Recent Development of Heterogeneous Information Networks: From Meta-paths to Meta-graphs

> Yangqiu Song Department of CSE, HKUST, Hong Kong



#### Homogeneous Graph/Networks



Transportation Network



Gene Network



Food Network

http://snap.stanford.edu/higher-order/higher-order-SM-science16.pdf

#### Heterogeneous Information Networks

109-2012 (UIUC)

- Yizhou Sun, Jiawei Har
  - Entity type mapping
  - Link type mapping:  $E \rightarrow R$



## Modern Social Media

- Entities: Person, Check-in location, Articles, etc.
- Relations: Friends, Like, Check-in, etc.



### Scholar Networks

- Entities: Paper, Venue, Author, Keyword, etc.
- Relations: Write, Attend, Contain, etc.



### Knowledge Graphs

• Example of entities and their relations:





### **Bio-medical Network**

- Entities: Gene, Patient, Drug, Disease, etc.
- Relations: Drug repurposing, Genotyping, etc.



http://web.cs.ucla.edu/~yzsun/Tutorials.htm https://sites.google.com/site/feiwang03/talks

### Problems in HIN

- Link Prediction
  - Homogeneous
  - Heterogeneous: recommendation
- Entity Typing/Profiling





• Similarity Search



#### Meta-Path: *Author-Paper-Author*

Abnormal kidney

physiology

Diabetes

isipidus

Decreased urine

Predictions

1 AQP1 2 AQP6 3 AQP5 4 MIP ... 40 MYBL2

Gene-Phenotyp

Gene-Gene

Predicted link

osmolailty

Response to self she

$\operatorname{Rank}$	Author	Score
1	Christos Faloutsos	1
2	Spiros Papadimitriou	0.127
3	Jimeng Sun	0.12
4	Jia-Yu Pan	0.114
5	Agma J. M. Traina	0.110
6	Jure Leskovec	0.096
7	Caetano Traina Jr.	0.096
8	Hanghang Tong	0.091
9	Deepayan Chakrabarti	0.083
10	Flip Korn	0.053

#### Christos' students or close collaborators

http://bigdata.ices.utexas.edu/project/gene-disease/ http://web.cs.ucla.edu/~yzsun/Tutorials.htm http://xren7.web.engr.illinois.edu/tutorial.html

# Explicit vs. Implicit "Flat" Semantics

• Explicit Semantic Analysis [Gabrilovich and Markovitch '06, '07, '09]

Represent	Barack Obama
tovt ac hag	Timeline of the presidency of Barack Obama (2009)
lexi as bag	Family of Barack Obama
of Wikipedia	Barack Obama citizenship conspiracy theories
titles	Barack Obama
titles	Barack Obama presidential primary campaign 2008

• Probabilistic Conceptualization [Song et al., '11,'15]



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## Explicit vs. Implicit "Flat" Semantics

- Implicit Semantic Analysis
  - SVD [Deerwester et al., JASIS'90]
  - PLSA [Hofmann, NIPS'99]
  - LDA [Blei et al., JMLR'03]
  - Word2vec [Mikolov et al., NIPS'13]





https://www.tensorflow.org/versions/r0.7/tutorials/word2vec/index.html

# Explicit vs. Implicit "Graph" Representation

- Graph Embedding
  - ISOMap [Tenenbaum et al., Science'00]
  - LLE [Roweis and Saul, Science'00]
  - Laplacian EigenMap [Belkin et al., NIPS'01]
  - (t)-SNE [Maaten and Hinton, JMLR'08]
  - Deepwalk [Perozzi et al., KDD'14]
  - LINE [Tang et al., WWW'15]
  - Node2vec [Grover and Leskovec, KDD'16]
- Knowledge Graph Embedding
  - TransE [Bordes et al., NIPS'13]
  - TransH [Wang et al., AAAI'14]
  - TransR [Lin et al., AAAI'15]
  - PathEmbedding [Guu et al., and Lin et al., EMNLP'15]
  - ATranB...



# Explicit vs. Implicit Representation

Representation	Implicit	Explicit
Flat/Homogenous	LDA, word2vec	ESA
Graph/Heterogeneous	TransE	

- From meta-path to meta-graphs
  - Semi-supervised learning [Jiang et al., IJCAI'17]
  - Recommendation [Zhao et al., KDD'17]
- Benefits
  - Have explicit semantics
    - Explainable
    - Knowledge discovery
  - Resolve different kinds of ambiguity

This talk

### What Semantics Can HIN Provide?



HIN network-schema: network with multiple object types and/or multiple link types.



### Meta-path, Commuting Matrix, and PathSim

• Meta-path defined over network schema.



- e.g., document->word binary occurrence matrix: W
- Un-normalized similarity:  $W^T W$ : dot product
  - Overall normalization: PathSim [Sun et al., VLDB'11]
  - Individual normalization: Path Ranking Algorithm [Lao et al., ML'10, EMNLP'11]

# What **Distinct** Semantics Can HIN Provide?

• The semantics of entities and their relations



- What can context cover?
- What cannot?

``New York'' vs. ``New York Times''

``George Washington'' vs. ``Washington''





### Entity Search

Who are most similar to Christos Faloutsos?
 – [Sun et al., 2011] (a) Path: APA





$\operatorname{Rank}$	$\operatorname{Author}$	$\mathbf{Score}$
1	Christos Faloutsos	1
2	Spiros Papadimitriou	0.127
3	Jimeng Sun	0.12
4	Jia-Yu Pan	0.114
5	Agma J. M. Traina	0.110
6	Jure Leskovec	0.096
7	Caetano Traina Jr.	0.096
8	Hanghang Tong	0.091
9	Deepayan Chakrabarti	0.083
10	Flip Korn	0.053

#### (c) Path: APTPA

Rank	Author	Score
1	Christos Faloutsos	1
2	Jian Pei	0.661
3	Srinivasan Parthasarathy	0.600
4	Jeffrey Xu Yu	0.587
5	Ming-Syan Chen	0.579
6	Jiawei Han	0.576
7	Mohammed Javeed Zaki	0.571
8	Hans-Peter Kriegel	0.563
9	Yannis Manolopoulos	0.548
10	Rakesh Agrawal	0.545

### What's Still Missing/Unachievable?

- Let's consider a random walk on graph
  - Construct n \* n adjacency matrix **M**
  - Normalize  $\mathbf{W} = \mathbf{D}^{-1/2} \mathbf{M} \mathbf{D}^{-1/2}$  (**D**: degree matrix))
  - One step random walk:  $\mathbf{p}^{t+1} = \mathbf{W} \mathbf{p}^t$
  - Stationary distribution follows:  $\mathbf{p} = \mathbf{W} \mathbf{p}$



### Personalized PageRank

- PageRank [Page et al., '98]
  - $\mathbf{p}^{t+1} = (\mathbf{\alpha}\mathbf{E} + (1-\alpha)\mathbf{W})\mathbf{p}^t$
  - With a probability to randomly/lazily jump
- Personalized PageRank/semi-supervised learning
  - [Haveliwala et al., TKDE'03, Jeh and Widom, WWW'03]
  - [Zhu et al., ICML'03, Zhou et al., NIPS'03]

$$- \mathbf{p}^{t+1} = \alpha \mathbf{q} + (1 - \alpha) \mathbf{W} \mathbf{p}^t$$

- With a probability to restart with a label: prior



### HIN: Path Constrained Random Walk

- In Path Ranking Algorithm
  - [Lao et al., ML'10, EMNLP'11]



### Meta-graph vs. Meta-path

• Meta-graph: [Fang et al., ICDE'16; Huang et al., KDD'16].



- We get a stationary distribution!



 $A_2$ 

### Application: Semi-supervised Text Classification



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Wang et al., AAAI'16

World Knowledge Specification: Unsupervised Semantic Parsing for Documents

Document Trump is the president of the United States of America

Semantic parsing is the task of mapping a piece of natural language text to a formal meaning representation.

#### Logic form *People.DonoldTrump* **¬** PresidentofCountry.*Country.USA*

- Motivation: [Berant et al. EMNLP'13] aim to train a parser from question/answer pairs on a large knowledge-base Freebase
  - Existing semantic parsing approaches, that require expert annotation
  - Scales to large scale knowledge-bases, supervised by the QA pairs
- We extend it to document analysis.

#### World Knowledge Specification: Unsupervised Semantic Parsing for Documents

Document Trump is the president of the United States of America



### Example Meta-paths in Text HIN



# Algorithm

- Input:
  - Partially labeled documents
  - HIN based on semantic parsing
- Algorithm:
  - Step 1: extract transition matrices of different meta-graphs
  - Step 2: run personalized random walk based semisupervised learning
  - Step 3: Ensemble of different meta-graph guided random walk
- Output:
  - Labels of all unlabeled data

## Ensemble

- Supervised learning (SVM)
  - Input: meta-graph generated labels (soft labels)
  - Output: ground truth labels (partially labeled ones)
- EM [Dawid and Skene, 1979]
  - E-step: estimate posterior of label assignment of each meta-graph label
  - M-step: estimate label cluster probabilities, and likelihood of label assignment of each meta-graph label
- Co-training [Wan et al., SDM'15]
  - Train the weight of each meta-graph
  - Update the label assignment of each random walk

	Meta-gra	aph 1	Meta-gra	aph 2			Meta-graph G		
	Label 1	Label 2	Label 1	Label 2			Label 1	Label 2	
Doc 1	0.9	0.1	0.1	0.8			0.9	0.2	
Doc 2	0.9	0.2	0.8	0.1			0.6	0.5	
Doc N	0.2	0.7	0.1	0.6			0.3	0.6	

#### Dataset

• 4 sub-datasets derived from 20-newsgroups and RCV1

		Doc	ument datase	ets	
20NewsGroup	Sub-datasets	#(Document)	#(word)	#(Entity)	#(Types)
	20NG-SIM	3,000	8,010	11,192	219
	20NG-DIF	3,000	9,182	13,297	251
	GCAG-SIM	3,596	11,096	10,540	233
	GCAT-DIF	2,700	13,291	13,179	261
RCV1-GCAT	Each su	b-datasets consis	sts of three si	milar or distinct	topics.

## Results

- BOW: bag-of-words
- Entity: entities extracted by semantic parsing
- NB: naïve Bayes
- SVM: support vector machines
- LP: label propagation
  - LP+Meta-graph: co-training [Wan et al., SDM'15]
  - KnowSim: unsupervised ensemble of meta-paths [Wang et al., ICDM'16]

	NB		SVM			LP		Semi <mark>IIN</mark>		Ensemble		
Settings Datasets	BOW	BOW+ Entity	BOW	BOW+ Entity	BOW+ Entity	Meta- path	Know- Sim	DWD Graph	Full- Graph	SVM	EM	Co- train
20NG-SIM 20NG-DIF GCAT-SIM GCAT-DIF	$39.02 \\ 43.74 \\ 71.24 \\ 56.60$	$\begin{array}{r} 48.46 \\ 57.24 \\ 71.24 \\ 56.66 \end{array}$	37.34 39.57 73.92 63.52	$\begin{array}{c} 49.67 \\ 55.71 \\ 74.64 \\ 63.91 \end{array}$	54.53 72.40 70.97 61.95	57.75 76.13 71.05 61.37	$56.87 \\ 77.14 \\ 60.59 \\ 51.64$	$\begin{array}{c} 48.94 \\ 61.31 \\ 79.14 \\ 64.32 \end{array}$	58.46 77.69 <b>81.02</b> 65.05	52.04 71.36 68.79 57.48	54.44 73.08 69.96 58.19	60.99 80.08 80.97 66.95

• We show our results of five labeled training data for each class. All the numbers are averaged accuracy (in percentage %) over 50 random trials.

## Results

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accuracy(%)

20NG-DIF



 ★
 LP KnowSim
 ... ▲...

 ★
 SemiHIN Full-Graph
 \_\_\_\_\_

 □
 SemiHIN DWD
 - + 

 □
 Ensemble-SVM
 ... ▼

 ▲
 Ensemble-EM
 - ▼ 

 ▲
 Ensemble-Co-train
 ▼

NB BOW+Entity  $- \times -$ 

SVM BOW -

LP Meta-Path … •

SVM BOW+Entity - = -

LP BOW+Entity -

# Explicit vs. Implicit "Graph" Representation

Representation	Implicit	Explicit				
Flat/Homogenous	LDA, word2vec	ESA				
Graph/Heterogeneous	TransE	This talk				

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  - Semi-supervised learning [Jiang et al., IJCAI'17]
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- Benefits
  - Have explicit semantics
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  - Resolve different kinds of ambiguous

### RS is Everywhere Nowadays



### **Typical Recommendation Problem**



### Matrix Factorization

- Matrix Factorization is one of the most popular methods for collaborative filtering
  - Given matrix  $R \in \mathbb{R}^{n*m}$
  - each row represents an user i
  - While each column an item j

$$MAE = \frac{\sum_{(i,j)\in\mathcal{R}_{test}} |R_{ij} - \hat{R}_{ij}|}{|\mathcal{R}_{test}|},$$
$$RMSE = \sqrt{\frac{\sum_{(i,j)\in\mathcal{R}_{test}} (R_{ij} - \hat{R}_{ij})^2}{|\mathcal{R}_{test}|}}.$$



# Other Existing Approaches

- Collaborative Filtering: Recommend items based only on the users past behavior
  - User based: find similar users for what they liked
  - Item based: find similar items which I have liked
- Content based: extract features for items
- Personalized learning to rank
- Demographic: user profiling
- Social recommendation: trust based
- Hybrid

### It's a Heterogeneous Information Network!



## A Typical Network Schema of Yelp

- R: reviews;
- U: users;
- B: business;
- Cat: category of item;
- Ci: city



#### Meta-graphs Extracted From Yelp



### Meta-graphs Extracted From Amazon



Brd: brand of item

### Compute a Similarity based on Meta-graph



Compute 
$$\mathbf{C}_{P_1}$$
:  $\mathbf{C}_{P_1} = \mathbf{W}_{RB} \cdot \mathbf{W}_{RB}^{\top}$ ;  
Compute  $\mathbf{C}_{P_2}$ :  $\mathbf{C}_{P_2} = \mathbf{W}_{RA} \cdot \mathbf{W}_{RA}^{\top}$ ;  
Compute  $\mathbf{C}_{S_r}$ :  $\mathbf{C}_{S_r} = \mathbf{C}_{P_1} \odot \mathbf{C}_{P_2}$ ;  
Compute  $\mathbf{C}_{M_9} = \mathbf{W}_{UR} \cdot \mathbf{C}_{S_r} \cdot \mathbf{W}_{UR}^{\top} \cdot \mathbf{W}_{UB}$ ;

How to Assemble Different Meta-graphs?

- Factorization Machine [Rendle ICDM'10, TIST'12]
  - One of the state-of-art recommendation model recent years.

$\bigcap$	Feature vector <b>x</b>														Ta	arg	et y						
<b>X</b> <sup>(1)</sup>	1	0	0		1	0	0	0		0.3	0.3	0.3	0		13	0	0	0	0	]		5	<b>y</b> <sup>(1)</sup>
<b>X</b> <sup>(2)</sup>	1	0	0		0	1	0	0		0.3	0.3	0.3	0		14	1	0	0	0			3	y <sup>(2)</sup>
<b>X</b> <sup>(3)</sup>	1	0	0		0	0	1	0		0.3	0.3	0.3	0		16	0	1	0	0			1	y <sup>(2)</sup>
<b>X</b> <sup>(4)</sup>	0	1	0		0	0	1	0		0	0	0.5	0.5		5	0	0	0	0			4	y <sup>(3)</sup>
<b>X</b> <sup>(5)</sup>	0	1	0		0	0	0	1		0	0	0.5	0.5		8	0	0	1	0			5	y <sup>(4)</sup>
<b>X</b> <sup>(6)</sup>	0	0	1		1	0	0	0		0.5	0	0.5	0		9	0	0	0	0			1	y <sup>(5)</sup>
<b>X</b> <sup>(7)</sup>	0	0	1		0	0	1	0		0.5	0	0.5	0		12	1	0	0	0			5	У <sup>(6)</sup>
	A	B Us	C ser		Т	NH	SW <u>Movie</u>	ST ;		TI Otl	NH her M	SW lovie	ST s rate	ed	Time	ΓL	NH _ast I	SW Novie	ST e rate	 ed			

Matrix Factorization (MF)+Factorization Machine (FM)

• For each meta-graph, do MF:

$$\min_{\mathbf{U},\mathbf{B}} \frac{1}{2} ||P_{\Omega}(\mathbf{U}\mathbf{B}^{\top} - \mathbf{R})||_{2}^{2} + \frac{\lambda_{u}}{2} ||\mathbf{U}||_{2}^{2} + \frac{\lambda_{b}}{2} ||\mathbf{B}||_{2}^{2}$$

- Given all MF latent features:
  - L meta-graphs
  - F dimension of MF

$$\mathbf{x}^{n} = \underbrace{\mathbf{u}_{i}^{(1)}, ..., \mathbf{u}_{i}^{(l)}, ..., \mathbf{u}_{i}^{(L)}}_{L \times F} \underbrace{\mathbf{b}_{j}^{(1)}, ..., \mathbf{b}_{j}^{(l)}, ..., \mathbf{b}_{j}^{(L)}}_{L \times F}$$

$$\hat{y}^n(\mathbf{w}, \mathbf{V}) = w_0 + \sum_{i=1}^d w_i x_i^n + \sum_{i=1}^d \sum_{j=i+1}^d \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i^n x_j^n,$$

### Automatic Meta-graph Selection

• The original cost function of FM

$$\min_{\mathbf{w},\mathbf{V}} \sum_{n=1}^{N} (y^n - \hat{y}^n(\mathbf{w},\mathbf{V}))^2$$
$$\hat{y}^n(\mathbf{w},\mathbf{V}) = w_0 + \sum_{i=1}^{d} w_i x_i^n + \sum_{i=1}^{d} \sum_{j=i+1}^{d} \langle \mathbf{v}_i, \mathbf{v}_j \rangle x_i^n x_j^n,$$

• + group lasso:

$$\Phi_{\mathbf{w}}(\mathbf{w}) = \sum_{l=1}^{2L} ||\mathbf{w}_l||_2$$

$$\Phi_{\mathbf{V}}(\mathbf{V}) = \sum_{l=1}^{2L} ||\mathbf{V}_l||_2$$

L meta-graphs

- In side meta-graph: L2 norm
- Between meta-graphs: L1 norm

nonmonotonous accelerated proximal gradient (nmAPG) algorithm [Li and Lin, NIPS'15]

### Datasets

Yelp-200k										
Relations(A-B)	Number	Number	Number	Avg Degrees						
Kelations(A-D)	of A	of B	of (A-B)	of A/B						
User-Business	36,105	22,496	191,506	5.3/8.5						
User-Review	36,105	191,506	191,506	5.3/1						
User-User	17,065	17,065	140,344	8.2/8.2						
Business-Category	22,496	869	67,940	3/78.2						
Business-Star	22,496	9	22,496	1/2,499.6						
Business-State	22,496	18	22496	1/1,249.8						
Business-City	22,496	215	22,496	1/104.6						
Review-Business	191,506	22,496	191,506	1/8.5						
Review-Aspect	191,506	10	955,041	5/95,504.1						
	Ama	azon-200k								
Polations(A-B)	Number	Number	Number	Avg Degrees						
Kelations(A-D)	of A	of B	of (A-B)	of A/B						
User-Business	59,297	20,216	183,807	3.1/9.1						
User-Review	59,297	183,807	183,807	3.1/1						
Business-Category	20,216	682	87,587	4.3/128.4						
Business-Brand	95,33	2,015	9,533	1/4.7						
Review-Business	183,807	20,216	183,807	1/9.1						
Review-Aspect	183,807	10	796,392	4.3/79,639.2						

## **Comparison Results**

Traditional Approaches		Amazon-200k	Yelp-200k	CIKM-Yelp	CIKM-Douban
	RegSVD	2.9656 (+60.0%)	2.5141 (+49.9%)	1.5323 (+27.7%)	0.7673 (+9.0%)
	FMR	1.3462 (+11.9%)	1.7637 (+28.6%)	1.4342 (+22.8%)	0.7524 (+7.2%)
	HeteRec	2.5368 (+53.2%)	2.3475 (+47.0%)	1.4891 (+25.6%)	0.7671 (+9.0%)
HIN Based	SemRec	-	1.4603 (+13.8%)	1.1559 (+4.2%)	0.7216 (+3.2%)
Approaches	FMG	1.1864	1.2588	1.1074	0.6985

- HeteRec [Yu et al., WSDM'14]:
  - Factorize each meta-path
  - Ensemble using the recovered matrices
  - Item-based CF

- SemRec [Shi et al., CIKM'15]:
  - Ensemble of original similarity matrices based on different metapaths
  - User based CF

	Amazon-200k	Yelp-200k	CIKM-Yelp	CIKM-Douban
Density	0.015%	0.024%	0.086%	0.630%

### Selected Meta-graphs for Yelp

		User	-Part	Item-Part			
		W	V	W	V		
Yelp	Important	$M_1 - M_4, M_6, M_8$	$M_1 - M_3, M_5, M_8$	$M_1 - M_5, M_8, M_9$	$M_3, M_8$		
	Useless	$M_5, M_7, M_9$	$M_4, M_6, M_7, M_9$	$M_{6}, M_{7}$	$M_1, M_2, M_4 - M_7, M_9$		



### Selected Meta-graphs for Amazon



### Scalability of Algorithm



# Collaborators

- He Jiang (HKUST)
- Huan Zhao (HKUST)
- Dik Lee (HKUST)
- Chenguang Wang (IBM)
- Ming Zhang (PKU)
- Yizhou Sun (UCLA)
- Jiawei Han (UIUC)
- Dan Roth (Upenn)

# Conclusion

Heterogeneous information networks as explicit semantic analysis

From meta-path to meta-graph analysis

Code released at <a href="https://github.com/HKUST-KnowComp/FMG">https://github.com/HKUST-KnowComp/FMG</a>

Thank You! 🙂

### Precision of Different Semantic Filtering



Wang et al., Incorporating World Knowledge to Document Clustering via Heterogeneous Information Networks. KDD'15. Wang et al., World knowledge as indirect supervision for document clustering. TKDD'16.

# Error Analysis of Semantic Filtering

Type of error	Example sentence	Number and percentage of errors					
		FBSF (805)	DFBSF (359)	CBSF (272)			
Entity Recognition	"Einstein 's theory of relativity explained mercury 's motion."	179 (22.2%)	129 (35.9%)	105 (38.6%)			
Entity Disambiguation	"Bill said all this to make the point that Christianity is eminently."	537 (66.7%)	182 (50.7%)	130 (47.8%)			
Subordinate Clause	"Bruce S. Winters, worked at United States Technologies Research Center, bought a Ford."	89 (11.1%)	48 (13.4%)	37 (13.6%)			

Finding #1: Entity disambiguation is the major error factor.

Entity disambiguation is a tough research problem in NLP community. The type information of relations are not sufficient to further prune out mismatching entities during semantic filtering process.

Finding #2: CBSF performs the best.

For example, by using context, the number of incorrect entities caused by disambiguation can be dramatically reduced.

### **Classification Results**

Average accuracy											
Model	Discrete					Embedding					
Settings	BC	W	BOW+ENTITY			Word2vec					
20NG-SIM	90.8	% 91.11%			91.67%						
20NG-DIF	96.66		% 96.90%			98.27%		Miko 2013	olov 3.		
GCAG-SIM	94.15		6 94.29			96.81%		Win	Window: 5		
GCAT-DIF	88.98		% 90.18%			90.64%		Dim	: 400		
Average accuracy											
Model	SVM <sup>HIN</sup>		SVM <sup>HIN</sup> +KnowSim				IndefSVM	-KnwoS	Sim		
Settings			DWD	C I	)WD+other MetaPaths		DWD	C	DWD+other MetaPaths		
20NG-SIM	91.60%		92.32%		92.68%		92.65%		93.38	8%	
20NG-DIF	97.20%		97.83%		98.01%		98.13%		98.45	%	
GCAG-SIM	94.82%		95.29%		96.04%		95.63%		98.10	%	
GCAT-DIF	91.19%		90.70%		91.88%		91.63%		93.51	.%	

Collective classification: Lu and Gatoor 2003; Kong et al. 2012