Statistical Sequence Modelling

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1. Adaptive Context Trees : Theory



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2. Adaptive Context Trees : Applications



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- 2. Adaptive Context Trees : Applications
- 3. Combining ACT with HMM?
- 4. From sequence modelling to classification...

Part 1

Adaptive Context Trees : Theory

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- A probabilistic model is a probability distribution over the set of sequences
- It can be used to compare two sequences or a sequence and a model

• A model is characterized by the conditional distribution P(Y | X) where X is the past, Y is the next character.

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• The number of parameters is exponential with D!

Context tree model

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- Maps any past sequence X into its longest suffix $\mathcal{S}(X)$
- A probability distribution θ_s is attached to each node $s \in \mathcal{S}$:

 $\overline{P_{\mathcal{S}}}_{,\theta}(Y \mid \overline{X}) = \theta_{\mathcal{S}(X)}(Y)$

The estimation issue

• Let $P(X \mid Y)$ an unknown probability distribution

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We observe an i.i.d. sample

$$\mathcal{E} = \{(X_1, Y_1), \dots, (X_N, Y_N)\}$$

• How to guess a good tree ${\mathcal S}$ and a good set of parameters θ from ${\mathcal E}?$

Adaptive Context tree model : the recipe

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2. Use \mathcal{E}_1 to estimate the parameters of every model S by: $\hat{P}_{\mathcal{S}}(Y \mid X) = \frac{\#\{i : s(X_i) = s(X) \text{ et } Y_i = Y\} + 1}{\#\{i : s(X_i) = s(X)\} + |\mathcal{A}|}$

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3. Chose a probability *a priori* on the set of trees $\pi(\mathcal{S})$

4. Use \mathcal{E}_2 to build a posterior distribution on the trees:

$$\rho(\mathcal{S}) = \frac{1}{Z} \pi(\mathcal{S}) \times \prod_{i \in \mathcal{E}_2} \hat{P}_{\mathcal{S}}(Y_i \mid X_i)^{\beta}$$

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5. The ACT estimator is finally:

$$\hat{P}(Y \mid X) = \sum_{\mathcal{S}} \rho(\mathcal{S}) \hat{P}_{\mathcal{S}}(Y \mid X)$$

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• The closeness of P(Y|X) and Q(Y|X) can be measured in conditional relative entropy

$$D(P||Q) = \sum_{(x,y)} P(x,y) \log \frac{Q(y|x)}{P(y|x)}$$

• For any unknown P the average loss of \hat{P} satisfies $E[D(P||\hat{P})] \leq \inf_{\mathcal{S},\theta} \left\{ D(P||P_{\mathcal{S},\theta}) + C\frac{|\mathcal{S}|}{N} \right\}$

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• C is an optimal constant

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- The implementation is efficient using a recursive algorithm (Context Tree Weighting method)
- The resulting distribution $\hat{P}(Y|X)$ is a mixture of all $P_{S,\theta}$ and not a particular one

Part 2

Adaptive Context Trees : Applications

Unsupervised Text clustering (1)

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Unsupervised Text clustering (1)

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• A pseudo-distance between T_1 et T_2 is:

$$d(T_1, T_2) = \ln \frac{\hat{Q}(\mathcal{E}'_1 \mid \mathcal{E}_1)}{\hat{Q}(\mathcal{E}'_2 \mid \mathcal{E}_1)} + \ln \frac{\hat{Q}(\mathcal{E}'_2 \mid \mathcal{E}_2)}{\hat{Q}(\mathcal{E}'_1 \mid \mathcal{E}_2)}$$

Unsupervised Text clustering (2)

Text Number	Extracted from
1-5	Wintson Churchill (<i>The Crossing</i>)
6-10	Joseph Conrad (<i>The Arrow of gold</i>)
11-15	Arthur Conan Doyle (<i>The hound of the Baskervilles</i>)
16-20	Karl Marx (<i>Manifesto of the communist party</i>)
21-25	Baruch Spinoza (<i>Political treatise</i>)
26-30	Jonathan Swift (<i>Gulliver's travel</i>)
31-35	Francois Marie Arouet Voltaire (<i>Candide</i>)
36-40	Virginia Woolf (<i>Night and day</i>)
Text database	

Distance between text n.23 (Spinoza) and other texts Text clustering (1.03 threshold)

Automatic text generation

talk.politics.mideast: associattements in the greeks who be neven exclub no bribedom of spread marinary s trooperties savi tack acter i ruthh jake bony soc.religion.christian: that must as a friend one jerome unimovingt ail serving are national atan cwru evid which done joseph in response of the wholeleaseriend

Biological sequences?

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- Approach already tested with good results for protein family prediction by Bejerano/Rona (RECOMB 1999) and Eskin/Grundy/Singer (RECOMB 2000)



ACT with HMM?

Definition of a CT-HMM (1)

• \mathcal{H} a finite set of hidden states

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• \mathcal{H} a finite set of hidden states

- $(S, \theta) = \{(S, \theta)_h, h \in \mathcal{H})\}$ a family of context tree models for each hidden state
- $\mu(h_2 \mid h_1)$ a transition probability

Definition of a CT-HMM (2)

• The CT-HMM distribution is:

 $P_{S,\theta,\mu}(H_{n+1}, X_{n+1} | H_{-\infty}^n, X_{-\infty}^n) = \mu(H_{n+1} | H_n) \times P_{(S,\theta)_{H_i}}(X_i | X_{-\infty}^n)$

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• It generalizes HMMs

• Let $x = (..., x_0, ..., x_N)$ a observed sequence, generated by an unknown model supposed to be well approached by a CT-HMM.

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- The classical approach (E-M algorithm) does not work
- How to guess a good $h = (h_1, \ldots, h_N)$?
- A good sequence can be seen as a one which reduces the complexity of the observed sequence

A mixture approach

• Let $\pi(S, d\theta, d\mu)$ a probability *a priori* on the models and parameters

A mixture approach

- Let $\pi(S, d\theta, d\mu)$ a probability *a priori* on the models and parameters
- The mixture probability sums up the information contained in all models:

$$P_w(X) = \sum_{H,S} \int_{\mu,\theta} P_{\mu,S,\theta}(X,H) \pi(d\mu,S,d\theta)$$

Selection by Minimum Description Length

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- $\log_2 P_w(x \mid h)$ to describe the observation x given a hidden sequence h
- MDL : Choose $h = \underset{h}{\operatorname{arg\,max}} P_w(h) \times P_w(x|h)$

Application : E Coli genome segmentation

Part 3

From modelling to classification

Classification ?

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- $X \in \mathcal{X}$ an objet
- $Y \in \mathcal{Y}$ a class (typically $\{1, \ldots, k\}$)
- Classifier = mapping $f : \mathcal{X} \to \mathcal{Y}$

• protein classification,

• protein classification, structure prediction ...

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(promoter-sequence based) gene classification...

• protein classification, structure prediction ...

- (promoter-sequence based) gene classification...
- functional classification of enzymes, binding pairs...

Classical approach in bioinformatics

• build probabilistic models

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- derive a score function

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- derive a score function
- classify according to maximum score

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• What about a seminar?