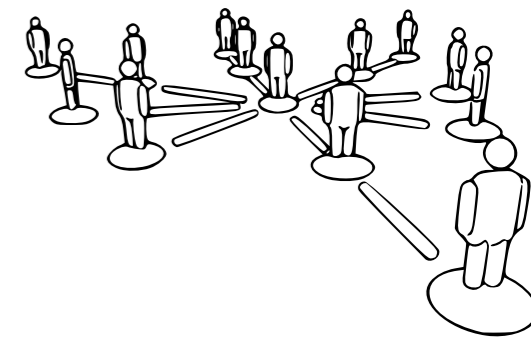


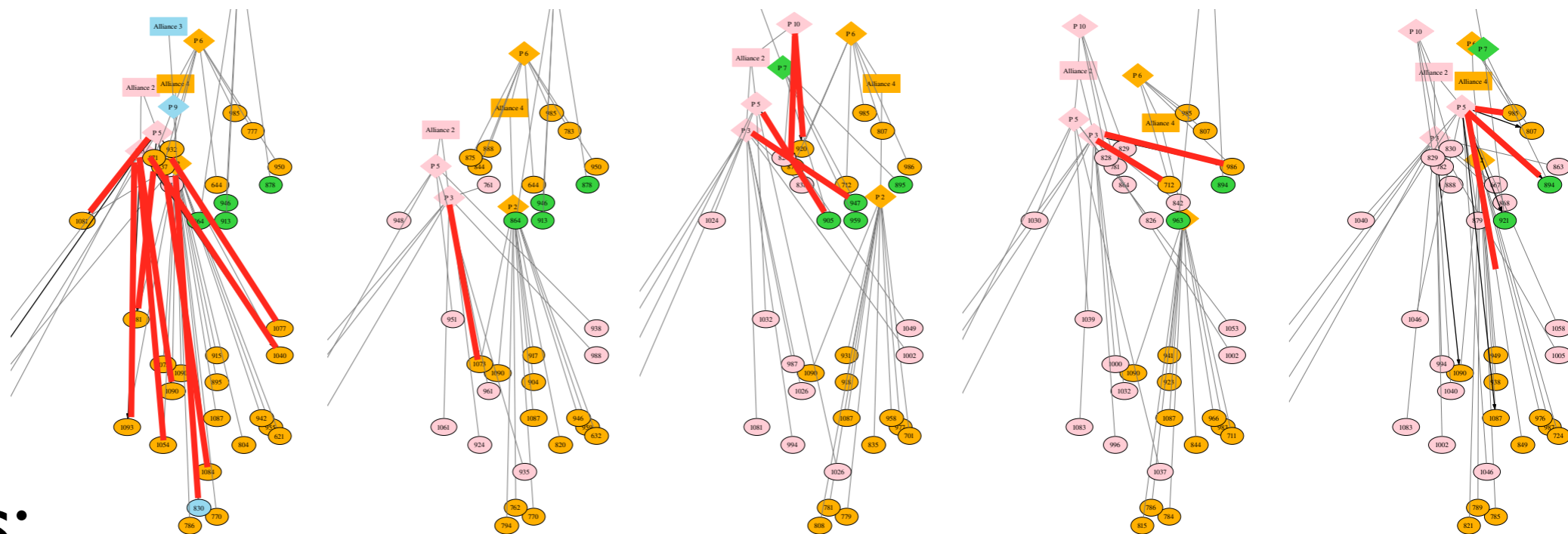
MLG-2008: Poster spotlights

1. CPT-L: an Efficient Model for Relational Stochastic Processes
Presenter: Ingo Thon
2. A graph-theoretic approach for reducing one-versus-one multi-class classification to ranking
Presenter: Willem Waegeman
3. Mining Common Semantic Patterns from Descriptions of Failure Knowledge
Presenter: Steven Kraines
4. Prediction of Molecular Substructures from Mass Spectrograms using Constraint Based Clustering
Presenter: Pieter-Jan Drouillon
5. Randomization Techniques for Statistical Significance Testing on Graphs
Presenter: Sami Hanhijärvi.
6. The Skew Spectrum of Graphs
Presenter: Risi Kondor
7. A Structured-Outputs Method for Prediction of Protein Function
Presenter: Michael Hamilton
8. A structured outputs method for predicting protein binding sites
Presenter: Michael Hamilton
9. The Sum-Over-Paths Covariance: A novel covariance measure between nodes of a graph
Presenter: Amin Mantrach
10. Training Non-linear Structured Prediction Models with Stochastic Gradient Descent
Presenter: Shankar Vembu

CPTL

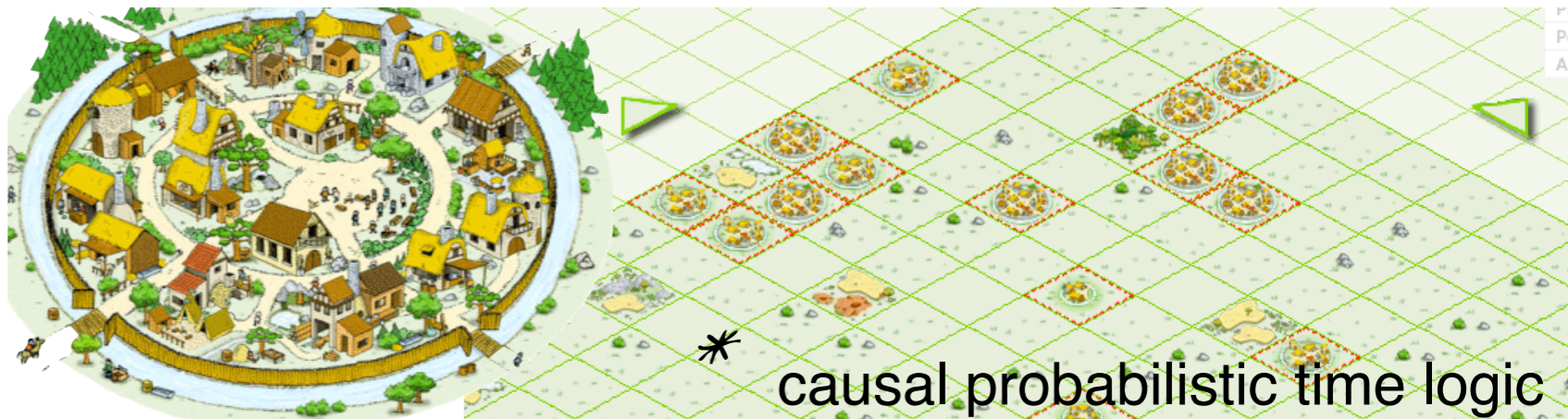


Problem: Model for Sequences of Relational Interpretations
Examples: Games, Dynamic of Social Networks,.....

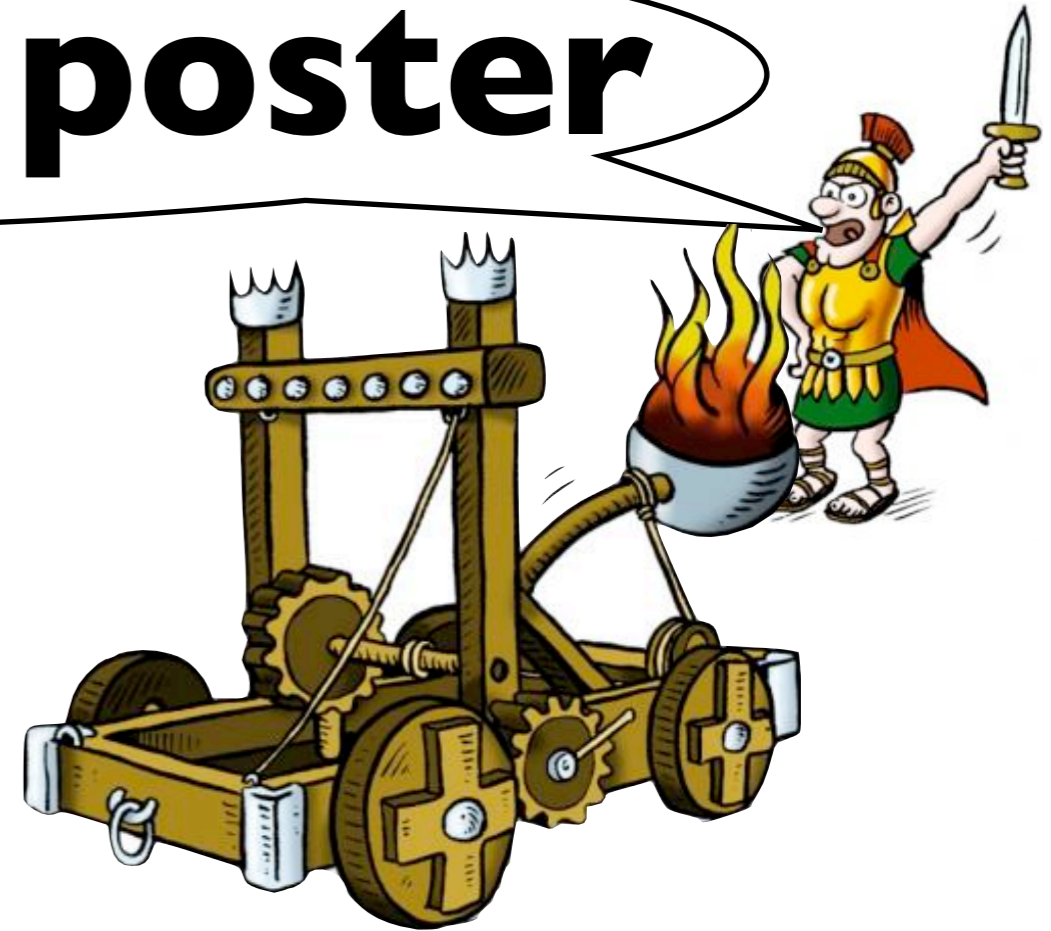


Applications:

- Game AI
- Network analysis
- fraud detection
- user support/advice



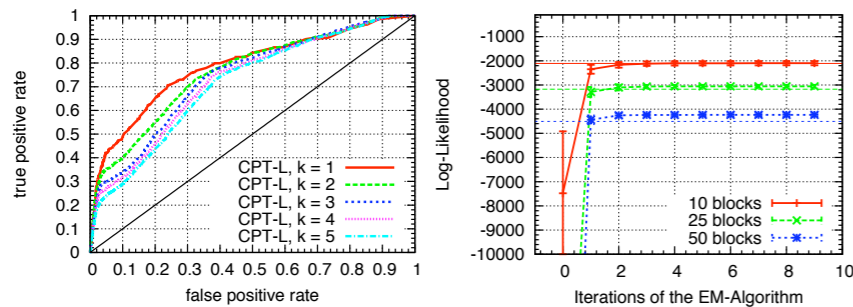
Come to our poster



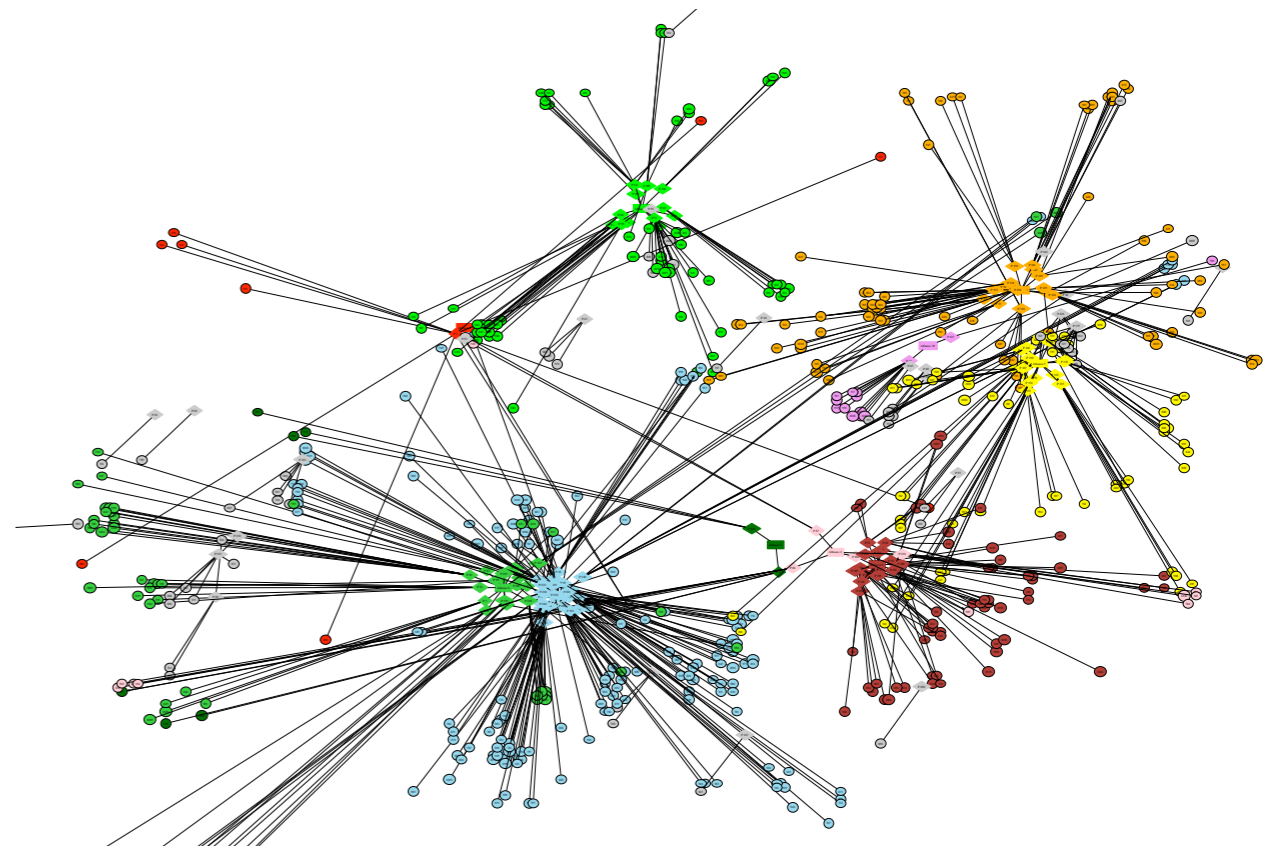
for more information about
- our model

$$\underbrace{b_1, \dots, b_n}_{\text{Body = Cause}} \rightarrow \underbrace{h_1 \vee \dots \vee h_m}_{\text{Head = Effect}} \vee \dots \vee p_m$$

- or experiments

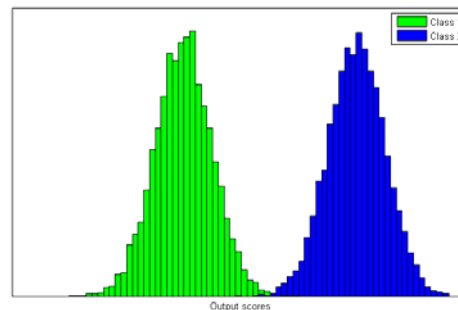
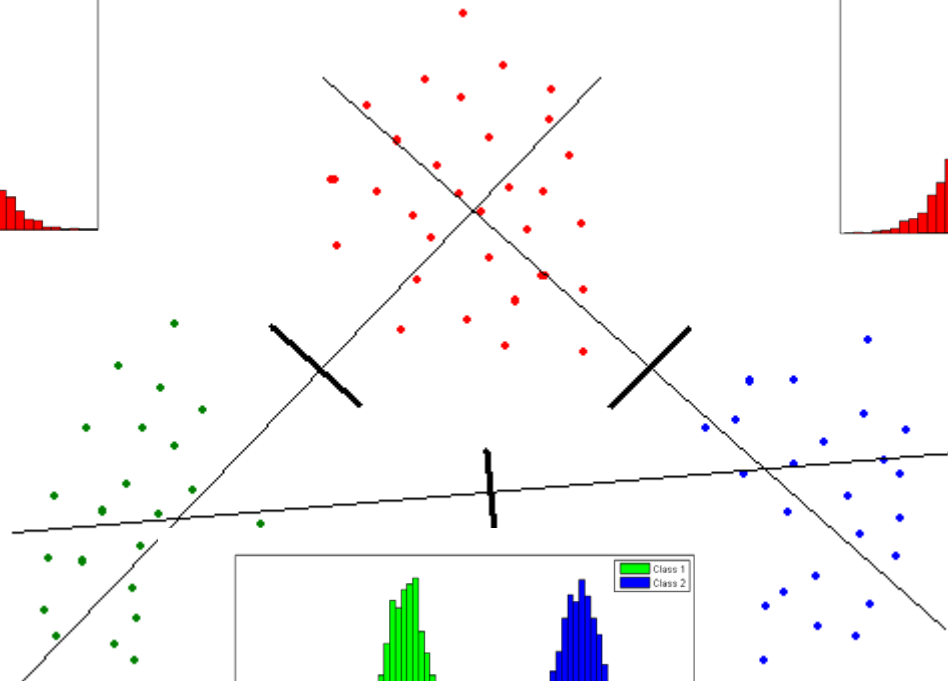
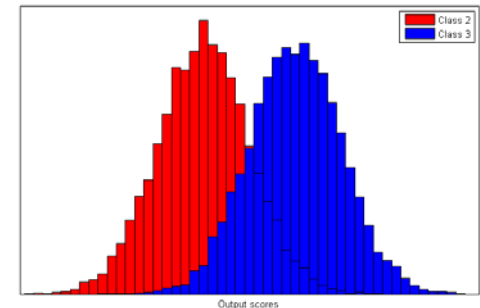
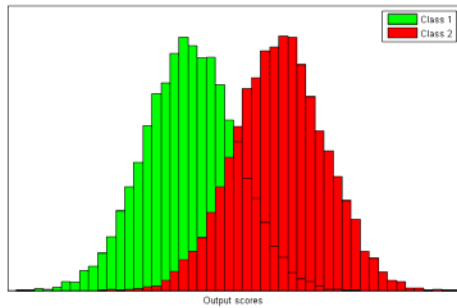


- or how to win in travian



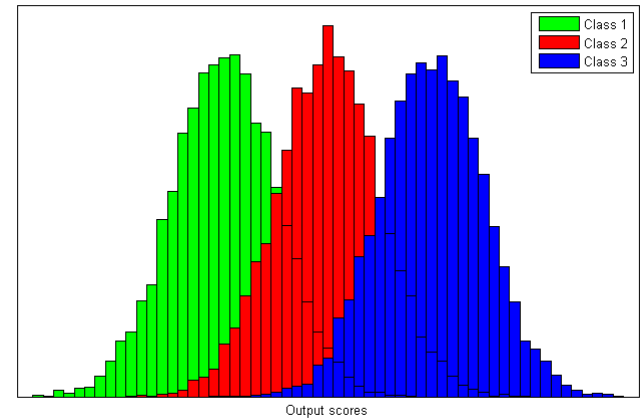
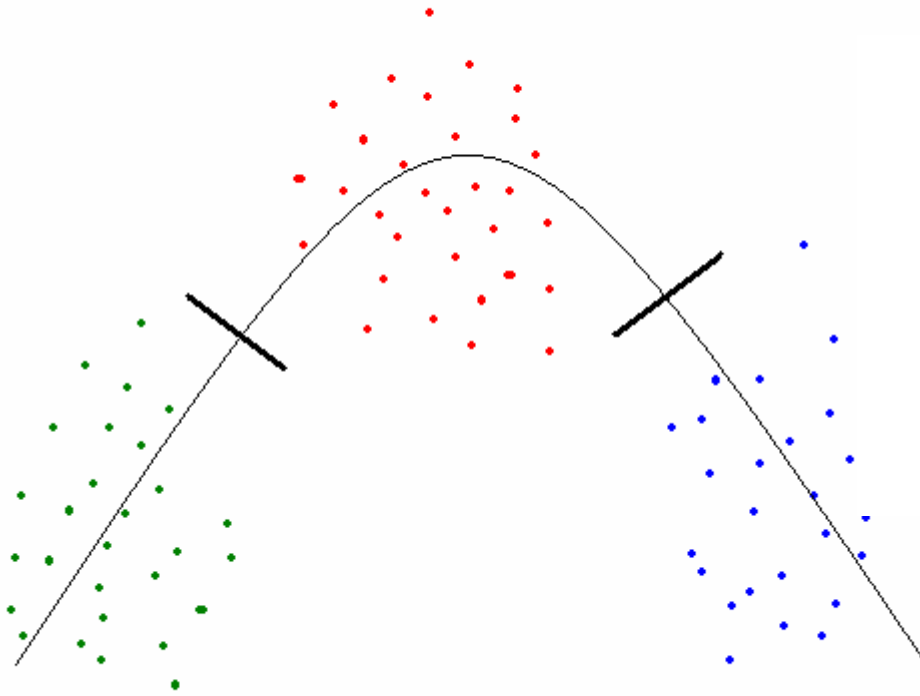
A graph-theoretic approach for reducing one-versus-one multi-class classification to ranking

Willem Waegeman
Ghent University



A graph-theoretic approach for reducing one-versus-one multi-class classification to ranking

Willem Waegeman
Ghent University



EKOSS

Expert Knowledge Ontology-based Semantic Search

Mining common semantic patterns from descriptions of failure knowledge

Steven Kraines , Weisen Guo

Science Integration Programme

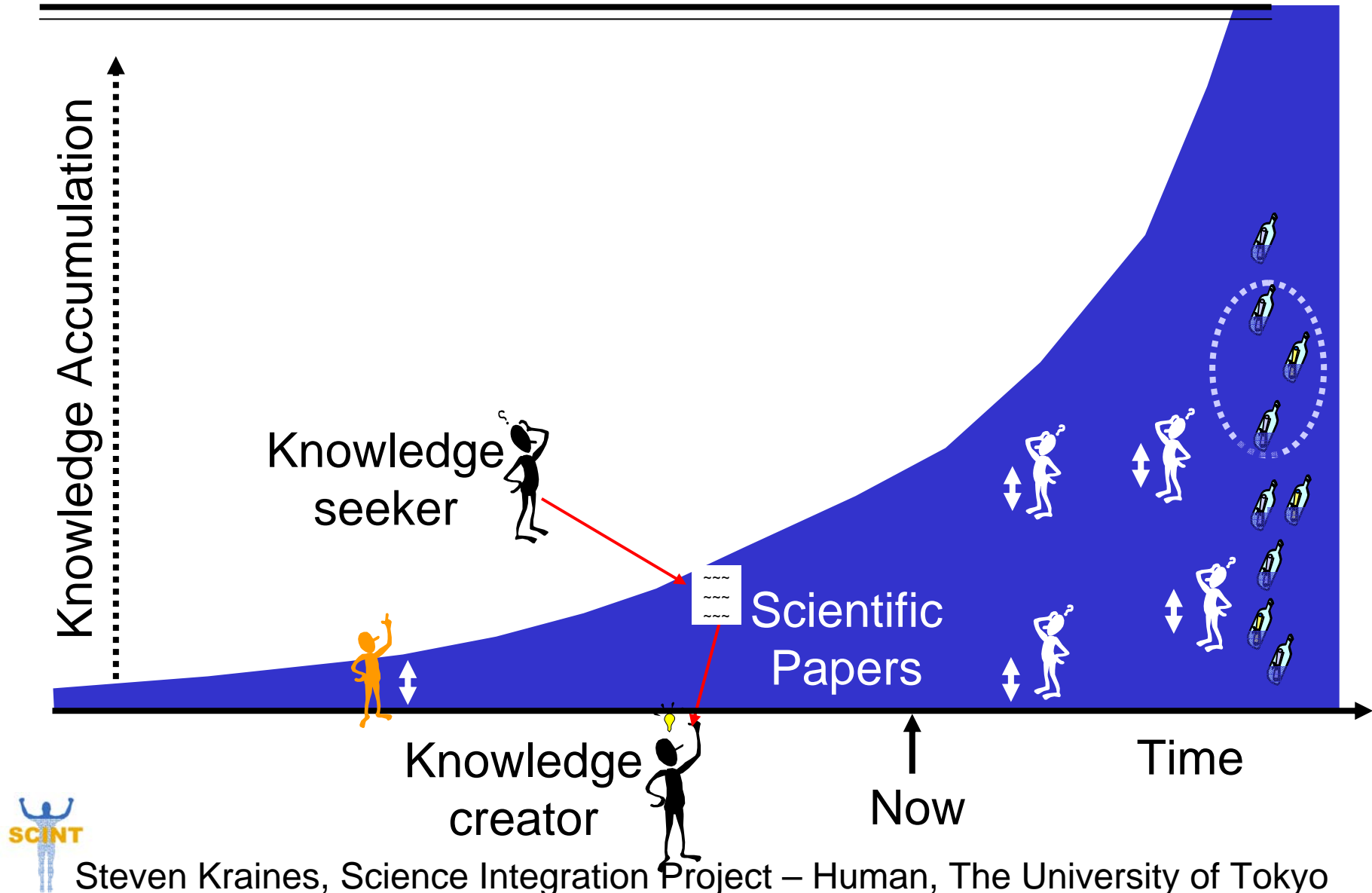
The University of Tokyo



Steven Kraines, Science Integration Project – Human, The University of Tokyo

The problem – the state of knowledge sharing in science

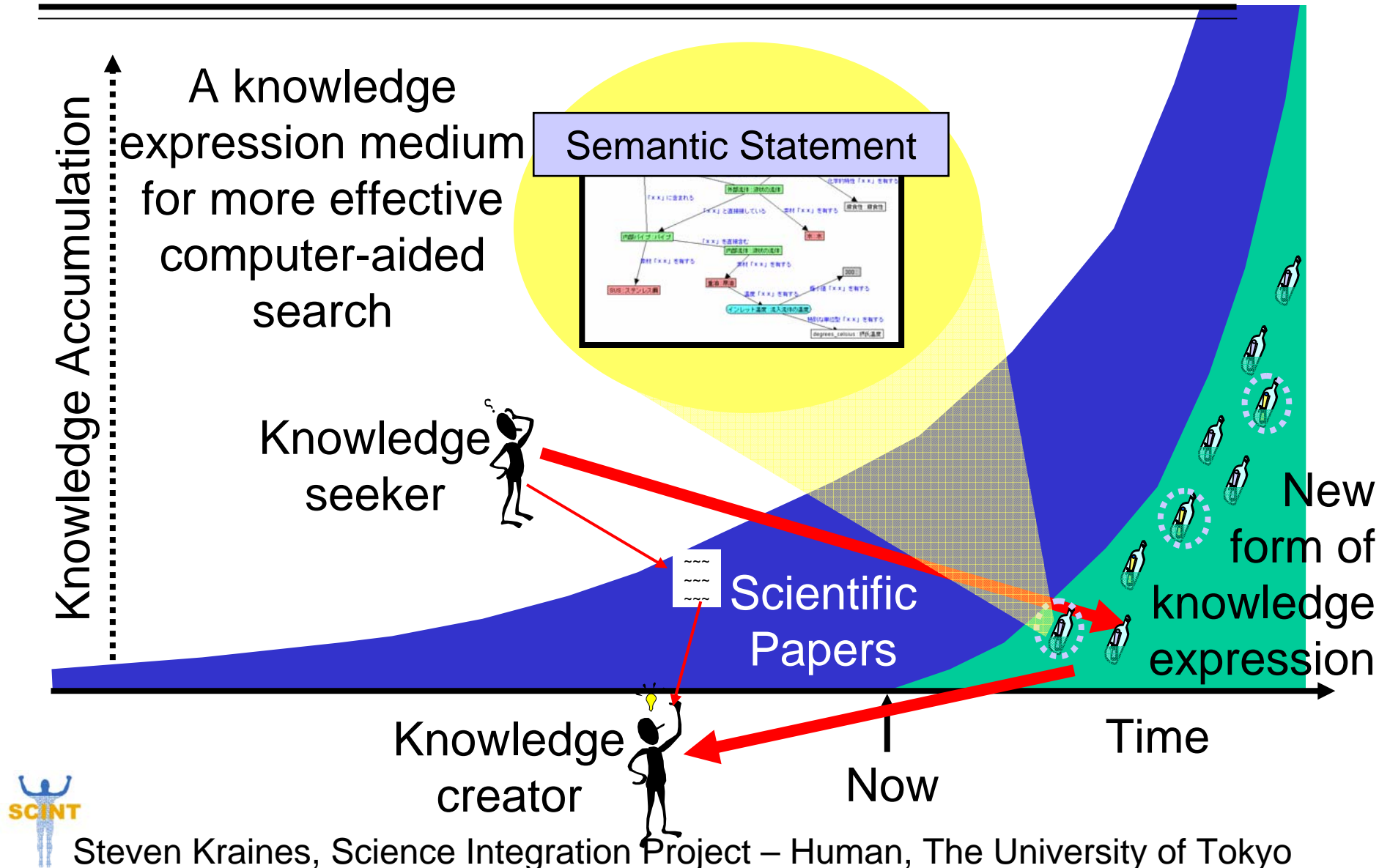
Explosive Increase in Scientific Knowledge



Steven Kraines, Science Integration Project – Human, The University of Tokyo

The problem – the state of knowledge sharing in science

Explosive Increase in Scientific Knowledge



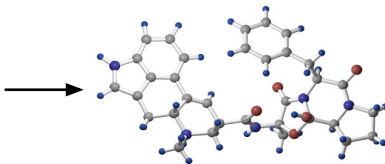
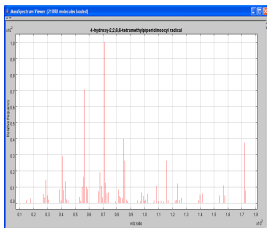
Prediction of Molecular Substructures from Mass Spectrograms using Constraint Based Clustering

Pieter-Jan Drouillon, Hendrik Blockeel

Prediction of Molecular Substructures from Mass Spectrograms using Constraint Based Clustering

Pieter-Jan Drouillon, Hendrik Blockeel

- Mass spectrogram
 - Molecule bombarded with electrons
 - Set of (m/z,frequency) couples
- Experts can predict parts of structures
- Idea: combine predictive clustering with constraints to predict substructures



Prediction of Molecular Substructures from Mass Spectrograms using Constraint Based Clustering

Pieter-Jan Drouillon, Hendrik Blockeel

Predictive clustering

- Input space X (mass spectrum): form well-separated clusters
- Output space Y (substructures): form coherent clusters
- Given example x on input space X
 - predict cluster it belongs to
 - given this cluster predict Y

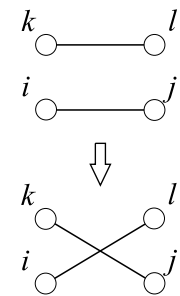
Add constraints with iterative process

- 1 cluster molecules based on mass spectra
- 2 Mine each cluster for specific substructures
- 3 Use these substructures to form clustering constraints
- 4 Repeat until no new substructures

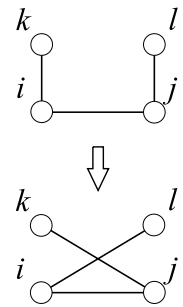
Randomization Techniques for Statistical Significance Testing on Graphs

- How to test statistical significance of graph mining results?
- Create random graphs by edge swaps
- Preserve user defined statistics, e.g.:
 - Degree distribution
 - Average clustering coefficient
- Are mining results a random effect in the data?

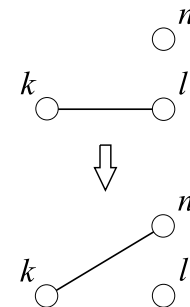
XSwap



LocalSwap



Flip



Can just 49 numbers characterize a graph?

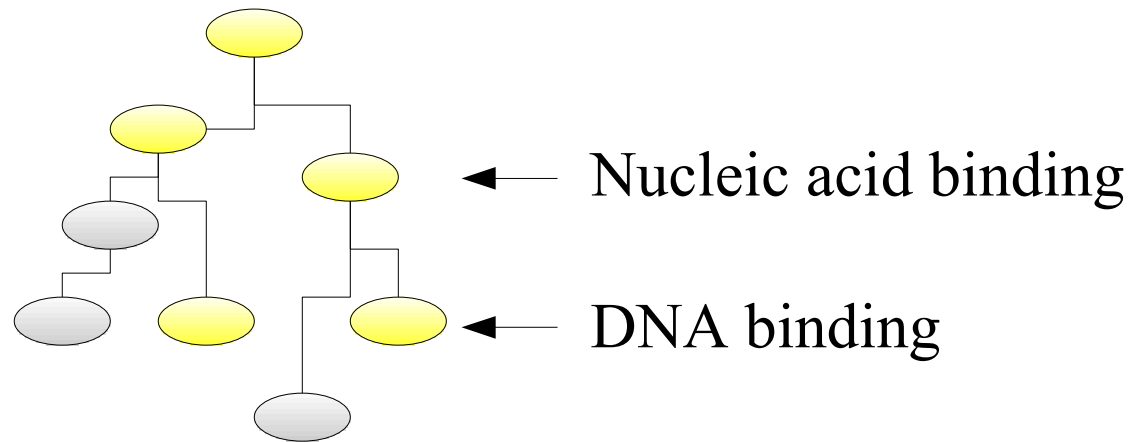
$$\hat{f}(\rho) = \sum_{\sigma \in \mathcal{S}_n} f(\sigma) \rho(\sigma) \quad \rho \in \mathcal{R}$$

“The skew spectrum of graphs”

Risi Kondor

Karsten Borgwardt

Protein Function Prediction



(0, 0, 1, 1, 1, 0, 1, 1)

- ◆ Nodes deeper in the tree specify more detail about the function
- ◆ Molecular function can be represented in vectorial form as a union of paths through the tree

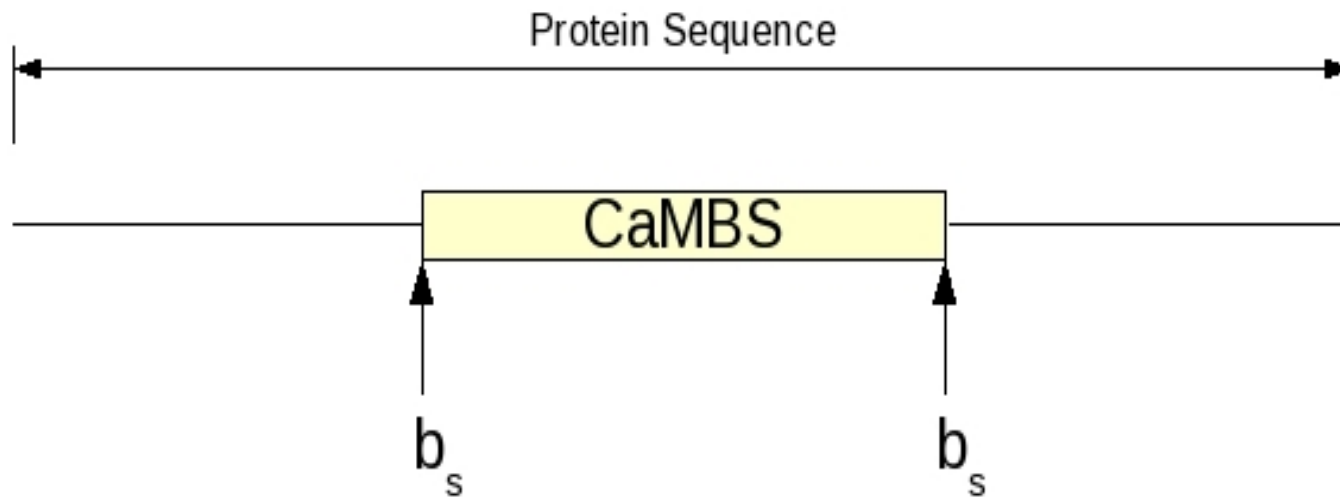
The Story

- Traditional methods transfer annotation based on sequence similarity
 - We approach the problem by learning the structure of the output space
 - Our results demonstrate that learning output space structure yields improved performance
-
-

Predicting Calmodulin Binding Sites

Michael Hamilton, Asa Ben-Hur, A.S.N Reddy

Colorado State University



- Special case of the label sequence problem
- Discriminant classifiers
 1. Sliding Windows (SVM)
 2. Structured Outputs (Perceptron)

Main Concepts

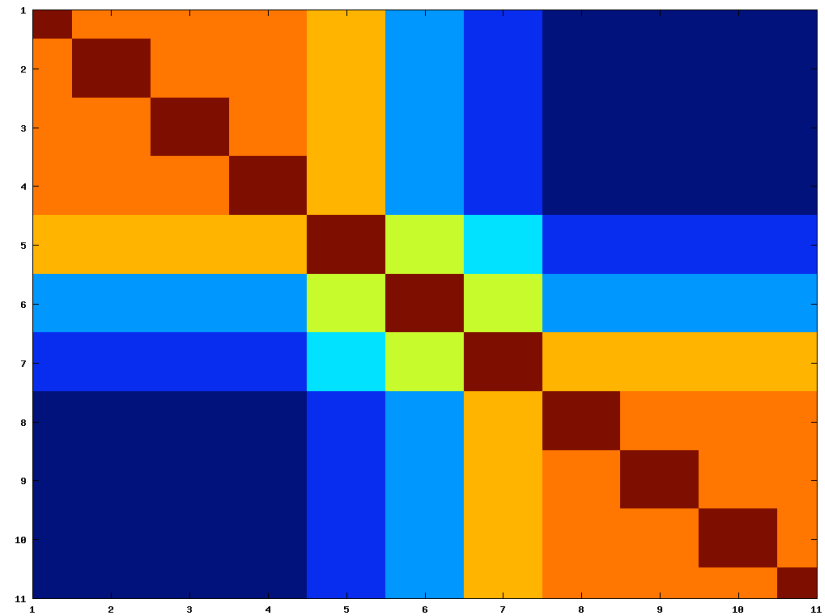
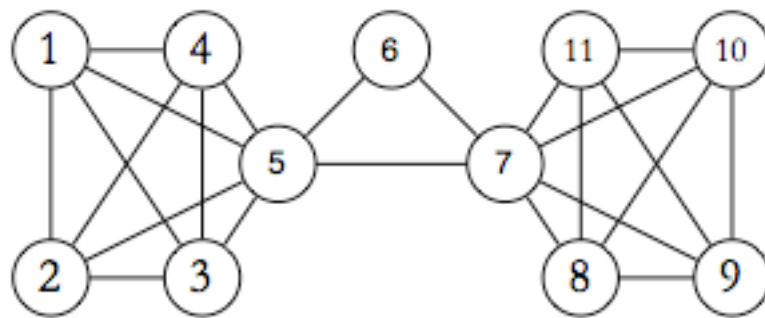
- Sliding window and structured output classifiers
- Kernels
- Benefits of structured outputs over sliding windows
 - Performance
 - Post-processing not required
- Other applications
- Future work



SoP measure

- Two nodes are **correlated** if they often lie on the same – preferably short – path;
- We consider the set of all paths between all pair of nodes :
 - Including **cycles**;
 - The set is possibly infinite
- It provides a **kernel** on a graph

Example



Training Non-Linear Structured Prediction Models with Stochastic Gradient Descent

Thomas Gärtner, Shankar Vembu



RHEINISCHE FRIEDRICH-WILHELMS-UNIVERSITÄT



Fraunhofer

Institut
Intelligente Analyse- und
Informationssysteme

Predicting Combinatorial Structures

- Dicycles, partially ordered sets, permutations, graphs
 - Route prediction on a street network
 - De novo drug design
- Existing structured prediction models (Taskar et al., 2005; Tsochantaridis et al., 2005) cannot be trained efficiently to predict these structures
- Standard assumptions (existence of separation oracle, decoding subroutine, certificate of optimality) are not met

Contributions

- Non-linear structured prediction model (unconstrained polynomially-sized quadratic program)
- Online training with stochastic gradient descent
- Approximation algorithms for predicting combinatorial structures
- Preliminary empirical results on multilabel classification and dicycle prediction