A Hybrid Construction of a Medical Decision Support System using Semantic Web and Machine Learning Techniques

(Atif Khan – PhD Seminar)

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University of Waterloo

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Motivation

Medical Decision Support Systems (MDSS)

- can a drug/procedure be administered to Alice?

Challenges

- information constraints – access, completeness
- expert knowledge – who is treating Alice
- temporal aspects – emergency medical scenarios

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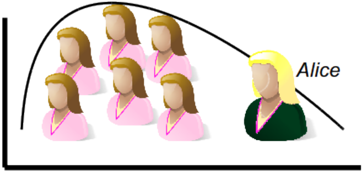
Motivation

Build a medical decision support system with the capability to handle the following *knowledge* features:

- black swan theory & Alice
- Alice's medical history
- nature of the drug/procedure
- expert knowledge
- information availability

⋮



Outline

Medical Decision Support Systems (MDSS)

Definition

computer systems designed to **impact clinician decision** making about **individual** patients.

(Berner, 2007)

Definition

clinical decision support systems **link** health **observations** with health **knowledge** to influence health choices by clinicians for **improved** health **care**.

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MDSS Classification (Berner, 2007)

Medical Decision Support Systems

- Knowledge-based MDSS
- Nonknowledge-based MDSS

Characteristics

Knowledge-based MDSS

- structured data representation *(schema)*
- knowledge is persisted in *data-stores*
- expert knowledge $\rightarrow$ system rules
  - heuristics based
  - evidence based
- reasoning capacity using *inference* engines

Nonknowledge-based MDSS

- learn from raw data (semi/un-structured)
- based on machine learning techniques
  - patterns in the data
  - past examples/cases
- learning capacity
- probabilistic prediction capability

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Advantages & Disadvantages

Knowledge-based MDSS

- quite capable and robust when the knowledge base is **complete**
- system made decisions are
  - based on logical rules/axioms
  - can be easily explained to end users ✓
  - can be verified using *logic proofs* ✓

Nonknowledge-based MDSS

- generally tolerant to noise ✓
- may mistake weaker signals in data as noise
- computationally expensive to build and maintain
  - require a *training* phase
  - specific to a line of inquiry
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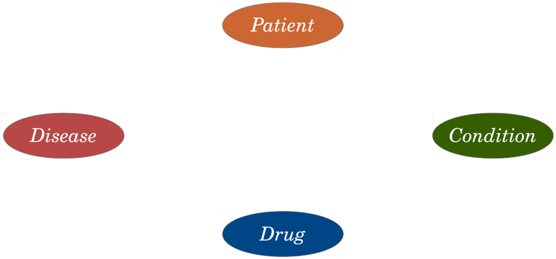

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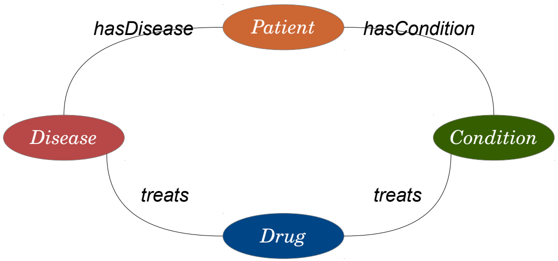

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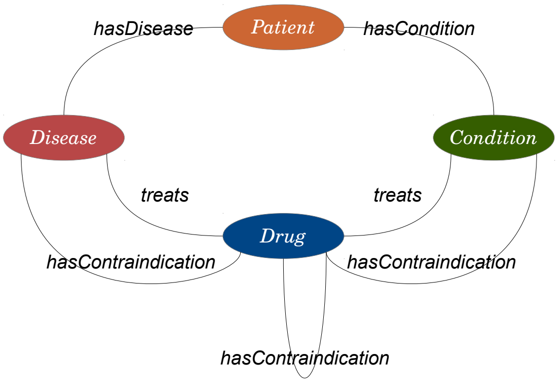

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Ontology

Let V be the set of structured vocabulary, and A_x axioms about V, which are formulated in formal language L.

An ontology is a *sign-system*: $ont = (L, V, A_x)$,

where, the symbols of V denote categories, and relations between categories or between their instances.

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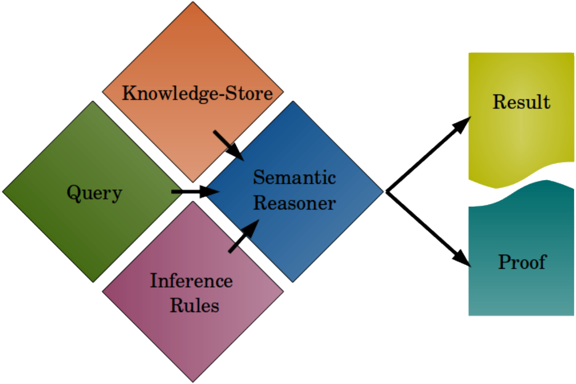
Knowledge Inference & Reasoning

Rules-based inference:

- discover implicit knowledge;
  $\{assertions\} \to \{implications\}$

Reasoning



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proof $\to$ based on first order logic, represents a unique traversal path through the knowledge graph

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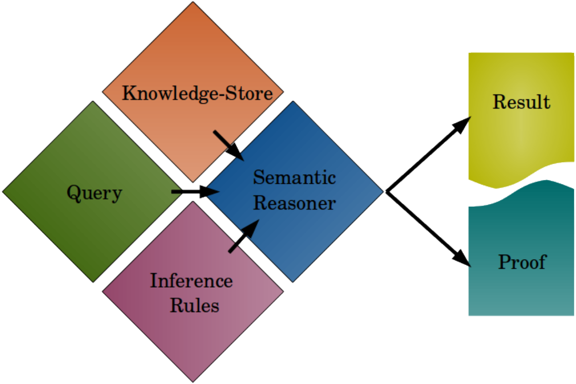

result $\rightarrow$ query answer

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based on first order logic, represents a unique traversal path through the knowledge graph

A Simple Example – Who has high blood pressure?

Knowledge Base

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:Alice  a  :Patient;  :hasSystolic 119;  :hasDiastolic 75.
:Kate   a  :Patient;  :hasSystolic 144;  :hasDiastolic 91.
:Dave   a  :Patient;  :hasSystolic 120;  :hasDiastolic 101.
:Bob    a  :Patient;  :hasCondition  :HighBloodPressure.
:John   a  : Patient.
```

Inference Rule

```
{?P a :Patient; :hasSystolic ?SYS. ?SYS math:greaterThan 140.}
=> {?P :hasCondition :HighBloodPressure}.

{?P a :Patient; :hasDiastolic ?DIA. ?DIA math:greaterThan 90.}
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Query

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_:WHO :hasCondition :HighBloodPressure.
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But what about John? → open vs. closed world assumptions.

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Machine Learning

Key Tasks:

- *classification*: predict the class of an instance of data
- *regression*: prediction of a numeric value

- *clustering*: group similar items together

Machine Learning

Key Tasks:

1. supervised learning
   - *classification*: predict the class of an instance of data
   - *regression*: prediction of a numeric value
2. unsupervised learning
   - *clustering*: group similar items together

Machine Learning

Our focus:

1. supervised learning
   - *classification*: predict the class of an instance of data

Machine Learning–Classification

Definition

Let X be the input space and Y be the output space.
Then a training set of examples can be defined as :
$D = \{(x_1, y_1), (x_2, y_2) \ldots (x_n, y_n)\}$.

The machine learning task is to induce a function $p : X \rightarrow Y$ that **best** explains the training data.

where,

best $\rightarrow$ minimizing "loss", via a loss function $L = f(p(x_i), y_i)$
$p(x_i)$ is predicted output, and y_i is actual output.
x_i is represented as a *feature* vector.

(Lin and Kolcz, 2012)

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Machine Learning–Classification: General Approach

Steps

- data collection & pre-processing
- data analysis (abnormal values, outliers etc.)
- feature selection & labelling
- train – build a classifier based on the training examples
- test – evaluate the classifier based on the test examples
- system integration of the classifier

Outline

Proposed Solution

Design Goals

1. **patient-centric**, evidence-based
2. automated (machine processable)
3. operate in constrained environments
4. decisions are easy to explain and validate
5. tolerant to noise in patient data → *information challenge*

Note: A knowledge-based MDSS meets 1-4 design objectives but fails to meet 5

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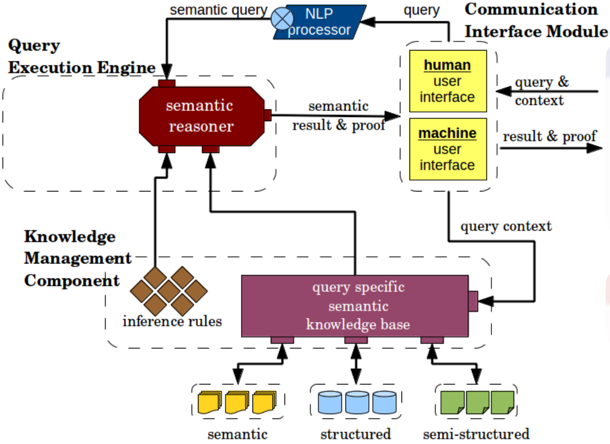

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- ontological data representation
- expert knowledge as inference rules
- logic-based decision making

Drawbacks

- susceptible to noise in data

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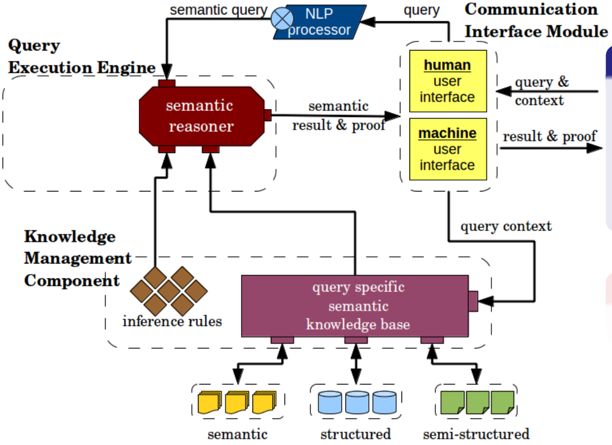

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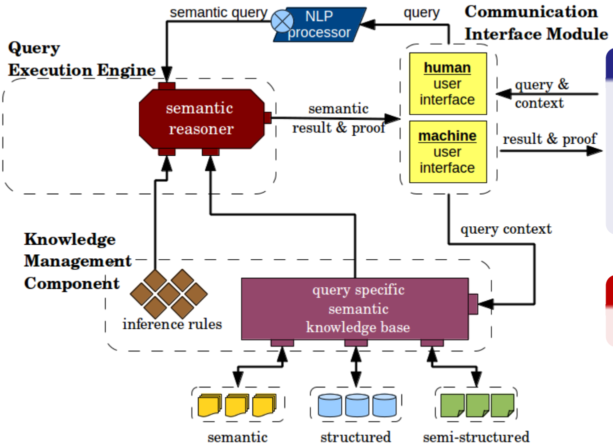

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Proposed Solution: Nonknowledge-based Engine

Recall: ML techniques are tolerant to noise

Design update: Replace semantic reasoner with a ML-based classifier

Validation strategy

- *line of inquiry*: drug prescription
- synthetic dataset: $\{Patient, Drug, Disease\}$
  - patient-to-drug interactions
  - drug-to-drug interactions
  - disease-to-drug interactions
- *result*: ML based classifiers performed poorly at prescribing the right drugs to the right patients

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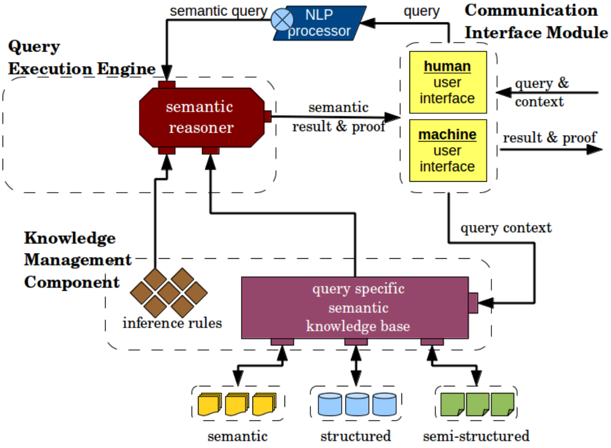

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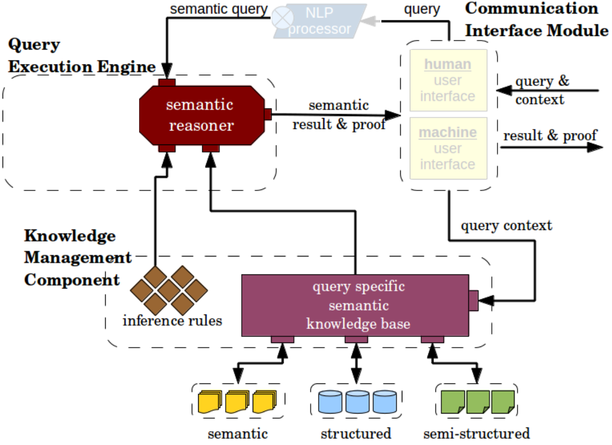

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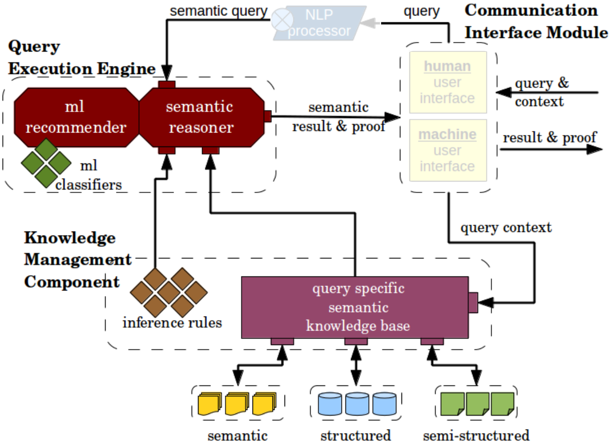

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Output: *result*, *proof*, *conf* confidence in the *result*.

reponse[*r*, *p*] = *reasoner*.doProof(*query*, *KB*, *rules*);
if *reponse*[*r*, *p*] *not empty* **then**
  return (*reponse.r*, *reponse.p*, 1.0);
end
noresult = inspectForFalseModel(*proof*);
unknownresult = inspectForCounterModel(*proof*);
if *noresult and not unknownresult* **then**
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//predict missing values
if *unknownresult* **then**
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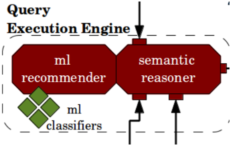

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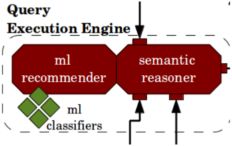

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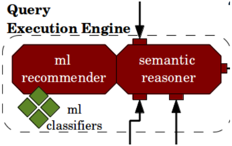
False model: deduction fails due to the facts themselves

Counter model: deduction fails due to incomplete facts



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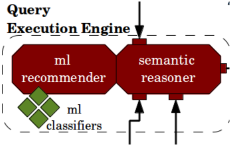


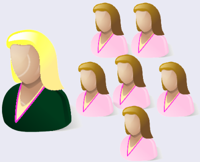
Outline

1. Background
2. Architecture
3. Experimental Validation
4. Conclusion

Experimental Validation

Line of Inquiry: *Sleeping pill prescription*

which patients can be prescribed what sleep medications?



prescribing sleep medication is not trivial

Dataset – BRFSS

Patient Records

- Behavioral Risk Factor Surveillance System (BRFSS)
  Center of Disease Control and Prevention
- 2010 dataset (records: 450K+ , features: 400+)
- multi-dimensional
  - demographic information
    (age, race, sex, geographic location)
  - medical information
    (cancer, asthma, mental illness,diabetes)
  - behavioural Information
    (alcohol consumption, drug use, sleep deprivation)

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Additional Datasets: Expert Knowledge

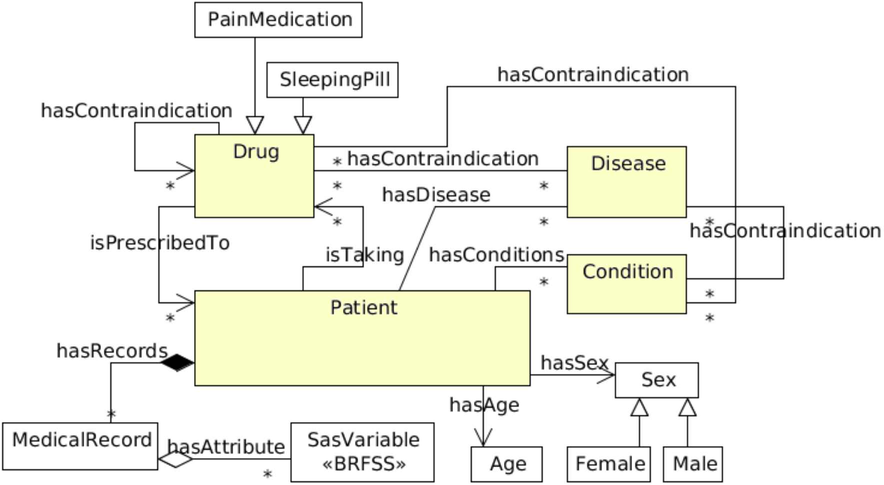
Mayo clinic sleeping pill prescription protocol

- describes expert rules dictating what sleeping drugs can be administered under a given set of medical conditions
- available online (HTML format)

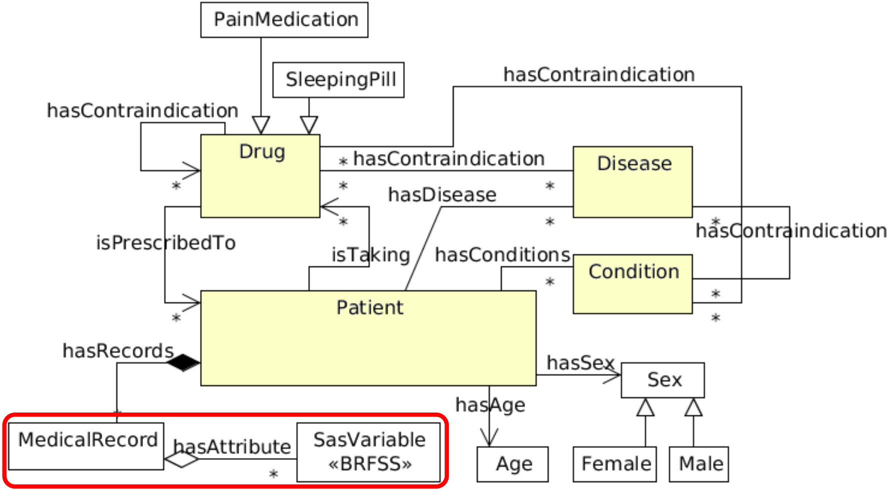
drug-to-drug interaction rules

- from *drug.com* online registry
- pain and sleeping medication interactions

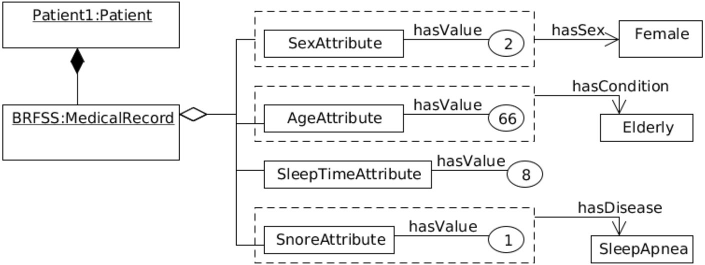
Ontological Knowledge Representation



Ontological Knowledge Representation



BRFSS Data to Patient Records

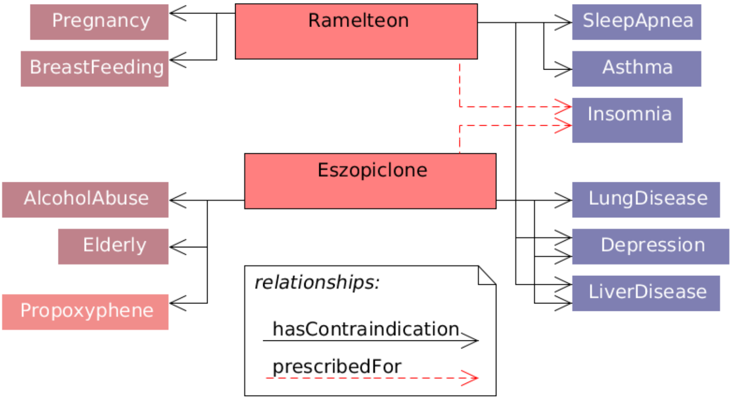


Data mapping

- BRFSS code book defined the **semantics** of the raw values
- the raw values were then mapped to **ontological concepts**

Expert Knowledge Representation

Mayo Clinic Sleeping Pill Prescription Protocol



Expert Knowledge Representation

Drug-to-Drug Interactions

```
:Propoxyphene a :Drug;
  :isPrescribedFor :Pain;
  :isContraIndictive :Eszopiclone.

:Wygesic a :Drug;
  :isPrescribedFor :Pain;
  :isContraIndictive :Eszopiclone.

:Trycet a :Drug;
  :isPrescribedFor :Pain;
  :isContraIndictive :Eszopiclone.

:Propacet100 a :Drug;
  :isPrescribedFor :Pain;
  :isContraIndictive :Eszopiclone.

:Aspirin a :Drug;
  :isPrescribedFor :Pain.

:Tylenol1 a :Drug;
  :isPrescribedFor :Pain.

:Tylenol2 a :Drug;
  :isPrescribedFor :Pain;
  :isContraIndictive
    :SleepingMedication.
```

N3 Tripple representation

Inference Rules

Drug-to-Drug Interactions

If a patient is taking an existing drug $D1$ and
$D1$ has contraindication to another drug $D2$
then drug $D2$ should not be prescribed to the patient

N3 Representation

```
{ ?P a :Patient.
  ?D1 a :Drug.
  ?D2 a :Drug.
  ?P :isTaking ?D1.
  ?D1 :hasContraIndication ?D2. } => {?P :cannotBeGiven ?D2}.
```

Inference Rules

Drug-to-Disease Interactions

If a patient has a condition that has a contraindication to a drug then the patient should not be given the drug

N3 Representation

```
{ ?P a :Patient .
  ?D a :Drug .
  ?P :hasDisease ?DIS .
  ?D :hasContraIndication ?DIS .} => {?P :cannotBeGiven ?D}.
```

Putting it All Together

DataSets

- BRFSS-2010
- Mayo Clinic sleeping pill prescription protocol
- sleeping pill-to-pain medication interaction

Knowledge engineering:

- Resource Description Framework (RDF)/Notation-3 (N3) based ontological model
- scenario specific ontology
- inference rules

Semantic Reasoner

- EulerSharp

Machine Learning toolkit

- Weka

Evaluation Criteria

Sensitivity

identify true positives

$$Sens = \frac{tp}{tp + fn}$$

Specificity

identify true negatives

$$Spec = \frac{tn}{tn + fp}$$

Balanced Accuracy

simple average of specificity and sensitivity

$$balAcc = \frac{Spec + Sens}{2}$$

where,
t_p = true positive,
f_p = false positive,
t_n = true negative,
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System Evaluation

3 Stage Experiment:

1. evaluate machine learning based MDSS on BRFSS patient dataset
2. introduce *information challenge*
3. evaluate the hybrid construction

Ex 1 – ML Evaluation

Goal

determine the best performing machine learning algorithm for BRFSS dataset to prescribe sleeping aids

Setup

1. **algorithms**: decision stump, C4.5-J8, Bagging and AdaBoost
2. **example data**: 50 different randomly selected training sets (of two sizes: 2500 exemplars and 5000 exemplars)
3. **features**: *information gain-based* feature selection algorithm (Yang and Pedersen, 1997) to select **30 features**
4. **labelling**: ground truth was established using the output of the knowledge-based reasoner **where possible**

Ex 1 – ML Evaluation

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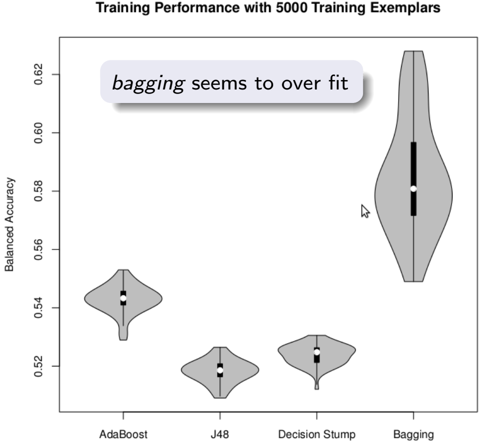
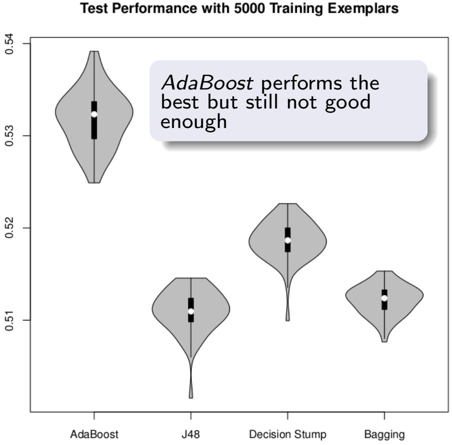




Ex 2 – Tolerance to Missing Information

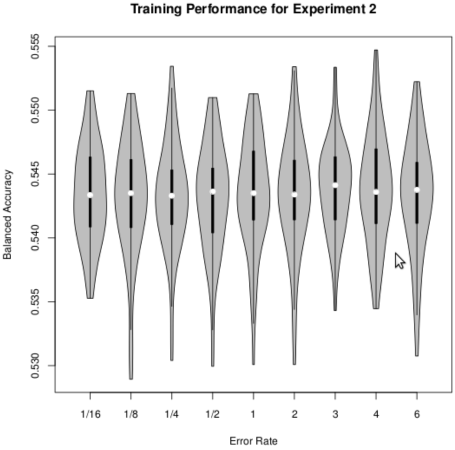
Goal

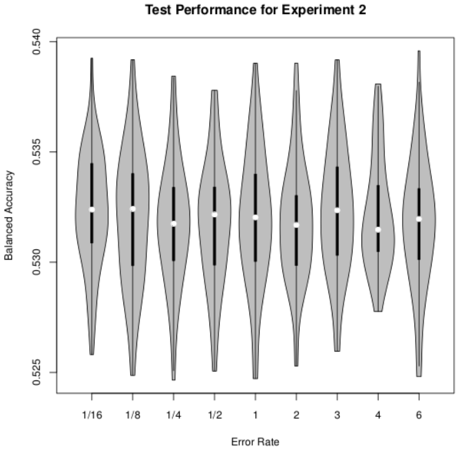
study the impact of data *missingness* (ϵ) for **AdaBoost** based classifiers

Setup

1. **noise $\rightarrow$ missing data**:
   removing known values from the patient records
2. **noise factor** ϵ: describes the probability of introducing noise at random across all insomnia related features
3. **information challenge**: for each value of ϵ,
   - create sample datasets
     (50 sets of 5000 exemplars from the noised data)
   - train AdaBoost based classifier

Ex 2 – Tolerance to Missing Information





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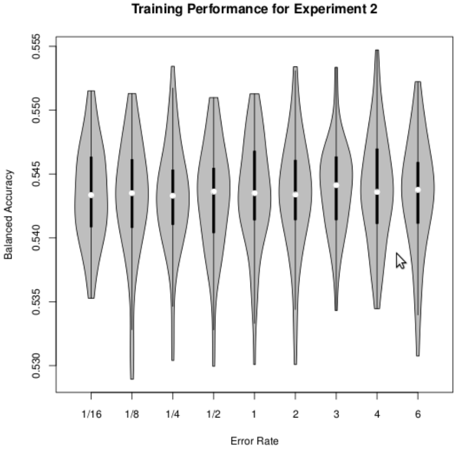

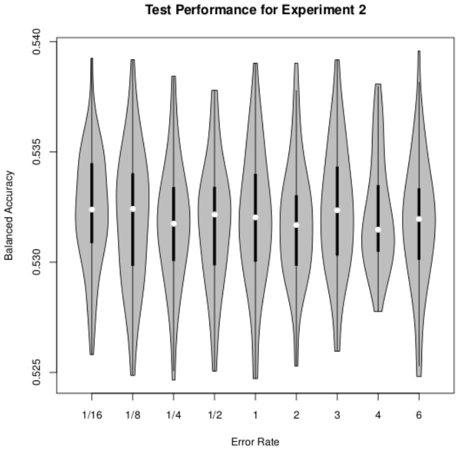

AdaBoost based classifiers are tolerant to 'missingness'

Ex 3 – Hybrid Construction Evaluation

Goal

hybrid construction to impute missing information

Data imputation:

$$R_{org} = \{f_1, f_2, f_3, f_4, f_5, f_6, f_7, f_8, f_9\}$$

$$R_{n\epsilon_i} = \{f_1, \square, f_3, f_4, \square, \square, f_7, f_8, f_9\}$$

$$R_{imp} = \{f_1, \mathbf{p_2}, f_3, f_4, \mathbf{p_5}, \mathbf{p_6}, f_7, f_8, f_9\}$$

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Ex 3 – Hybrid Construction Evaluation

Setup

For a given ϵ:

1. transform $R_{org} \rightarrow R_{n\epsilon}$
2. from $R_{n\epsilon}$ generate an example dataset for training and testing
3. R_{org} is used for establishing ground truth for labelling
4. learn an AdaBoost classifier for each missing feature to impute
5. predict the missing value using the feature classifier
6. observe the impact of *missingness* on the knowledge-based MDSS

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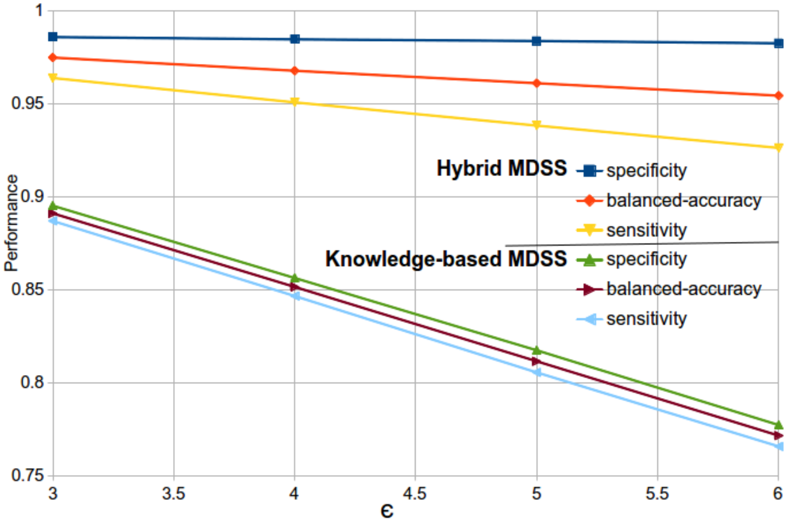
6. observe the impact of *missingness* on the knowledge-based MDSS

repeated for top four ϵ values

Ex 3 – Hybrid Construction Evaluation



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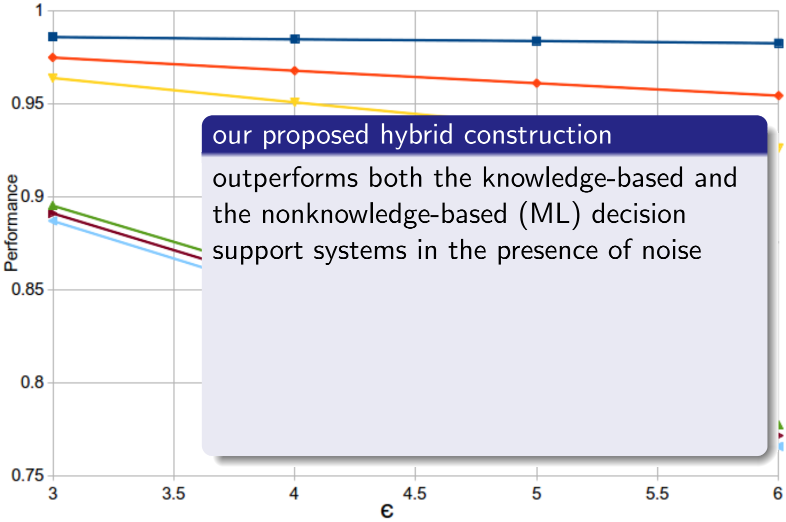

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outperforms both the knowledge-based and the nonknowledge-based (ML) decision support systems in the presence of noise

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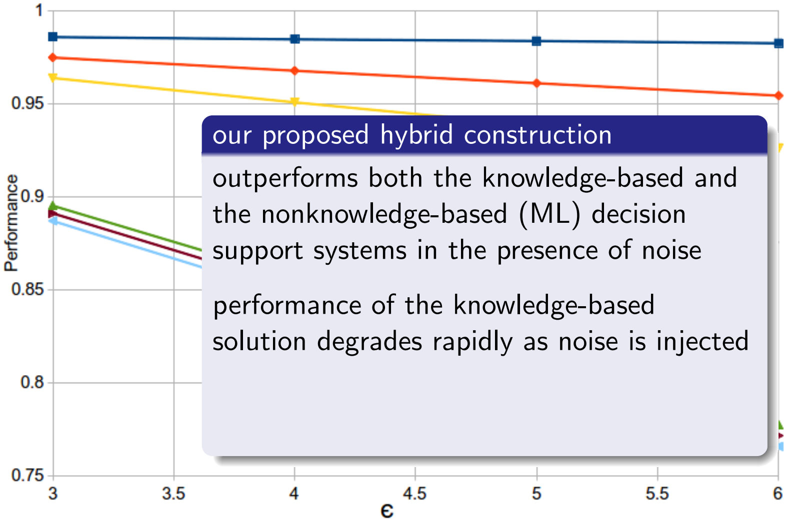

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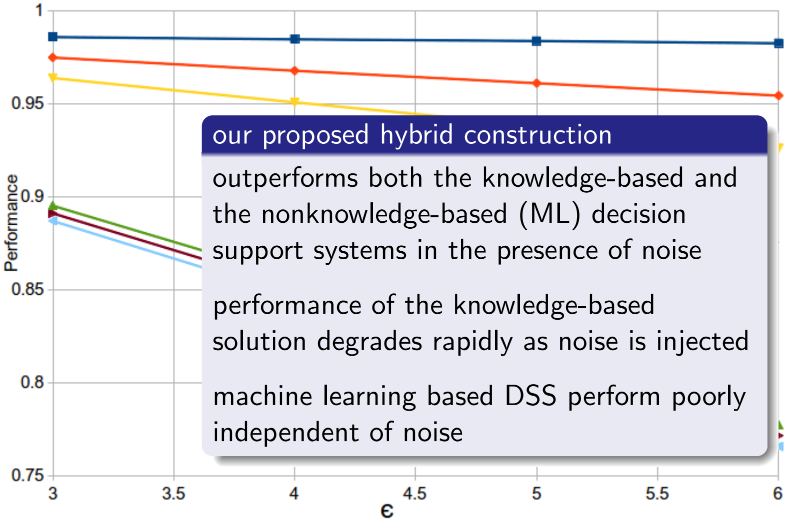

our proposed hybrid construction

- outperforms both the knowledge-based and the nonknowledge-based (ML) decision support systems in the presence of noise
- performance of the knowledge-based solution degrades rapidly as noise is injected
- machine learning based DSS perform poorly independent of noise

Outline

Conclusion

Hybrid Construction for MDSS

- demonstrated the value of a hybrid MDSS that combines ontological and machine learning approaches on real-world datasets
- the hybrid construction fulfils all design goals

Future Work

1. **False Information**
    - missing vs. false information
      (what if the patient provides wrong details)
    - the hybrid construction fulfils all design goals
2. **Confidence Estimations**
3. **POC**
    - deployable implementation

Thank You!

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[1] E.S. Berner. *Clinical decision support systems: theory and practice*. Springer Verlag, 2007.

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[6] Y. Yang and J. O. Pedersen. “A comparative study on feature selection in text categorization”. In: *Proceedings of ICML-97, 14th International Conference on Machine Learning*. 1997, pp. 412–420.