Maximum Likelihood vs. Least Squares for Estimating Mixtures of Truncated Exponentials

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INFORMS, Seattle, November 2007

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Motivation.

- The MTE (Mixture of Truncated Exponentials) model.
- Maximum Likelihood (ML) estimation for MTEs.
- Least Squares (LS) estimation of MTEs.
- Experimental analysis.
- Conclusions.

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• Graphical models are a common tool for decision analysis.

- Problems in which continuous and discrete variables interact are frequent.
- A very general solution is the use of MTE models.
- When learning from data, the only existing method in the literature is based on least squares.
- The feasibility of ML estimation seems to be worth studying.

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Bayesian networks



D.A.G.

- The nodes represent random variables.
- Arc \Rightarrow dependence.

$$p(\mathbf{x}) = \prod_{i=1}^n p(x_i | \pi_i) \ \mathbf{x} \in \Omega_{\mathbf{X}}$$

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 $p(x_1, x_2, x_3, x_4, x_5) = p(x_1)p(x_2|x_1)p(x_3|x_1)p(x_5|x_3)p(x_4|x_2, x_3)$.

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Definition (MTE potential)

X: mixed *n*-dimensional random vector. Y = (Y₁,..., Y_d),
 Z = (Z₁,...,Z_c) its discrete and continuous parts. A function f : Ω_X → ℝ₀⁺ is a Mixture of Truncated
 Exponentials potential (MTE potential) if for each fixed value y ∈ Ω_Y of the discrete variables Y, the potential over the continuous variables Z is defined as:

$$f(\mathbf{z}) = a_0 + \sum_{i=1}^m a_i \exp\left\{\sum_{j=1}^c b_i^{(j)} z_j
ight\}$$

for all $\mathbf{z} \in \Omega_{\mathbf{Z}}$, where a_i , $b_i^{(j)}$ are real numbers.

Also, *f* is an MTE potential if there is a partition *D*₁,..., *D_k* of Ω_Z into hypercubes and in each *D_i*, *f* is defined as above.

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Example

Consider a model with continuous variables X and Y, and discrete variable Z.



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Example

One example of conditional densities for this model is given by the following expressions:

 $f(x) = \begin{cases} 1.16 - 1.12e^{-0.02x} & \text{if } 0.4 \le x < 4 \\ 0.9e^{-0.35x} & \text{if } 4 < x < 19 \end{cases}.$

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$$f(z|x) = \begin{cases} 0.3 & \text{if } z = 0, \ 0.4 \le x < 5 \ , \\ 0.7 & \text{if } z = 1, \ 0.4 \le x < 5 \ , \\ 0.6 & \text{if } z = 0, \ 5 \le x < 19 \ , \\ 0.4 & \text{if } z = 1, \ 5 \le x < 19 \ . \end{cases}$$

The learning task involves three basic steps:

- Determination of the splits into which Ω_X will be partitioned.
- Determination of the number of exponential terms in the mixture for each split.
- Estimation of the parameters.

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Why ML?

- Well developed core theory.
- Good asymptotic properties under regularity conditions.
- Several procedures connected to Bayesian networks rely on ML estimations.

Problems for applying ML to MTEs

- The likelihood equations cannot be solved for the MTE model.
- Numerical methods are slow and potentially unstable.

Question

Can the LS estimates be used as approximations to the ML ones?

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- Empiric density approximated by a histogram.

Improved version

V. Romero, R. Rumí, A. Salmerón (2006) Learning hybrid Bayesian networks using mixtures of truncated exponentials. *International Journal of Approximate Reasoning* **42**:54-68.

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Learning MTEs from data

• The split points are determined observing the extreme and inflexion points.

- The number of points (*N*) to locate is established beforehand.
- The *N* higher changes from concavity/convexity or increase/decrease are selected.
- The number of exponential terms can be determined beforehand or decided during the parameter estimation procedure.

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Target density

$$f(x) = k + ae^{bx} + ce^{dx}$$

• Assume we have initial estimates a_0 , b_0 and k_0 .

c and d are estimated by fitting to points (x, w), where

$$\mathbf{w} = \mathbf{y} - \mathbf{a}_0 \exp{\{\mathbf{b}_0 \mathbf{x}\}} - \mathbf{k}_0$$

a function

$$w = c \exp\{dx\} ,$$

minimising the weighted mean squared error.

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Taking logarithms, the problem reduces to linear regression:

 $\ln \{w\} = \ln \{c\} \exp \{dx\} = \ln \{c\} + dx ,$

that can be written as

$$w^* = c^* + dx$$

where $c^* = \ln \{c\}$ and $w^* = \ln \{w\}$.

The solution is

$$(c^*, d) = \arg\min_{c^*, d} \sum_{i=1}^n (w_i^* - c^* - dx_i)^2 f(x_i)$$

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The solution can be obtained by analytical means:

$$= \frac{\left(\sum_{i=1}^{n} w_i x_i f(x_i)\right) - d\left(\sum_{i=1}^{n} x_i f(x_i)\right)^2}{\left(\sum_{i=1}^{n} x_i f(x_i)\right)}$$

 $d = \frac{\left(\sum_{i=1}^{n} w_i f(x_i)\right) \left(\sum_{i=1}^{n} x_i f(x_i)\right) - \left(\sum_{i=1}^{n} f(x_i)\right) \left(\sum_{i=1}^{n} w_i x_i f(x_i)\right)}{\left(\sum_{i=1}^{n} x_i f(x_i)\right)^2 - \left(\sum_{i=1}^{n} f(x_i)\right) \left(\sum_{i=1}^{n} x_i^2 f(x_i)\right)}$

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• Once *a*, *b*, *c* and *d* are known, we go for *k*:

$$f^*(x) = k + ae^{\{bx\}} + ce^{\{dx\}}$$

where $k \in \mathbb{R}$ should be such that minimises the error

$$E(k) = \sum_{i=1}^{n} \frac{(f(x_i) - ae^{bx_i} - ce^{dx_i} - k)^2 f(x_i)}{n} ,$$

This is optimised for

$$\hat{k} = \frac{\sum_{i=1}^{n} (f(x_i) - ae^{bx_i} - ce^{dx_i})f(x_i)}{\sum_{i=1}^{n} f(x_i)}$$

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• The contribution of each exponential term can be refined. Assume that we have an estimated model

$$\hat{f}(x) = \hat{a}_0 e^{\hat{b}_0 x} + \hat{c}_0 e^{\hat{d}_0 x} + \hat{k}_0$$
 .

 The impact of the second exponential term can be determined by introducing a factor *h* in the regression equation, for a sample (x, y), given by

$$\mathbf{y} = \hat{\mathbf{a}}_0 \mathbf{e}^{\hat{\mathbf{b}}_0 \mathbf{x}} + h\hat{\mathbf{c}}_0 \mathbf{e}^{\hat{\mathbf{d}}_0 \mathbf{x}} + \hat{\mathbf{k}}_0$$
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and the value of *h* is computed by least squares, obtaining

$$h = \frac{\sum_{i=1}^{n} (y_i - \hat{a}_0 e^{\hat{b}_0 x_i} - \hat{k}_0) (e^{\hat{d}_0 x_i}) f(x_i)}{\sum_{i=1}^{n} \hat{c}_0 e^{2\hat{d}_0 x_i} f(x_i)}$$

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Initialising a, b and k

- The initial values of *a*, *b* and *k* can be arbitrary, but a good selection of them can speed up the convergence of the method.
- These values can be initialised fitting a curve
 y = a exp {bx} to the modified sample by exponential regression, and computing k as before.
- Another alternative is to force the empiric density and the initial model to have the same derivative.

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Experimental setting

• Tested distributions:

- Normal.
- Log-normal.
- χ^2 .
- Beta.
- MTE.
- Sample size: 1000.
- Split points detection:
 - ML: Manually determined.
 - LS: Automatic detection.

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Graphical comparison: MTE

Artificial 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

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Graphical comparison: Log-normal

LogNormal 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

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Graphical comparison: χ^2

Chi 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

Graphical comparison: Normal (2 splits)

Normal 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

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Graphical comparison: Normal (4 splits)

Normal 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

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Graphical comparison: Beta

Beta 1000 Sample Size



Black=Original, Red=LSE, Blue=ML

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Graphical comparison: Beta, kernel fitting



Beta 1000 Sample & Kernel values

Comparison Kernel values vs LSE (red)

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Comparison in terms of likelihood

	Artificial	χ^2	Beta	Normal-2	Normal-4	Log-normal
ML	-2263.132	160.687	-2685.765	-1373.499	-1364.643	-1398.300
LS	-2293.473	90.234	-2726.950	-1533.889	-1404.747	-1451.568

Comparison through a two-sided paired *t*-test

- Including all the data: p = 0.02039.
- Excluding the Beta: p = 0.05418.

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Conclusions

- LS highly dependent on the empirical density (kernel or histogram).
- LS and ML very close except for the Beta case.
- ML reaches higher likelihood values.
- LS efficient from a computational point of view.

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- ML reaches higher likelihood values.
- LS efficient from a computational point of view.

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• Refining LS estimation.

More exhaustive comparison with ML.

• Extension to the conditional case.

• Possible mixed approach ML and LS.

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