequence patterns of the RFN elements, together with construction of protein trees, allowed for identification of several horizontal transfer events.

Analysis of the biotin regulon lead to identification of a regulatory signal common to bacteria and archaea; this is the first observation of this kind. We demonstrated that conserved base pairs in regulatory signals form more contacts with recognizing proteins and suggested a method for identification of amino acid residues responsible for the specificity of recognition of DNA sites and ligands in large families of transcription factors.

A new recognition rule for identification of T-boxes was constructed based on comparative computer analysis of known examples. The search new T-boxes produced new biological results; this is the first attempt of complete characterization of a global RNA-based regulatory system.

New attenuators in alpha- beta-and gamma-proteobacteria were identified using analysis of RNA structures and other relevant features such as candidate leader peptides, and relative positions of the Shine-Dalgarno boxes and start codons.

Complete analysis of the glycerol-3-phosphate regulons (GlpR repressor from the DeoR family) in the genomes of proteobacteria led to identification new regulatory signals that are palindromic in gamma-proteobacteria from the Enterobacteriaceae and Pasteurellaceae families and tandem repeats in alpha- and beta-proteobacteria.

A problem of influence of the players' knowledge level and its form on creating the optimal strategies in games connected with stochastic dynamic systems with discrete time (Nash equilibrium) is studied. It was shown that additional information and favorable external conditions can have a negative impact on the game results. However, for the cooperative behavior of the players in the same situations both increase of the knowledge and improvement of external conditions always lead to the players' payoffs. Developed methods are implemented in computer algorithms.

The general properties of categories of information transformers (IT) were investigated as a monoidal category of special kind. The key concept in construction of such category as Kleisly category is a functor T that takes an object A to an object TA of all "distributions on A ", and a natural transformation which assigns an "independent joint distribution" to a pair of "distributions". Necessary and sufficient conditions for a derived Kleisly category to satisfy the axioms for a monoidal category of ITs were obtained.

There were studied measurement systems that are described by an integral operator on a plane, which is invariant with respect to the group of motions on a plane. The problem of construction of an optimum measurement-computer system was studied. It was shown that adequate consideration of invariance reduces the problem on a plane to a one-dimensional Fredholm equation on an interval. Developed methods are implemented in computer algorithms.

Well known hypothesis: that fragments of the intuitionistic propositional logic defined by limitation on the number of variables used are decidable by a polynomial algorithm is refuted. This hypothesis was also formulated for standard modal logics with PSPACE-complete problem of decidability. This hypothesis was also refuted for modal logics, namely, it was proved that the condition of PSPACE-completeness for K, K4 logics are ensured by constant formulas, and for S4, Crz, GL logics – by formulas with one variable.

The complexity of decidability for modal logic of statements on consistency in formal arithmetic (GLLin logic) with limitation on the number of variables is studied. It is proved that its constant fragment is polynomial decidable, and one variable formulas fragment have NP-complete problem of satisfiability (unprovability).

The problem of reducibility of Borel and countably determined equivalence relations in nonstandard domains is studied. It is proved that reducibility relation between such equivalence is determined by the relative rate of growth of confinal sequences in initial segments which induce the monads. In particular, any two equivalence relations induced by countably confinal monads are comparable by Borel reducibility.

A generalization of Gilbert geometric form theorem on basis was obtained. The sense of this generalization is in the replacement of the notion of "polynom" to more general notion of "quasipolynom" from variables x_1, x_2, \dots, x_k . By quasipolynom we mean a polynom from x_1, x_2, \dots, x_k and expressions $F(x_1), F(x_2), \dots, F(x_k)$, and also of derivatives $F'(x_1), \dots, F'(x_k), \dots, F^{(i)}(x_1), \dots, F^{(i)}(x_k)$. It is proved that for any infinite sequence S of quasipolynoms of x_1, x_2, \dots, x_k there exists such a number c that for almost all polynoms $p=F(x)$ for any point $a=\langle x_1, x_2, \dots, x_k \rangle$ either all polynoms in $S(p)$ equal 0 in the point a or some polynom from $S(p)$ having number not greater than c is not equal to 0 in the point a (phrase "for almost all" means that for any polynom it is always possible to change its coefficients as little as possible so)

Well-known universal (for stationary ergodic sources) data compression algorithms (for example Lempel-Ziv algorithms) have a property of asymptotic optimality. In particular, for almost every infinite data sequence generated by a source with unknown statistics the average length of the code sequence on one bit of input sequence tends to entropy of the source when the block-length tends to infinity. Non-robustness property for such algorithms is proved in the case when ergodicity is violated. We used a notion of deficiency of randomness as a measure of dissimilarity between probability distribution and data sequence. The robustness property for more specific sources is proved: Lempel-Ziv algorithm is robust on any sequence generated by Markov chains if the deficiency of randomness of this sequence grows as $o(n)$.

A theoretical ground for Minimum Description Length principle (MDL) was given. Assume that we are given some data x (we may assume that x is a finite binary sequence). We want to find a best hypothesis explaining x . By definition a hypothesis is a probability distributions on the set of all binary strings. Assume that the description complexity of any explanation must not increase a given number a . MDL principle suggests to define the best hypothesis as that minimizing the difference $K(P) - \log_2(P(x))$. It is proved (with P. Vytanyi) that this hypothesis is the best, i.e. it also

minimizes the randomness deficiency of x with respect to P (among all hypothesis of complexity at most a).

The a priori measure of any set is at least 2 to the power of minus complexity of its implicit description. It is proved that an inverse inequality holds: the square of the measure of any set is at most the same value. This was already known with the cube in place of the square (Solovay's theorem).

The members took part as invited speakers at the conferences and schools:

- International Summer School in Functional Genomics "From Genome To Life. Structural, Functional and Evolutionary Approaches", Cargese, Corsica, July, 2002.
- Modern Logik: theory, history and applications, Sankt-Petersburg, 2002.
- Fourth conference Advances in Modal Logic, Toulouse, 2002.
- Nonstandard methods and applications in mathematics. Pisa, Italy, 10-16 June 2002.
- Logic Colloquium 2002, ASL European Summer meeting. Munster, Germany, 2002, August 3-10.
- Workshop on Descriptive Set Theory, Analysis, and Dynamical Systems. Fields Institute, Toronto, Canada, 2002, Oktober 6-12.
- Fourth International Conference «Problems of control and modelling in the complex systems», Samara, 2002, June 17-23.
- The third international conference on bioinformatics of genome regulation and structure, BGRS'2002, Novosibirsk, Russia, 2002, July 14-20.
- Computational Learning Theory, Australia, Sydney, 2002, January.

International cooperation: Vuppertal (Germany), Bonn (Germany), Royal Holloway College (London university), CWI (Amsterdam, The Netherlands), Provence university (Marseille), Dagshtul (Germany), Vienna university (Austria), AstraZeneca (Boston), NCBI (Bethesda, USA), Int. Summer School (Cargese, France), MIT (Boston), Lawrence Berkeley National Laboratory (Беркли), Stanford University (США).

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PUBLICATIONS IN 2002

Articles

1. Вьюгин В.В., Любецкий В.А. О некоторых способах отбора горизонтально перенесенных генов на основе филогенетических данных // Электронный научный журнал "Информационные процессы". 2002. Т. 2. № 1. С. 120-140. (<http://www.jip.ru>).
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