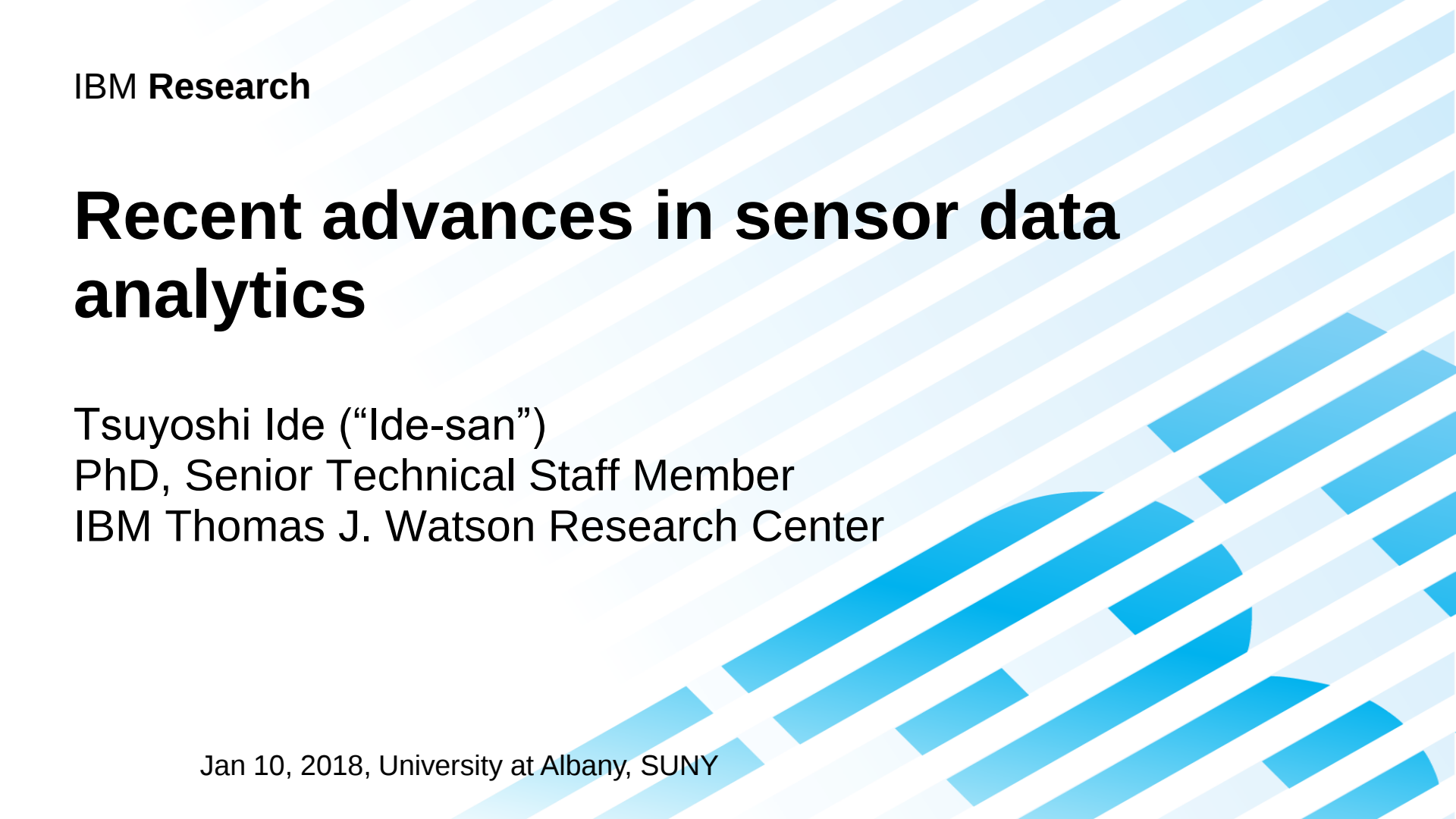




IBM Research

Recent advances in sensor data analytics

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PhD, Senior Technical Staff Member

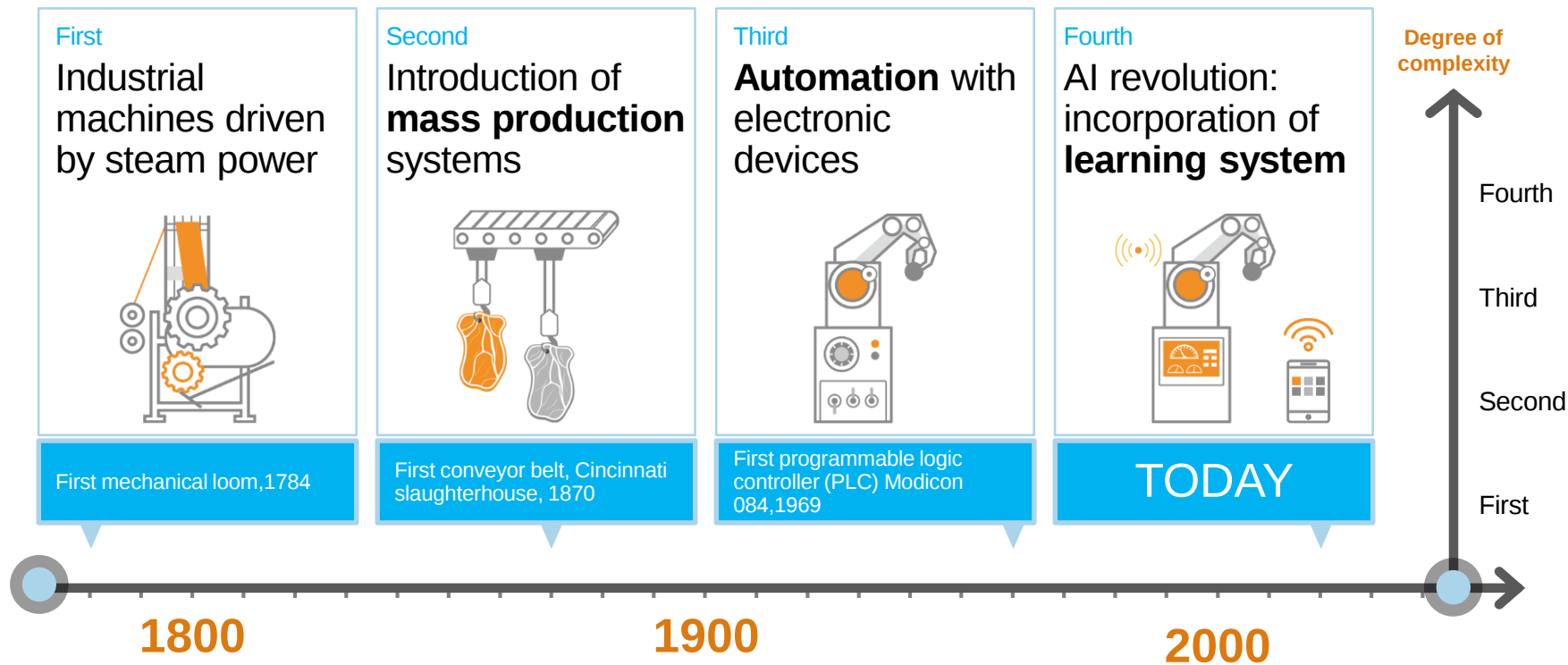
IBM Thomas J. Watson Research Center

Jan 10, 2018, University at Albany, SUNY

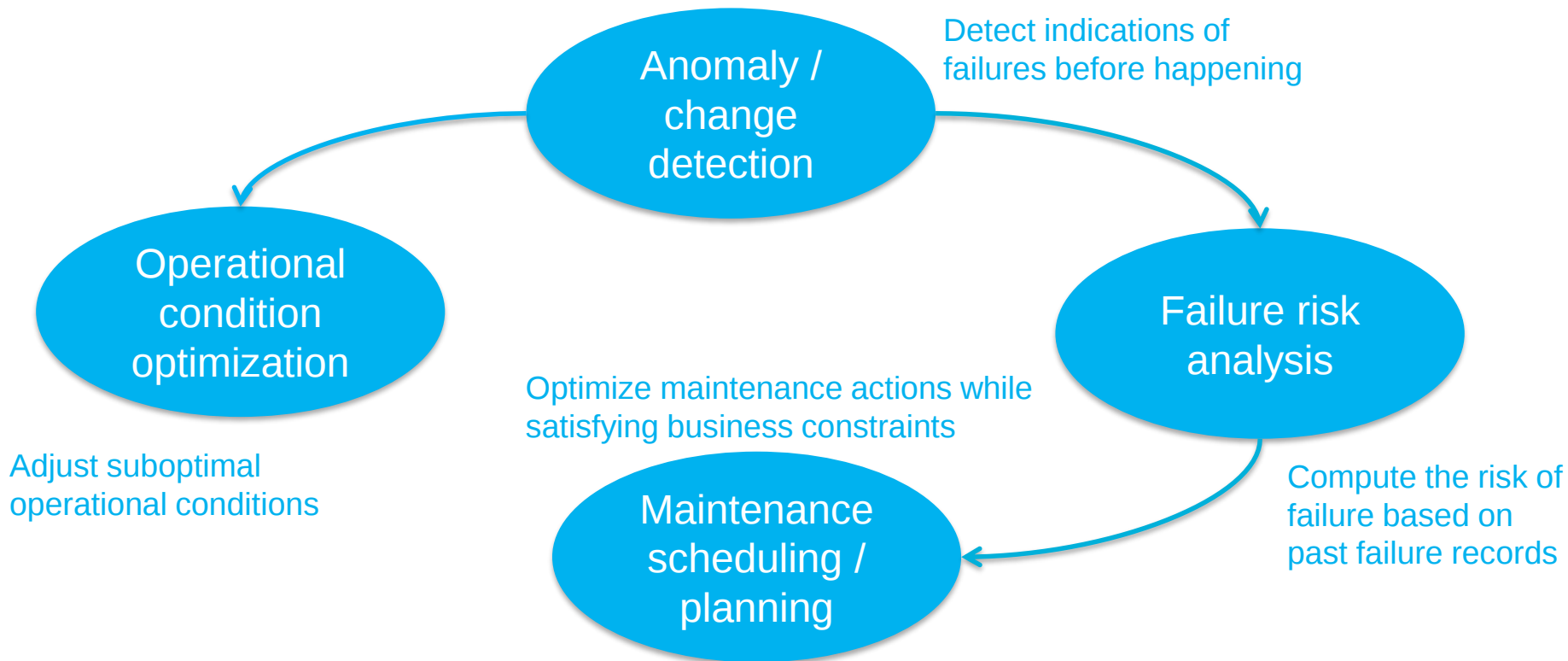
Agenda

- General challenges in Cognitive Manufacturing
- Change detection using directional statistics
 - T. Ide et al., IJCAI 16
- Multi-task multi-modal models for collective anomaly detection
 - T. Ide et al., ICDM 17
- Summary and future work

Cognitive Manufacturing is IBM's research initiative to address Industry 4.0



Key technical areas of Cognitive Manufacturing: Sensor data analytics plays a key role



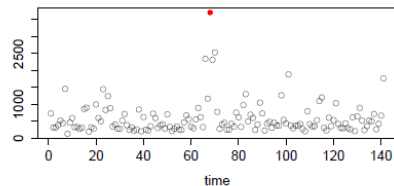
General challenges: No “one-size-fits-all” algorithm

■ Example in anomaly detection

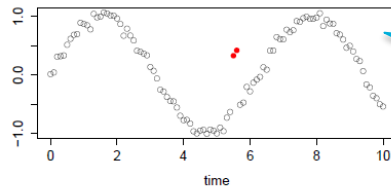
- “Happy families are all alike; every unhappy family is unhappy in its own way.” - *Anna Karenina*, Leo Tolstoy

Examples of anomalies

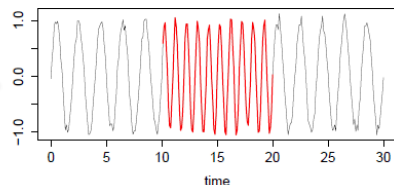
outliers (from i.i.d. samples)



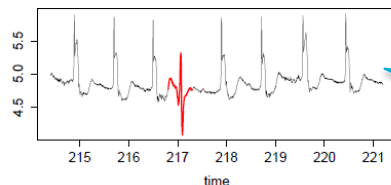
outliers (from auto-correlated samples)



change points



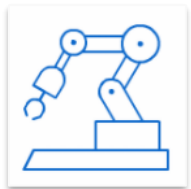
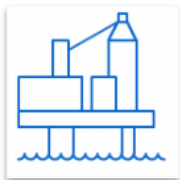
discords



General challenges: Business requirements often drive extension of existing approaches



...



...



...

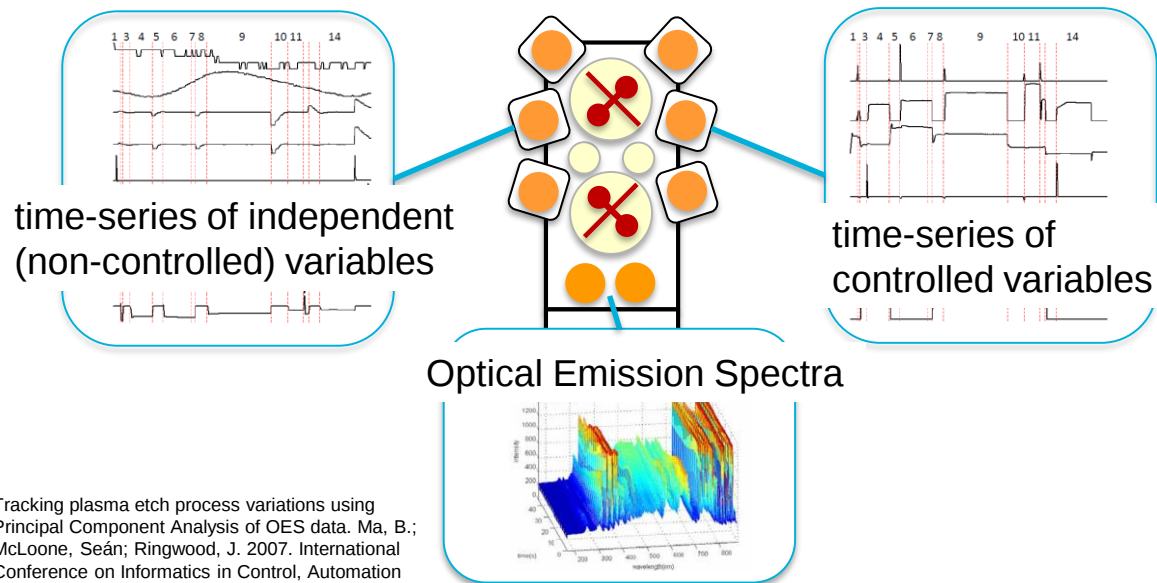


■ Example: corporate-level asset management with anomaly detection

- Typically assets are managed as a cohort
 - ✓ 10s of off-shore oil production systems
 - ✓ 100s of industrial robots
 - ✓ 1000s of electric vehicles in a certain area
- How can we leverage the commonality between assets to build an anomaly detection solution for individual assets?

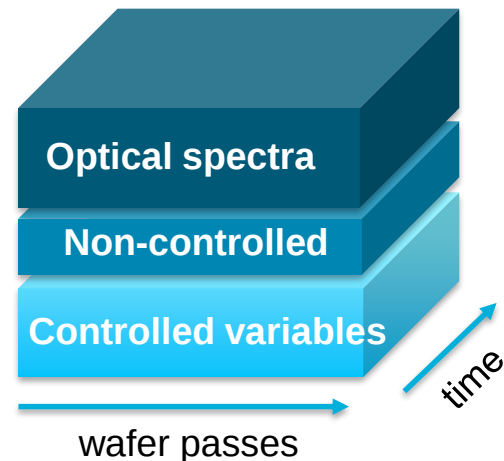
General challenges: Complex internal structure may exist in one measurement

Example from semiconductor manufacturing (etching)



Tracking plasma etch process variations using Principal Component Analysis of OES data. Ma, B.; McLoone, Seán; Ringwood, J. 2007. International Conference on Informatics in Control, Automation and Robotics (ICINCO 2007), Angers, France.

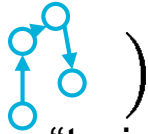
Each wafer pass is a higher-order tensor, rather than a vector

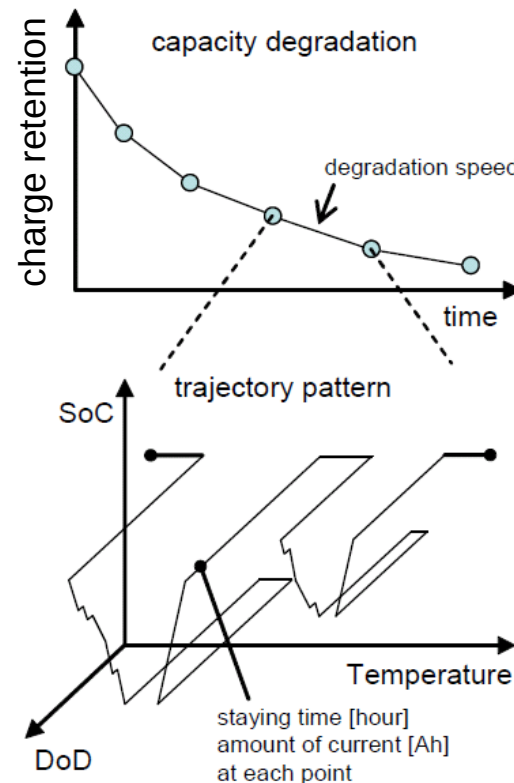


General challenges: Ready-to-use solution to your problem might not even exist

- Example: Charge retention (~ battery life) prediction of electric vehicle batteries
 - Depends on the entire history of battery usage
 - Battery usage is represented as a complex trajectory of a multi-dimensional space
- Charge retention prediction task should be formulated as “trajectory regression”

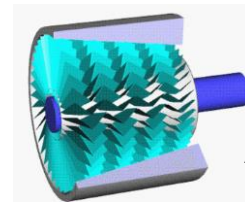
charge retention $y = f(\text{trajectory})$



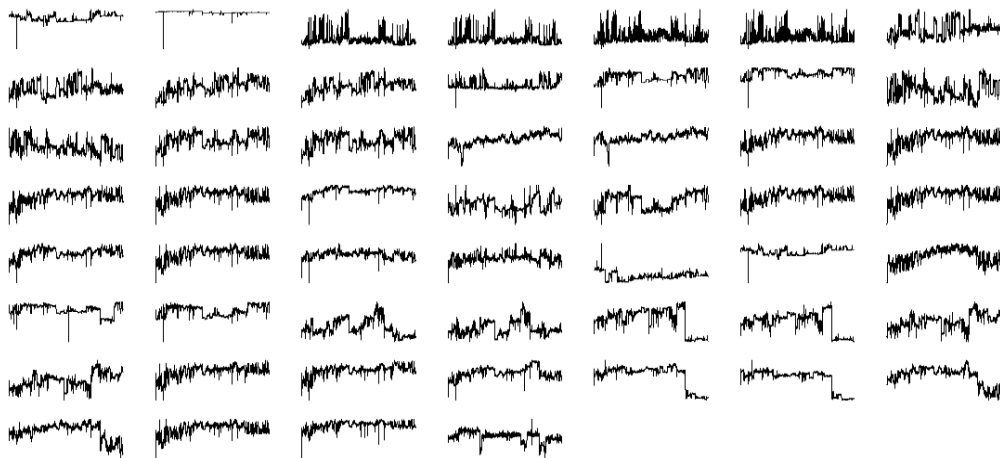


General challenges: Ground truth may not be available. Some degrees of freedom are usually latent

- Example: sensor data of a compressor of oil production system
 - Data taken under a normal operational condition
 - Noisy, nonstationary, heterogeneous, high-dimensional ...
- Hard to pinpoint what is indicative of malfunction



Axial compressor
(Source: Wikipedia)

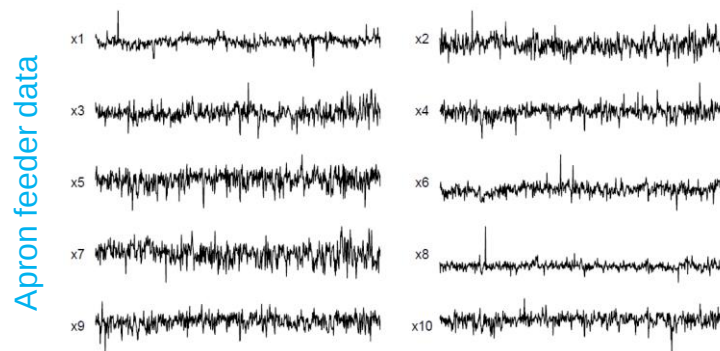


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Continuous operation of conveyor systems is critical in the mining industry

- **Business goal:** Ensure continuous operation of conveyor system (“apron feeder”) by detecting early indications of failures
- **Data:** Physical sensor data from conveyors and motors
 - Every several seconds over ~ 1 year
 - Sensors include: Gearbox temperatures, motor power consumptions, apron speed, etc.
- **Challenge:** Conveyor system is subject to significant fluctuation in load. Hard to characterize the normal operation
 - Mined crude ore never come in a uniform size



(simulation data)

Problem setting: change detection from multivariate noisy time-series data

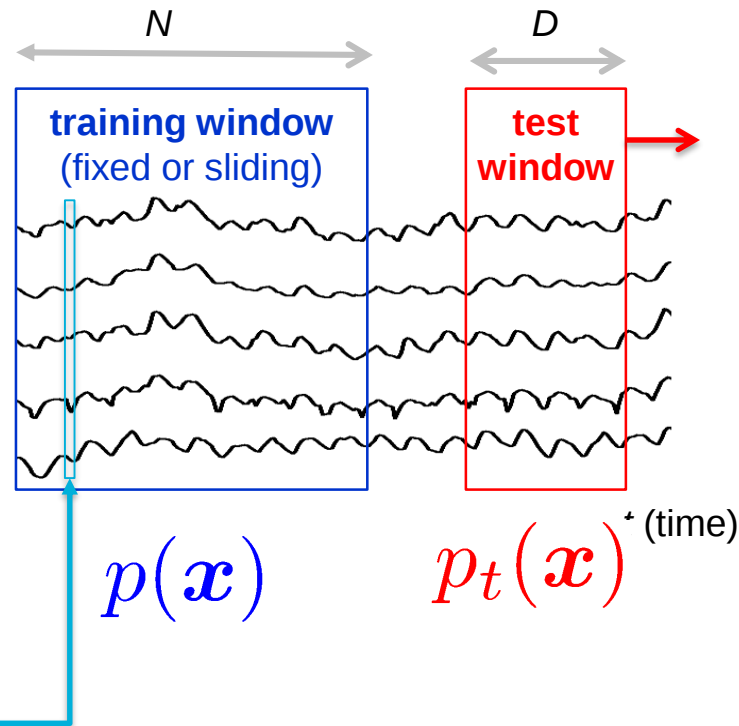
- Change = difference between $p(\mathbf{x})$ and $p_t(\mathbf{x})$
 - $\mathbf{x}$: M -dimensional *i.i.d.* observation
 - $p(\mathbf{x})$: p.d.f. estimated from training window
 - $p_t(\mathbf{x})$: p.d.f. estimated from the test window at time t

- Assume a sequence of i.i.d. vectors

- Training data in the training window

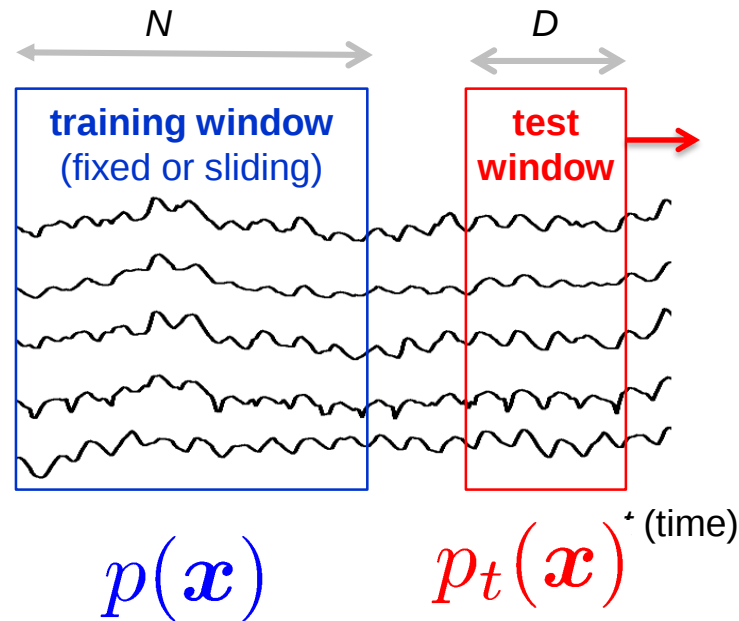
$$\{\mathbf{x}^{(1)}, \dots, \mathbf{x}^{(t)}, \dots, \mathbf{x}^{(N)}\}$$

time index (or sample index)



Problem setting: change detection from multi-variate noisy time-series data

- Question 1: What kind of model should we use for the probability density?
- Question 2: How can we quantify the difference between the densities?



We use von Mises-Fisher distribution to model $p(\mathbf{x})$ and $p_t(\mathbf{x})$

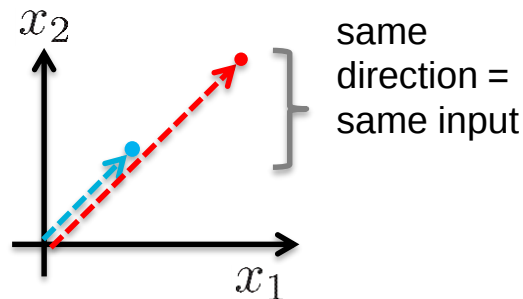
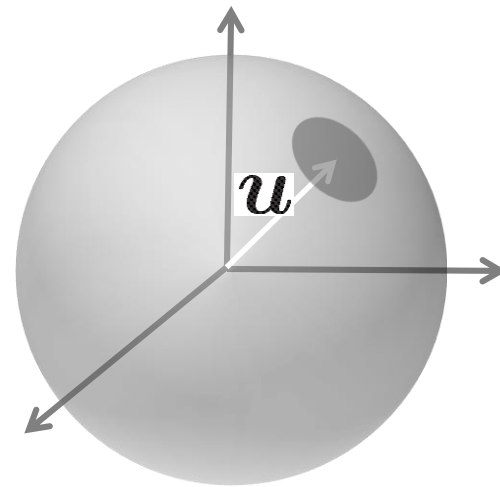
- vMF distribution: “Gaussian for unit vectors”

$$p(\mathbf{z} \mid \mathbf{u}, \kappa) = c_M(\kappa) \exp(\kappa \mathbf{u}^\top \mathbf{z})$$

- $\mathbf{z}$: random unit vector of $\|\mathbf{z}\| = 1$
- $\mathbf{u}$: mean direction
- κ : “concentration” ($\sim$ precision in Gaussian)
- M : dimensionality
- We are concerned only with the direction of observation $\mathbf{x}$:

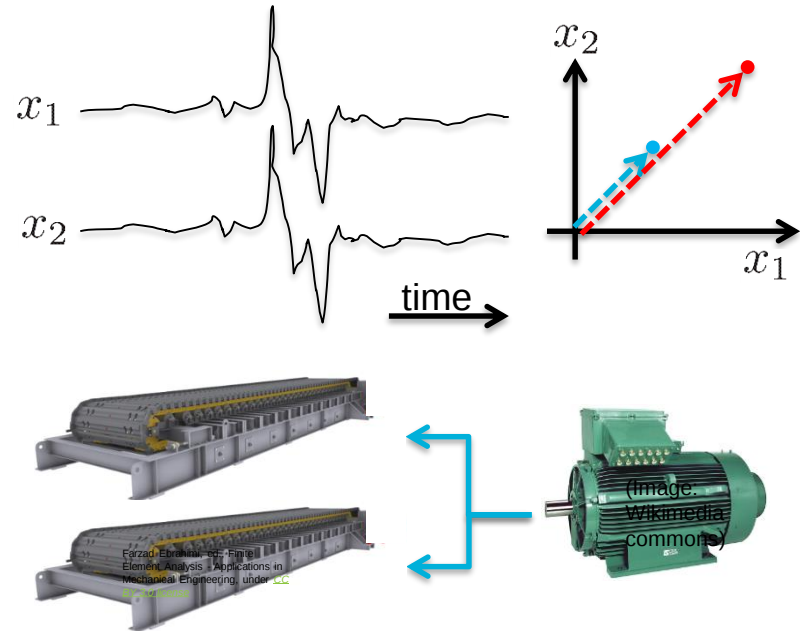
$$\mathbf{z} = \frac{\mathbf{x}}{\|\mathbf{x}\|}$$

- Normalization is always made
- Do not care about the norm



Normalization is useful to suppress multiplicative noise

- Real mechanical systems often incur **multiplicative** noise
 - Example: two belt conveyors operated by the same motor
- Normalization of vector is simple but powerful method for noise reduction



Mean direction $\mathbf{u}$ is learned via maximum likelihood. Introduce sample weight to down-weight contaminated ones

- Weighted likelihood function

$$L(\mathbf{u}, \kappa) = \sum_{n=1}^N w^{(n)} b^{(n)} \{ \ln c_M(\kappa) + \kappa \mathbf{u}^\top \mathbf{z}^{(n)} \}$$

$\|\mathbf{x}^{(n)}\|_2$ (normalization factor)

sample weight

- Regularization over sample weights

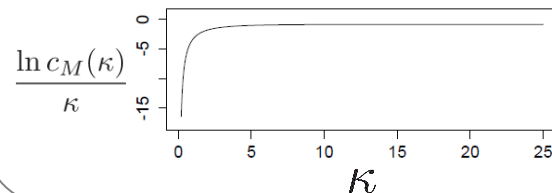
$$R(\mathbf{w}) = \frac{1}{2} \|\mathbf{w}\|_2^2 + \nu \|\mathbf{w}\|_1$$

encourage sparsity

- Parameters are learned by solving

$$(\mathbf{u}^*, \mathbf{w}^*) = \arg \max_{\mathbf{u}, \mathbf{w}} \{ L(\mathbf{u}, \kappa) + \lambda R(\mathbf{w}) \}$$

The term related to κ is less important. κ is treated as a given constant.



Multiple patterns (directions) can be obtained by coupling maximum likelihood equations

- Find orthogonal sequence of the mean direction $\mathbf{u}_1, \mathbf{u}_2, \dots, \mathbf{u}_m$ by coupling the weighted regularized maximum likelihood

$$(\mathbf{u}_1^*, \mathbf{w}_1^*) = \arg \max_{\mathbf{u}_1, \mathbf{w}_1} \{L(\mathbf{u}_1, \kappa) + \lambda R(\mathbf{w}_1)\}$$

$$(\mathbf{u}_2^*, \mathbf{w}_2^*) = \arg \max_{\mathbf{u}_2, \mathbf{w}_2} \{L(\mathbf{u}_2, \kappa) + \lambda R(\mathbf{w}_2)\}$$

$$\vdots$$

$$(\mathbf{u}_m^*, \mathbf{w}_m^*) = \arg \max_{\mathbf{u}_m, \mathbf{w}_m} \{L(\mathbf{u}_m, \kappa) + \lambda R(\mathbf{w}_m)\}$$

Orthogonality
condition

$$\mathbf{u}_i^\top \mathbf{u}_j = \delta_{i,j}$$

Kronecker
delta

Iterative sequential algorithm for the coupled maximum likelihood

$$\mathbf{w}_1 \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \mathbf{u}_1$$

$$\mathbf{w}_2 \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \mathbf{u}_2 \perp \mathbf{u}_1$$

$$\vdots$$

$$\mathbf{w}_m \begin{array}{c} \curvearrowright \\ \curvearrowleft \end{array} \mathbf{u}_m \perp \mathbf{u}_i$$

$(i = 1, \dots, m - 1)$

- For each i , $\mathbf{w}_i$ and $\mathbf{u}_i$ are solved iteratively until convergence
- Analytic solution exists in each step
- Results in very simple fixed point equations

Derived fixed-point iteration algorithm

■ Example: $i = 1$

Given $\mathbf{w}_1$, solve

$$\max_{\mathbf{u}_1} \{ \kappa \mathbf{u}_1^\top \mathbf{X} \mathbf{w}_1 \} \quad \text{s.t.} \quad \mathbf{u}_1^\top \mathbf{u}_1 = 1$$

Given $\mathbf{u}_1$, solve

$$\min_{\mathbf{w}_1} \left\{ \frac{1}{2} \|\mathbf{w}_1 - \frac{\mathbf{q}}{\lambda}\|_2^2 + \nu \|\mathbf{w}_1\|_1 \right\}$$

$$\mathbf{q} \equiv \ln c_M \mathbf{b} + \kappa \mathbf{X}^\top \mathbf{u}_1$$

This Lasso problem is solved analytically

Algorithm 1 RED algorithm.

Input: Initialized $\mathbf{w}$. Regularization parameters λ, ν . Concentration parameter κ . The number of major directional patterns m .

Output: $\mathbf{U} = [\mathbf{u}_1, \dots, \mathbf{u}_m]$ and $\mathbf{W} = [\mathbf{w}_1, \dots, \mathbf{w}_m]$.

for $j = 1, 2, \dots, m$ **do**

while no convergence **do**

$$\mathbf{u}_j \leftarrow \kappa [\mathbf{I}_M - \mathbf{U}_{j-1} \mathbf{U}_{j-1}^\top] \mathbf{X} \mathbf{w}_j \quad (17)$$

$$\mathbf{u}_j \leftarrow \text{sign}(\mathbf{u}_j^\top \mathbf{X} \mathbf{w}_j) \frac{\mathbf{u}_j}{\|\mathbf{u}_j\|_2} \quad (18)$$

$$\mathbf{q}_j \leftarrow \gamma \mathbf{b} + \kappa \mathbf{X}^\top \mathbf{u}_j \quad (19)$$

$$\mathbf{w}_j \leftarrow \text{sign}(\mathbf{q}_j) \odot \max \left\{ \frac{|\mathbf{q}_j|}{\lambda} - \nu \mathbf{1}, \mathbf{0} \right\} \quad (20)$$

end while

end for

Return $\mathbf{U}$ and $\mathbf{W}$.

Theoretical property: The algorithm is reduced to the “trust-region subproblem” in $\nu \rightarrow 0$

Theorem 2. *When ν tends to 0, the nonconvex problem (5) is reduced to an optimization problem in the form of*

$$\min_{\mathbf{u}} \{ \mathbf{u}^\top \mathbf{Q} \mathbf{u} + \mathbf{c}^\top \mathbf{u} \} \quad \text{s.t.} \quad \mathbf{u}^\top \mathbf{u} = 1, \quad (23)$$

Useful to initialize
the iterative
algorithm

which has a global solution obtained in polynomial time.

Proof. The non-convex optimization problem (23) is known as the trust region subproblem. For polynomial algorithms to the global solution, see [Sorensen, 1997; Tao and An, 1998; Hager, 2001; Toint *et al.*, 2009]. Here we show how the algorithm is reduced to the trust region subproblem.

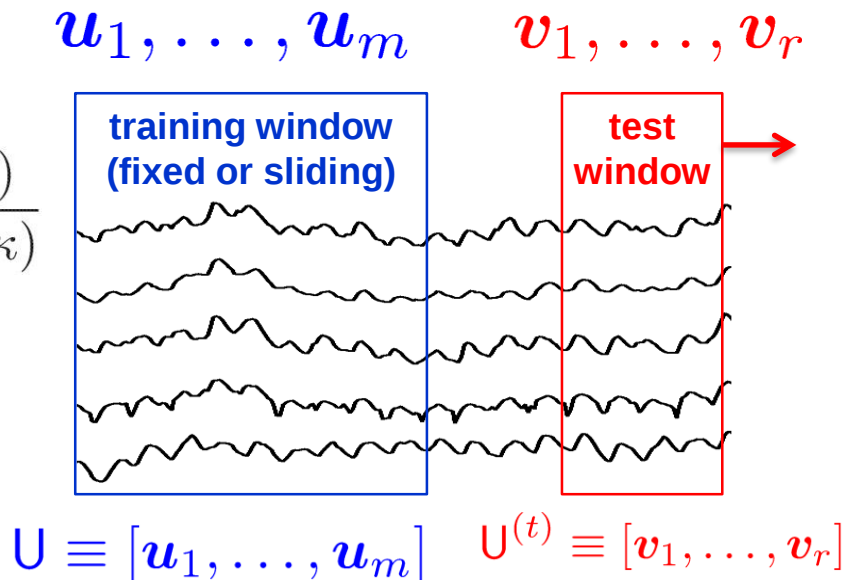
Change score as parameterized Kullback-Leibler divergence

- With extracted directions, define the change score at time t as

$$a^{(t)} = \min_{\mathbf{f}, \mathbf{g}} \int dx \overset{\text{vMF dist.}}{\mathcal{M}(\mathbf{x} | \mathbf{U} \mathbf{f}, \kappa)} \ln \frac{\overset{\text{vMF dist.}}{\mathcal{M}(\mathbf{x} | \mathbf{U} \mathbf{f}, \kappa)}}{\overset{\text{vMF dist.}}{\mathcal{M}(\mathbf{x} | \mathbf{U}^{(t)} \mathbf{g}, \kappa)}}$$

$$\mathbf{f}^\top \mathbf{f} = 1, \mathbf{g}^\top \mathbf{g} = 1$$

- Concisely represented by the top singular value of $\mathbf{U}^\top \mathbf{U}^{(t)}$



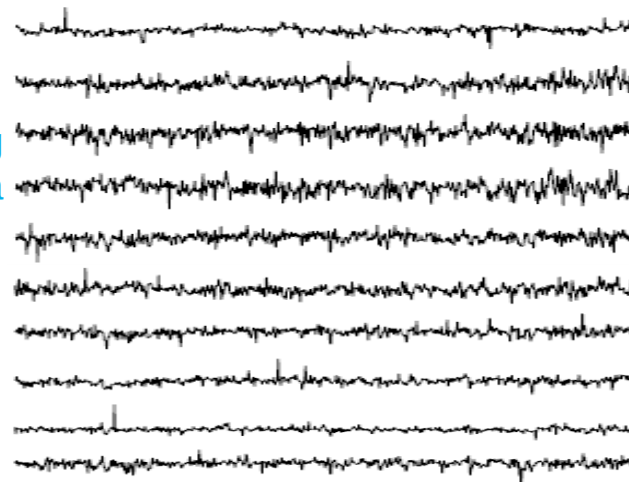
Experiment: Failure detection of ore belt conveyors

- vMF formulation successfully suppressed very noisy non-Gaussian noise of multiplicative nature
- ~40% of samples were automatically excluded from the model
- Better than alternatives
 - PCA, Hotelling T²
 - Stationary subspace analysis [Blythe et al., 2012]

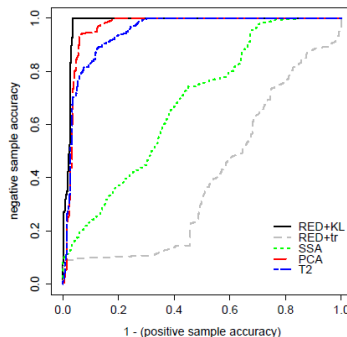
Learned
sample
weights



Training
data



(simulation data)



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Wish to build a collective monitoring solution

System 1
(in New Orleans)



⋮

System s



⋮

System S
(in New York)



- You have many similar but not identical industrial assets
- You want to build an anomaly detection model for each of the assets
- Straightforward solutions have serious limitations
 - 1. Treat the systems separately. Create each model individually
 - ✓ Suffers from lack of fault examples
 - 2. Build one universal model by disregarding individuality
 - ✓ Model fit is not good

Practical requirements: Need to capture both commonality and individuality

System 1
(in New Orleans)



⋮

System s

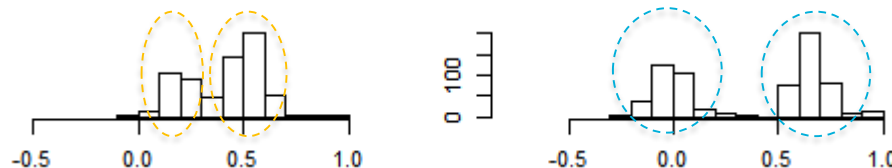


⋮

System S
(in New York)

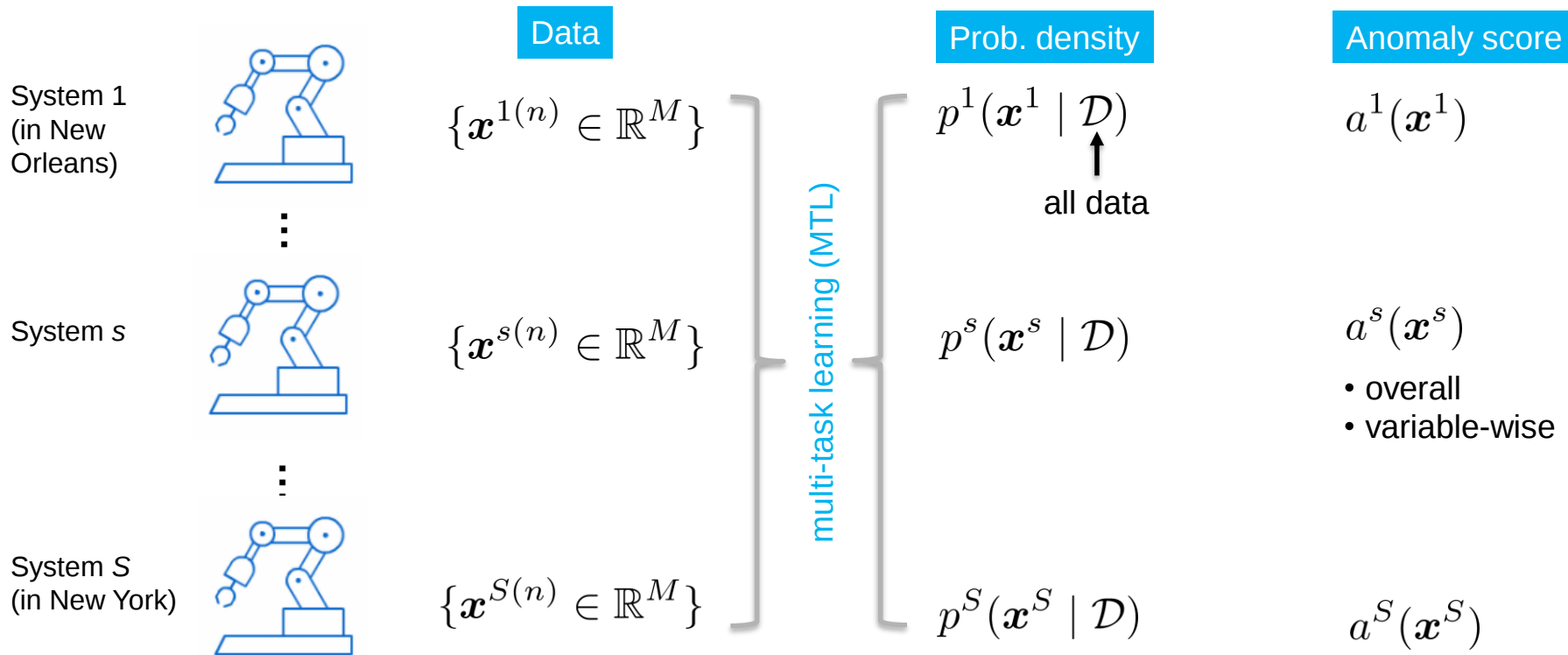


- Capture both individuality and commonality
- Automatically capture multiple operational states
 - Real-world is not single-peaked / single-modal



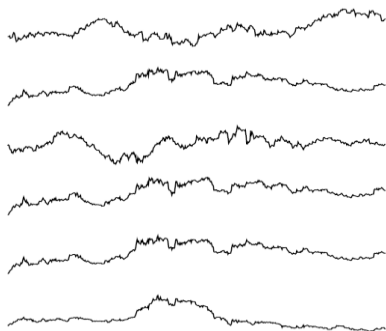
- Be robust to noise
- Be highly interpretable for diagnosis purposes

Formalizing the problem as multi-task density estimation for anomaly detection

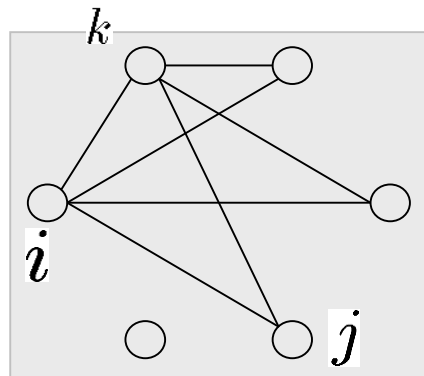


Use Gaussian graphical model (GGM)-based anomaly detection approach as the basic building block

Multi-variate data



Sparse graphical model



$$\max_{\Lambda} \{ \ln \det \Lambda - \text{tr}(\Sigma \Lambda) - \rho \|\Lambda\|_1 \}$$

sample covariance

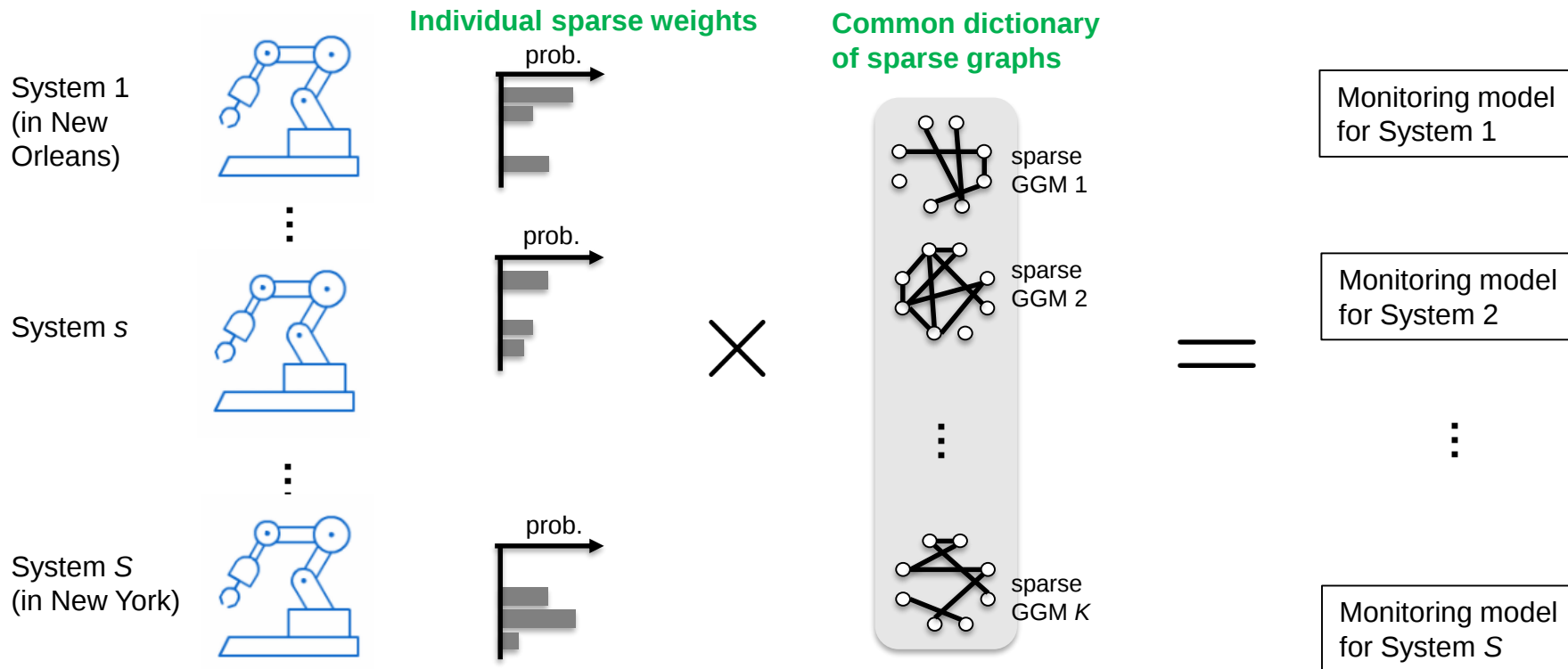
training data

Anomaly score

$$a(\mathbf{x}) = \begin{cases} -\ln p(\mathbf{x} \mid \mathcal{D}) & \text{Overall score} \\ -\ln p(x_i \mid \mathbf{x}_{-i}, \mathcal{D}) & \text{Variable-wise score} \end{cases}$$

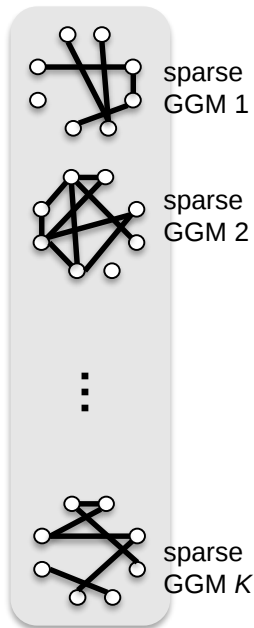
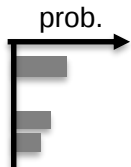
[Ide+ SDM09] [Ide+ ICDM16]

Basic modeling strategy: Combine common pattern dictionary with individual weights



Basic modeling strategy: Resulting model will be a sparse mixture of sparse GGM

System s



GGM=Gaussian Graphical Model

Monitoring model for System s

Gaussian mixture

$$= \sum_{k=1}^K \pi_k^s \mathcal{N}(\mathbf{x}^s \mid \boldsymbol{\mu}^k, (\boldsymbol{\Lambda}^k)^{-1})$$

Sparse mixture weights

(= automatic determination of the number of patterns)

Sparse Gaussian graphical model

Propose a Bayesian multi-task model with two sparsity-enforcing priors

- Observation model (for the s -th task)
 - Gaussian mixture with task-dependent weight
$$\prod_{k=1}^K \mathcal{N}(\mathbf{x}^s \mid \boldsymbol{\mu}^k, (\Lambda^k)^{-1})^{z_k^s}$$
- Sparsity enforcing priors (non-conjugate)
 - Laplace prior for the precision matrix
 - Bernoulli prior for the mixture weights
$$p(\Lambda^k) = \left(\frac{\rho}{4}\right)^{M^2} \exp\left(-\frac{\rho}{2} \|\Lambda^k\|_1\right)$$

$$p(\boldsymbol{\pi}^s) = p_0^{\|\boldsymbol{\pi}^s\|_0} (1 - p_0)^{G - \|\boldsymbol{\pi}^s\|_0}$$
- Conjugate prior on $\{\boldsymbol{\mu}^k\}$ and $\{\mathbf{z}^s\}$

$$p(\boldsymbol{\mu}^k \mid \Lambda^k) = \mathcal{N}(\boldsymbol{\mu}^k \mid \mathbf{m}^0, (\lambda_0 \Lambda^k)^{-1})$$

$$p(\mathbf{z}^s \mid \boldsymbol{\pi}^s) = \prod_{k=1}^K (\pi_k^s)^{z_k^s}$$

Maximizing log likelihood using variational Bayes combined with point-estimation

- Complete log likelihood

$$L = \underbrace{\sum_{s=1}^S \sum_{n=1}^{N_s} \sum_{k=1}^K \ln \mathcal{N}(\mathbf{x}^{s(n)} | \boldsymbol{\mu}^k)^{z^{s(n)}}}_{\text{Likelihood by the obs. model}} + \underbrace{\sum_{k=1}^K \text{Lap}(\Lambda^k | \rho) p(\boldsymbol{\mu}^k | \Lambda^k) + \sum_{s=1}^S z^{s(n)} \ln \pi_k^s + \sum_{s=1}^S \ln p(\boldsymbol{\pi}^s)}_{\text{Prior distributions}}$$

- Use VB for $\{\boldsymbol{\mu}^k\}, \{z^{s(n)}\}$
- Use point-estimate for $\{\Lambda^k\}, \{\boldsymbol{\pi}^s\}$
 - Results in two convex optimization problems

Maximizing log likelihood using variational Bayes combined with point-estimation

- Update sample weights

- Update cluster weights

- Update precision matrices

- Update other parameters

Use new semi-closed form solution

$$\max_{\pi^s} \left\{ \sum_{k=1}^K c_k^s \ln \pi_k^s - \tau \|\pi^s\|_0 \right\}$$

The ratio of samples assigned to the k -th cluster

s.t. $\|\pi^s\|_1 = 1.$

Solved by graphical lasso [Friedman 08]

$$\max_{\Lambda^k} \left\{ \ln |\Lambda^k| - \text{Tr}(\Lambda^k Q^k) - \frac{\rho}{N_k} \|\Lambda^k\|_1 \right\}$$

total # of samples assigned to the k -th cluster

Solving the L_0 -regularized optimization problem for mixture weights

- Conventional VB approach without L_0 regularization on π_k^s is problematic
 - Claimed to get a sparse solution [Corduneanu+ 01]
 - But mathematically π_k^s cannot be zero due to logarithm
- We re-formalized the problem as a convex mixed-integer programming
 - A semi-closed form solution can be derived ($\rightarrow$ see paper)

$$\max_{\boldsymbol{\pi}^s} \left\{ \sum_{k=1}^K c_k^s \ln \pi_k^s \right\}$$
$$\text{s.t. } \|\boldsymbol{\pi}^s\|_1 = 1.$$

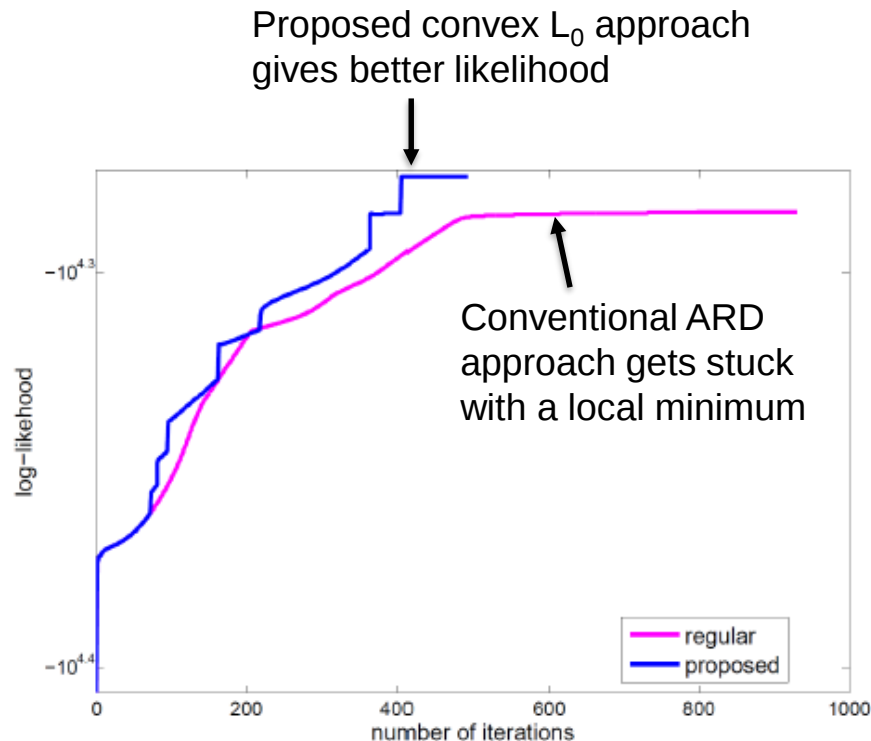
$$\max_{\boldsymbol{\pi}^s, \mathbf{y}^s} \sum_{k=1}^K \{c_k^s \ln \pi_k^s - \tau y_k^s\} \quad \text{s.t.} \quad \sum_{k=1}^K \pi_k^s = 1,$$
$$y_k^s \geq \pi_k^s - \epsilon, \quad y_k^s \in \{0, 1\} \quad \text{for } k = 1, \dots, K,$$

Comparison with possible alternatives

		Interpretability	Noise reduction	Fleet-readiness	Multi-modality
Our work [Ide et al. ICDM 17]		Yes	Yes	Yes	Yes
(single) sparse GGM	[Ide et al. SDM 2009, Ide et al. ICDM 2016]	Yes	Yes	No	No
Gaussian mixtures	[Yamanishi et al., 2000; Zhang and Fung, 2013; Gao et al., 2016]	Limited	Limited	No	Yes
Multi-task sparse GGM	[Varoquaux et al., 2010; Honorio and Samaras, 2010; Chiquet et al., 2011; Danaher et al., 2014; Gao et al., 2016; Peterson et al., 2015].	Yes	Yes	Yes	No
Multi-task learning anomaly detection	[Bahadori et al., 2011; He et al., 2014; Xiao et al., 2015]	No	(depends)	Yes	No

Experiment (1): Learning sparse mixture weights

- Conventional ARD approach sometimes gets stuck with local minima
 - ARD = automatic relevance determination
 - Often less sparse than the proposed convex L_0 approach
- Typical result of log likelihood vs VB iteration count →

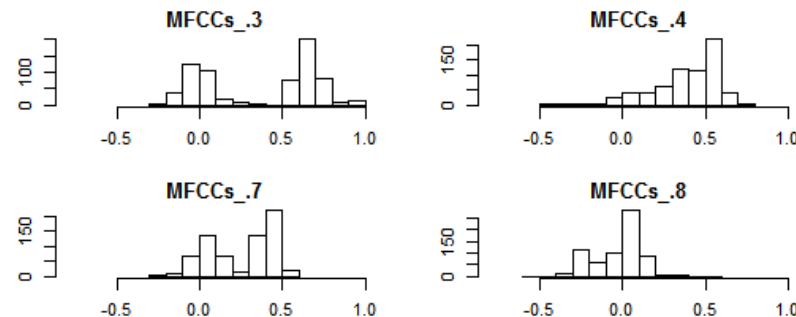


Experiment (2): Learning GGMs and detecting anomalies

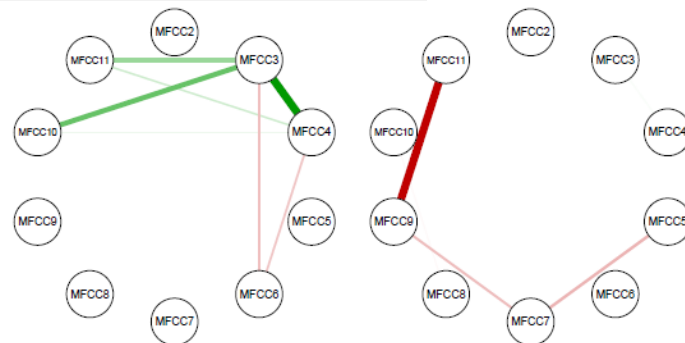


- “Anuran Calls” (frog voice) data in UCI Archive
 - Multi-modal (multi-peaked)
 - Voice signal + attributes (species, etc.)
- Created 10-variate, 3-task dataset
 - Use the species of “*Rhinellagranulosa*” as the anomaly
- Results
 - Two non-empty GGMs are automatically detected starting from $K=9$
 - Clearly outperformed single-modal MTL alternative in anomaly detection
 - ✓ Group graphical lasso, fused graphical lasso

Example of variable-wise distribution



Automatically learned GGMs



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- Change detection using directional statistics
 - T. Ide et al., IJCAI 16
- Multi-task multi-modal models for collective anomaly detection
 - T. Ide et al., ICDM 17
- Summary and future work

Summary and ongoing work

- Industrial sensor data have many interesting features that call for new machine learning formulation
- Introduced two recent works on anomaly detection
 - Feature extraction method based on von Mises-Fisher distribution
 - Bayesian multi-task density estimation with double sparsity
- Ongoing/future work

Discussion: What is the potential of deep learning in cognitive manufacturing?

Thank you!

(For ref.) Algorithm for sparse structure learning

- Assume graphical Gaussian model

$$p(\mathbf{x}|\Lambda) = \mathcal{N}(\mathbf{x}|\mathbf{0}, \Lambda^{-1}) = \frac{\det(\Lambda)^{1/2}}{(2\pi)^{M/2}} \exp\left(-\frac{1}{2}\mathbf{x}^\top \Lambda \mathbf{x}\right)$$

- Put a Laplace prior on Lambda

$$p(\Lambda) = \prod_{i,j=1}^M \frac{\rho}{2} \exp\left(-\rho|\Lambda_{i,j}|\right)$$

rho: constant controlling the strength of prior

- MAP (Maximum a posteriori) estimation for Lambda

$$\begin{aligned} \Lambda^* &= \arg \max_{\Lambda} \left\{ \ln p(\Lambda) \prod_{n=1}^N p(\mathbf{x}^{(n)}|\Lambda) \right\} \\ &= \arg \max_{\Lambda} \{ \ln \det \Lambda - \text{tr}(S\Lambda) - \rho \|\Lambda\|_1 \} \end{aligned}$$

S: sample covariance matrix

For the detail, see, T. Ide et al., "Proximity-Based Anomaly Detection using Sparse Structure Learning," Proc. SIAM Intl Conf. on Data Mining 2009 (SDM 09).

(For ref.) Anomaly scoring algorithm (for outlier analysis)

- Define the outlier score for the i -th variable as

$$\text{score}_i(\mathbf{x}|\Lambda) \equiv -\ln p(x_i|x_1, \dots, x_{i-1}, x_{i+1}, \dots, x_M, \Lambda)$$

- Lambda represents a sparse structure
 - p is p.d.f. defined by the graphical Gaussian model
- Final result: Anomaly score of the i -th variable
 - Only variables connected to the i -th variable play a role

$$\text{score}_i(\mathbf{x}|\Lambda) = \frac{1}{2} \ln \frac{2\pi}{\Lambda_{i,i}} + \frac{1}{2\Lambda_{i,i}} \left(\sum_{j=1}^M \Lambda_{i,j} x_j \right)^2$$

Title: Recent advances in sensor data analytics

- Abstract:
- Sensor data analytics is one of the major application fields of data mining and machine learning. Typically taking real-valued time-series data from physical sensors as the input, its problem setting includes a variety of tasks depending on the application domain, not limited to the traditional regression and classification.
- This talk will first introduce technical challenges in industrial sensor data analytics. Then it will cover recent developments in machine learning algorithms in sensor data analytics. Major topics include change detection using directional statistics and multi-task extension of graph-based anomaly detection.