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Semantic Breakthrough in Drug Discovery

Bin Chen
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THE SEMANTIC WEB: THEORY AND TECHNOLOGY
Ying Ding and Paul Groth, *Series Editors*

Semantic Breakthrough In Drug Discovery Huijun Wang

Clifford Lane



Semantic Breakthrough In Drug Discovery Huijun Wang:

Semantic Breakthrough in Drug Discovery Bin Chen,Huijun Wang,Ying Ding,David Wild,2022-06-01 The current drug development paradigm sometimes expressed as One disease one target one drug is under question as relatively few drugs have reached the market in the last two decades Meanwhile the research focus of drug discovery is being placed on the study of drug action on biological systems as a whole rather than on individual components of such systems The vast amount of biological information about genes and proteins and their modulation by small molecules is pushing drug discovery to its next critical steps involving the integration of chemical knowledge with these biological databases Systematic integration of these heterogeneous datasets and the provision of algorithms to mine the integrated datasets would enable investigation of the complex mechanisms of drug action however traditional approaches face challenges in the representation and integration of multi scale datasets and in the discovery of underlying knowledge in the integrated datasets The Semantic Web envisioned to enable machines to understand and respond to complex human requests and to retrieve relevant yet distributed data has the potential to trigger system level chemical biological innovations Chem2Bio2RDF is presented as an example of utilizing Semantic Web technologies to enable intelligent analyses for drug discovery Table of Contents Introduction Data

Representation and Integration Using RDF Data Representation and Integration Using OWL Finding Complex Biological Relationships in PubMed Articles using Bio LDA Integrated Semantic Approach for Systems Chemical Biology Knowledge Discovery Semantic Link Association Prediction Conclusions References Authors Biographies [The Epistemology of](#)

[Intelligent Semantic Web Systems](#) Mathieu d'Aquin,Enrico Motta,2022-05-31 The Semantic Web is a young discipline even if only in comparison to other areas of computer science Nonetheless it already exhibits an interesting history and evolution This book is a reflection on this evolution aiming to take a snapshot of where we are at this specific point in time and also showing what might be the focus of future research This book provides both a conceptual and practical view of this evolution especially targeted at readers who are starting research in this area and as support material for their supervisors From a conceptual point of view it highlights and discusses key questions that have animated the research community what does it mean to be a Semantic Web system and how is it different from other types of systems such as knowledge systems or web based information systems From a more practical point of view the core of the book introduces a simple conceptual framework which characterizes Intelligent Semantic Web Systems We describe this framework the components it includes and give pointers to some of the approaches and technologies that might be used to implement them We also look in detail at concrete systems falling under the category of Intelligent Semantic Web Systems according to the proposed framework allowing us to compare them analyze their strengths and weaknesses and identify the key fundamental challenges still open for researchers to tackle **Natural Language Processing for the Semantic Web** Diana Maynard,Kalina

Bontcheva,Isabelle Augenstein,2022-05-31 This book introduces core natural language processing NLP technologies to non

experts in an easily accessible way as a series of building blocks that lead the user to understand key technologies why they are required and how to integrate them into Semantic Web applications Natural language processing and Semantic Web technologies have different but complementary roles in data management Combining these two technologies enables structured and unstructured data to merge seamlessly Semantic Web technologies aim to convert unstructured data to meaningful representations which benefit enormously from the use of NLP technologies thereby enabling applications such as connecting text to Linked Open Data connecting texts to each other semantic searching information visualization and modeling of user behavior in online networks The first half of this book describes the basic NLP processing tools tokenization part of speech tagging and morphological analysis in addition to the main tools required for an information extraction system named entity recognition and relation extraction which build on these components The second half of the book explains how Semantic Web and NLP technologies can enhance each other for example via semantic annotation ontology linking and population These chapters also discuss sentiment analysis a key component in making sense of textual data and the difficulties of performing NLP on social media as well as some proposed solutions The book finishes by investigating some applications of these tools focusing on semantic search and visualization modeling user behavior and an outlook on the future

Semantic Mining of Social Networks Jie Tang, Juanzi Li, 2022-06-01 Online social networks have already become a bridge connecting our physical daily life with the web based information space This connection produces a huge volume of data not only about the information itself but also about user behavior The ubiquity of the social Web and the wealth of social data offer us unprecedented opportunities for studying the interaction patterns among users so as to understand the dynamic mechanisms underlying different networks something that was previously difficult to explore due to the lack of available data In this book we present the architecture of the research for social network mining from a microscopic point of view We focus on investigating several key issues in social networks Specifically we begin with analytics of social interactions between users The first kinds of questions we try to answer are What are the fundamental factors that form the different categories of social ties How have reciprocal relationships been developed from parasocial relationships How do connected users further form groups Another theme addressed in this book is the study of social influence Social influence occurs when one s opinions emotions or behaviors are affected by others intentionally or unintentionally Considerable research has been conducted to verify the existence of social influence in various networks However few literature studies address how to quantify the strength of influence between users from different aspects In Chapter 4 and in 138 we have studied how to model and predict user behaviors One fundamental problem is distinguishing the effects of different social factors such as social influence homophily and individual s characteristics We introduce a probabilistic model to address this problem Finally we use an academic social network ArnetMiner as an example to demonstrate how we apply the introduced technologies for mining real social networks In this system we try to mine knowledge from both the informative publication network and the

social collaboration network and to understand the interaction mechanisms between the two networks The system has been in operation since 2006 and has already attracted millions of users from more than 220 countries regions

Social Semantic Web Mining Tope Omitola, Sebastián A. Ríos, John G. Breslin, 2022-06-01 The past ten years have seen a rapid growth in the numbers of people signing up to use Web based social networks hundreds of millions of new members are now joining the main services each year with a large amount of content being shared on these networks tens of billions of content items are shared each month With this growth in usage and data being generated there are many opportunities to discover the knowledge that is often inherent but somewhat hidden in these networks Web mining techniques are being used to derive this hidden knowledge In addition the Semantic Web including the Linked Data initiative to connect previously disconnected datasets is making it possible to connect data from across various social spaces through common representations and agreed upon terms for people content items etc In this book we detail some current research being carried out to semantically represent the implicit and explicit structures on the Social Web along with the techniques being used to elicit relevant knowledge from these structures and we present the mechanisms that can be used to intelligently mesh these semantic representations with intelligent knowledge discovery processes We begin this book with an overview of the origins of the Web and then show how web intelligence can be derived from a combination of web and Social Web mining We give an overview of the Social and Semantic Webs followed by a description of the combined Social Semantic Web along with some of the possibilities it affords and the various semantic representation formats for the data created in social networks and on social media sites Provenance and provenance mining is an important aspect here especially when data is combined from multiple services We will expand on the subject of provenance and especially its importance in relation to social data We will describe extensions to social semantic vocabularies specifically designed for community mining purposes SIOCM In the last three chapters we describe how the combination of web intelligence and social semantic data can be used to derive knowledge from the Social Web starting at the community level macro and then moving through group mining meso to user profile mining micro

Entity Resolution in the Web of Data Vassilis Christophides, Vasilis Efthymiou, Kostas Stefanidis, 2022-05-31 In recent years several knowledge bases have been built to enable large scale knowledge sharing but also an entity centric Web search mixing both structured data and text querying These knowledge bases offer machine readable descriptions of real world entities e g persons places published on the Web as Linked Data However due to the different information extraction tools and curation policies employed by knowledge bases multiple complementary and sometimes conflicting descriptions of the same real world entities may be provided Entity resolution aims to identify different descriptions that refer to the same entity appearing either within or across knowledge bases The objective of this book is to present the new entity resolution challenges stemming from the openness of the Web of data in describing entities by an unbounded number of knowledge bases the semantic and structural diversity of the descriptions provided across domains

even for the same real world entities as well as the autonomy of knowledge bases in terms of adopted processes for creating and curating entity descriptions The scale diversity and graph structuring of entity descriptions in the Web of data essentially challenge how two descriptions can be effectively compared for similarity but also how resolution algorithms can efficiently avoid examining pairwise all descriptions The book covers a wide spectrum of entity resolution issues at the Web scale including basic concepts and data structures main resolution tasks and workflows as well as state of the art algorithmic techniques and experimental trade offs

Knowledge Graphs Aidan Hogan,Eva Blomqvist,Michael Cochez,Claudia d'Amato,Gerard de Melo,Claudio Gutierrez,Sabrina Kirrane,Jose Emilio Labra Gayo,Roberto Navigli,Sebastian Neumaier,Axel Polleres,Sabbir Rashid,Anisa Rula,Antoine Zimmermann,Lukas Schmelzeisen,Axel-Cyrille Ngonga Ngomo,Juan Sequeda,Steffen Staab,2022-06-01 This book provides a comprehensive and accessible introduction to knowledge graphs which have recently garnered notable attention from both industry and academia Knowledge graphs are founded on the principle of applying a graph based abstraction to data and are now broadly deployed in scenarios that require integrating and extracting value from multiple diverse sources of data at large scale The book defines knowledge graphs and provides a high level overview of how they are used It presents and contrasts popular graph models that are commonly used to represent data as graphs and the languages by which they can be queried before describing how the resulting data graph can be enhanced with notions of schema identity and context The book discusses how ontologies and rules can be used to encode knowledge as well as how inductive techniques based on statistics graph analytics machine learning etc can be used to encode and extract knowledge It covers techniques for the creation enrichment assessment and refinement of knowledge graphs and surveys recent open and enterprise knowledge graphs and the industries or applications within which they have been most widely adopted The book closes by discussing the current limitations and future directions along which knowledge graphs are likely to evolve This book is aimed at students researchers and practitioners who wish to learn more about knowledge graphs and how they facilitate extracting value from diverse data at large scale To make the book accessible for newcomers running examples and graphical notation are used throughout Formal definitions and extensive references are also provided for those who opt to delve more deeply into specific topics

Library Linked Data in the Cloud Carol Jean Godby,Shenghui Wang,Jeffrey K. Mixer,2022-06-01 This book describes OCLC s contributions to the transformation of the Internet from a web of documents to a Web of Data The new Web is a growing cloud of interconnected resources that identify the things people want to know about when they approach the Internet with an information need The linked data architecture has achieved critical mass just as it has become clear that library standards for resource description are nearing obsolescence Working for the world s largest library cooperative OCLC researchers have been active participants in the development of next generation standards for library resource description By engaging with an international community of library and Web standards experts they have published some of the most widely used RDF datasets representing library

collections and librarianship This book focuses on the conceptual and technical challenges involved in publishing linked data derived from traditional library metadata This transformation is a high priority because most searches for information start not in the library nor even in a Web accessible library catalog but elsewhere on the Internet Modeling data in a form that the broader Web understands will project the value of libraries into the Digital Information Age The exposition is aimed at librarians archivists computer scientists and other professionals interested in modeling bibliographic descriptions as linked data It aims to achieve a balanced treatment of theory technical detail and practical application

Ontology Engineering

Elisa F. Kendall, Deborah L. McGuinness, 2022-05-31 Ontologies have become increasingly important as the use of knowledge graphs machine learning natural language processing NLP and the amount of data generated on a daily basis has exploded As of 2014 90% of the data in the digital universe was generated in the two years prior and the volume of data was projected to grow from 3.2 zettabytes to 40 zettabytes in the next six years The very real issues that government research and commercial organizations are facing in order to sift through this amount of information to support decision making alone mandate increasing automation Yet the data profiling NLP and learning algorithms that are ground zero for data integration manipulation and search provide less than satisfactory results unless they utilize terms with unambiguous semantics such as those found in ontologies and well formed rule sets Ontologies can provide a rich schema for the knowledge graphs underlying these technologies as well as the terminological and semantic basis for dramatic improvements in results Many ontology projects fail however due at least in part to a lack of discipline in the development process This book motivated by the Ontology 101 tutorial given for many years at what was originally the Semantic Technology Conference SemTech and then later from a semester long university class is designed to provide the foundations for ontology engineering The book can serve as a course textbook or a primer for all those interested in ontologies

Demystifying OWL for the Enterprise Michael Uschold, 2022-05-31 After a slow incubation period of nearly 15 years a large and growing number of organizations now have one or more projects using the Semantic Web stack of technologies The Web Ontology Language OWL is an essential ingredient in this stack and the need for ontologists is increasing faster than the number and variety of available resources for learning OWL This is especially true for the primary target audience for this book modelers who want to build OWL ontologies for practical use in enterprise and government settings The purpose of this book is to speed up the process of learning and mastering OWL To that end the focus is on the 30% of OWL that gets used 90% of the time Others who may benefit from this book include technically oriented managers semantic technology developers undergraduate and post graduate students and finally instructors looking for new ways to explain OWL The book unfolds in a spiral manner starting with the core ideas Each subsequent cycle reinforces and expands on what has been learned in prior cycles and introduces new related ideas Part 1 is a cook's tour of ontology and OWL giving an informal overview of what things need to be said to build an ontology followed by a detailed look at how to say them in OWL This is illustrated using a healthcare example Part 1

concludes with an explanation of some foundational ideas about meaning and semantics to prepare the reader for subsequent chapters Part 2 goes into depth on properties and classes which are the core of OWL There are detailed descriptions of the main constructs that you are likely to need in every day modeling including what inferences are sanctioned Each is illustrated with real world examples Part 3 explains and illustrates how to put OWL into practice using examples in healthcare collateral and financial transactions A small ontology is described for each along with some key inferences Key limitations of OWL are identified along with possible workarounds The final chapter gives a variety of practical tips and guidelines to send the reader on their way

Validating RDF Data Jose Emilio Labra Gayo, Eric Prud'hommeaux, Iovka Boneva, Dimitris Kontokostas, 2022-05-31 RDF and Linked Data have broad applicability across many fields from aircraft manufacturing to zoology Requirements for detecting bad data differ across communities fields and tasks but nearly all involve some form of data validation This book introduces data validation and describes its practical use in day to day data exchange The Semantic Web offers a bold new take on how to organize distribute index and share data Using Web addresses URIs as identifiers for data elements enables the construction of distributed databases on a global scale Like the Web the Semantic Web is heralded as an information revolution and also like the Web it is encumbered by data quality issues The quality of Semantic Web data is compromised by the lack of resources for data curation for maintenance and for developing globally applicable data models At the enterprise scale these problems have conventional solutions Master data management provides an enterprise wide vocabulary while constraint languages capture and enforce data structures Filling a need long recognized by Semantic Web users shapes languages provide models and vocabularies for expressing such structural constraints This book describes two technologies for RDF validation Shape Expressions ShEx and Shapes Constraint Language SHACL the rationales for their designs a comparison of the two and some example applications

Linked Data Visualization Laura Po, Nikos Bikakis, Federico Desimoni, George Papastefanatos, 2022-05-31 Linked Data LD is a well established standard for publishing and managing structured information on the Web gathering and bridging together knowledge from different scientific and commercial domains The development of Linked Data Visualization techniques and tools has been followed as the primary means for the analysis of this vast amount of information by data scientists domain experts business users and citizens This book covers a wide spectrum of visualization issues providing an overview of the recent advances in this area focusing on techniques tools and use cases of visualization and visual analysis of LD It presents the basic concepts related to data visualization and the LD technologies the techniques employed for data visualization based on the characteristics of data techniques for Big Data visualization use tools and use cases in the LD context and finally a thorough assessment of the usability of these tools under different scenarios The purpose of this book is to offer a complete guide to the evolution of LD visualization for interested readers from any background and to empower them to get started with the visual analysis of such data This book can serve as a course textbook or a primer for all those interested in LD and data visualization

Web Data

APIs for Knowledge Graphs Albert Meroño-Peñuela, Pasquale Lisena, Carlos Martínez-Ortiz, 2022-05-31 This book describes a set of methods architectures and tools to extend the data pipeline at the disposal of developers when they need to publish and consume data from Knowledge Graphs graph structured knowledge bases that describe the entities and relations within a domain in a semantically meaningful way using SPARQL Web APIs and JSON To do so it focuses on the paradigmatic cases of two middleware software packages grlc and SPARQL Transformer which automatically build and run SPARQL based REST APIs and allow the specification of JSON schema results respectively The authors highlight the underlying principles behind these technologies query management declarative languages new levels of indirection abstraction layers and separation of concerns explain their practical usage and describe their penetration in research projects and industry The book therefore serves a double purpose to provide a sound and technical description of tools and methods at the disposal of publishers and developers to quickly deploy and consume Web Data APIs on top of Knowledge Graphs and to propose an extensible and heterogeneous Knowledge Graph access infrastructure that accommodates a growing ecosystem of querying paradigms

Designing and Building Enterprise Knowledge Graphs Juan Sequeda, Ora Lassila, 2022-05-31 This book is a guide to designing and building knowledge graphs from enterprise relational databases in practice It presents a principled framework centered on mapping patterns to connect relational databases with knowledge graphs the roles within an organization responsible for the knowledge graph and the process that combines data and people The content of this book is applicable to knowledge graphs being built either with property graph or RDF graph technologies Knowledge graphs are fulfilling the vision of creating intelligent systems that integrate knowledge and data at large scale Tech giants have adopted knowledge graphs for the foundation of next generation enterprise data and metadata management search recommendation analytics intelligent agents and more We are now observing an increasing number of enterprises that seek to adopt knowledge graphs to develop a competitive edge In order for enterprises to design and build knowledge graphs they need to understand the critical data stored in relational databases How can enterprises successfully adopt knowledge graphs to integrate data and knowledge without boiling the ocean This book provides the answers

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01-06-2024,

Reviewing **Semantic Breakthrough In Drug Discovery Huijun Wang**: Unlocking the Spellbinding Force of Linguistics

In a fast-paced world fueled by information and interconnectivity, the spellbinding force of linguistics has acquired newfound prominence. Its capacity to evoke emotions, stimulate contemplation, and stimulate metamorphosis is actually astonishing. Within the pages of "**Semantic Breakthrough In Drug Discovery Huijun Wang**," an enthralling opus penned by a highly acclaimed wordsmith, readers set about an immersive expedition to unravel the intricate significance of language and its indelible imprint on our lives. Throughout this assessment, we shall delve into the book's central motifs, appraise its distinctive narrative style, and gauge its overarching influence on the minds of its readers.

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