Structure vs. Property: Algorithms and Models

Thesis of Habilitation

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Contents

Rezumat

Teza 'Structură vs. proprietate: algoritmi şi modele' a fost scrisă ca o abordare transdisciplinară care uneşte împreună conceptele de matematică şi informatică pentru a rezolva probleme în chimie. Principala problemă tratată este de utilizare a structurii chimice pentru a explica proprietăţi (fizice, chimice) şi activităţi (biologice) de compuşi.

Noi folosim modele şi algoritmi tot timpul, dar cel mai dificil nu este de a folosi, ci a-i proiecta şi / sau a-i recunoaşte. Având în vedere acest lucru, teza a fost scrisă ca o instruire in recunoaşterea şi proiectarea lor, şi, prin urmare, ar putea părea prea structurată.

Primul capitol, *De la observaţie la experiment, şi la model*, provine dintr-o introspecţie despre proiectarea experimentelor, cele care ne furnizează date brute, şi din care extragem modele, tipare şi relaţii între observabile noastre şi el poate fi considerat situat la baza următoarelor.

Al doilea capitol, *Reprezentare cu formule şi proprietăţi*, defineşte materialul nostru de cercetare în timp ce al treilea capitol, *Nivele de reprezentare* sintetizează legăturile cheie între structura şi proprietatea compuşilor chimici. Un rezultat original este dat la sfârşitul său, şi este despre legătura dintre răspândirea clorofilelor în organisme vii şi eficienţa lor în conversia energiei solare.

Capitolul al patrulea, *Topologie şi geometrie moleculară*, defineşte reprezentarea informaţională a structurii chimice şi este o punte spre metodele noastre de cercetare. Acesta conţine, de asemenea, o serie de rezultate originale privind dezvoltarea şi utilizarea de instrumente de topologie moleculară pentru a investiga structura chimică.

Capitolul al cincilea, *Teoria reacţiilor chimice şi a echilibrului*, discută despre a doua utilizare a modelării matematice în chimie, pentru studiul cineticii de reacţie. Implementări soft uşor de făcut sunt furnizate.

Capitolul al şaselea, *Separare în amestecuri de solvenţi: metoda triunghiului lui Snyder*, asigură legătura dintre teoria soluţiilor şi utilizarea de modele pentru a estima faza optimă realizată în cromatografie. Aplicaţii ale unor modele derivate aici sunt oferite în capitolul 16.

Capitolul al şaptelea, *Analiza variabilelor binare şi multinomiale: intervale binomiale de încredere*, este o întoarcere înapoi la provocarea de a utiliza funcţia de măsurare, discutată în primul capitol. Anume, acest capitol (care conţine rezultate originale de asemenea), ia primul nivel al funcţiei de măsurare (în scală binară şi multinominală) şi oferă soluţii pentru a exprima încrederea la expresii care conţin rapoarte binare (atunci când sunt utilizate pentru a măsura asocieri între observabile).

Capitolul 8, *Analiza variabilelor ordinale: statistica rangurilor*, ia al doilea nivel al funcţiei de măsurare (pe scale de ordine) şi oferă soluţii pentru a exprima tăria asocierii monotone.

Capitolul 9, *Analiza de regresie liniară: modele liniare*, ia ultimul nivel de măsurare (pe scala raport) și oferă alternative de analiză pentru cel mai important model de asociere: al asociației liniare. Două rezultate originale sunt prezentate aici: despre generalizarea distribuțiilor Gauss și Laplace și utilizarea acesteia pentru a evalua tipul de eroare experimentală, iar celălalt este cu privire la alternativele în analiza de asociere liniară.

Capitolul 10, *Relații structură-activitate: metoda familiilor de descriptori*, dă contribuția mea principală la dezvoltarea metodelor de analiză a legăturii dintre structura și proprietatea compușilor chimici.

Capitolul 11, *Reducerea complexității de calcul: proiectarea și utilizarea de algoritmi genetici*, dă contribuția mea principală la proiectarea de algoritmi genetici pentru a găsi euristic relațiile structură-activitate.

Capitolul 12, *Aplicații de analiza distribuției populației*, oferă o serie de rezultate originale obținute implicând analiza distribuției populației din care provine un eșantion.

Capitolul 13, *Aplicații de teoria grafurilor și analiză statistică*, oferă o serie de rezultate originale în teoria grafurilor, teoria informației, și statistică aplicată, precum și utilizarea lor pentru a evalua relația dintre structura și proprietatea compușilor chimici.

Capitolul 14, *Aplicații de proiectare soft*, descrie pe scurt rezultatele de la dezvoltarea și evaluarea software-ului pentru efectuarea cercetărilor.

Capitolul 15, *Aplicații de meta-euristici*, subliniază rezultatele obținute din utilizarea unei contingențe de strategii de evoluție la studiul evoluției supervizate de algoritmi genetici.

Capitolul 16, *Analiza factorilor în separarea din amestecuri de solvenți*, subliniază rezultatele obținute din analiza a factorilor intrinseci care apar la separarea cromatografică de compuși chimici.

Capitolul 17, *Dinamica chimicalelor*, discuta patru rezultate originale obținute atunci când dinamica a produselor chimice a făcut obiectul cercetării.

Următoarele trei capitole (18, 19, și 20, numite *Relații structură-activitate cu familii de descriptori moleculari (1)*, *(2)*, și *(3)*) structurează principalele rezultate obținute din utilizarea familiilor de descriptori moleculari pentru căutarea relațiilor dintre structura și proprietatea compușilor chimici.

Capitolul 21, *Subiect de interes: proiectarea de algoritmi și modele*, explică planurile mele pentru dezvoltarea în continuare pe acest subiect-cheie asumat: proiectarea de algoritmi și modele, implementarea programelor și obținerea de ecuații pentru a corela structura cu proprietatea.

Capitolul 22, *Planurile de acțiune*, oferă o serie de acțiuni identificate, și, prin urmare probabil să urmeze planul asumat de dezvoltare.

Summary

'*Structure vs. Property: Algorithms and Models*' thesis has been written as a transdisciplinary approach joining together concepts of mathematics and informatics to solve problems in chemistry. The main problem treated is the use of the chemical structure to explain measured (physical, chemical) properties and (biological) activities of the compounds.

We use models and algorithms all the time, but the most difficult is not to use, but to design and/or recognize them. Having this in mind, the thesis has been written as training for their recognition and design, and therefore it may seem too structured.

First chapter, *From observation to experiment, and to model*, comes from a introspection about the experimental design, the one which we provide raw data, and from which we extract models, patterns and relations between our observables and may be considered the basis for the following.

The second chapter, *Representation with formulas and properties*, defines our researching material while the third chapter, *Representation levels* synthesizes the key links between the structure and the property of the chemical compounds. An original result is given at the end of its, and is about the link between the spread of the chlorophylls in living organisms and their efficiency in converting the solar energy.

The fourth chapter, *Molecular topology and geometry*, defines the informational representation of the chemical structure and is a bridge to our methods of research. It contains also a series of original results about the developing and the use of molecular topology tools to investigate the chemical structure.

The fifth chapter, *Theory of chemical reactions and equilibrium*, discuss the second using of mathematical modelling in chemistry, for study of the reaction kinetics. Software implementations easy to do are provided.

The sixth chapter, *Separation in solvent mixtures: Snyder triangle's method*, provides the link between the theory of solutions and the use of models to estimate the optimum mobile phase in chromatography. Applications of the models derived here are given in Chapter 16.

The seventh chapter, *Binary and multinomial variables analysis: binomial confidence intervals*, is a turning back to the challenge of measurement function use, discussed in the first chapter. Namely, this chapter (containing original results too), takes the first level of the measurement function (on binary and multinomial scales) and provides solutions to express the confidence for expressions containing binary ratios (when are used to measure the association between observables).

Chapter 8, *Ordinal variables analysis: ranks statistic*, takes the second level of the measurement function (on ordinal scales) and provides solutions to express the strength of the

monotonic association.

Chapter 9, *Linear regression analysis: linear models*, takes the last level of measurement (on ratio scales) and provides analysis alternatives for the most important model of association: the linear association. Two original results are given here: about the generalization of the Gauss and Laplace distributions and its use to assess the type of the experimental error, and the other is about the alternatives in linear association analysis.

Chapter 10, *Structure-activity relationships: families of descriptors method*, gives my main contribution at developing of the methods of analysis the link between the structure and the property of the chemical compounds.

Chapter 11, *Reducing computing complexity: projecting and using of genetic algorithms*, gives my main contribution at the design of genetic algorithms for heuristic finding of structure-activity relationships.

Chapter 12, *Population distribution analysis applications*, gives a series of original results obtained involving the analysis of population distribution from which a sample was drawn.

Chapter 13, *Graph theory and statistical analysis applications*, gives a series of original results in graph theory, information theory, and applied statistic, as well as their use to assess the relation between the structure and the property of the chemical compounds.

Chapter 14, *Software design applications*, briefly describes the results from development and assessment of the software for conducting researches.

Chapter 15, *Meta-heuristics applications*, points out the results obtained from the use of a contingency of evolution strategies to the study of the evolution supervised by genetic algorithms.

Chapter 16, *Analysis of factors in separating from solvent mixtures*, point out the results obtained from the analysis of intrinsic factors occurring at the chromatographic separation of chemical compounds.

Chapter 17, *Chemicals dynamics applications*, discuss four original results obtained when dynamics of chemicals was the subject of research.

Following three chapters (18, 19, and 20, named *Structure-activity relationships with families of molecular descriptors (1)*, *(2)*, and *(3)*) structures the main results obtained from the use of the families of molecular descriptors to provide relations between the structure and the property of the chemical compounds.

Chapter 21, *Subject of interest: design of algorithms and models*, explain my plans for further development on this assumed key subject: design of algorithms and models, implementation of programs and obtaining of equations for relating the structure with the property.

Chapter 22, *Action plans*, gives a series of identified actions, and thus probable to follow the assumed plan of development.

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RYBALKO, Paul SAAB, Wayne SALAMON, Boris SAMORODOV, Hiroki SATO, Bernhard SCHMIDT, Søren SCHMIDT, Wolfram SCHNEIDER, Ed SCHOUTEN, Cy SCHUBERT, David SCHULTZ, Michael SCHEIDELL, Jens SCHWEIKHARDT, Stanislav SEDOV, Hans Petter SELASKY, Johan van SELST, Lev SEREBRYAKOV, Gregory Neil SHAPIRO, Wesley SHIELDS, Norikatsu SHIGEMURA, Hidetoshi SHIMOKAWA, Shteryana SHOPOVA, Vanilla I. SHU, Ashish SHUKLA, Mike SILBERSACK, Bruce M. SIMPSON, Jordan SISSEL, Dmitry SIVACHENKO, Sergey SKVORTSOV, Florian SMEETS, Gleb KURTSOU, Gleb SMIRNOFF, Ken SMITH, Dag-Erling C. SMØRGRAV, Maxim SOBOLEV, Brian SOMERS, Stacey SON, Suleiman SOUHLAL, Ulrich SPÖRLEIN, Mohan SRINIVASAN, Vsevolod STAKHOV, Ryan STEINMETZ, Lawrence STEWART, Randall R. STEWART, Murray STOKELY, Ryan STONE, Søren STRAARUP, Marius STROBL, Carlo STRUB, Munechika SUMIKAWA, Cheng-Lung SUNG, Ryusuke SUZUKI, Shinsuke SUZUKI, Yoshihiro TAKAHASHI, Sahil TANDON, Tomonari TAKATSU, Seigo TANIMURA, Romain TARTIÈRE, Sylvio Cesar TEIXEIRA, Ion-Mihai TETCU, Mikhail TETERIN, Gordon TETLOW, Lars THEGLER, David THIEL, Fabien THOMAS, Thierry THOMAS, Andrew THOMPSON, Florent THOUMIE, Yar TIKHIY, Jilles TJOELKER, Andreas TOBLER, Ganbold TSAGAANKHUU, Michael TUEXEN, Andrew TURNER, Oleksandr TYMOSHENKO, Hajimu UMEMOTO, Stephan UPHOFF, Yvan VANHULLEBUS, Alberto VILLA, Nicola VITALE, Jack F. VOGEL, Ivan VORAS, Bernd WALTER, Stefan WALTER, Kai WANG, Takanori WATANABE, Robert WATSON, Adam WEINBERGER, Christian WEISGERBER, Peter WEMM, Doug WHITE, Nathan WHITEHORN, Martin WILKE, Steve WILLS, Garrett WOLLMAN, Michael C. WU, Jörg WUNSCH, David XU, Maksim YEVMENKIN, Pyun YONGHYEON, Marko ZEC, Bjoern A. ZEEB, Alexey ZELKIN, Sepherosa ZIEHAU, Andrej ZVEREV, 1993 (and to date). FreeBSD: a free Unix-like operating system. Internet: The FreeBSD Foundation. URL: http://freebsd.org

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From prologue to epilogue

January 30, 2012:
   Thesis 'Structure vs. Property: Algorithms and Models' was submitted to the office for habilitation accreditation management;

July 24, 2012:
   The evaluation of the thesis begins;

August 30, 2012:
   Accepting of the thesis of habilitation for public defense;

September 24, 2012:
   Public defending of the thesis; favorable resolution of the committee:
   ÷ Prof. Dr. Mircea V. DIUDEA (President, Chemistry, Babeş-Bolyai University);
   ÷ Prof. Dr. Ion NEDA (Chemistry, Braunschweig University of Technology);
   ÷ Prof. Dr. Dusanka JANEZIC (Chemistry & Mathematics, National Institute of Chemistry Ljubljana);
   ÷ Prof. Dr. Adrian PETRUŞEL (Mathematics, Babeş-Bolyai University);
   ÷ Assoc. Prof. Lehel CSATO (Informatics, Babeş-Bolyai University);

December 11, 2012:
   Validation of the national scientific council with the proposal of the field: Chemistry;

April 18, 2013:
   Resort ministry order confirming the resolution and allowing the use of the title: PhD Advisor in Chemistry;

April 30, 2013:
   Information about the resolution to the Technical University of Cluj-Napoca;

May 8, 2013:
   I was informed about the resolution;

May 20, 2013:
   I applied to use PhD Advising right under the frame of the Doctoral School of Babeş-Bolyai University;

July 11, 2013:
   I received the acceptance for PhD Advising under the frame of the Doctoral School of Babeş-Bolyai University;

August 3, 2014:
   No open positions for PhD studies in the 2013 year for me under the frame of the Doctoral School of Babeş-Bolyai University;

(from) August 4, 2014:
   2014 is the year in which I start to have open positions for PhD studies.

Lorentz JÄNTSCHI
June 10, 2013; Updated on July 12, 2013; Updated on August 3, 2013; Updated on September 25, 2014.