Project Proposal

Element database and Analytical system

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Motivation and Background

Access to affordable, healthy, and nutritious food is among the key determinants of health [1]. Chemical elements are important for nutrition and health. Elements can be essential or beneficial for health because they are the components of major structural components in the body (Ca, P, S), they help maintenance of electrochemical equilibria, activation, or signaling (Ca, K, Mg, Na), or they are components of enzymes or hormones (Co, Cr, Cu, Fe, I, Mn, Mo, Ni, Se, Sn, V, Zn) [2]. More than 20 elements are considered as toxic risk (Ag, As, Au, Be, Bi, Cd, Ce, Ch, Co, Cu, Fe, Ga, Hg, Mn, Ni, Pb, Pt, Sb, Sn, Te, Th, U, V, and Zn) and seven of them are considered as high-risk (As, Al, Cd, Cr, Fe, Hg, and Pb) [3]. The improvements in instrumentation, such as inductively coupled plasma mass spectrometry (ICP-MS) and advanced computational algorithms enabled accurate and affordable measurement of more than 70 elements at reasonable cost [4] even in tiny concentrations (as low as one part in 10^{15}). Elemental profiles in various foods enable the assessment of safety, security, and quality of food as well as prevention of food crime [5]. Data representing elemental composition in various foods data are accumulating at an accelerating speed, but these data are scattered across literature and various web sites and are not available in a unified information system. Professor Brusic and colleagues have proposed such a database and analysis systems whereby complex food data (field measurements, geographic location, weather data, pollution, etc.) are combined with elemental profile measurements and stored in a database and analyzed to trace the origin and assess the quality and safety of foods [6]. This project will focus on the design and implement the database and analysis system of elemental profiles in foods. This product will use software engineering process, to deliver the proposed software product as a functional prototype. The team will analyze user requirements for the prototype and develop a complete set of SE project requirements, design the system, and implement a database and analytical tools (including functionalities for search, visualization, basic statistical analysis, and classification tasks). The analysis will include feature selection for classification using Artificial Neural Networks and Support Vector Machines.

Aims and Objectives

This project focusses on applied computer science – we will use computer science techniques and methods to solve a real-life scientific problem. The overall aim of this project is the establishment of database of chemical element profiles in foodstuffs that will be combined with statistical and machine learning tools to enable data analysis, including classification of food samples by origin, chemical profile, and nutritional or health properties.

Specific aims:

1. **Data.** Data collection cleaning and standardization will be performed to provide the content of the database. Data will be collected from literature, company catalogues, data repositories, and directly from the researchers.
2. **Background knowledge**. Metadata will be developed to assist in understanding the type of samples and help classify them. Standardized nomenclature and ontologies will be used whenever possible. Reference values of elemental concentrations for various foods will be established to allow identification of contaminants, measurement artefacts and out-of-range elements (harmful, or nutrients).
3. **Database and analysis system.** The software product will have the following elements:
    a. Software (user interface, database, analysis system, help pages, and visualization module)
    b. Testing and maintenance components (these will be basic for a prototype)
4. **Project process.** Project documents will include
    a. Initial project proposal (this document, it will be updated regularly)
    b. Project Charter document
    c. User requirements and project assumptions
    d. Project plan
    e. Other software engineering related documents
    f. Interim reports, and final report
    g. Demonstration cases
    h. Documentation and presentations as outlined in the handbook

Project Plan

Software development will utilize Spiral Model of software development [7]. The main risk of this project will be the delay in the development and implementation of the database – it will be mitigated through iterative improvement of the software solution, rigorous application of software engineering practices, and implementation of formal methods of managing and monitoring progress using ISO software quality principles [8]. The emphasis of this project is the development of robust software prototype that will fulfill the scientific need for elemental analysis in foods, since currently there is no such solution in existence. The theoretical technological and engineering aspects of the software development will be considered and

deployed as a secondary priority in this project. Specific tasks in this project are:

Preparatory and process tasks
1.1 Complete and submit project proposal (this document)
1.2 Prepare Project Charter document
1.3 Clarify user requirements and project assumptions
1.4 Develop project plan
1.5 Develop and implement process monitoring and control plan
1.6 Prepare other software engineering related documents as needed
1.7 Demonstration cases
1.8 Documentation and presentations as outlined in the handbook

Software development
2.1 Develop standardized data format and define metadata
2.2 Collect raw data and transform into standardized format
2.3 Design and implement database
2.4 Develop and implement analysis tools
2.5 Integrate system
2.6 Test, correct, and validate software
2.7 Iterate process until acceptance criteria are satisfied

Reporting and publication
3.1 Provide weekly incremental progress reports and short monthly written reports
3.2 Complete and submit interim reports as required
3.3 Develop a plan and schedule for preparing the final report, preliminary and revised
3.4 Prepare and deliver presentation (deadline ??? ??, 2019)
3.4 Write and submit the final report (deadline ??? ??, 2019)

References

1. World Health Organization. Health Impact Assessment. The Determinants of Health. 26 June 2013 < www.who.int/hia/evidence/doh/en/index3.html >.
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3. Yasuda H, Yasuda Y, Tsutsui T. Estimation of autistic children by metallomics analysis. Scientific reports. 2013 Feb 4;3:1199.
4. ICP Mass Spectrometry. *The 30-Minute Guide to ICP-MS*. Technical Note, Perkin-Elmer Instruments, 2001.
5. Manning L, Soon JM. Food safety, food fraud, and food defense: a fast evolving literature. Journal of food science. 2016 Apr;81(4):R823-34.
6. Danezis GP, Tsagkaris AS, Brusic V, Georgiou CA. Food authentication: state of the art and prospects. Current Opinion in Food Science. 2016 Aug 1;10:22-31.
7. Boehm BW. A spiral model of software development and enhancement. Computer. 1988 May;21(5):61-72.
8. Dugalic B, Mishev A. ISO Software Quality Standards and Certification. InBCI (Local) 2012 (pp. 113-116).

Project schedule and deliverables

This chart is based on the activities detailed in the Project Plan section.
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