# Information Theoretic Novelty Detection

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# Outline of the talk

1. Novelty Detection
   - General Definitions
   - Maximum Likelihood Approach for i.i.d. data
2. Information Theoretic Novelty Detection
   - Gaussian
   - Mixture of Gaussians
   - Autoregressive Time Series
3. Conclusions and Future Works

# Novelty Detection

## Novelty/Outlier

*"an observation that deviates so much from other observations as to arouse suspicion that it was generated by a different mechanism."*
D. Hawkins

# Novelty Detection

Novelty/Outlier detection can be used for two different reasons:

- reduce their impact in the modeling stage (outlier rejection)
- flag events/detect changes in order to take decisions on the system (novelty detection)

Two types of novelties:

- Event based (Additive Outliers)
- Model based (Innovative Outliers)

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# Novelty Detection

Novelty detection is employed in many fields:

- Mechanical Engineering (Fault detection)
- Condition Monitoring
- Hydrology
- Surveillance

Approaches:

- Neural networks
- Extreme value theory
- Support Vector methods
- Statistical approaches (Frequentist and Bayesian)

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# Novelty Detection

The performances of novelty detection systems can be measured by means of:

- Accuracy
- False Positive and False Negative rates

In every application it is important to balance the cost of False Negatives and False Positives.

# Novelty Detection

- Modeling the system in a training stage
- Training set:

$$X = \{x_1, \ldots, x_n\}$$

- The model describes what is "normal", on the basis of the training set $X$

# Maximum Likelihood Approach for i.i.d. data

- Assume a parametric form for $p(x)$, i.e. $p(x) = p(x|\theta)$
- Likelihood

$$L = \prod_{i=1}^{n} p(x_i|\theta)$$

- ML approach leads to an estimate $\hat{\theta}$ of $\theta$
- a test point can be tested using quantiles

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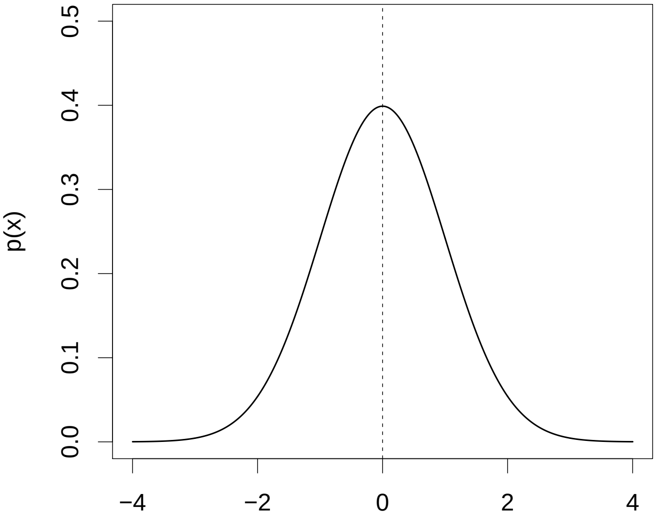
# Example



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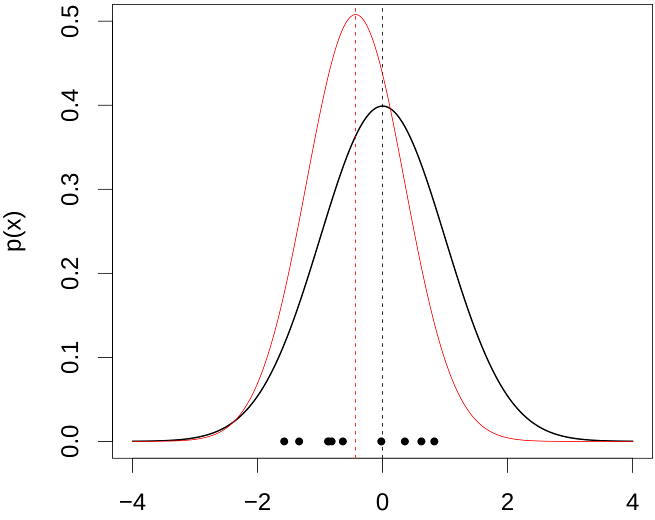

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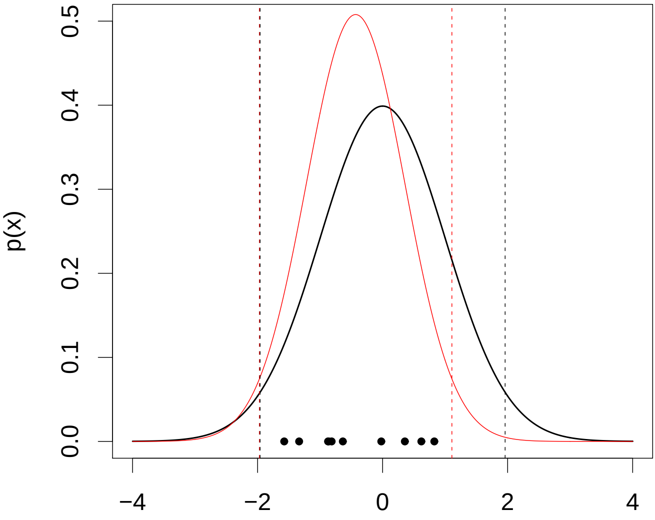

# Information Theoretic Novelty Detection

We recast the novelty detection problem in the framework of information theory

- i.i.d. data:
  - Gaussian case (univariate and multivariate)
  - Mixture of Gaussians (univariate and multivariate)
- time series (linear autoregressive)

# Kullback Leibler divergence

- Definition:

$$\mathrm{KL}\left[p||q\right] = \int p(x) \log \left[ \frac{p(x)}{q(x)} \right] dx$$

- it measures the dissimilarity between probability distributions
- it is not symmetric and it does not obey to the triangular inequality

# Information theoretic measure for novelty detection - i.i.d. case

We denote with $x_*$ a new data point from the same model
We propose to evaluate the expected information content of $x_*$ as a measure of novelty

- $p(x|\hat{\theta})$ with $\hat{\theta}$ estimated on $X$
- $p(x|\hat{\theta}_*)$ with $\hat{\theta}_*$ estimated on $X \cup \{x_*\}$
- Kullback Leibler divergence between $p(x|\hat{\theta})$ and $p(x|\hat{\theta}_*)$

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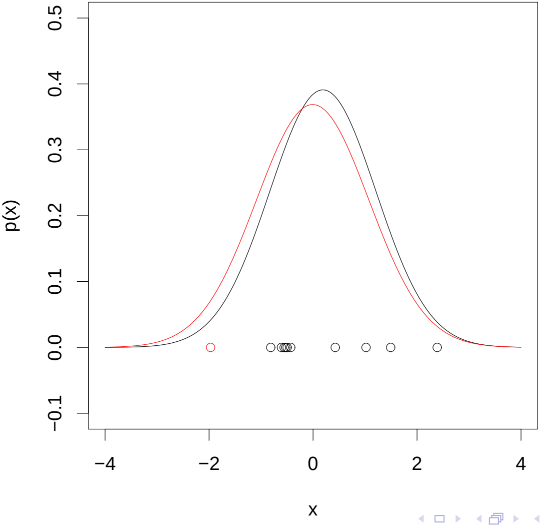
# KL divergence - Example



## Univariate Gaussian Case

- $x_i \sim \mathcal{N}(m, s^2)$
- We introduce:

$$\hat{z} = \frac{(x_* - \hat{m})}{\hat{s}}$$

- The KL divergence results in:

$$\mathrm{KL} = f(n, \hat{z}^2)$$

- The distribution of $\hat{z}^2$ is known:

$$\hat{z}^2 = \frac{(x_* - \hat{m})^2}{\hat{s}^2} \sim \left(\frac{n+1}{n-1}\right) F_{(1,n-1)}$$

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# Univariate Gaussian Case - $F$-test

- The analysis of $\hat{z}^2$ leads to the $F$-test
- The thresholds for novelty can be set by using the quantiles of an $F_{(1,n-1)}$ with the desired different rejection rates
- a test point can be tested comparing its $\hat{z}^2$ score with the thresholds
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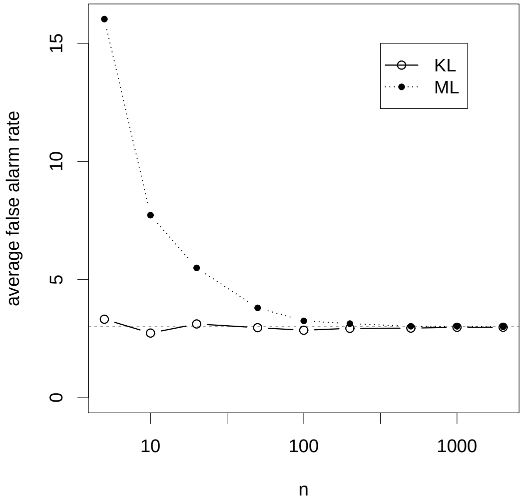
# Univariate Gaussian Case - Experimental comparison

- Generate a training set of $n$ points from a $\mathcal{N}(m, s^2)$;
- Generate $10^6$ test points from the same $\mathcal{N}(m, s^2)$;
- Compute the number of outliers (false alarm rate);
- Repeat 200 times, and average the false alarm rate.

# KL vs ML - Univariate Gaussian



# Multivariate Gaussian Case

- Training data:

$$\mathbf{x}_i \sim \mathcal{N}(\mathbf{m}, S)$$

- Introduce:

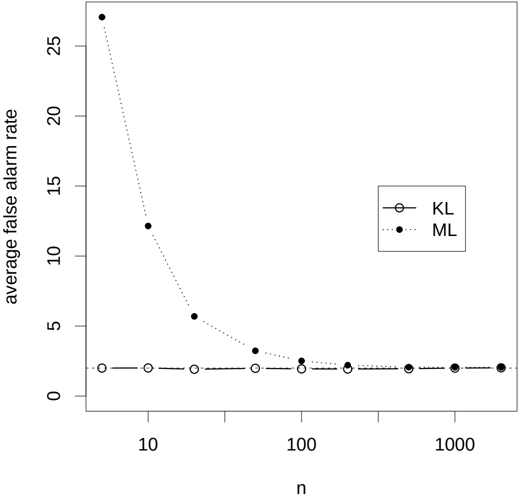
$$\hat{z}^2 = (\mathbf{x}_* - \hat{\mathbf{m}})^T \hat{S}^{-1} (\mathbf{x}_* - \hat{\mathbf{m}})$$

- The KL divergence results in:

$$\mathrm{KL} = f(n, \hat{z}^2)$$

- Again, the KL divergence does not depend on the statistics!!

# KL vs ML - Multivariate Gaussian



# Information Theoretic Novelty Detection

Based on the connection between the information theoretic approach and statistical testing in the Gaussian case, we propose two extensions:

- Mixture of Gaussians (univariate and multivariate)
- time series (linear autoregressive)

# Mixture of Gaussians

- Pdf:

$$p(x|\theta) = \sum_{k=1}^{c} \pi_k \mathcal{N}(x|m_k, s_k^2)$$

- KL divergence between:
  - $p(x|\hat{\theta})$ the mixture learned on $X$ (for example using the EM algorithm)
  - $p(x|\hat{\theta}^*)$ the mixture learned starting from $p(x|\hat{\theta})$ and EM step on $X \cup \{x_*\}$
- No closed form for the KL divergence between two mixtures!!

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# Approximation of the KL divergence

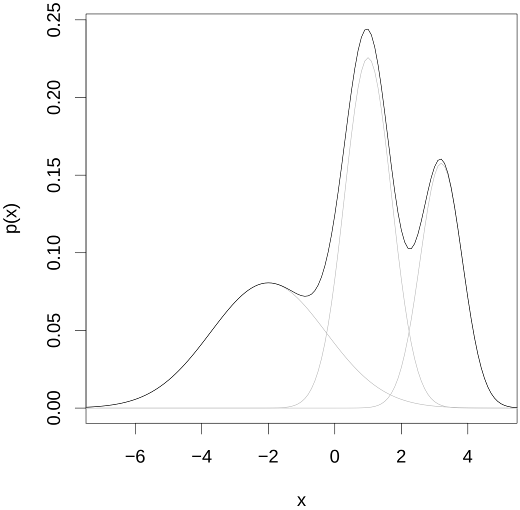
- Two-stage approximation
  - second order approximation of the logarithm

$$p(x|\hat{\theta}^*) = p(x|\hat{\theta}) + \delta p(x|\hat{\theta})$$

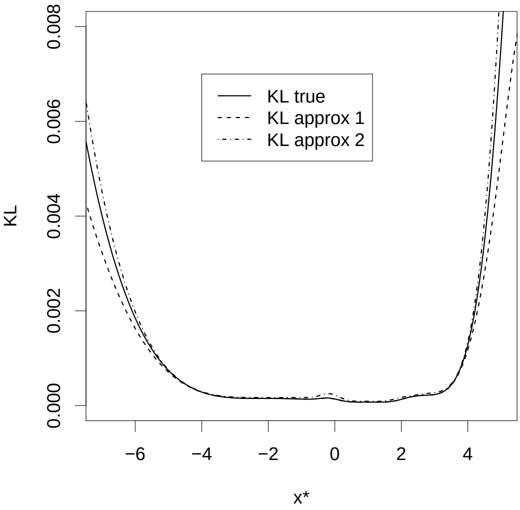
$$\log\left[\frac{p(x|\hat{\theta})}{p(x|\hat{\theta}^*)}\right] = -\log\left[1 + \frac{\delta p(x|\hat{\theta})}{p(x|\hat{\theta})}\right]$$

  - crisp responsibilities

# Example - the pdf



# Example - the approximation



# Mixture of Gaussian - KL divergence

- the approximation of the KL divergence is:

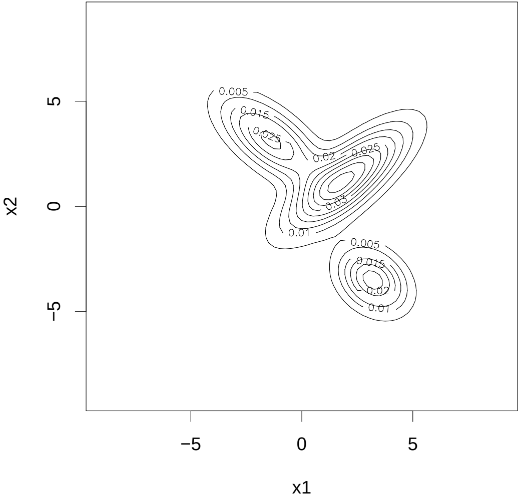
$$\mathrm{KL} = f(n, \hat{z}_k^2, \hat{\pi}_k, \hat{s}_k)$$

where:

$$\hat{z}_k^2 = \frac{(x_* - \hat{m}_k)^2}{\hat{s}_k^2}$$

- Monte Carlo simulation to obtain the quantiles of the KL divergence
- We can take into account the variability of the means and the variances!!

# Mixture of Gaussian - Results



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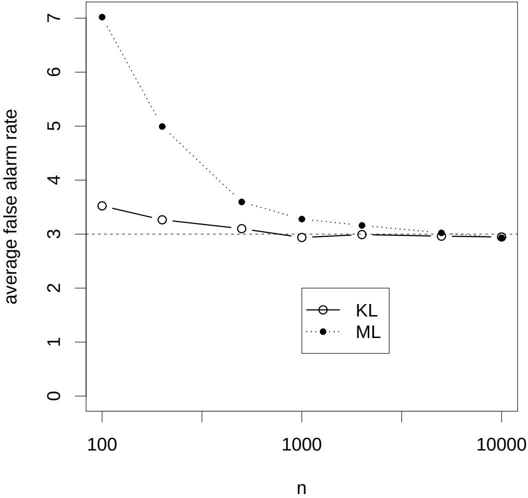

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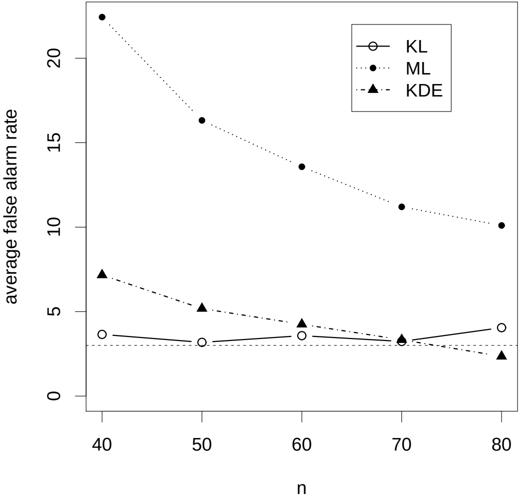

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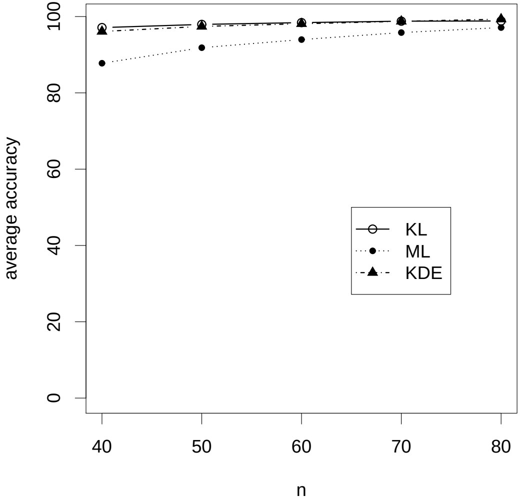

# Autoregressive model - AR($d$)

- In many applications the i.i.d. assumption is not valid
- A well established framework for modeling temporal correlation in a series of observation is given by autoregressive models:

$$x_{t+1} = \boldsymbol{\alpha}^{\mathrm{T}} \mathbf{x}_t + \varepsilon_{t+1} + \mu$$

- $\boldsymbol{\alpha} = (\alpha_1, \ldots, \alpha_d)$
- $\mathbf{x}_t = (x_t, x_{t-1}, \ldots, x_{t-d+1})$
- $\varepsilon_{t+1} \sim \mathcal{N}(0, \gamma^2)$ and i.i.d.
- $\mu$ allows to model series with any mean value $m$

# Autoregressive model - Parameter Estimation

$$c_k = \mathrm{E}[(x_i - m)(x_{i-k} - m)] \qquad k = 1, \ldots, d$$

Introducing the vector $\mathbf{c} = (c_1, c_2, \ldots, c_d)^{\mathrm{T}}$ and the matrix $C$:

$$C = \begin{pmatrix} c_0 & c_1 & \cdots & c_{d-1} \\ c_1 & c_0 & \cdots & c_{d-2} \\ \vdots & \vdots & \ddots & \vdots \\ c_{d-1} & c_{d-2} & \cdots & c_0 \end{pmatrix}$$

we see that:

$$\alpha = C^{-1}\mathbf{c}$$

# Autoregressive model - Parameter Estimation

Once we have $\hat{\boldsymbol{\alpha}}$, we can estimate the other parameters of the model $\mu$ and $\gamma$.
Let's focus on $\hat{\gamma}^2$

$$\hat{\gamma}^2 = \frac{1}{n-d} \sum_{i=d}^{n-1} \left( x_{i+1} - \hat{\boldsymbol{\alpha}}^{\mathrm{T}} \mathbf{x}_i - \hat{\mu} \right)^2 = \frac{1}{n-d} \sum_{i=d}^{n-1} \hat{\varepsilon}_{i+1}^2$$

In a ML approach to novelty detection we test a new data point on the basis of $\hat{\gamma}^2$

# Autoregressive model - Information theoretic measure

- Updated version of the parameters when we add a new data point $x_*$: $\hat{\alpha}_*$, $\hat{\mu}_*$, and $\hat{\gamma}_*^2$
- Information content of $x_*$ in the null hypothesis that it has been generated from the same model:

$$\mathrm{KL}\left[\mathcal{N}(\varepsilon|0,\hat{\gamma}^2)\|\mathcal{N}(\varepsilon|0,\hat{\gamma}_*^2)\right] = f\left(\frac{\hat{\gamma}_*^2}{\hat{\gamma}^2}\right)$$

# Approximating the KL divergence

Let's focus on the ratio $\frac{\hat{\gamma}_*^2}{\hat{\gamma}^2}$

- Write the estimated parameters as their true values plus a term that is given by the fact that the estimation is based on a finite set of observations. For $\boldsymbol{\alpha}$, for example:

$$\hat{\boldsymbol{\alpha}} = \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha} \qquad \hat{\boldsymbol{\alpha}}_* = \boldsymbol{\alpha} + \Delta\boldsymbol{\alpha}_*$$

- Substitute these relations into $\hat{\gamma}^2$ and $\hat{\gamma}_*^2$
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# Approximating the KL divergence

The ratio becomes a function of this form:

$$\frac{\hat{\gamma}_*^2}{\hat{\gamma}^2} \simeq \frac{n-d}{n-d+1}\left[1 + \frac{\Delta}{\sum_{i=d}^{n-1} \varepsilon_{i+1}^2}\right]$$

where:

$$\Delta = \varepsilon_*^2 + \text{correction terms}$$

# Approximating the KL divergence

- The leading term of the ratio $\frac{\Delta}{\sum_{i=d}^{n-1} \varepsilon_{i+1}^2}$ is therefore:

$$\frac{\varepsilon_*^2}{\sum_{i=d}^{n-1} \varepsilon_{i+1}^2} \sim \frac{1}{n-d} F_{(1,n-d)}$$

- We propose this approximation:

$$\frac{\Delta}{\sum_{i=d}^{n-1} \varepsilon_{i+1}^2} \sim \tau \frac{1}{n-d} F_{(1,n-d)}$$

- We compute $\tau$ to match the expected value of the $F$-distribution with the actual distribution of the ratio $\frac{\Delta}{\sum_{i=d}^{n-1} \varepsilon_{i+1}^2}$

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Finally, the test we propose is:

$$\frac{\hat{\gamma}_*^2}{\hat{\gamma}^2} = \frac{n-d}{n-d+1}\left[1 + \tau \frac{1}{n-d} F_{(1,n-d)}\right]$$

$$\tau = 1 + 2\frac{d}{(n-d)} + \frac{2}{n}(1 - \sum_i \hat{\alpha}_i)^2 - \frac{2}{n}(1 - \sum_i \hat{\alpha}_i)$$

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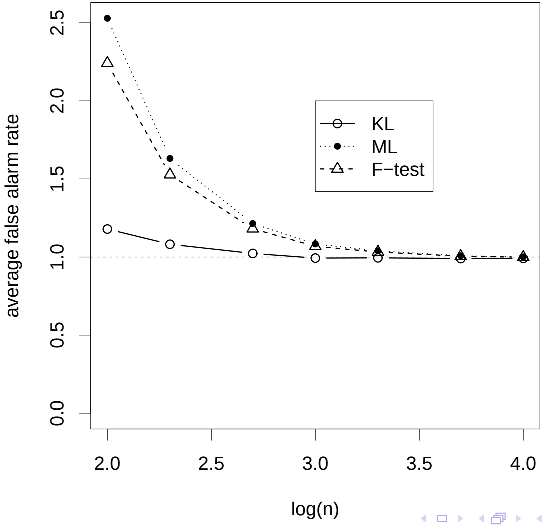
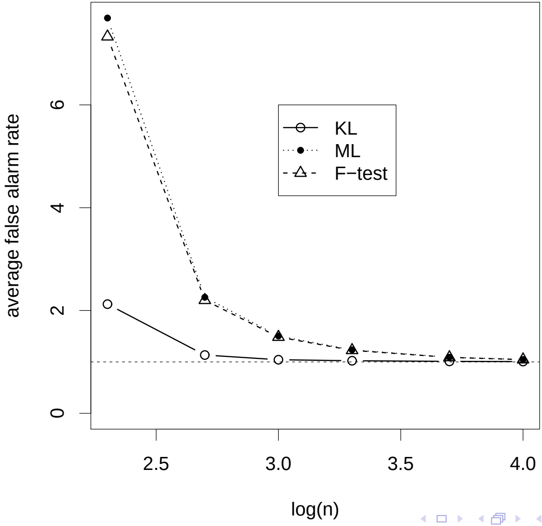
# AR(10) - Results



# AR(50) - Results



# Conclusions and Future Works

- We recast novelty detection in the framework of information theory
- Important connections with statistical testing
- Control of the false positive rate even for small data sets
- Model selection is crucial
- Extension to the exponential family (?)
- Regularization (?)
- Extend to model based novelties

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# Contacts & References

- email: m.filippone@dcs.shef.ac.uk
- web: http://www.dcs.shef.ac.uk/~filippone/
- papers:

[1] M. Filippone, G. Sanguinetti. **Information theoretic novelty detection**. *Pattern Recognition*, to appear.

[2] M. Filippone and G. Sanguinetti. **Novelty detection in autoregressive models using information theoretic measures**. Technical Report CS-09-06, Department of Computer Science, University of Sheffield, July 2009.

Thank You!