

# Learning for Information Extraction in Biomedical and General Domains

Makoto MIWA <makoto-miwa@toyota-ti.ac.jp>

Associate Professor, Toyota Technological Institute

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# Self-introduction



Japanese chess “shogi”

I started  
NLP here

Main research  
topics on IE

- 2008 Ph.D. thesis on “AI in computer games”
- 2008-2011
  - Researcher, Tsujii laboratory, the University of Tokyo
- 2011-2014
  - Research Associate, NaCTeM, the University of Manchester
  - Visiting researcher, Tsuruoka laboratory, the University of Tokyo
- 2014-
  - Associate Processor, Computational Intelligence laboratory, Toyota Technological Institute (TTI)
  - Visiting Researcher, Artificial Intelligence Research Center, National Institute of Advanced Industrial Science and Technology (AIST)

PPI  
extraction  
(AkaneRE)

Event  
extraction  
(EventMine,  
PathText)

Joint entity  
& relation  
extraction  
(JointER,  
LSTM-ER)

# Toyota Technological Institute (TTI)



- Located in Nagoya (in between Osaka and Tokyo), Japan
- Founded in 1981 by Toyota Motors Cooperation
- TTI-C (Toyota Technological Institute at Chicago) is a sister university of TTI and TTI-C is founded by TTI in 2003



# Acknowledgements

- Most contents are from collaboration with my colleagues at





豊田工業大学  
知能数理研究室

# Europe PMC EvidenceFinder [Black et al., 2016]



EvidenceFinder

Europe PMC

EvidenceFinder

mdm2

## Results

Results: [All citations for keyword search \(6592\)](#) | [Full text articles \(140\)](#)

Sort by: | Date




1 2 3 4 5 6



Results 1 - 25 of 140

### The role of miR-18b in **MDM2**-p53 pathway signaling and melanoma progression.

(PMCID:PMC3601951) Free resource 

Dar AA, Majid S, Rittsteuer C, de Semir D, Bezrookove V, Tong S, Nosrati M, Sagebiel R, Miller JR 3rd, Kashani-Sabet M

J Natl Cancer Inst [2013, 105(6):433-442]

Cited: 14 times

#### Extracts relevant to your question

- In addition, substantial downregulation of **MDM2** protein levels was observed following miR-18b overexpression, indicating the posttranscriptional regulation of **MDM2** by targeting its 3'UTR.

### MicroRNA-145 targets the metalloprotease ADAM17 and is suppressed in renal cell carcinoma patients.

(PMCID:PMC3579323) Free resource 

Doberstein K, Steinmeyer N, Hartmetz AK, Eberhardt W, Mittelbronn M, Harter PN, Juengel E, Blaheta R, Pfeilschifter J, Gutwein P

Neoplasia [2013, 15(2):218-230]

Cited: 7 times

#### Extracts relevant to your question

- Particularly, the regulation of the p53 repressor **MDM2** by **miR-145** could play a major role for the changes in cell cycle, chemoresistance, and proliferation [58].

## Ask a question

### What regulates mdm2? (140)

- What inhibits mdm2? (193)
- What induces mdm2? (162)
- What expresses mdm2? (149)
- What increases mdm2? (116)
- What activates mdm2? (109)
- What binds mdm2? (108)
- What binds to mdm2? (108)
- What affects mdm2? (95)
- What is inhibited by mdm2? (94)
- What does mdm2 bind to? (84)
- What is regulated by mdm2? (81)
- What does mdm2 result in? (77)
- What affects mdm2? (75)
- What interacts with mdm2? (73)

## Results

Results: All citations for keyword

**The role of miR-18**  
(PMCID:PMC3601  
Dar AA, Majid S, R  
3rd, Kashani-Sabe  
J Natl Cancer Inst  
Cited: 14 times

### Extracts relevant

- In addition, su
- indicating the

**MicroRNA-145 tar**  
**carcinoma patient**  
(PMCID:PMC3579  
Doberstein K, Steir  
R, Pfeilschifter J, C  
Neoplasia [2013, 1  
Cited: 7 times

### Extracts relevant

- Particularly, th
- cycle, chemor

## Ask a question

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EvidenceFinder

Europe PMC



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Results 1 - 25 of 140

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EvidenceFinder



mdm2



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Neurofibromatosis type 2 tumor suppressor protein, NF2, induces proteasome-mediated degradation of JC virus T-antigen in human glioblastoma.

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# PathText (CellDesigner Plug-in) [Miwa et al., 2013a]

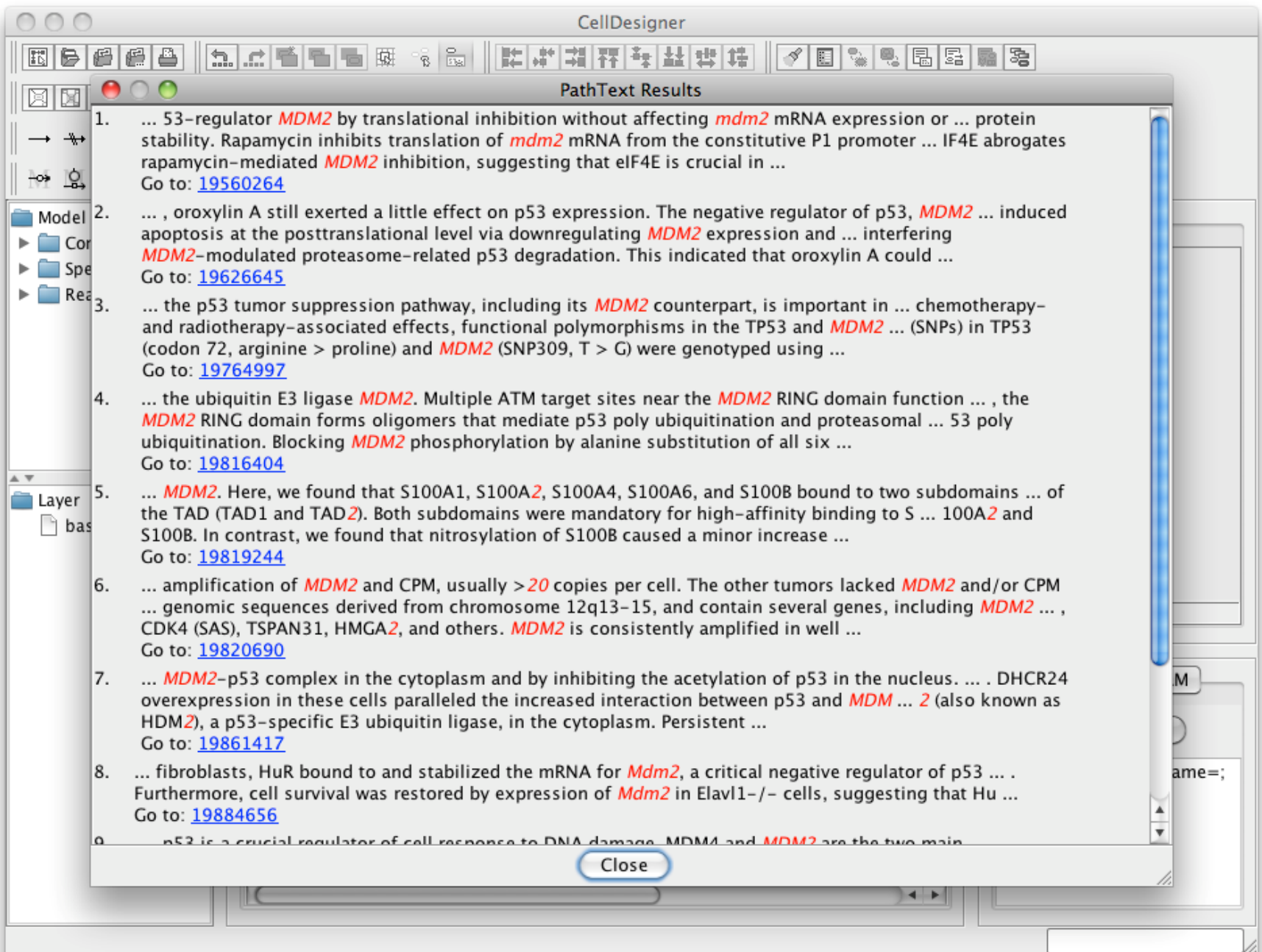
CellDesigner:  
Pathway editor in  
systems biology

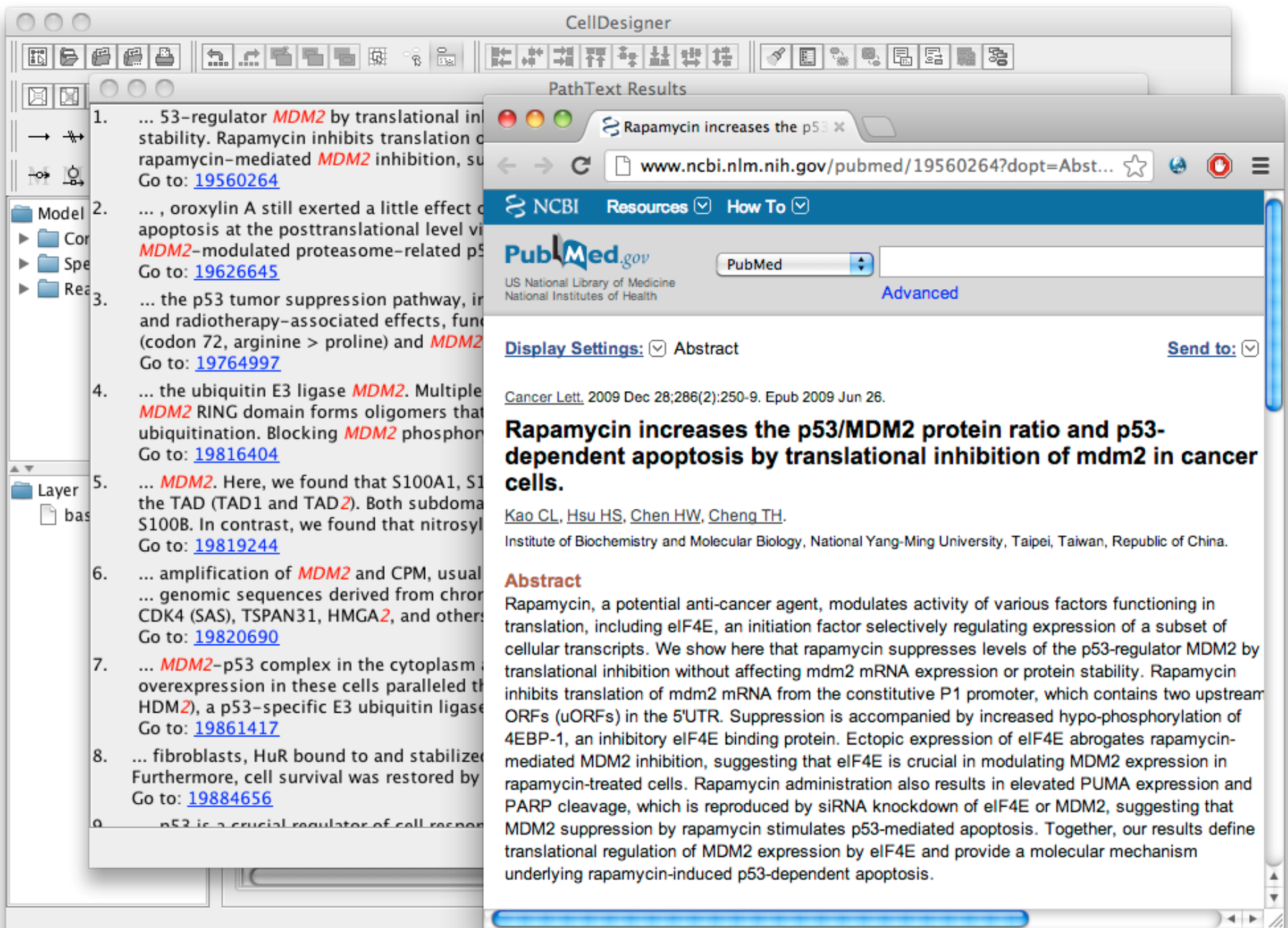
The screenshot shows the CellDesigner software interface. The main window displays a pathway diagram with a green box labeled 'lys P53' and a yellow box labeled 'Mdm2'. A blue arrow labeled 're26' points from 'lys P53' to 'Mdm2'. A context menu is open over the 're26' arrow, listing various actions such as 'Add Anchor Point', 'Remove Anchor Point', 'Adjust Connection To Orthogonal', 'Change Identity...', 'Edit Reaction...', 'Edit KineticLaw...', 'Reaction Notes...', 'Change Color & Shape...', 'Add Text', 'Import KineticLaw from SABIO-RK...', 'PathText', and 'Get References for Reaction'. The 'PathText' option is highlighted in blue. Below the screenshot, there are two blue callout boxes. The first box contains the text 'Import KineticLaw from SABIO-RK...' and 'PathText'. The second box contains the text 'Get References for Reaction'.

Import KineticLaw from SABIO-RK...  
PathText

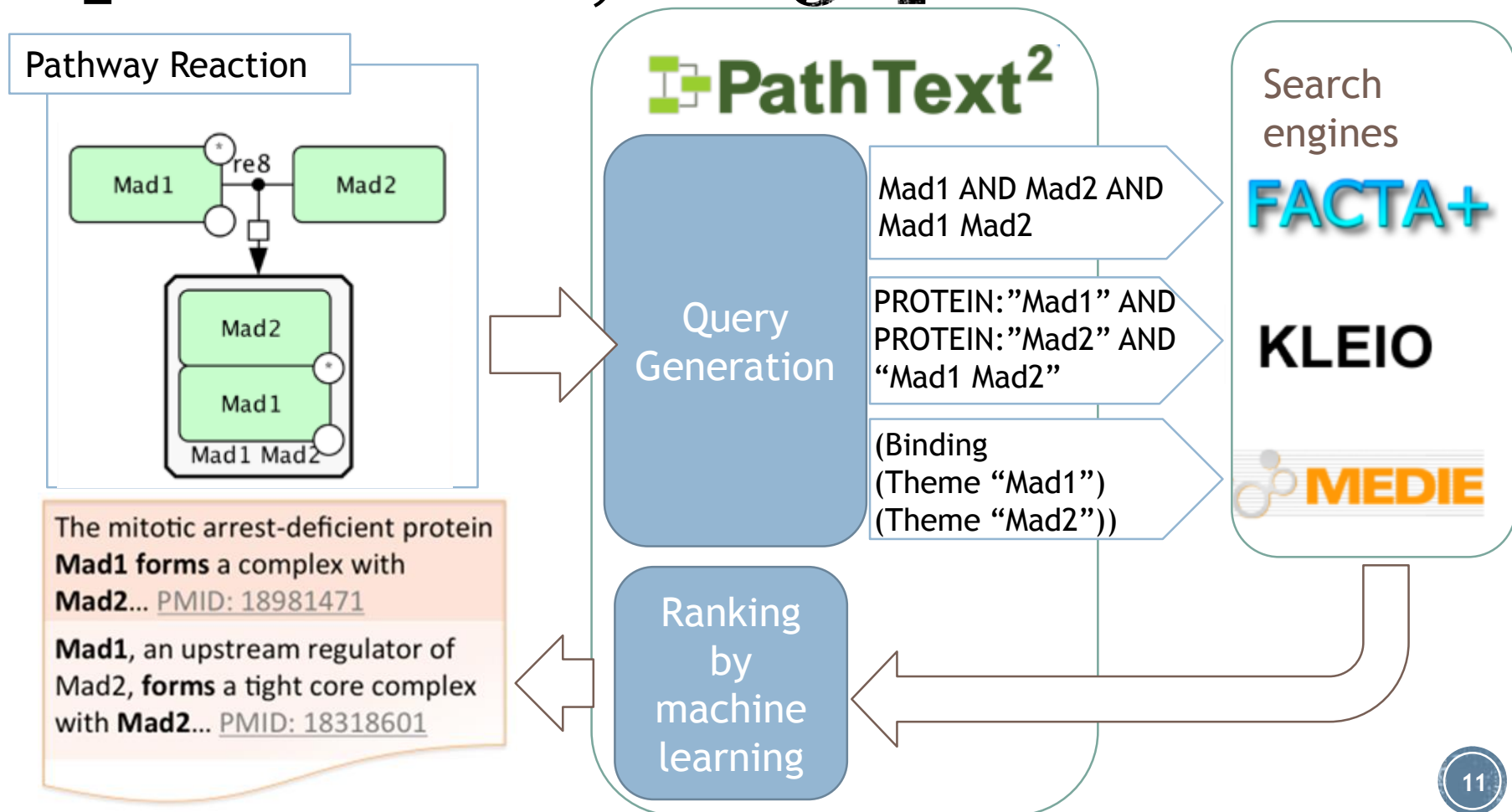
Get References for Reaction



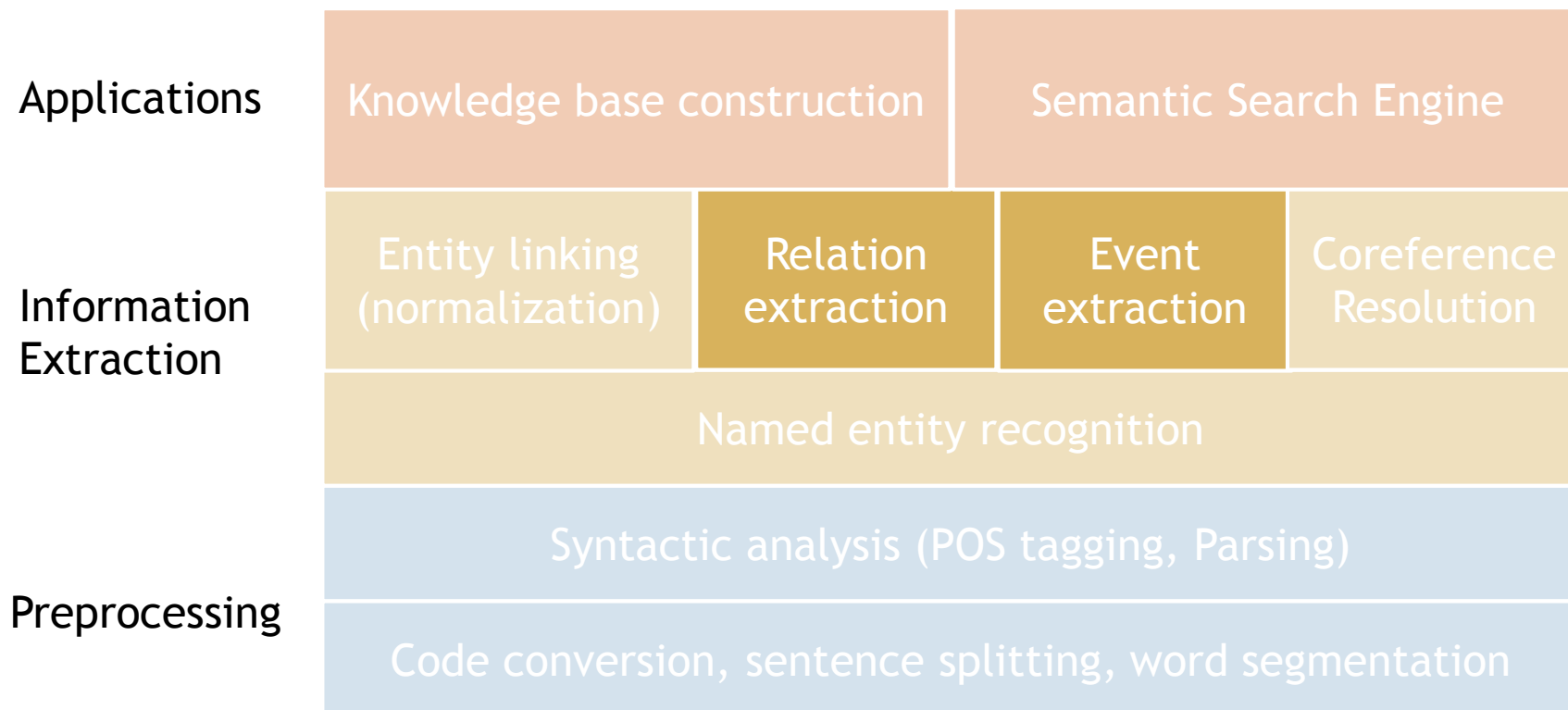




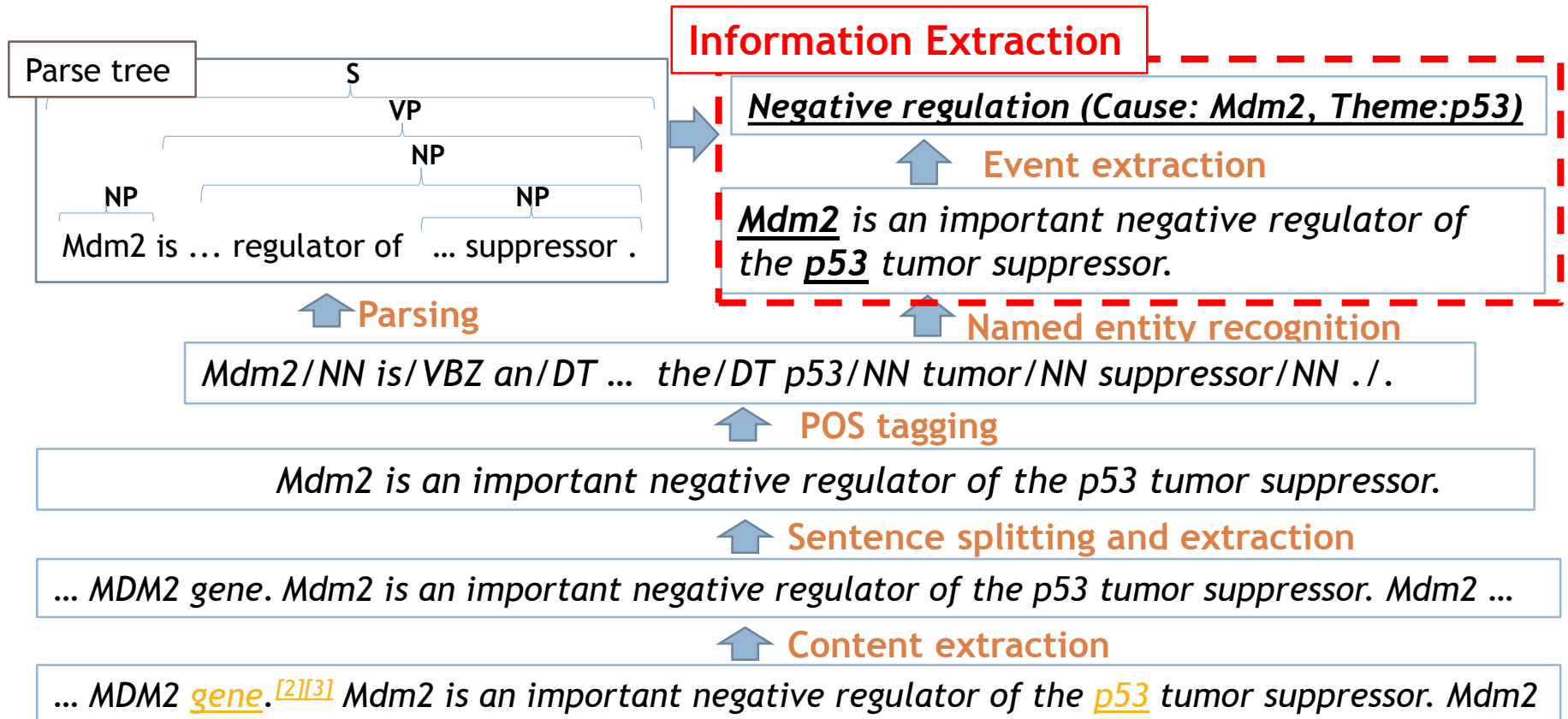
# PathText: semantic search engine using extracted events [Miwa et al., 2013a]



# Workflow in Information Extraction



# Workflow in Information Extraction



<http://en.wikipedia.org/wiki/Mdm2>

# Why you should research information extraction?

- The goal is clear
    - Close to practical applications
  - Close to several syntactic and semantic tasks
    - They learn how to use basic NLP tools, e.g., parsers, during development
    - They can move to a variety of related tasks, e.g., NER, co-reference, SRL.
  - Complex enough to try a variety of ML methods, but not too complex
    - From simple classifiers to structured learning, and deep learning.
    - Un- or semi-supervised methods can also be considered.
  - Clear evaluation metrics and task settings as for recent tasks
- ➔ Good research targets especially for novices in NLP, TM, and ML



# Target problems in this talk

Supervised machine learning (ML) for extracting semantic structures (relations and events) from texts

- Extracting not only terms/words but also *structures related to them*
  - ⇔ Sometime events are single words in knowledge discovery
- Structures need to be linked to some parts of texts as *evidence*
  - ⇔ MUC and knowledge discovery methods often ignore the evidence
- Annotated data and target structures are **manually** built
  - ⇔ Distantly (or weakly) supervised methods from knowledge bases may not align with the structures

# Outline

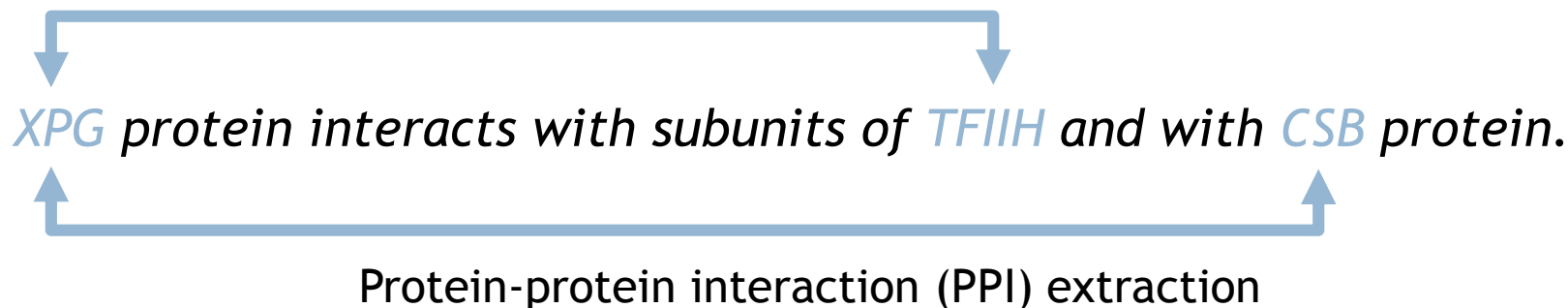
- Introduction
- Overview of IE tasks
  - General vs Biomedical
- Challenges/considerations in building IE systems
  - Machine learning problems
  - Deep learning
- Our joint entity and relation extraction models
- Conclusion



# Overview of IE tasks

# Relation extraction/classification

- Extracting static binary relationships between given entities/nominals
  - Few tasks deal with dynamic and/or n-ary relationships
    - e.g., BB and SeeDev in BioNLP-ST 2016



# Classification-based relation extraction (AkaneRE)

- Classifying each target pair as a specific relation or not
  - Pros: easy, fast
  - Cons: no consideration on interactions between relations
- Pairs are represented as *feature vectors* or with multiple *kernels*.

*XPG* protein interacts  
with subunits of *TFIIH*  
and with *CSB* protein.

(XPG, TFIIH)  
(XPG, CSB)  
(TFIIH, CSB)

(XPG, TFIIH, ✓)  
(XPG, CSB, ✓)  
(TFIIH, CSB, ✗)

Enumerate all  
possible pairs

Classify each  
pair using  
classifiers

[Miwa et al., 2009]

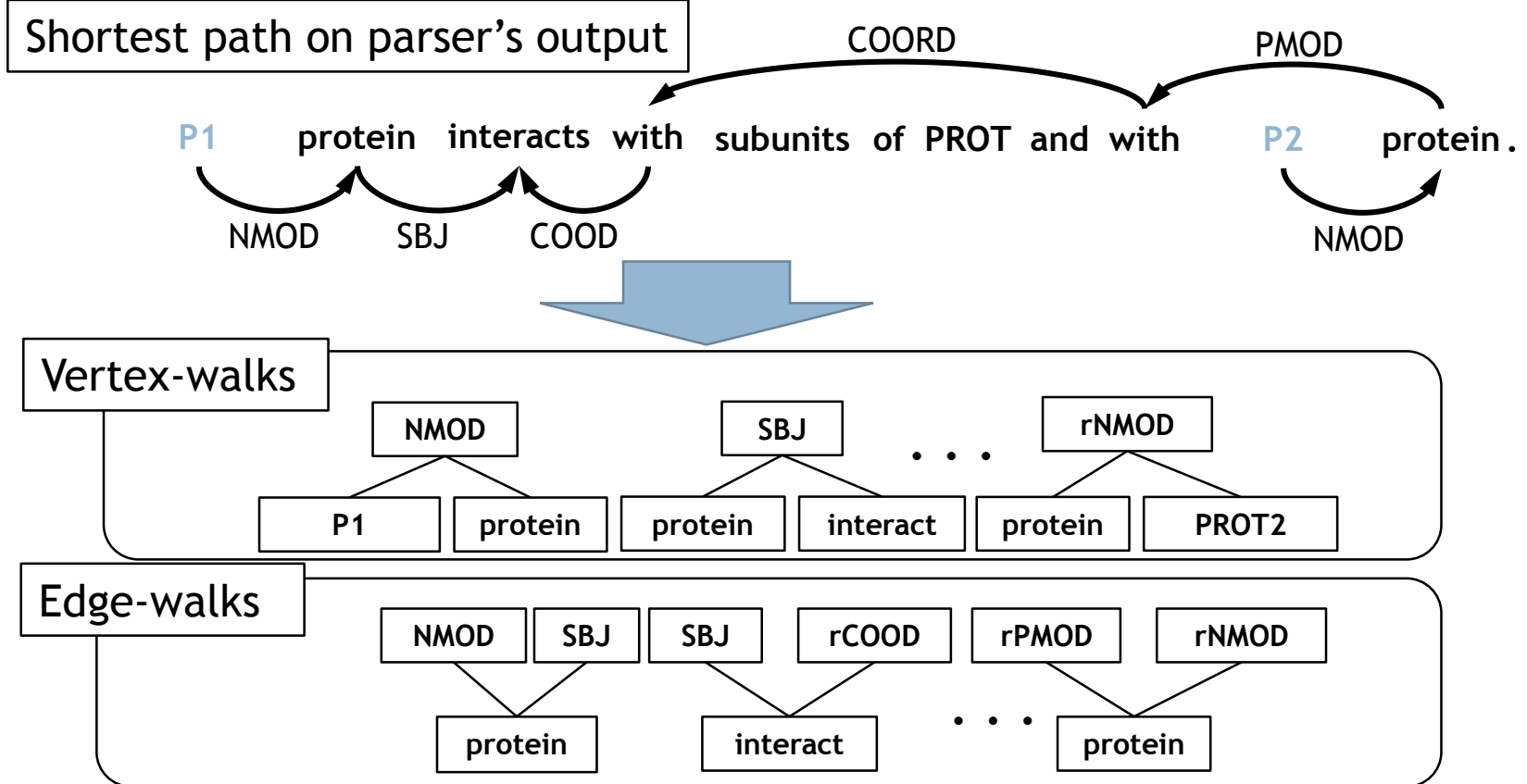
# Example of features for relation extraction: bag-of-words (BoW)

P1 protein interacts with multiple subunits of PROT and with P2 protein .

position	features (lemma, frequency, position to a pair)
Before the pair	-
in the Middle of the pair	PROT_M:1, and_M:1, interact_M:1, multiple_M:1, of_M:1, protein_M:1, subunit_M:1, with_M:2
After the pair	protein_A:1

- Features are usually designed as pair-dependent
- Bio-tasks often blind named entities

# Example of features for relation extraction: shortest path (SP) between a pair



# Other common features/kernels

- Lexical features
  - Character n-grams, part-of-speech

- Contextual features

[Miwa et al., 2009]

- Kernels
  - Shortest path kernel
  - Tree kernels
  - Graph kernel

System	F1-scores on AImed (%)
AkaneRE (BoW+SP)	63.2
AkaneRE (BoW+SP+Graph)	64.2

- BoW+SP produces close to the state-of-the-art performance (if we ignore deep learning-based methods)

# Major relation extraction tasks

Biomedical

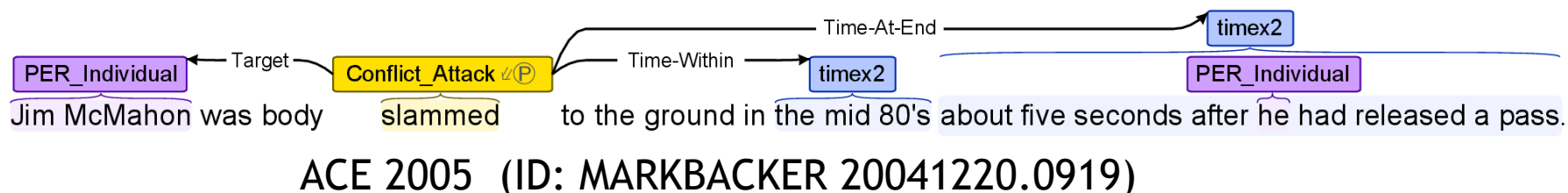
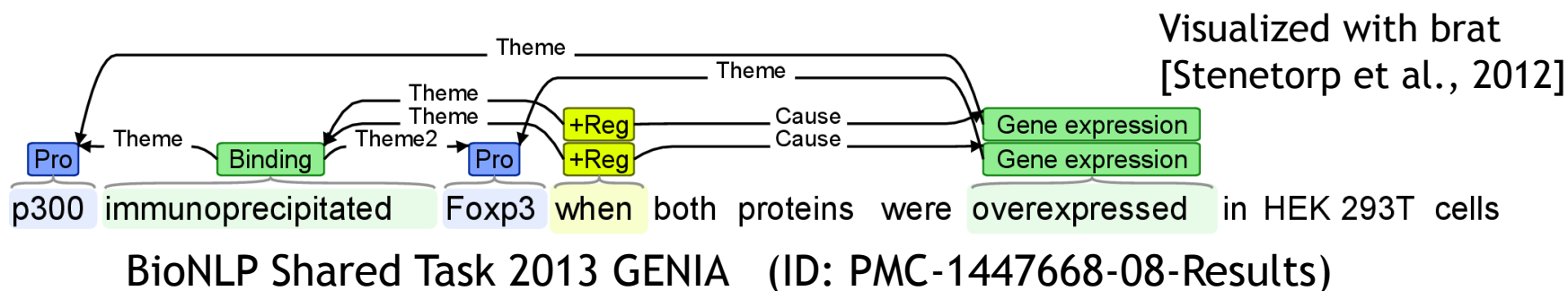
General

	AIMed (PPI)	DDI-Extraction 2013	ACE2005	SemEval-2010 Task 8
#types	1	4	6 (18 subtypes)	9
directed?	No	No	Yes	Yes
participants	NEs (1 type)	NEs (4 types)	Entities (7 types)	Nominals
Eval. target	relations	typed relations	relations, types	types
metric	CV macro-F1, AUC	Type macro-F1	micro-F1	Type macro-F1

- In Bio domain, relations are often undirected and defined between NEs
  - NEs are often *blinded* in biomedical relation extraction
- SemEval-2010 Task 8 is pure relation classification task (one pair/sentence)
- The differences are minor and same classification methods are applicable, but evaluation metrics are different among tasks
  - Note: evaluation metrics for PPI and ACE2005 are not always same among papers

# Event extraction

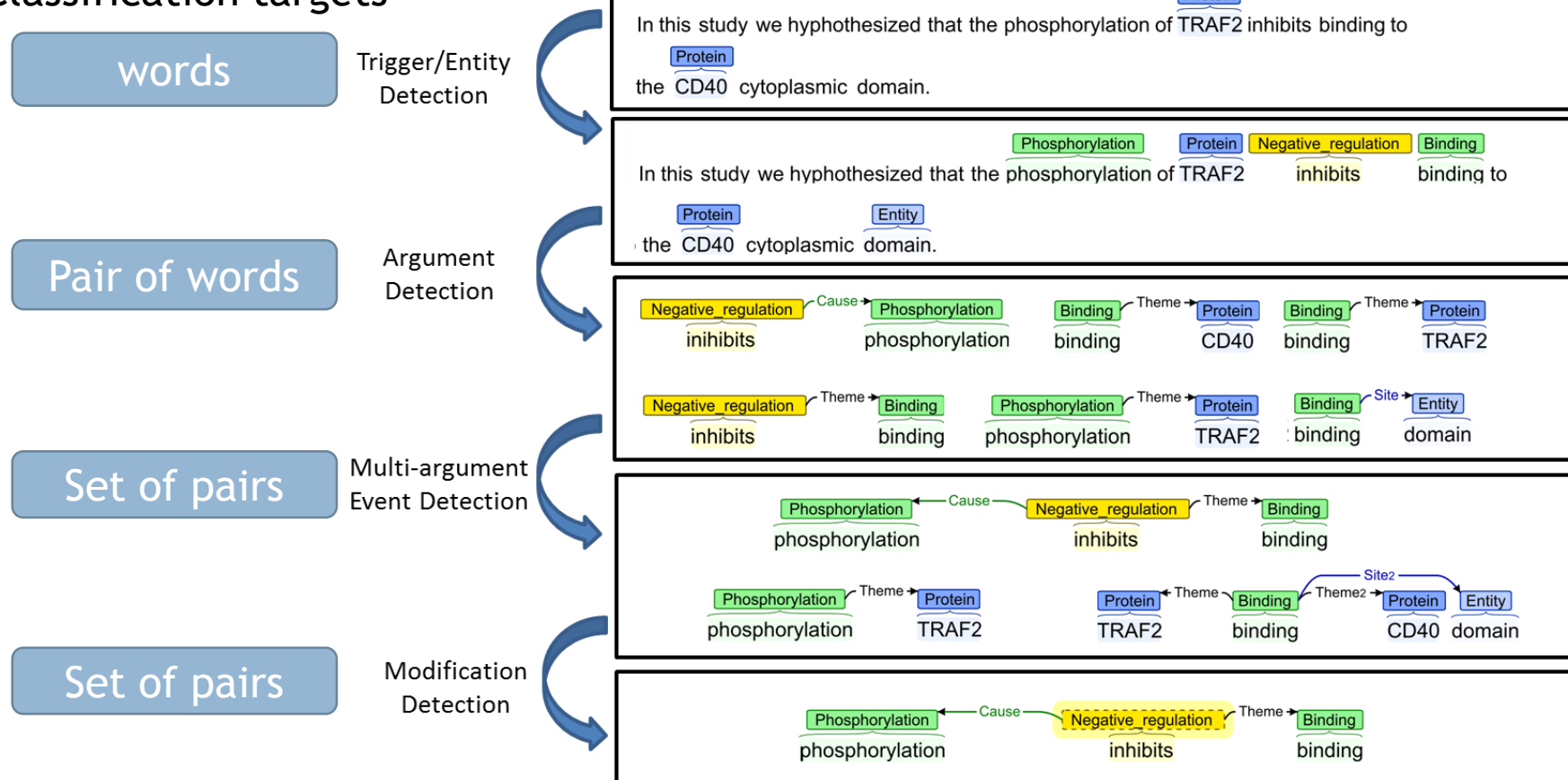
- Extracting dynamic (given) entity state changes and their relationships
  - An event usually consists of a trigger and their typed arguments





# Pipeline-based event extraction (EventMine)

## Classification targets



# Comparison between ACE2005 (General) and GENIA2013 (Bio)

## [Miwa et al., 2014a]

		ACE2005	GENIA2013
type	#event types	8 types / 33 subtypes	13 types
	#entity types	13 types / 53 subtypes	2 types
	#argument role types	35 types	7 types
	argument types	Entity/Nominal/Value/Time	Entity
structure	Max # of arguments	11	4
	Nested events	None	Possible
	Overlaps of events	None	Possible
	Correspondences of arguments	None	Possible

- ACE defines more entity types with a hierarchy
- ⇔ GENIA in shared task has fewer, flat types
- ACE events have more arguments with flat structure

# Comparison between ACE2005 (General) and GENIA2013 (Bio)

		ACE2005	GENIA2013
task	Entity	Given	Partially given
	Entity name	Given	Not available
	Entity attributes	Given	Not available
	Entity coreference	Given	Not given
	Evaluation	Trigger/Role	Event (nested events are broken down)

- ACE provides rich entity information and performs break-down evaluation (due to many arguments)
- Since definitions on event structures are different (flat vs nested), flat ACE event extraction methods are not directly applicable to nested GENIA 2013 events
- Both employs micro-averaged F1 scores

# Application of biomedical event extraction system EventMine to general events

F1-scores (%)

	GENIA2013 (Bio)	ACE05 (General)
EventMine	52.71	52.1
Li et al. (2013) (General)	-	52.7
EVEX (Bio)	50.97	-

- EventMine was originally developed for BioNLP tasks, but it also performs well on ACE05
  - Little domain knowledge
  - Not over-tuned to some specific domain
- Biomedical event extraction system can be easily applied to general domain tasks

# Summaries in overview

- Basic relation/event extraction systems can be built using classifiers
- Building general IE systems on both bio- and general tasks is not so difficult if we consider the differences including
  - blinded named entities
  - directed relations, and
  - nested events
- Discussions
  - Why do we need to reinvent the methods for almost the same tasks?
  - Can we share strong baseline systems?

# Challenges / considerations in building IE systems

# Challenges in relation / event extractions (1)

- Ambiguity in analyzing phrase structures
  - >80% of core arguments in GENIA events are covered by the subjects or direct/indirect objects of trigger verbs [Nhung et al., 2015]
  - Disambiguation needs knowledge on contexts outside of the target sentences, and some of them relate to coreference
    - Coreference seems to be a major source of low performance, but the performance on ACE05 is not high with coreference information

*the induction of IL-10. → Gene expression*

*the induction of IL-10 production by Th1 cells → Regulation*

# Challenges in relation / event extractions (2)

- Variety in expressions

*IL-10 production*  
*The induction of IL-10*  
*ability to express IL-10*  
*IL-10-producing Th1 cells*

*tyrosine phosphorylation of STAT1*  
*phosphorylation of STAT1 on tyrosine*  
*STAT1 tyrosine phosphorylation*  
*phosphorylation of tyrosine on STAT1*  
*phosphorylation on tyrosine of STAT1*



- ML-based systems entrust these to features and ML methods
- Other enhancements are also important for performance
  - ➔ I will overview problems and their practical solutions for high performance system, to get to the research baseline



# Machine learning-related problems

- Highly imbalanced problems
  - Most pairs are not related (negative)
- Different types of features with different scales
  - E.g., binary features, count-based features, length-based features
- Many features but relatively few instances (compared to other simple tasks)
  - NEs (2,000 abstracts in NLPBA2004) or parsing (~2,500 stories in PTB)
  - Relation/event corpora are less consistent than NE corpora *in nature*
- Pipeline-specific problems

# Alleviating imbalanced problems

- High accuracy (ML objectives) does not always mean high F-scores (metrics)

	#positive instances	#negative instances
AlMed	1,000	4,832
DDI 2013 (train)	4,020	23,772

- Rule-based filters of negative instances [Chowdhury et al., 2012]
  - Easy and simple rules work well on some tasks
  - Rules depend on the task, and may not be generalized well
- Weighting / Under-sampling frequent-type instances [Miwa et al, 2012]
  - Preparing two hyper-parameters for positive and negative instances

$$\min_w \frac{1}{2} R(w) + C_p \sum_p L(w, x_p) + C_n \sum_n L(w, x_n), L: \text{loss}, R: \text{regularizer}$$

# Robustness against different scales of values

- Larger values are strongly regularized, and they are not learned well

$$\min_w \frac{1}{2} \|w\|^2 + \sum_i L(w, x_i)$$

- Normalization [Miwa et al., 2009]
  - Normalizing each sub-vector (n-gram, dependency, etc.) of a feature vector, and then globally normalizing the entire vector
    - $x = \frac{x'}{\|x'\|}, x' = \left( \frac{x_1}{\|x_1\|}, \frac{x_2}{\|x_2\|}, \dots \right)$
  - c.f. “unit kernel” in kernel-based methods, “batch normalization” and “layer normalization” in deep learning
- Scaling
  - Scaling each value with its maximum absolute value

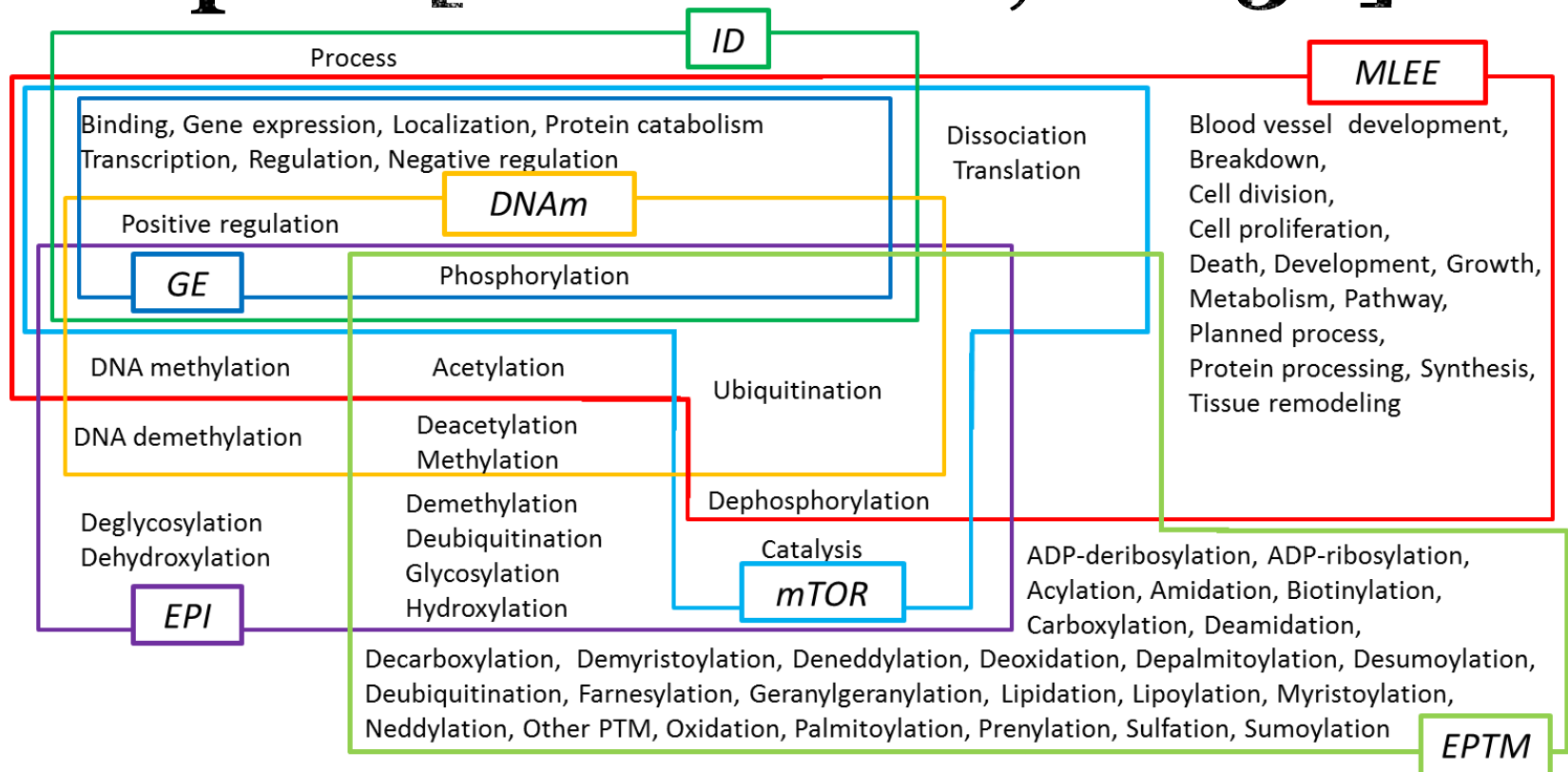
# Addressing many features problems

- Should we consider *bias-variance trade-off* and select features?  $\Leftrightarrow$   
We do not know representative features, so an IE model with manually-selected features can easily underfit to training data
- Regularization
  - Regularization can well adjust the trade-off
  - AkaneRE and EventMine almost overfit the training data (close to 100% accuracy)
- Feature hashing
  - Memory cost reduction with slight performance loss
    - In EventMine, feature space (with hundreds of millions features) are condensed by hashing to  $2^{20}$  (~1 million)

# Addressing few instance problems

- Multi-task learning/domain adaptation/transfer learning
  - Several *different* corpora for PPIs and events [Miwa et al., 2009, Miwa et al., 2013b]
    - Different in definitions of types, domains, etc
  - Incorporating distant supervision, e.g., domain database
- Semi-supervised learning
  - Self-training/bootstrapping
  - Incorporating unsupervised information via word embeddings [Li et al., 2015]
    - Note: direct incorporation of word embeddings can hurt the performance of traditional systems [Guo et al., 2014]
- Adding domain features from thesaurus
  - ⇔ We hide entity names in biomedical IE, so we have no way to use them for entities.

# Event extraction from partially overlapping corpora [Miwa et al., 2013b]



Seven corpora annotates different, but overlapping events

# Event extraction from partially overlapping corpora[Miwa et al., 2013b]

- Method
  - Create training sets by unifying training instances in several corpora with removing unreliable examples
  - Train a single model on all the training sets
- Results
  - A model trained on multiple corpora outperforms all the individual models

	GENIA	ID	EPI	MLEE	DNAm	EPTM	mTOR
Individual	56.28	57.69	48.68	52.11	72.4	44.0	47.1
Multiple	57.28	59.06	54.35	52.76	76.0	50.0	51.0

# Pipeline-specific problems

- Jack-knifing (cross-validation) on the training set
  - A system trained on gold annotations is biased and does not work well on predicted annotations.
    - Since the system never see wrong annotations, or it needs to fit to the annotations that are hard to be predicted
  - ➔ Using prediction results by jack-knifing
- Tuning strategy of pipeline modules
  - Missing annotations in earlier stages cannot be recovered in the latter stages
  - Keeping too many unreliable instances, however, causes highly imbalanced problems



# Incorporating deep learning (1)

- Convolutional or recurrent neural networks (CNN or RNN) methods often produce the best performance in several tasks
  - SemEval-2010 Task 8
    - Many DL-based models for relation classification
    - Best shared task system 82.2% (SVM) → 88.0% (CNN) [Wang et al., 2016]
  - AIMed (PPI)
    - AkaneRE 65.2% (SVM) → 72.4% (CNN) [Quan et al., 2016]
  - DDI Extraction 2013
    - 67.0% (SVM) [Kim et al., 2015] → 70.5% (CNN) [Quan et al., 2016]
  - ACE Event
    - 52.7% (Structured perceptron) [Li et al., 2014] → 55.4% (RNN) [Nguyen et al., 2016]

# Incorporating deep learning (2)

- High performance often without external resources
  - We don't know what made this performance boosting, and we may get better with external resources
- Semi-supervised learning by incorporating pre-trained embeddings
  - Unlike feature-based learning, no preprocessing on embeddings is required
- Easy to build parameter-sharing models
  - Recent deep learning frameworks are quite helpful
    - Dynet, Chainer, Tensorflow, Theano, Keras, etc.

# Incorporating deep learning (3)

- High computational costs
  - Can we apply the model to PubMed?
- High tuning costs
  - Parameters, model architectures, etc.
  - Performance is not stable due to non-convexity, parallelization, etc., and most results are not completely reproducible
  - The performance highly depends on tuning, and the comparison is quite difficult. (the models are good? Or the tuning is good?)
- Almost impossible to analyze what is learned
  - Feature engineering is less magical than model engineering

# Minor points in building IE systems (1)

- Mismatches in automated preprocessing
  - Entities do not match linguistic units like words, phrases, or sentences
  - Relations can be inter-sentential due to errors in sentence splitting
- Selection of preprocessing modules including tokenizers, sentence splitters, parsers, stemmers, and named entity recognizers, etc.
  - Parser comparison on event extraction [Miwa et al., 2010] shows that the parsers and formats affect a lot (> 5 percent points) in F-score

# Minor points in building IE systems (2)

- Data formats and conversions
  - byte offsets (old ascii systems) vs character offsets (recent UTF-8 systems)
  - XML (GENIA, Bioinfer, DDI, etc.) vs standoff (brat)
- Configurability and usability
  - Applicable to other tasks without changing the codes

# Summary

- In developing ML-based systems, we need to solve many problems that seem not to be essential for NLP/TM
  - Their handlings affect the performance in a non-negligible way
- Discussion
  - How can we evaluate each individual method?
  - What is solved and what is remaining problem?
    - Analysis on the state-of-the-art results is required

# Joint entity and relation extraction

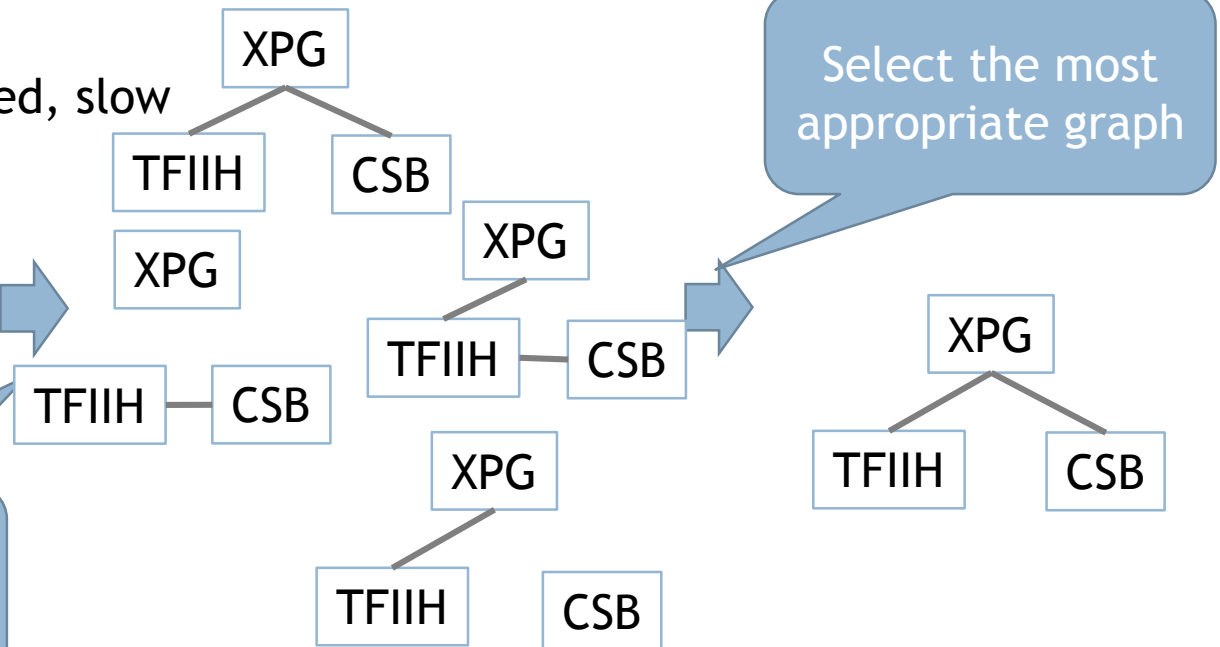
# Joint entity and relation extraction

- Extract a relation graph from a target sentence
  - Pros: treatment of interactions among entities and relations, no pipeline

- Cons: complicated, slow

*XPG* protein interacts with subunits of *TFIIH* and with *CSB* protein.

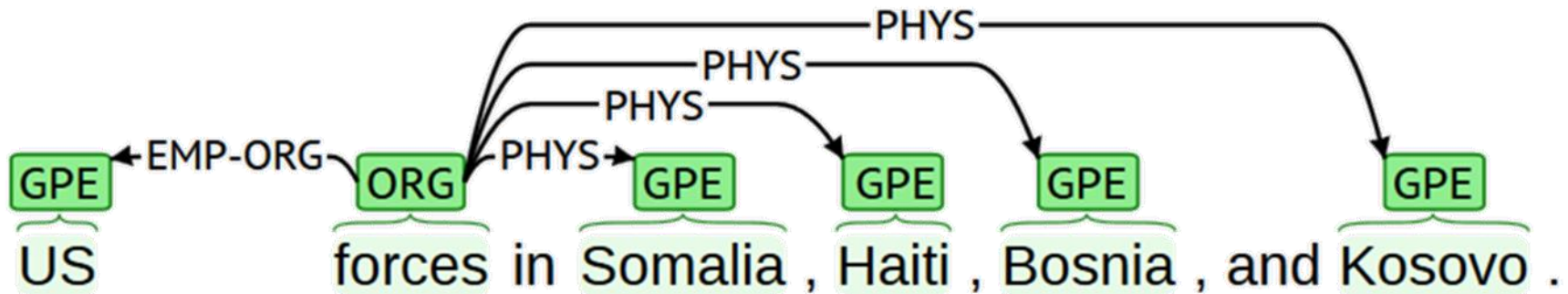
Consider (implicitly) all possible relation graphs





# Joint entity and relation extraction [Miwa et al., 2014b]

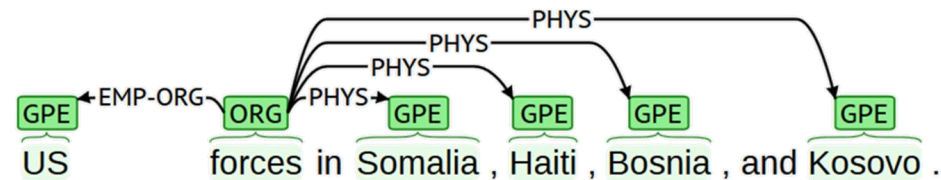
- Search-based structured prediction with global features
  - Features among multiple relations
    - E.g., “Somalia” and “Haiti” are in coordination, and they have “PHYS” relations with “forces”



[Li et al., 2014] proposed similar approach

# Joint entity and relation extraction

- Joint representation by table representations
- Filling table cells one by one with search-based structured learning



US	GPE							
forces	EMP-ORG	ORG						
in	⊥	⊥	⊥					
Somalia	⊥	<PHYS	⊥	GPE				
Haiti	⊥	<PHYS	⊥	⊥	GPE			
Bosnia	⊥	<PHYS	⊥	⊥	⊥	GPE		
and	⊥	⊥	⊥	⊥	⊥	⊥	⊥	
Kosovo	⊥	<PHYS	⊥	⊥	⊥	⊥	⊥	GPE
	US	forces	in	Somalia	Haiti	Bosnia	and	Kosovo

# Joint entity and relation extraction

- Joint learning performs well on relation extraction, but not entity
  - Entity detection performance dropped since the performance was tuned for relation extraction performance

	Entity	Relation
Pipeline	81.8	57.7
Joint	81.3	61.2

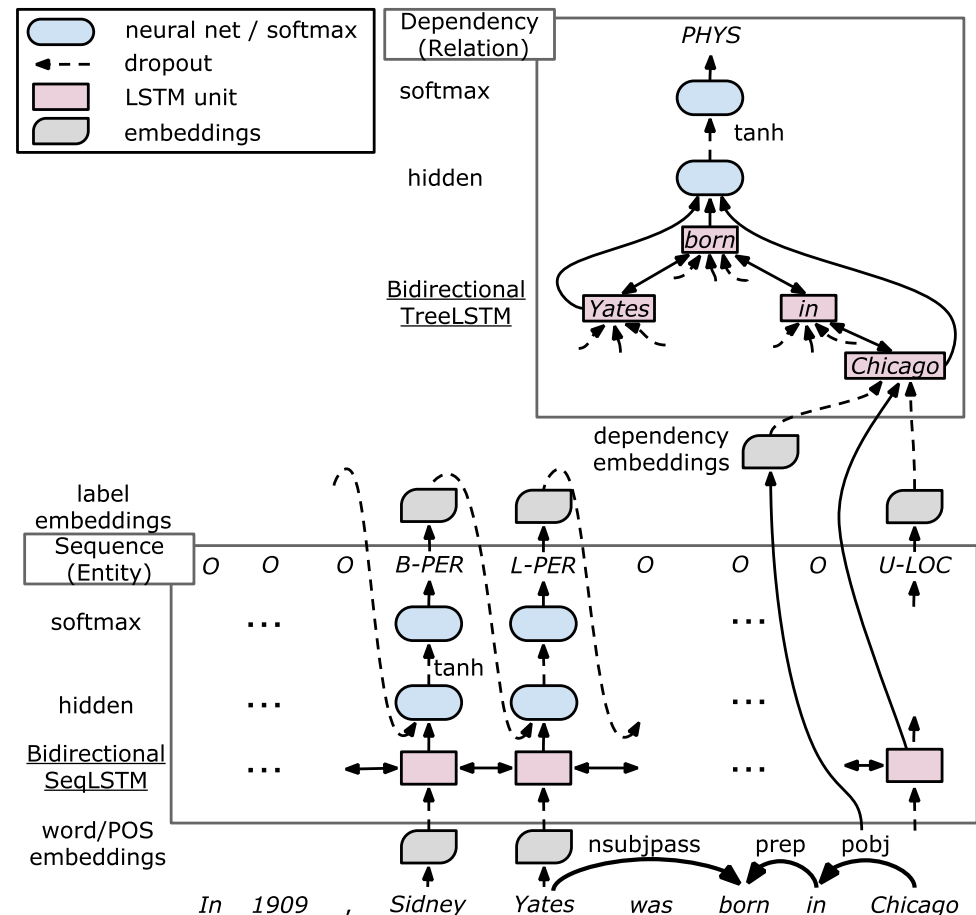
F1-scores on CoNLL04 (%)

- The joint system may find more relation-related entities than the pipeline does

Available at <https://github.com/tticoin/JointER>

# Deep learning-based entity and relation extraction [Miwa et al., 2016]

- Stacked RNN-based approach
  - Entity sequential LSTM-RNNs on word sequence
  - Relation tree LSTM-RNNs on parse tree
- Not structured prediction, but end-to-end approach
  - No structured margin loss, no beam search
  - Shared parameters among prediction tasks



# Deep learning-based entity and relation extraction

- Deep learning-based greedy model outperforms feature-based structured learning model in a significant margin
- Deep learning can push forward the state-of-the-art, but the performance is still not high enough

	Entity	Relation
Miwa et al., 2016	83.4	55.6
Li et al., 2014	80.8	49.5

F1-scores on ACL2005 Relation (%)

Available at  
<https://github.com/tticoin/LSTM-ER>

➔ What can we import from traditional feature-based models?

# Summary

- Joint entity & relation extraction models show better performance on relation extraction, and with deep learning, the performance was boosted
- Discussion
  - How can we analyze the model in detail?
  - Since deep learning models are flexible, we can incorporate external knowledge and information (e.g., database, distant supervision, multi-task learning)
    - We should relax the restriction on blinded named entities, since using word embeddings will keep generality

# Conclusions

- I introduced our work from simple classification models to deep learning models, along with several problems to consider
  - We need to find a solid way to analyze errors
- Please try our models at our github:  
<https://github.com/ttcoin/>

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