Machine Learning for Data Exploration and Generation

Charles Sutton University of Edinburgh and the Alan Turing Institute 13 June 2017

http://bit.ly/sutton-ml-exploration

Google: "charles sutton" talks —> find this talk



The Alan Turing



Ingineering and Physical Sciences Research Council

Prediction: A small part of a big picture



Towards an Artificial Intelligence for Data Science

Data understanding



When you get a new data set....

- What's in it?
- What's wrong with it?
- What should I do with it?

Automating exploratory data analysis?

Contradiction in terms?

A task in visual analytics

Scalability a challenge



Our theme

Summarise data with probabilistic ML Visualize resulting patterns Patterns are "first class citizens" of model

Exploratory data analysis

Data analysts are like cats.

- 1. Want to explore their data
- 2. Don't know what they want.



Machine learning for analysts

Whose information need is not explicit

Whose domain knowledge is difficult to encode

Explore data via learned patterns

... not just for dummies!



Mining Patterns

[Fowkes & Sutton, KDD 2016]

[Fowkes & Sutton, PKDD 2016]

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Association Rules (def'n)



Association rule mining:

Find set of all rules



Database of transactions

Why? Exploratory data analysis

Association Rules (alg)

1. Identify all frequent item sets



via exhaustive search (APriori, FP-Growth, etc.)

2. For each item set, consider all possible partitions



3. Rank the resulting list (e.g., by confidence) and enjoy

Pathologies

List of association rules unwieldy, difficult to understand

Procedure as a whole is statistically incoherent.

Essentially just repeated counting

Redundancy





frequent,

so are all 14 nontrivial subsets. (Association rules "filter" item sets)

"Free riders"

If both of these



have support >> M and independent



usually still support > M

(Confidence and lift do not fix this!)

Rare itemsets

Strongly associated but rare: Not a frequent itemset



e.g., champagne, caviar [Hastie et al., 2009]

Alternative: Interesting Itemsets

Optimise the collection of itemsets as a whole, rather than each in isolation





choose ${\mathcal I}$ to best fit data

 ${\cal I}$ are the *interesting* itemsets

(unlike frequent itemsets, these are suitable for data analysis)

Interesting Sequence Mining

define a goodness measure on a set of patterns

Minimum description length

[Vreeken et al, 2011; Tatti and Vreeken, 2012; Lam et al 2014]

Use patterns to define a compression algorithm for database Search for patterns that best compress

Probabilistic methods

[Fowkes and Sutton, KDD 2016, PKDD 2016]

Use patterns to define a probability distribution over database Search for patterns that maximise database probability

(actually isomorphic; see MacKay, 2003)

Sequences more meaningful, less redundant

Also, see tiling: [Geerts, Goethals, and Mielikäinen, 2004]

Model

To sample a transaction, 1. For each itemset, sample $z_S \sim \text{Bernoulli}(\pi_S)$.

2. Deterministically set

$$X = \bigcup_{z_s=1} S.$$





Inference / Learning

${\rm Infer}\; z \; {\rm from}\; X$

$$\max_{\mathbf{z}} \sum_{S \in \mathcal{I}} z_S \ln\left(\frac{\pi_S}{1 - \pi_S}\right) + \ln(1 - \pi_S)$$

s.t.
$$\sum_{S \mid i \in S} z_S \ge 1 \quad \forall i \in X$$
$$z_S \in \{0, 1\} \quad \forall S \in \mathcal{I}$$

NP-hard but submodular (weighted set cover) use greedy algorithm

Infer \mathcal{I}

Structural EM

Propose new itemset SAdd S to model Re-infer \mathcal{Z} Check if cost improved

"Implicit regularization"

Redundancy

Average distance between itemsets in one ranked list (symmetric distance, higher is better)

	Plants	Mammals	ICDM	Uganda	
Interesting Itemsets	3.50	5.30	3.66	3.72	
KRIMP	1.53	2.02	2.22	2.24	
CHARM	1.53	1.52	1.47	1.45	

Facebook posts

_			
	IIM	MTV	KRIMP
-	soul, rest, peace	heal, jesus, amen	whi, ?
	chris, brown	god , amen	?, !
	bebe, cool	2,4	2,4
	airtel, red	whi, $?$	wat, $?$
	everi, thing	god, heal	time, !
	time, wast	2, !	soul, rest, peace

Trending









public Ugandan pages

[courtesy John Quinn, UN Global Pulse]

Plants

KRIMP







Plants

IIM









Frequent Sequence Mining

Return all patterns with >= given support Support of pattern: Number of database sequences that contain it

bdbafec bcea edafc aefb bdaefc

Database of sequences

[Agrawal and Srikant, 1995; Wang and Han, 2004]

Sequence patterns (e.g. minimum support = 3)

d a f c

bafc

ae

be

e c

Problem: Frequent can be trivial!

Fundamental Pathologies



Spurious correlation

Support(\mathbf{a}) = 90% Support(\mathbf{d}) = 90%

... but independent ...

d a

Pattern at 81% min_support

Freerider

a f c real pattern Support(d) = 90%

adfc

for high enough min_support

Effect: Redundant list of patterns

Probabilistic Sequence Mining

[Fowkes and Sutton, KDD 2016]

Sampled database sequence

Define a distribution P(database | patterns)



probability of generating X, zfrom this process

Probabilistic Sequence Mining

[Fowkes and Sutton, KDD 2016]

Model:

$$p(X, \mathbf{z} | \mathbf{\Pi}) = \frac{1}{|\mathcal{P}|} \prod_{S \in \mathcal{I}} \prod_{m=0}^{|\pi_S|-1} \pi_{S_m}^{[z_S=m]}$$



```
Use greedy algorithm to \max_{z} \log p(z|X, \mathcal{I}) (extension of weighted set cover)
```

Probabilistic Sequence Mining

[Fowkes and Sutton, KDD 2016]

[b c e]: 0.3, 0.7

: 0.0, 1.0

:0.7,0.3

: 0.3, 0.7

Output of inference

bdcedff eedfff dfddff



| d f]

[ef]

[df]

Т.

Learning step: Infer ${\cal I}$

Update probabilities (average of *z*)

Propose new patterns Add to model See if probability increases

Formally: Structural Expectation Maximization



Application to Software Engineering

[Fowkes & Sutton, FSE 2016]

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Modern development is layers of libraries

Average Java file on Github: Imports from 2.1 packages outside project
45% of files import an external package (Not counting java.* javax.* sun.*)

> Github Java corpus (Allamanis and Sutton, 2013) 13000+ projects with at least one fork, 2M+ Java files <u>http://groups.inf.ed.ac.uk/cup/javaGithub/</u> (heuristic analysis)



Frequent Sequence Mining

Each transaction: client method

Each element: a method call to an API method

bdbafec bcea edafc aefb bdaefc dafc bafc ae be be

Database of sequences

Sequence patterns (e.g. minimum support = 3)

For API Mining...

TwitterFactory.<init> TwitterFactory.getInstance

TwitterFactory.<init> Twitter.setOAuthConsumer

Top 10 API patterns from pure sequence mining (BIDE)

Status.getUser Status.getText

auth.AccessToken.<init>
Twitter.setOAuthAccessToken

TwitterFactory.<init> TwitterFactory.getInstance Twitter.setOAuthConsumer Twitter.setOAuthAccessToken TwitterFactory.getInstance Twitter.setOAuthConsumer

TwitterFactory.<init> TwitterFactory.getInstance Twitter.setOAuthConsumer

TwitterFactory.<init> Twitter.setOAuthAccessToken

TwitterFactory.<init> TwitterFactory.getInstance Twitter.setOAuthAccessToken

TwitterFactory.getInstance Twitter.setOAuthAccessToken

TwitterFactory.<init> Twitter.setOAuthConsumer Twitter.setOAuthAccessToken

Previous Approach: Cluster before/after

[Zhong et al, 2009; Dang et al 2013]

Probabilistic API Miner (PAM)

Interesting sequence mining for API mining

ConfigurationBuilder.<init> ConfigurationBuilder.setOAuthConsumerKey ConfigurationBuilder.setOAuthConsumerSecret ConfigurationBuilder.setUseSSL ConfigurationBuilder.build TwitterFactory.<init> TwitterFactory.getInstance

ConfigurationBuilder.<init> ConfigurationBuilder.setOAuthConsumerKey ConfigurationBuilder.setOAuthConsumerSecret ConfigurationBuilder.setOAuthAccessToken ConfigurationBuilder.setOAuthAccessTokenSecret ConfigurationBuilder.build TwitterFactory.<init> TwitterFactory.getInstance

ConfigurationBuilder.<init> ConfigurationBuilder.setOAuthConsumerKey ConfigurationBuilder.setOAuthConsumerSecret ConfigurationBuilder.build TwitterFactory.<init> TwitterFactory.getInstance TwitterFactory.getOAuthRequestToken RequestToken.getAuthenticationURL private FinchTwitterFactory(Context context) { mContext = context: installHttpResponseCache(); ConfigurationBuilder configurationBuilder = new ConfigurationBuilder(); configurationBuilder.setOAuthConsumerKey(ConsumerKey.CONSUMER_KEY); configurationBuilder.setOAuthConsumerSecret(ConsumerKey.CONSUMER_SECRET); configurationBuilder.setUseSSL(true); Configuration configuration = configurationBuilder.build(); mTwitter = new TwitterFactory(configuration).getInstance() brk3 / finch public Twitter getTwitterInstance() { ConfigurationBuilder cb = new ConfigurationBuilder(): cb.setOAuthConsumerKey(Keys.consumerKey); cb.set0AuthConsumerSecret(Keys.consumerSecret); cb.set0AuthAccessToken(mSettings.getString("accessToken", null)); cb.setOAuthAccessTokenSecret(mSettings.getString("accessSecret", null)); TwitterFactory tf = new TwitterFactory(cb.build()); return tf.getInstance(); jrupac/CleanTwitter orivate void startOAuth() { ConfigurationBuilder configurationBuilder = new ConfigurationBuilder(); configurationBuilder.set0AuthConsumerKey(Const.CONSUMER_KEY); configurationBuilder.set0AuthConsumerSecret(Const.CONSUMER_SECRET); twitter = new TwitterFactory(configurationBuilder.build()).getInstance(); requestToken = twitter.getOAuthRequestToken(Const.CALLBACK_URL); Toast.makeText(this, "Please authorize this app!", Toast.LENGTH_LONG).show(); this.startActivity(new Intent(Intent.ACTION_VIEW, Uri.parse(requestToken.getAuthenticationURL() + "&force_login=true"))); } catch (TwitterException e) {
 e.printStackTrace(); 🗘 katahirado/tsubunomi Corpus

Sequence database

Probabilistic sequence mining

Data

Target projects: 17 Java libraries, all that: Library source on Github Library in top 1000 Github projects Called by >50 other methods on Github At least 10k lines of example/ code Total: Over 300k lines of example code

Client methods: all that called any targets 967 client projects Total: Over 4M lines of client code

Experimental Questions

Quality

Match to "held-out" client code

Match to examples from library developers

Measure: sequence overlap, precision, recall

Redundancy

Why? Ease of use, diversity

Measure: number of containing sequences

All results averaged over the 17 libraries

Handwritten Examples



Why Low Recall?

API mining bad, or examples incomplete?

- Match test set to examples: is test set covered?
- 73% of client API sequences not covered
- 36% of examples used in client code
- Manual error analysis
 - 3 random projects, top 5 unmatching patterns
 - 7 referred to API method not in examples
 - 3 referred to API class not in examples

Prevalence in Client Code



Example: twitter4j

PAM

MAPO [Zhong et al, '09]

UPMiner [Wang et al, '13]

TwitterFactory. <init> TwitterFactory.getInstance</init>	TwitterFactory. <init> TwitterFactory.getInstance</init>	TwitterFactory. <init> TwitterFactory.getInstance</init>
TwitterFactory. <init> TwitterFactory.getInstance Twitter.setOAuthConsumer Twitter.setOAuthAccessToken</init>	Status.getUser Status.getText	TwitterFactory.getInstance Twitter.setOAuthConsumer
Status.getUser Status.getText	ConfigurationBuilder. <init> ConfigurationBuilder.build</init>	TwitterFactory. <init> TwitterFactory.getInstance Twitter.setOAuthConsumer</init>
AccessToken.getToken AccessToken.getTokenSecret	ConfigurationBuilder. <init> TwitterFactory.<init></init></init>	Status.getUserStatus.getText
ConfigurationBuilder. <init> ConfigurationBuilder.build TwitterFactory.<init> TwitterFactory.getInstance</init></init>	ConfigurationBuilder. <init> ConfigurationBuilder.setOAuthConsu merKey</init>	Twitter.setOAuthConsumer Twitter.setOAuthAccessToken

: two main types of twitter initialization call





Super-Fast Neural Network Topic Modelling

[Srivastava and Sutton, ICLR 2017]

http://bit.ly/sutton-ml-exploration

Topic Models



motherboard meg printer quadra hd windows processor vga mhz connector armenian genocide turks turkish muslim massacre turkey armenians armenia greek voltage nec outlet circuit cable wiring wire panel motor install season nhl team hockey playoff puck league flyers defensive player israel israeli lebanese arab lebanon arabs civilian territory palestinian militia

Topic Models: The Industry



- New topic model means new inference algorithm
- MCMC general but slow; variational fast but not as general, and lower quality topics

Recognition Networks

[Hinton et al, 1995]

Inference network



Appx posterior

Variational autoencoder [Kingma and Welling, 2013]

 $L(\gamma, \phi \mid \alpha, \beta) = -D_{KL} \left[q(\theta, z \mid \gamma, \phi) \mid | p(\theta, z \mid \alpha) \right] + \mathbb{E}_{q(\theta, z \mid \gamma, \phi)} \left[\log p(\mathbf{w} \mid z, \theta, \alpha, \beta) \right]$

How to make it work

- Discrete variables
 - Marginalize them out
- Dirichlet difficult to reparameterize
 - Use Laplace approximation [MacKay, 1998]
- Topic collapsing (a bad local minimum)
 - High momentum in ADAM [Kingma and Ba, 2014]
 - Batch normalization [loffe and Szegeti, 2015]

Deriving new models



LDA

$$p(w_n | \theta, \beta) = \sum_k \theta_k p(w_n | z_n = k, \beta)$$

ProdLDA
 $p(w_n | \theta, \beta) \propto \prod_k p(w_n | z_n = k, \beta)^{\theta_k}$

Very simple change to LDA, but hasn't been seen before. Why?

- Before, I would have derived a variational inference algorithm
- Now, change one line of code

Evaluation

# topics	ProdLDA	LDA NVLDA	LDA DMFVI	LDA Collapsed Gibbs	NVDM
50	0.24	0.20	0.11	0.17	0.08
200	0.19	0.12	0.06	0.14	0.06

Topic coherence (20 Newsgroups)

# topics	ProdLDA	LDA NVLDA	LDA DMFVI	LDA Collapsed Gibbs	NVDM
50	0.14	0.07	-	0.04	0.07
200	0.12	0.05	-	0.06	0.05

Topic coherence (RCV1)

Look Ma, no inference!

# Topics	Inference Network Only	Inference Network + Optimization
50	1172	1162
200	1168	1151

Test set perplexity (20 Newsgroups)

Accurate topic inference on new topic with one pass of a feedforward neural network

VEEGAN: Reducing Mode Collapse in Generative Adversarial Learning

http://bit.ly/sutton-ml-exploration

Generative Adversarial Networks

Classical probabilistic modelling



Input





Explicit model





Density value

Implicit probabilistic modelling



Sampling procedure for $p_{\theta}(x)$

How to train?

Can't use maximum likelihood. There is no likelihood!

Instead define a game



1 if x came from generator 0 if x came from data

Optimize

 $\max_{\omega} \min_{\gamma} \mathcal{O}_{GAN}(\omega, \gamma) := E_z \left[\log D_{\omega}(G_{\gamma}(z)) \right] + E_x \left[\log \left(1 - D_{\omega}(x) \right) \right]$

Mode Collapse

Example from 2D mixture of Gaussians





Samples from GAN

VEEGAN: Adding an Autoencoder



Detecting mode collapse



Not detecting mode collapse

Problem: How to train F_{θ} ?

VEEGAN objectives



Generator network $G_{\gamma}(z)$



Discriminator network $D_{\omega}(x)$



Autoencoder

VEEGAN algorithm

Algorithm 1 VEEGAN training

$$\begin{array}{ll} \text{i: while not converged do} \\ \text{2:} & \text{for } i \in \{1 \dots N\} \text{ do} \\ \text{3:} & \text{Sample } z^i \sim p_0(z) \\ \text{4:} & \text{Sample } x^i_g \sim q_\gamma(x|z_i) \\ \text{5:} & \text{Sample } x^i_g \sim p_\theta(z_g|x_i) \\ \text{6:} & \text{Sample } z^i_g \sim p_\theta(z_g|x_i) \\ \text{7:} & g_\omega \leftarrow -\nabla_\omega \frac{1}{N} \sum_i \log \sigma \left(D_\omega(z^i, x^i_g) \right) + \log \left(1 - \sigma \left(D_\omega(z^i_g, x^i) \right) \right) \\ \text{8:} \\ \text{9:} & g_\theta \leftarrow \nabla_\theta \frac{1}{N} \sum_i d(z^i, x^i_g) \\ \text{10:} \\ \text{11:} & g_\gamma \leftarrow \nabla_\gamma \frac{1}{N} \sum_i D_\omega(z^i, x^i_g) + \frac{1}{N} \sum_i d(z^i, x^i_g) \\ \text{12:} \\ \text{13:} & \omega \leftarrow \omega - \eta g_\omega; \theta \leftarrow \theta - \eta g_\theta; \gamma \leftarrow \gamma - \eta g_\gamma \\ \end{array} \right) \\ \text{Perform SGD updates for } \omega, \theta \text{ and } \gamma \\ \end{array}$$

Examples of generated images



Celebrity faces

Examples of generated images



CIFAR-10 natural images



Help cats explore!

Machine Learning for Data Exploration Charles Sutton, University of Edinburgh



- Akash Srivastava
- Lazar Valkov
- Chris Russell
- Michael Gutmann





Neural topic modelling



VEEGANs

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