

Statistical Machine Learning Approaches to Change Detection

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 - Thesis: Statistical Machine Learning Approaches to Change Detection
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Learning from Data

The era of big data is coming.

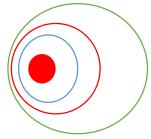


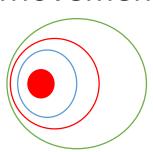
- Without interpretation, raw data make no sense to human.
- Machine learning helps make sense out of data.

The Human Learning in Astronomy A brief history

- Learning Constellations
 - Patterns of Stars
 - Predicting warfare, harvest

- Patterns of Planetary Movements
 - Tycho Brahe's data
 - Kepler's law

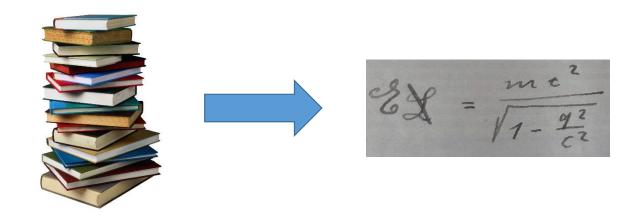




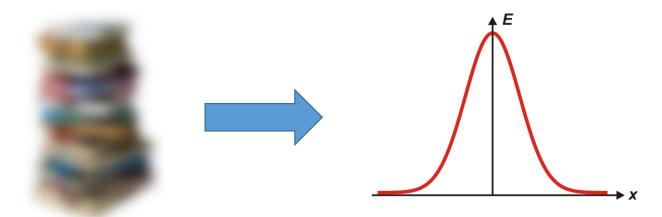
- Newton Laws
 - Predicting the movements of new planets = ma



Statistical Machine Learning



Data is so big, so we look for compressive rules (patterns).



Data involving uncertainty, we prefer statistical patterns.

However, Data is Always Changing!

Patterns learned today may be useless tomorrow.



Everyday, 20% Google queries have never been seen before¹.

Learning pattern changes are also important.



Red spots are detected changes on NASA satellite images, reflecting the heaviest damages after super typhoon Haiyan struck Philippines on Nov. 8 2013 ².

We need a new paradigm of machine learning.

1. http://certifiedknowledge.org/blog/are-search-queries-becoming-even-more-unique-statistics-from-google

2. http://www.nasa.gov/content/goddard/haiyan-northwestern-pacific-ocean/#.Uq3u6vQW2So

Two Paradigms of Machine Learning



Static Learning: Data do not change

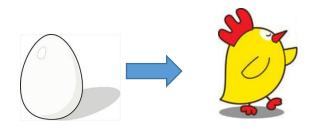
(p.5)

Supervised

Predict Future: p(y|x)Classification, Regression (Duda et al., 2001, Bishop, 2006)

Unsupervised

Learn Patterns: p(x)Clustering, Anomaly Detection
(Murphy, 2012, Shaw-Taylor & Cristianini, 2004)



Dynamic Learning: Data are shifting

Supervised

Predict future under data shifts $p(y'|x'), p \neq p'$

e.g. Transfer learning (Sugiyama et al., 2012)

Unsupervised

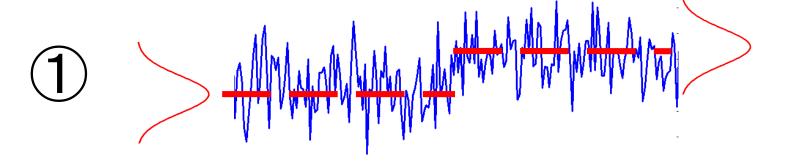
Learn changes of patterns p/q or p-q, $p \neq q$

Change detection

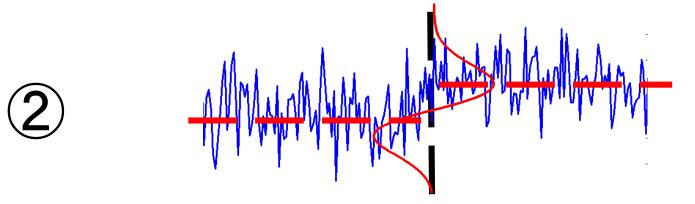
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Two Ways of Learning Changes

Separated Learning Approach



Direct Learning Approach

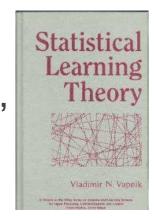


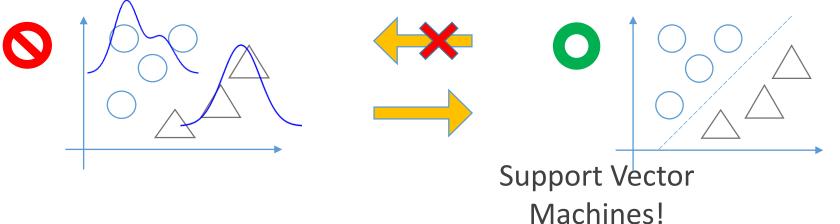
Which one is the best?

Vapnik's Principle

(Vapnik, Statistical Learning Theory, 1998)

- Generally, we prefer ② to ① because of **Vapnik's** principle.
- "When solving a problem of interest, one should not solve a more general problem as an intermediate step."

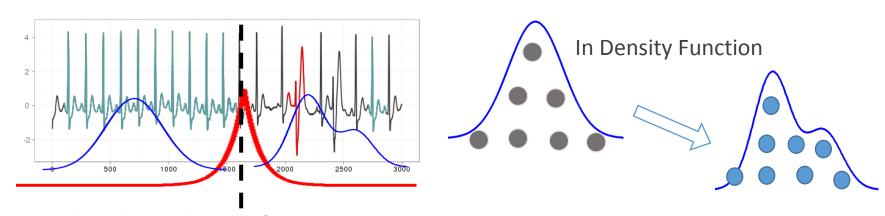




Unsupervised Change Detection

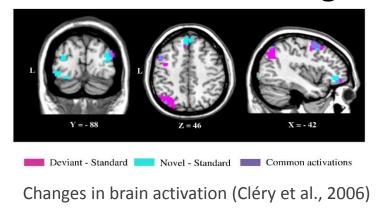
(p.10)

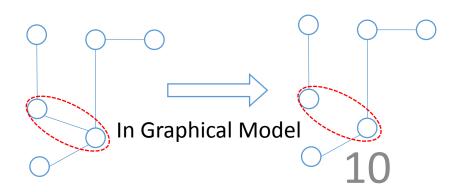
Has it been changed? Distributional Change Detection



Heartbeat disorder detection, from JMOTIF project.

What has been changed? Structural Change Detection

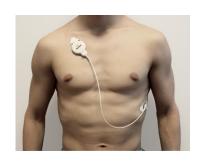




Chapter 2, Distributional Change Detection

- 1. Background & Existing Methods
- 2. Problem Formulation
- 3. Divergence based Change-point Score
- 4. Experiments

Changes in Time-series



Health monitoring

e.g. Kawahara et al., 2012



Engineering fault detection

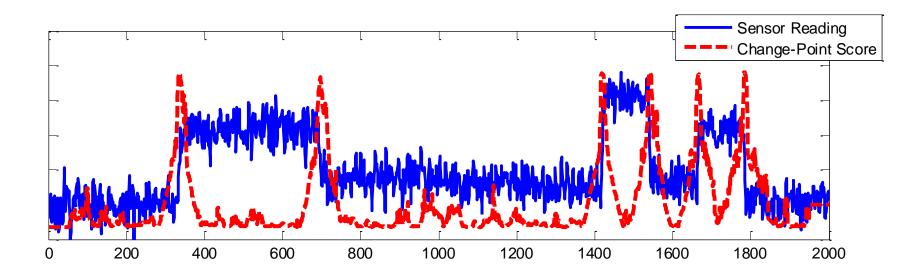
e.g. Keogh et al., 2005



Network intrusion detection

e.g. Takeuchi et al., 2006

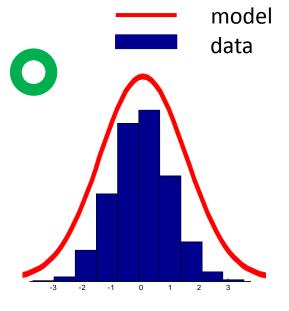
Distributional Change Detection in Time-series

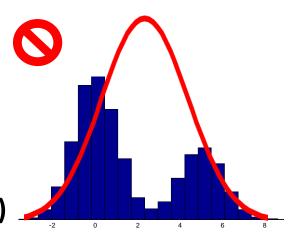


- Objective: Detecting abrupt changes lying among time-series data
- Change-point score: Plausibility of changes that have happened
- Metrics: True positive rate, false positive rate, and detection delay

Existing Methods

- Model based Methods:
 - Auto Regressive (AR)
 - (Takeuchi and Yamanishi, 2006)
 - Autoregressive model with Gaussian noise.
 - Singular Spectrum Transformation (SST)
 - (Moskvina and Zhigljavsky, 2003)
 - Subspace Identification (SI)
 - (Kawahara et al., 2007)
 - State Space model with Gaussian noise.
- Model-free Methods:
 - One-class Support Vector Machine (OSVM)
 - (Desobry et al., 2005)
 - Density Ratio based Methods (KLIEP)
 - KLIEP (Kawahara & Sugiyama, 2009)
 - No model assumption.





Model based methods fail to characterize data when model mismatches.

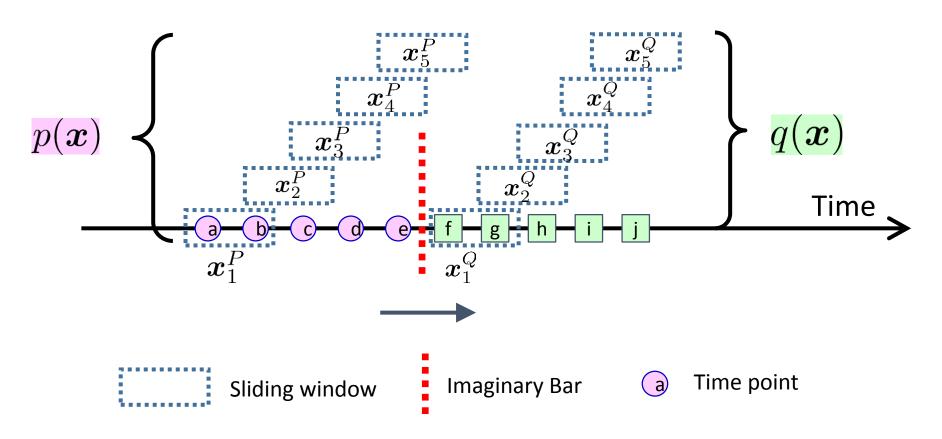
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Chapter 2, Distributional Change Detection

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Formulate Problem from Time-series

- Construct samples by using sliding window.
- An imaginary bar in the middle divides samples into two groups.
- Assume two groups of samples are from p and q.



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Divergence based Change Point Detection

- Need a **measure of change** between p(x) and q(x).
- f-divergence is a **distance** from p to q.

(Ali and Silvey, 1966)

$$\mathrm{D}[p\|q] = \int f \left(rac{p(oldsymbol{x})}{q(oldsymbol{x})}
ight) q(oldsymbol{x}) \, \mathrm{d}oldsymbol{x} \quad egin{array}{l} f ext{is convex} \ f(1) = 0 \end{array}$$

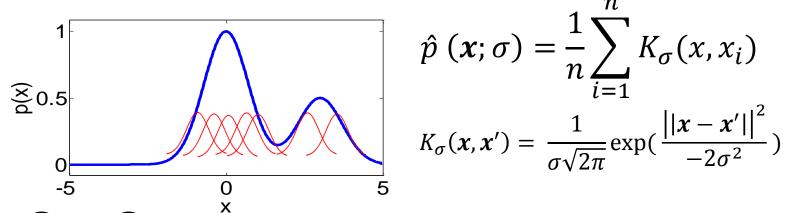
- f is a function of a ratio between two **probability** density functions (p and q).
- D[p||q] is asymmetric, thus we symmetrized it:

$$D[p||q] + D[q||p]$$

Density Estimation

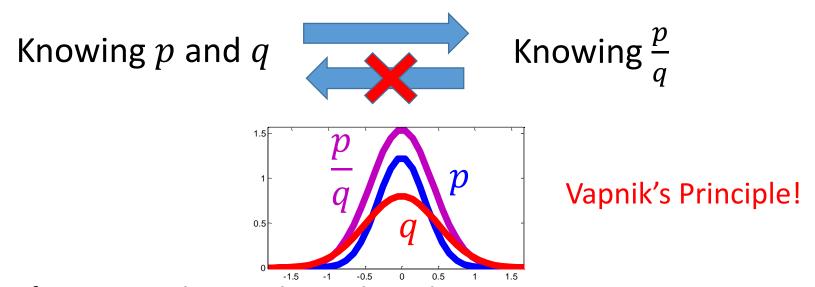
A naive way is a two step approach:

• e.g. Kernel Density Estimation (Csörgo & Horváth 1988)



- 1 or 2 is carried out without taking care of the ratio.
 - Error may be magnified after the division.

Density Ratio Estimation



• Direct Density Ratio Estimation (Sugiyama et al., 2012).

$$rac{p(oldsymbol{x})}{q(oldsymbol{x})}pprox\hat{r}(oldsymbol{x};oldsymbol{ heta})=\sum_{i}^{n} heta_{i}K_{\sigma}(oldsymbol{x},oldsymbol{x}_{i})$$

• By plugging in estimated density ratio, we may obtain various *f*-divergences.

Kullback-Leibler Divergence as Change-point Score (p.22)

We may have different choices for change-point score:

Kullback-Leibler Divergence (Kullback and Leibler, 1951)

$$\mathrm{KL}[p||q] = \int p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} d\boldsymbol{x}$$

- Has been applied, and promising results were obtained.
 Kawahara & Sugiyama, SDM 2009
- Density ratio can be obtained via Kullback-leibler Importance Estimation Procedure (KLIEP) (Sugiyama, et al., NIPS 2008).
 - Optimization for density ratio is convex!
 - Slow, less robust

Pearson Divergence as Change-point Score (pp.24)

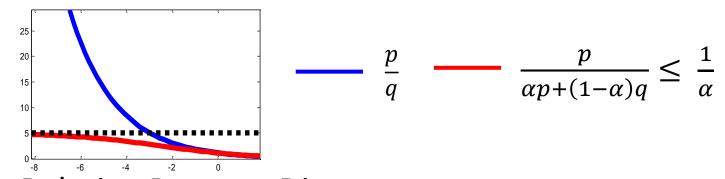
- The log term in Kullback-leibler divergence can go infinity if $\frac{p(x)}{q(x)} = 0$.
- Pearson Divergence (Pearson, 1900)

$$PE[p||q] = \frac{1}{2} \int q(\boldsymbol{x}) \left(\frac{p(\boldsymbol{x})}{q(\boldsymbol{x})} - 1 \right)^2 d\boldsymbol{x}$$

- Density ratio can be obtained via unconstrained Least Square Importance Fitting (uLSIF) (Kanamori, et al., JMLR 2009).
- Solution has an analytic form.
- Fast, relatively robust!

Relative Pearson Divergence as Change-point Score (pp.26)

- The density ratio may go unbounded.
- Bounded Density Ratio -> Relative Density Ratio



• Relative Pearson Divergence (Yamada, et al., NIPS 2011)

$$PE_{\alpha}[p||q] = PE[p||\alpha p + (1 - \alpha)q]$$

$$= \frac{1}{2} \int (\alpha p(\mathbf{x}) + (1 - \alpha)q(\mathbf{x})) \left(\frac{p(\mathbf{x})}{\alpha p(\mathbf{x}) + (1 - \alpha)q(\mathbf{x})} - 1\right)^{2} d\mathbf{x}$$



Divergences as Change-point Scores (Summary) (pp.22-28)

Kullback-Leibler Divergence (via KLIEP):

$$\widehat{\mathrm{KL}} := rac{1}{n} \sum_{i=1}^n \log \hat{r}(m{x}_i)$$
 Existing method

Previous Work: Kawahara & Sugiyama, 2009

Pearson Divergence (via uLSIF):

$$\widehat{PE} := -\frac{1}{2n} \sum_{i=1}^{n} \hat{r}(x_i')^2 + \frac{1}{n} \sum_{i=1}^{n} \hat{r}(x_i) - \frac{1}{2}$$

Relative Pearson Divergence (via RuLSIF):

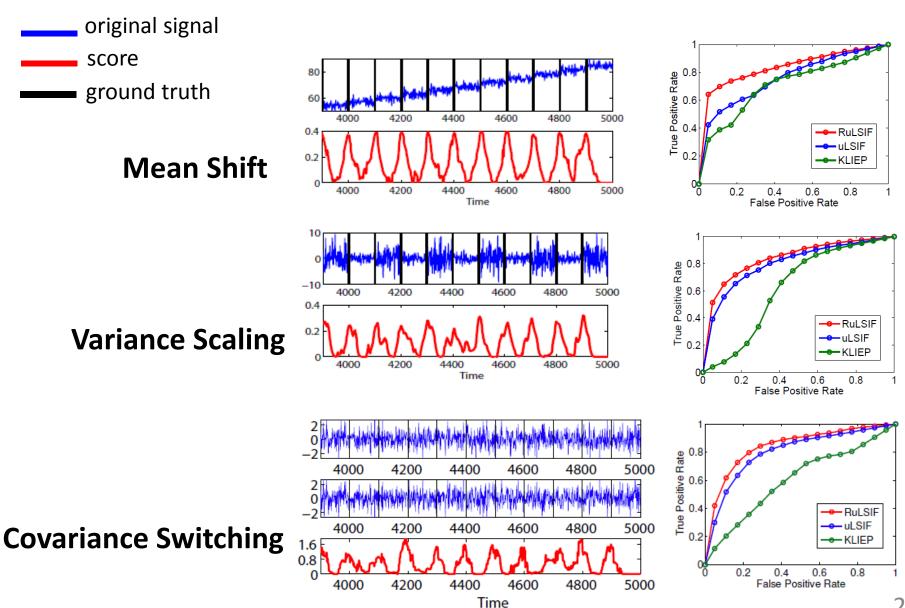
$$\widehat{PE}_{\alpha} = -\frac{\alpha}{2n} \sum_{i=1}^{n} \hat{r}(\boldsymbol{x}_{i})^{2} - \frac{1-\alpha}{2n} \sum_{i=1}^{n} \hat{r}(\boldsymbol{x}'_{i})^{2} + \frac{1}{n} \sum_{i=1}^{n} \hat{r}(\boldsymbol{x}_{i}) - \frac{1}{2} \boldsymbol{J}_{\alpha}$$

Robust

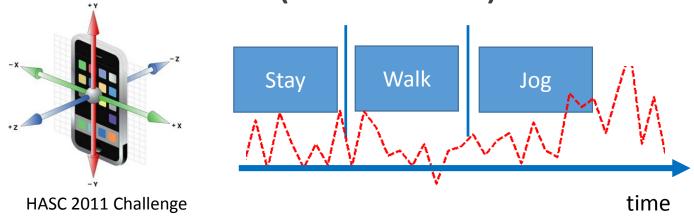
Chapter 2, Distributional Change Detection

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Experiments (Synthetic)

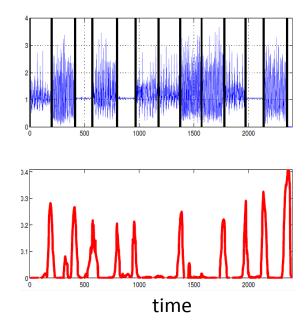


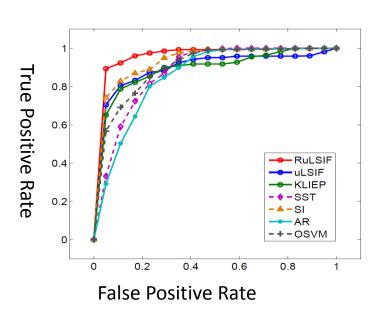
Experiments (Sensor)



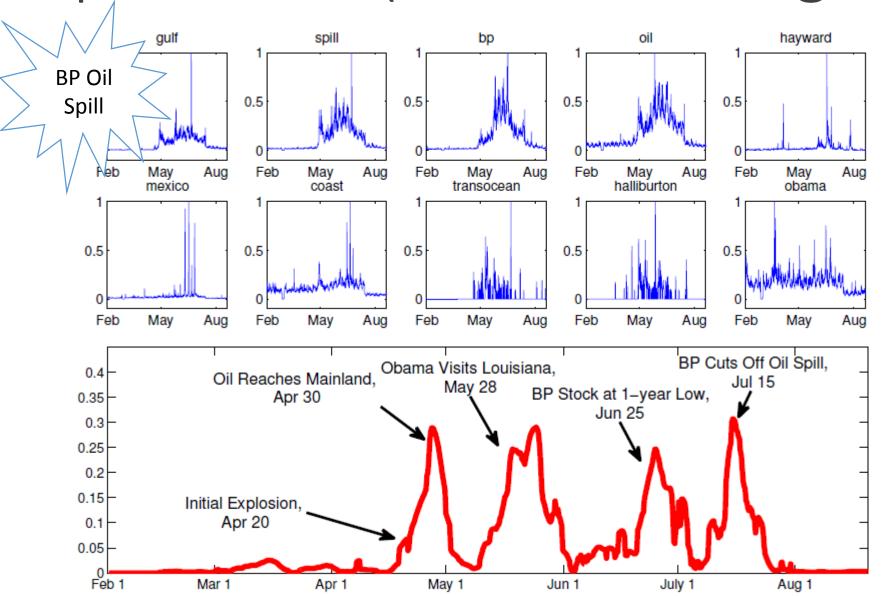
Mobile *Sensor* data, measured in 20 seconds, recording human activity.

Task: Segmenting the activities. e.g. walk, jogging, stairs up/down...





Experiments (Twitter Messages)



Conclusion

 A robust and model-free method for distributional change detection in time-series data was proposed.

 The proposed method obtained the leading performance in various artificial and real-world experiments.

Chapter 3, Structural Change Detection

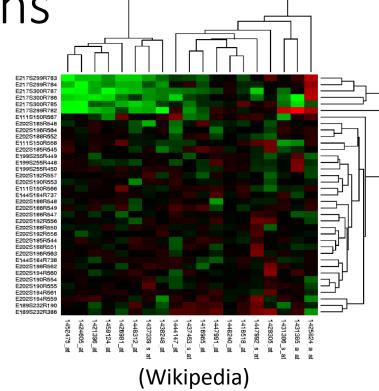
- 1. Background
- 2. Separate Estimation Methods
- 3. Proposed Methods
- 4. Experiments

Patterns of Interactions

 Genes regulate each other via gene network.

 Brain EEG signals may be synchronized in a certain pattern.

 However, such patterns of interactions may be changing!

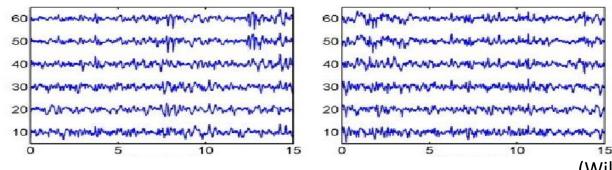




Structural Change Detection

• Interactions between features may change. $\mathbf{x} = (x^{(1)}, \dots, x^{(d)})^{\mathrm{T}}$

$$\{\boldsymbol{x}_i^P\}_{i=1}^n \overset{\text{i.i.d.}}{\sim} p(\boldsymbol{x}) \qquad \{\boldsymbol{x}_i^Q\}_{i-1}^n \overset{\text{i.i.d.}}{\sim} q(\boldsymbol{x})$$



(Williamson et al., 2012)

The change of brain signal correlation at two different experiment intervals.

- e.g. Interactions between some genes may be activated,
 - but only under some conditions.
- "apple" may co-occur with "banana" quite often in cookbook,
 - but not in IT news.

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Chapter 3, Structural Change Detection

- 1. Background
- 2. Existing Methods
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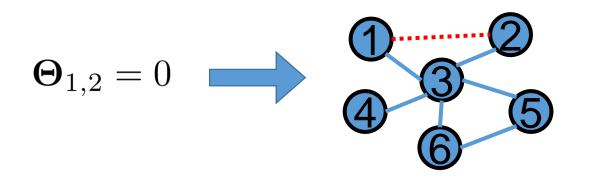
Gaussian Markov Networks (GMNs)

- The interactions between random variables can be modelled by Markov Networks.
- Markov Networks (MNs) are undirected Graphical Models.
- The simplest example of MN is a Gaussian MN:

$$p(\boldsymbol{x}; \boldsymbol{\Theta}) = \frac{\det(\boldsymbol{\Theta})^{1/2}}{\left(2\pi\right)^{d/2}} \exp\left(-\frac{1}{2} \boldsymbol{x}^{\top} \boldsymbol{\Theta} \boldsymbol{x}\right)$$

$$\mathbf{x} = (x^{(1)}, x^{(2)}, \dots, x^{(d)})$$
 $\mathbf{\Theta}$ is the inverse covariance matrix

We can visualize the above MN using an undirected graph.



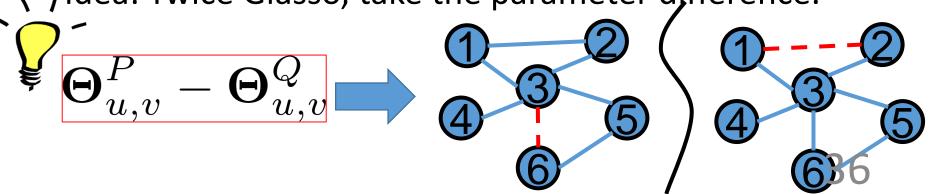
Estimating Separate GMN

Tibshirani, JRSS 1996; Friedman et al., Biostatistics 2008

- Recall, we would like to detect changes between MNs.
- Changes can be found once the structure of two separate GMNs are known to us.
- Estimating Sparse GMNs can be done via **Graphical Lasso (Glasso)**.

$$\max_{\mathbf{\Theta}^P} \sum_{i=1}^n \log p(\mathbf{x}_i^P; \mathbf{\Theta}^P) - \lambda^P \|\mathbf{\Theta}^P\|_1$$

、•, Idea: Twice Glasso, take the parameter difference.



Glasso: Pros and Cons

©Pros:

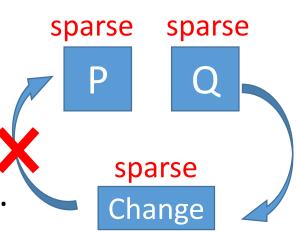
- Statistical properties are well studied.
- Off-the-shelf software can be used.
- Sparse change is produced.

Cons:

- Cannot detect high-order correlation.
- Not clear how to choose hyper-parameters.
- Does not work if p or q is dense.



Can we combine two optimizations into one?



Semi-direct Approach (Fused-lasso)

• We can impose sparsity directly on $\Theta_{u,v}^P - \Theta_{u,v}^Q$, using **Fused-lasso (Flasso)** (Tibshirani et al., 2005).

Consider the following objective:

$$\max_{\pmb{\theta}} \ell(\pmb{x}^P, \pmb{\Theta}^P) + \ell(\pmb{x}^Q, \pmb{\Theta}^Q) - \lambda \|\pmb{\Theta}^P - \pmb{\Theta}^Q\|_1$$
 Gaussian Gaussian (Zhang & Wang, UAI2010)

- \odot We don't have to assume p or q is sparse.
- © Sparsity control is much easier than Glasso.

Nonparanormal (NPN) Extension

Liu et al., JMLR 2009

- Gaussian assumption is too restrictive.
- However, considering general non-Gaussian model can be computationally challenging.
- We may consider a method half-way between Gaussian and non-Gaussian.
- Non-paranormal (NPN).

$$p(\boldsymbol{x}; \boldsymbol{\Theta}) = \frac{\det(\boldsymbol{\Theta})^{1/2}}{(2\pi)^{d/2}} \exp\left(-\frac{1}{2}\boldsymbol{f}(\boldsymbol{x})^{\top}\boldsymbol{\Theta}\boldsymbol{f}(\boldsymbol{x})\right) \prod_{i=1}^{d} |f_i'(x^{(i)})|$$

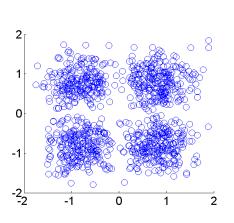
$$\mathbf{x} = (x^{(1)}, x^{(2)}, \dots, x^{(d)})$$

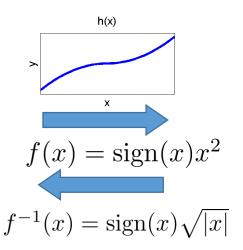
$$\mathbf{f}(\mathbf{x}) = (f_1(x^{(1)}), f_2(x^{(2)}), \dots, f_d(x^{(d)}))$$

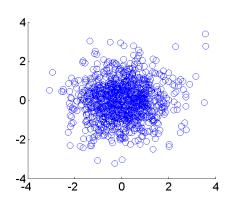
 f_k : Monotone, differentiable function

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Nonparanormal (NPN) Extension







- More flexible than Gaussian methods, still tractable.
- (3) However, NPN extension is still restrictive.

Non-Gaussian Log-linear Model

Pairwise Markov Network

$$p(\boldsymbol{x};\boldsymbol{\theta}) = \frac{1}{Z(\boldsymbol{\theta})} \exp \left(\sum_{u \geq v} \boldsymbol{\theta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)}) \right)$$

• **f** are feature vectors.

$$f: \mathcal{R}^2 \to \mathcal{R}^b$$

Gaussian: $f_{gau}(x, y) = xy$

Nonparanormal: $f_{npn}(x, y) = f(x)f(y)$

Polynomial: $f_{poly}(x, y) = [x^k, y^k, x^{k-1}y ..., x, y, 1]$

- The normalization term $Z(\theta)$ is generally intractable.
 - Gaussian or Nonparanormal models are exceptions.

The Normalization Issue

$$Z(\boldsymbol{\theta}) = \int \exp\left(\sum_{u \geq v} \boldsymbol{\theta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right) d\boldsymbol{x}$$

- However, for a generalized Markov Network, there is no closed-form for $Z(\theta)$.
- Importance Sampling (IS):

$$Z(\boldsymbol{\theta}) = \int p_{\text{inst}}(\boldsymbol{x}) \frac{\exp\left(\sum_{u \geq v} \boldsymbol{\theta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right)}{p_{\text{inst}}(\boldsymbol{x})} d\boldsymbol{x}$$

- IS can be used to extend both Glasso and Flasso.
 - IS-Glasso, IS-Flasso.

Chapter 3, Structural Change Detection

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Modeling Changes Directly

 $oldsymbol{ heta}$ Recall, our interest is: $oldsymbol{eta}_{u,v} := oldsymbol{ heta}_{u,v}^P - oldsymbol{ heta}_{u,v}^Q$

• The ratio of two MNs naturally incorporates the $\theta_{u,v}^P - \theta_{u,v}^Q$!

$$\frac{p(\boldsymbol{x};\boldsymbol{\theta}^{P})}{q(\boldsymbol{x};\boldsymbol{\theta}^{Q})} \propto \exp\left(\sum_{u \geq v} (\boldsymbol{\theta}_{u,v}^{P} - \boldsymbol{\theta}_{u,v}^{Q})^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right)$$

$$= \exp\left(\sum_{u \geq v} \boldsymbol{\beta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right)$$

So, model the **ratio** directly!

Modeling Changes Directly

Density ratio model:

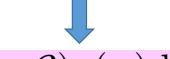
$$r(\boldsymbol{x}; \boldsymbol{\beta}) = \frac{1}{N(\boldsymbol{\beta})} \exp\left(\sum_{u \geq v} \boldsymbol{\beta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right)$$

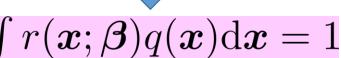
The normalization term is:

$$N(\boldsymbol{\beta}) = \int q(\boldsymbol{x}) \exp\left(\sum_{u \geq v} \boldsymbol{\beta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)}, x^{(v)})\right) d\boldsymbol{x}$$

To ensure:

$$\hat{p} = q(\mathbf{x})r(\mathbf{x}, \hat{\boldsymbol{\beta}})$$







Sample average approximation
Also works when integral has no closed form!

$$\frac{1}{n} \sum_{i}^{n} \exp \left(\sum_{u \geq v} \boldsymbol{\beta}_{u,v}^{\top} \boldsymbol{f}(x^{(u)Q}, x_{\boldsymbol{45}}^{(v)Q}) \right)$$

Estimating Density Ratio

Sugiyama et al., NIPS 2007

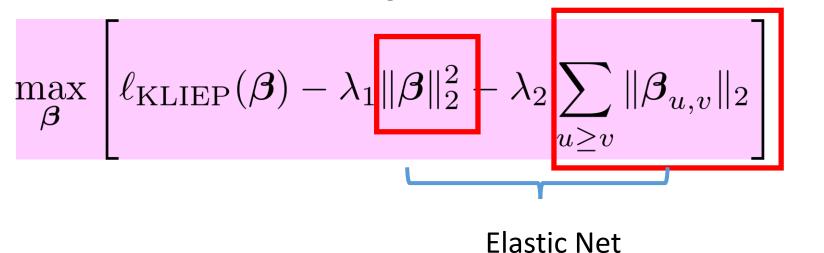
Kullback-Leibler Importance Estimation Procedure (KLIEP):

$$\underset{\boldsymbol{\theta}}{\operatorname{argmin}} \operatorname{KL}[p||\hat{p}] = \int p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{\hat{p}(\boldsymbol{x})} d\boldsymbol{x} \\
= \int p(\boldsymbol{x}) \log \frac{p(\boldsymbol{x})}{q(\boldsymbol{x})\hat{r}(\boldsymbol{x})} d\boldsymbol{x} \quad \hat{p}(\boldsymbol{x}) = q(\boldsymbol{x})\hat{r}(\boldsymbol{x}) \\
= \operatorname{Const.} - \int p(\boldsymbol{x}) \log \hat{r}(\boldsymbol{x}; \boldsymbol{\beta}) d\boldsymbol{x} \\
\underset{\boldsymbol{\theta}}{\operatorname{argmax}} \ell_{\operatorname{KLIEP}}(\boldsymbol{\beta}) = \frac{1}{n} \sum_{i=1}^{n} \log \hat{r}(\boldsymbol{x}_i; \boldsymbol{\beta})$$

Unconstrained convex optimization!

Sparse Regularization

L2 regularizers Group lasso regularizer

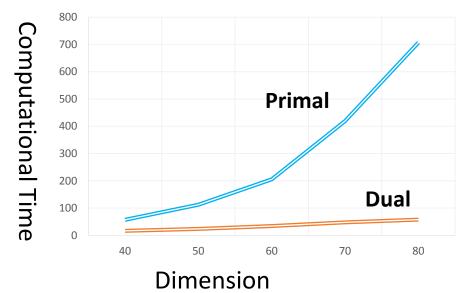


- Impose sparsity constraints on each factor $oldsymbol{eta}_{u,v}$.
 - equals to impose sparsity on changes.
- So finally, we can obtain a β with group sparsity!

The Dual Formulation p. 57

When dimensionality is high, the dual formulation is preferred.

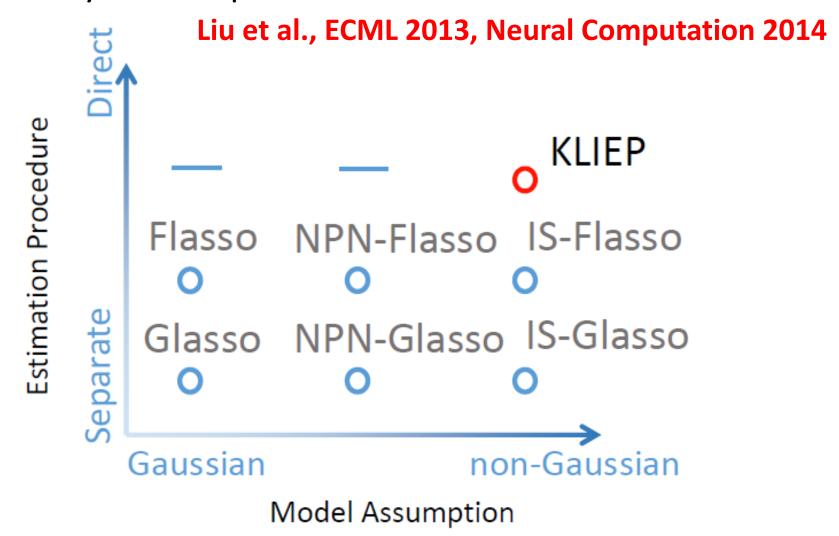
$$\min_{\boldsymbol{\alpha} = (\alpha_1, \dots, \alpha_{n_Q})^{\top}} \sum_{i=1}^{n_Q} \alpha_i \log \alpha_i + \frac{1}{\lambda_1} \sum_{u \geq v} \max(0, \|\boldsymbol{\xi}_{u,v}\| - \lambda_2)^2$$
subject to $\alpha_1, \dots, \alpha_{n_Q} \geq 0$ and
$$\sum_{i=1}^{n_Q} \alpha_i = 1,$$



$$oldsymbol{ heta}_{u,v} = egin{cases} rac{1}{\lambda_1} \left(1 - rac{\lambda_2}{\|oldsymbol{\xi}_{u,v}\|}
ight) oldsymbol{\xi}_{u,v} & ext{if } \|oldsymbol{\xi}_{u,v}\| > \lambda_2, \ oldsymbol{0} & ext{if } \|oldsymbol{\xi}_{u,v}\| \leq \lambda_2. \end{cases}$$

$$egin{aligned} m{\xi}_{u,v} &= m{g}_{u,v} - m{H}_{u,v} m{lpha}, \ m{H}_{u,v} &= [m{f}(x_1^{(u)Q}, x_1^{(v)Q}), \dots, m{f}(x_{n_Q}^{(u)Q}, x_{n_Q}^{(v)Q})], \ m{g}_{u,v} &= rac{1}{n_P} \sum_{i=1}^{n_P} m{f}(x_i^{(u)P}, x_i^{(v)P}). \end{aligned}$$

Summary: Comparison between Methods

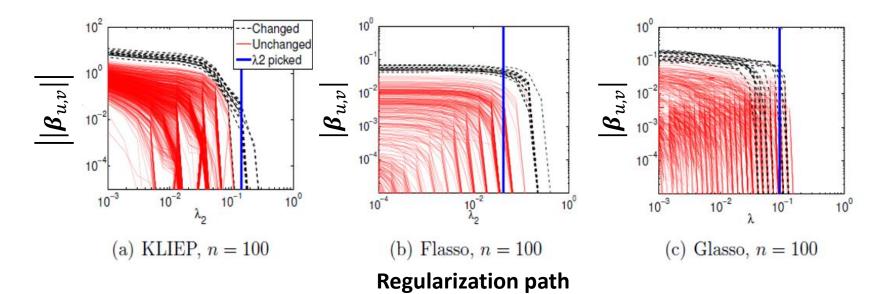


 The Illustration of methods on model assumption and estimation procedure

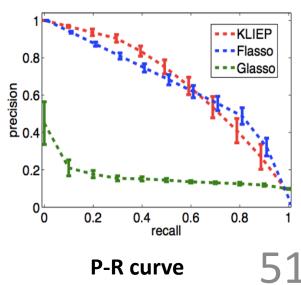
Chapter 3, Structural Change Detection

- 1. Background
- 2. Existing Methods
- 3. Proposed Methods
- 4. Experiments

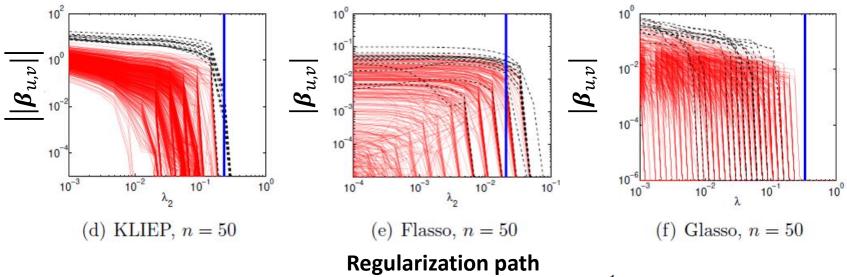
Gaussian Distribution (n = 100, d = 40)



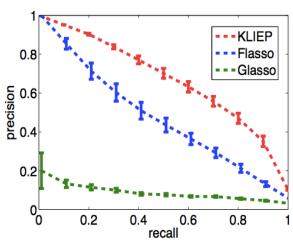
- Start from 40 dimensional GMN with random correlations.
- Randomly drops 15 edges.
- Precision and Recall curves are averaged over 20 runs.



Gaussian Distribution (n = 50, d = 40)

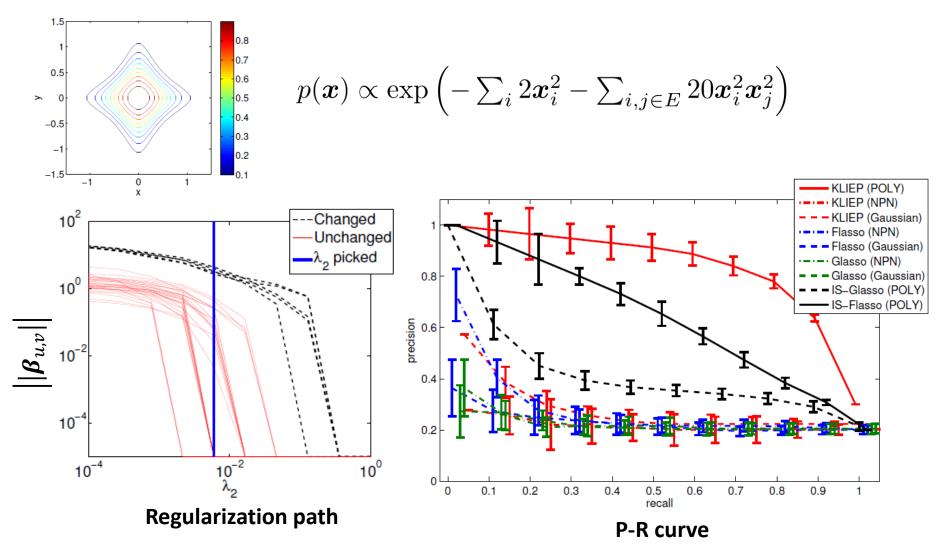


- Start from 40 dimensional GMN with random correlations.
- Randomly drops 15 edges.
- Precision and Recall curves are averaged over 20 runs.



P-R curve

Diamond Distribution (n = 5000, d = 9)



The proposed method has the leading performance.

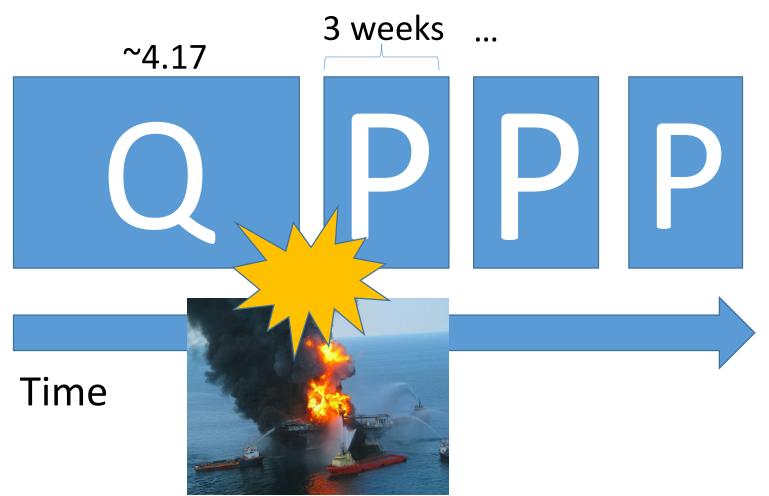
Twitter Dataset



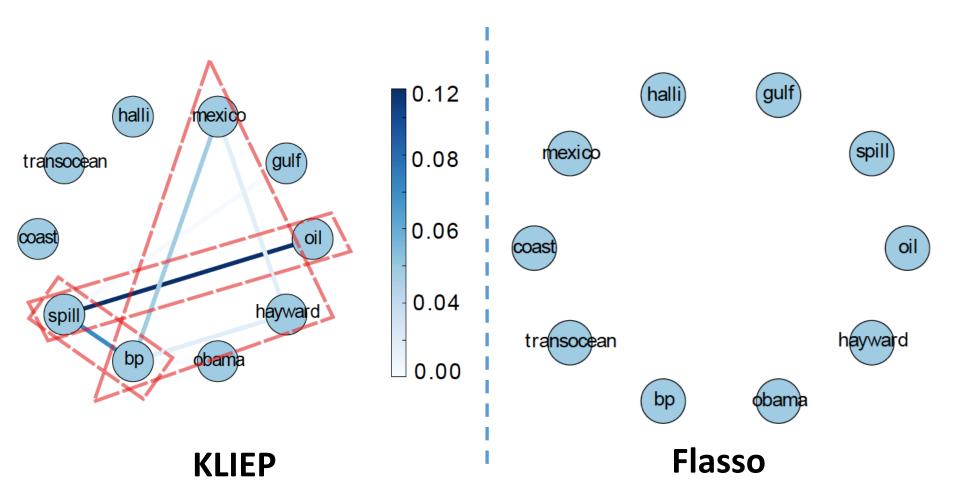
source: Wikipedia

- We choose the Deepwater Horizon oil spill as the target event.
 - Samples are the frequencies of 10 related keywords over time.
 - Detecting the change of co-occurrences on keywords before and after a certain event.

Twitter Dataset (pp. 68-72)



The Change of Correlation From 7.26-9.14



Small # of samples, severe over-fitting of Flasso!

Conclusion

 We proposed a direct structural change detection method for Markov Networks.

 The proposed method can handle non-Gaussian data, and can be efficiently solved using primal or dual objective.

 The proposed method showed the leading performance on both artificial and real-world datasets