2019 ACM SIGKDD International Conference on Knowledge Discovery and Data Mining

#### Modern MDL meets Data Mining Insight, Theory, and Practice



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#### About the presenters



#### Jilles Vreeken









#### About this tutorial

Approximately 3.5 hours long

Extensive, but incomplete introduction to

- MDL theory
- MDL practice in data mining
- naturally a bit biased

#### Schedule

8:00am	Opening
8:10am	Introduction to MDL

MDL in Action

9:30am

8:50am

-break—

10:00amStochastic Complexity11:00amMDL in Dynamic Settings





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8:00am	
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10:00am	

——break ———

Introduction to MDL

10:00amStochastic Complexity11:00amMDL in Dynamic Settings

**MDL** in Action

Opening





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# Part 1 Introduction to MDL



Jilles Vreeken

### Induction by Simplicity

*"The simplest description of an object is the best"* 

### Kolmogorov Complexity

 $K_U(x) = \min_{y} \{ l(y) \mid U(y) \text{ halts and } U(y) = x \}$ 

The Kolmogorov complexity of a binary string xis the length of the shortest program  $y^*$ for a universal Turing Machine Uthat generates s and halts.

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### Ultimately Impractical

#### Kolmogorov complexity K(x), or rather, the Kolmogorov optimal program $x^*$ is not computable.

## We can approximate it from above, but, this is not very practical.

(simply not enough students to enumerate all Turing machines)

#### We can approximate it through off-the-shelf compressors, yet, this has serious drawbacks.

(big-O, what structure does a compressor reward, etc)

#### A practical variant

A more viable alternative is the **Minimum Description Length** principle

*"the best model is the model that gives the best lossless compression"* 

There are two ways to motivate MDL

- we'll discuss both at a high level
- then go into more details on what MDL is and can do

#### Two-Part MDL

The Minimum Description Length (MDL) principle

given a set of hypotheses  $\mathcal{H}$ , the best hypothesis  $H \in \mathcal{H}$ for given data D is that H that minimises

 $L(H) + L(D \mid H)$ 

in which

L(H) is the length, in bits, of the description of H

 $L(D \mid H)$  is the length, in bits, of the description of the data when encoded using H

#### Bayesian Learning

Bayes tells us that

$$\Pr(H \mid D) = \frac{\Pr(D \mid H) \times \Pr(H)}{\Pr(D)}$$

This means we want the *H* that maximises Pr(H | D). Since Pr(D) is the same for all models, we have to maximise  $Pr(D | H) \times Pr(H)$ 

> Or, equivalently, minimise  $-\log(\Pr(H)) - \log(\Pr(D \mid H))$

#### From Bayes to MDL

So, Bayesian Learning means minimising  $-\log(\Pr(H)) - \log(\Pr(D \mid H))$ 

Shannon tells us that the —log transform takes us from probabilities to **optimal prefix-code lengths** 

This means we are actually minimizing

 $L(H) + L(D \mid H)$ 

for some encoding *L* for *H* resp.  $D \mid H$  corresponding to distribution Pr

#### Bayesian MDL

If we want to do MDL this way – i.e., being a Bayesian – we need to specify

- a prior probability Pr(M) on the models, and
- a conditional probability Pr(D|M) on data given a model

What are reasonable choices?

#### What Distribution to Use?

For the data, this is 'easy': a maximum likelihood model

• a maximum entropy model for  $Pr(D \mid M)$  makes most sense

For the models, this is 'harder', we could, e.g., use

- 'whatever the expert says is a good distribution', or
- an uninformative prior on *M*, or
- (a derivative of) the universal prior from algorithmic statistics

These are not easy to compute, query, and **ad hoc**.

In MDL we say, if we are going to be ad hoc, let us do so **openly** and use **explicit universal encodings** 

### Information Criteria

MDL might make you think of either

Akaike's Information Criterion (AIC)

 $k - \ln(\Pr(D|H))$ 

or the **Bayesian Information Criterion** (BIC)

$$\frac{k}{2}\ln(n) - \ln(\Pr(D|H))$$

### Information Criteria

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k - L(D|H)

or the **Bayesian Information Criterion** (BIC)

$$\frac{k}{2}\ln(n) - L(D|H)$$

### Information Criteria

MDL might make you think of either

Akaike's Information Criterion (AIC)

 $L_{AIC}(H) = k$ 

or the Bayesian Information Criterion (BIC)

$$L_{BIC}(H) = \frac{k}{2}\ln(n)$$

We, however, **do not** assume that all parameters are created equal, we take their complexity into account

#### From Kolmogorov to MDL

Both Kolmogorov complexity and MDL are based on compression. Is there a relationship between the two?

Yes.

We can derive **two-part MDL** from Kolmogorov complexity. We'll sketch here how.

### Objects and Sets

Recall that in Algorithmic Information Theory we are looking for (optimal) descriptions of **objects**.

One way to describe an object is

- describe a set of which it is a member
- point out which of these members it is.

In fact, we do this all the time

- the beach (i.e., the set of all beaches)
- over there (pointing out a specific one)

### Algorithmic Statistics

#### We have, a set S

- which we call a model
- which has complexity K(S)

#### and an object $x \in S$

- *S* is a model of *x*
- the complexity of pointing out x in S is the complexity of x given S, i.e. K(x | S)

Obviously,

 $K(x) \le K(S) + K(x \mid S)$ 

#### So?

#### Algorithmic Information Theory states that

- every program that outputs x and halts encodes the information in x
- the smallest such program encodes only the information in *x*

If x is a data set, i.e. a random sample, we expect it has

- epistemic structure, "true" structure; captured by *S*
- aleatoric structure, "accidental" structure; captured by x | S

We are hence interested in that model S that minimizes K(S) + K(x | S)

which is surprisingly akin to two-part MDL

#### More detail

For K(S)

 this is simply the length of the shortest program that outputs S and halts; i.e., a generative model of x

For  $K(x \mid S)$ 

 if x is a typical element of S there is no more efficient way to find x in S than by an index, i.e., K(x | S) ≈ log(|S|)

### Kolmogorov's Structure Function

This suggests a way to discover the best model.

Kolmogorov's structure function is defined as

$$h_x(i) = \min_{S} \{ \log(|S|) \mid x \in S, K(S) \le i \}$$

That is, we start with very simple – in terms of complexity – models and gradually work our way up

#### The MDL function

This suggests a way to discover the best model.

Kolmogorov's structure function is defined as

$$h_x(i) = \min_{S} \{ \log(|S|) \mid x \in S, K(S) \le i \}$$

which defines the MDL function as

 $\lambda_x(i) = \min_{S} \{ K(S) + \log(|S|) \mid x \in S, K(S) \le i \}$ 

We try to find the minimum by considering increasingly complex models.

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Say we have a string x = 0101110000110100011of 10 zeroes and 10 ones

Suppose  $\mathcal{H}$  consists of these binomials, e.g.  $p_1 = 0.1, p_2 = 0.2, p_3 = 0.5$ 

 $L(x | p_1) = -10 \log p_1 - 10 \log(1 - p_1) = 34.7 \text{ bits}$   $L(x | p_2) = -10 \log p_2 - 10 \log(1 - p_2) = 26.4 \text{ bits}$  $L(x | p_3) = -10 \log p_3 - 10 \log(1 - p_3) = 20.0 \text{ bits}$ 

Suppose x = 0101110000110101011, and  $\mathcal{H} = \{p_1 = 0.1, p_2 = 0.2, p_3 = 0.5\}$ 

Without prior preference over  $H \in \mathcal{H}$  $L(H) = \log |\mathcal{H}|$ 

> $L(p_1) + L(x | p_1) = 36.3$  bits  $L(p_2) + L(x | p_2) = 28.0$  bits  $L(p_3) + L(x | p_3) = 21.6$  bits

Suppose x = 0101110000110101011, and  $\mathcal{H} = \{p_1 = 0.1, p_2 = 0.2, p_3 = 0.5\}$ 

$$L(p_1) + L(x | p_1) = 36.3$$
 bits  
 $L(p_2) + L(x | p_2) = 28.0$  bits  
 $L(p_3) + L(x | p_3) = 21.6$  bits

However, when you receive  $L(p_1)$  you know that  $p_2$  and  $p_3$  were disregarded by the sender as these did not lead to a minimal description.

Suppose x = 0101110000110101011, and  $\mathcal{H} = \{p_1 = 0.1, p_2 = 0.2, p_3 = 0.5\}$ 

> $L(p_1) + L(x | p_1) = 36.3$  bits  $L(p_2) + L(x | p_2) = 28.0$  bits  $L(p_3) + L(x | p_3) = 21.6$  bits

Models  $H \in \mathcal{H}$  will only be used for data where they are optimal within the model class! Two-part MDL ignores this, it wastes bits!

#### Crude MDL

The Minimum Description Length (MDL) principle

given a set of hypotheses  $\mathcal{H}$ , the best hypothesis  $H \in \mathcal{H}$ for given data D is that H that minimises

 $L(H) + L(D \mid H)$ 

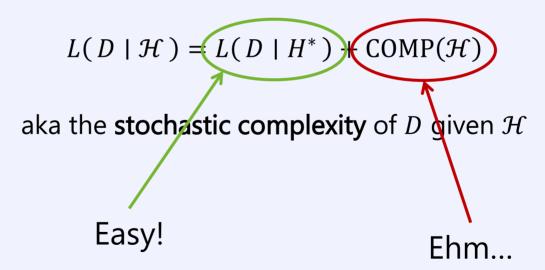
in which

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#### Refined MDL

The main intuition, coming from crude MDL: L(H) is ad hoc, so we want to get rid of it, but keeping only  $L(D \mid H)$  is going to give us a bad time, as maximising likelihood leads to overfitting.



#### Universal Codes

What Universal codes do we know?

- the two-part code (iff minimax guarantees, or large sample)
- prequential plug-in codes
- Bayesian mixtures codes (Jeffrey's prior)
- Normalised Maximum Likelihood (NML)

Each of these have quite a different nature, hence different coding schemes, but all lead to very similar  $L(D \mid \mathcal{H})$ .

Normalized Maximum Likelihood (Shtarkov, 1987)

$$L(D \mid \mathcal{H}) = -\log \frac{P(D \mid H^* \in \mathcal{H})}{\sum_{D' \in \mathcal{D}} P(D' \mid H' \in \mathcal{H})}$$

Interpretation:

The more special D is with respect to  $\mathcal{H}$ , the shorter its code.

One nasty detail, the normalization: Enumerating every possible *D*' requires many PhD students, calculating the maximum likelihood *H*' for every *D*', even more so.

#### Crude in Practice

Refined MDL is **only** defined for a small set of cases. Computing stochastic complexity is possible for **even fewer**.

Hence, in practice, as much as we may dislike it in theory, we often have to resort to crude MDL.

However, as long as we're **aware of the biases** of the encoding, that's **not a bad thing**.

In fact, as in two-part MDL we can steer our encoding towards models we (intuitively) like better, and hence for data mining purposes two-part MDL is a very often a good friend indeed.

### MDL is a principle

MDL is **not** a single method

• it's a **general principle** for doing inductive inference

The main adage: fewer bits is better

- encode the data universally that is, without external input, only consider the data at hand
- ideally, uphold minimax optimality properties, try to make sure your encoding is never much worse than the best

Try to avoid, as much as possible, ad hoc biases

be explicit about those that exist