Variational Inference of Joint Models using Multivariate Gaussian Convolution Processes

Xubo Yue, Ph.D. Student
Raed Al Kontar, Assistant Professor

The University of Michigan, Ann Arbor

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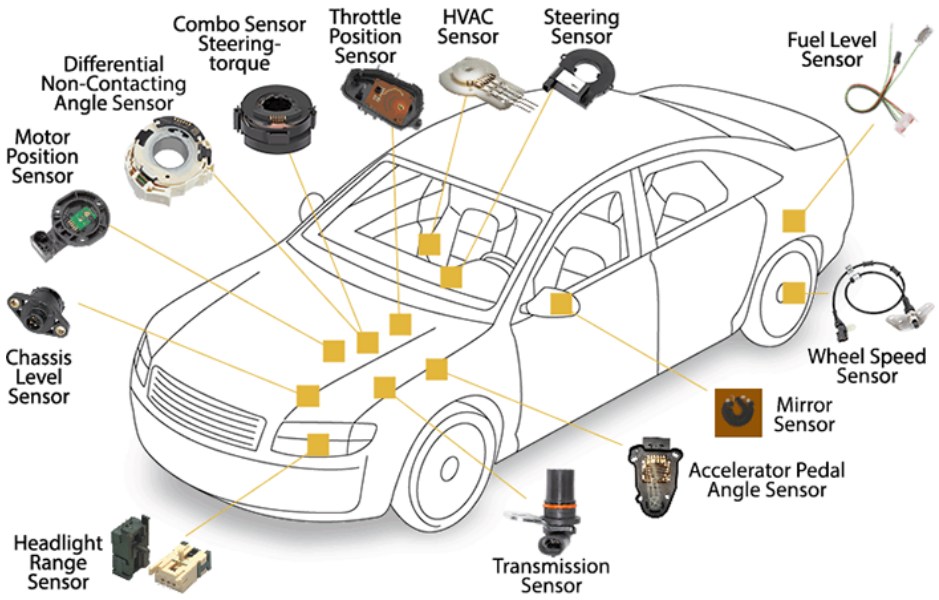
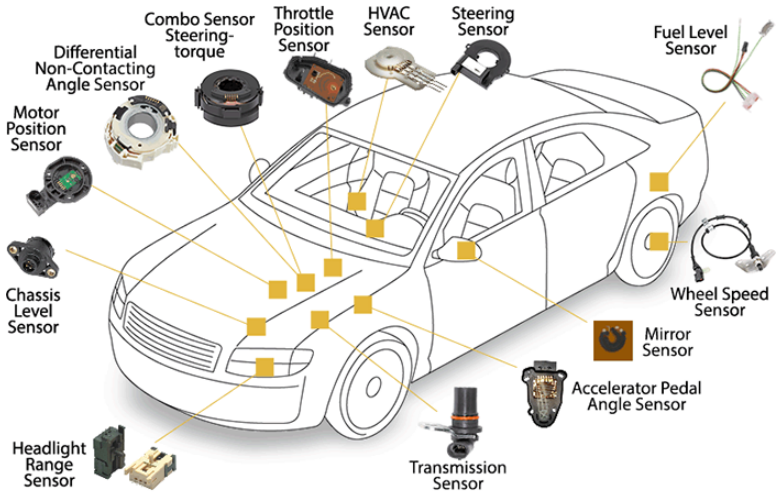
Signal Measurement Time-series Data



https://www.raypcb.com/the-schematic-diagram-of-automotive-sensor-signal-conditioning/
http://clipart-library.com/cartoon-vehicle-cliparts.html

Background

Time-series Data



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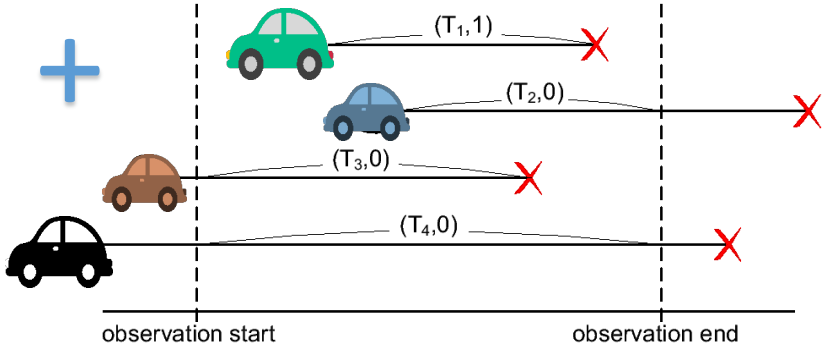
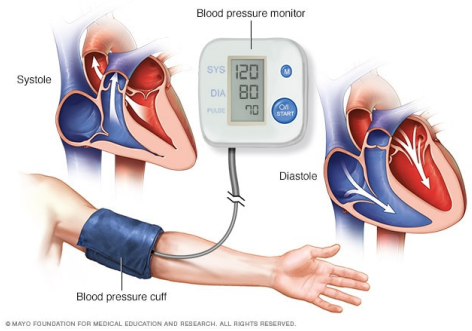
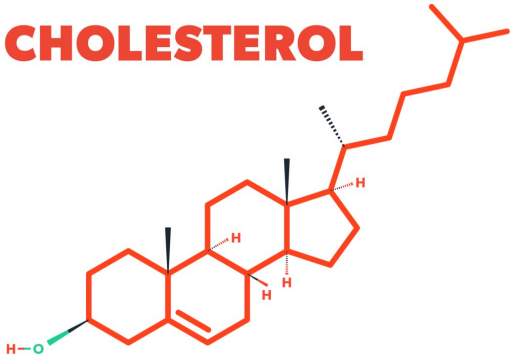


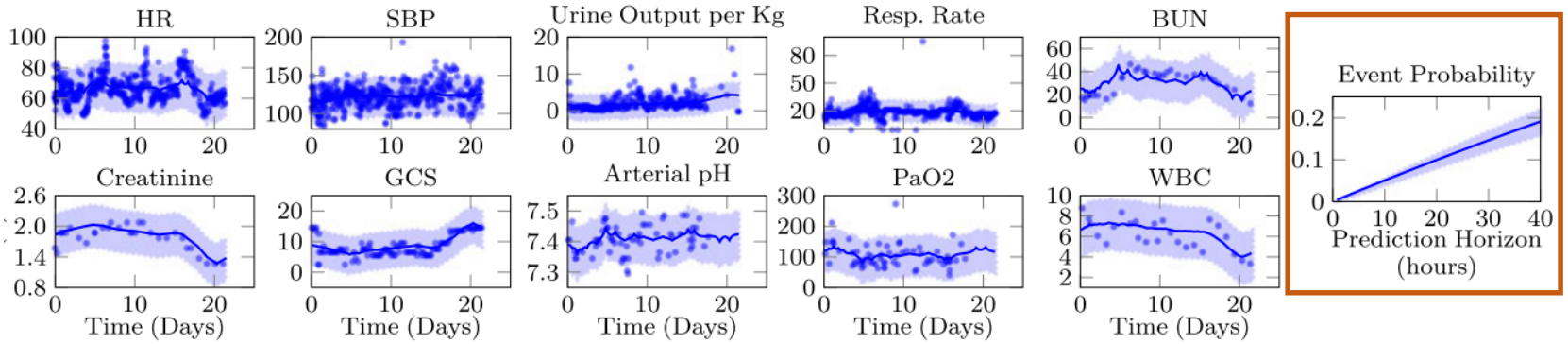
Lifetime Data

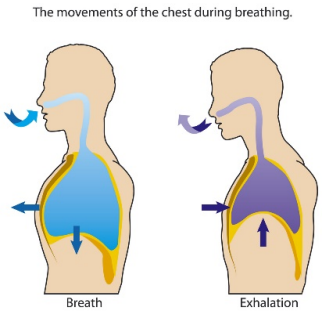
https://www.raypcb.com/the-schematic-diagram-of-automotive-sensor-signal-conditioning/
http://clipart-library.com/cartoon-vehicle-cliparts.html

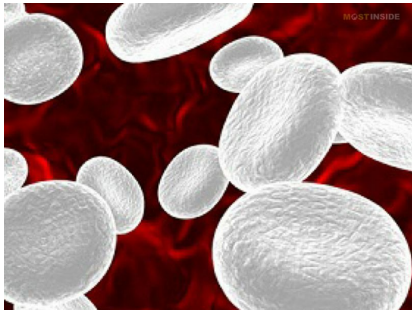
Background











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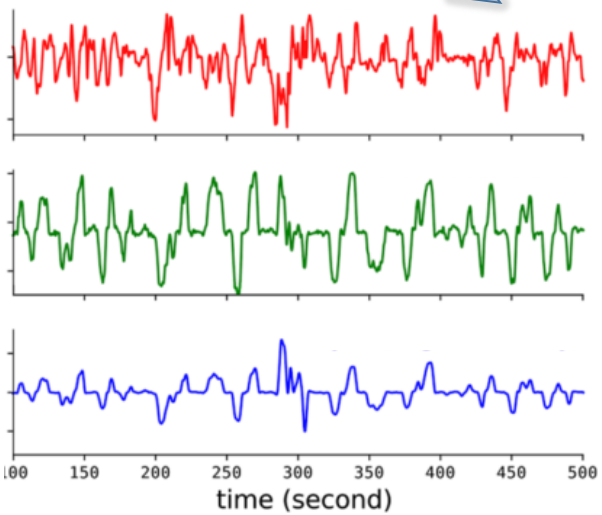
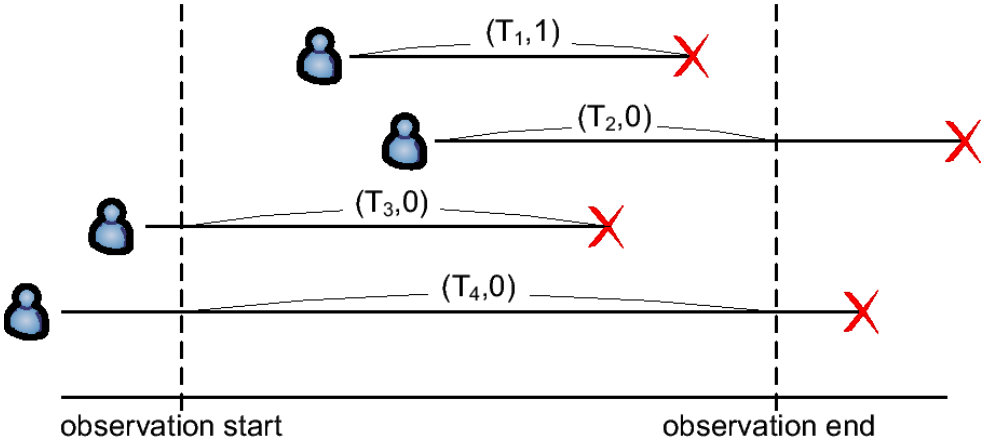
Background

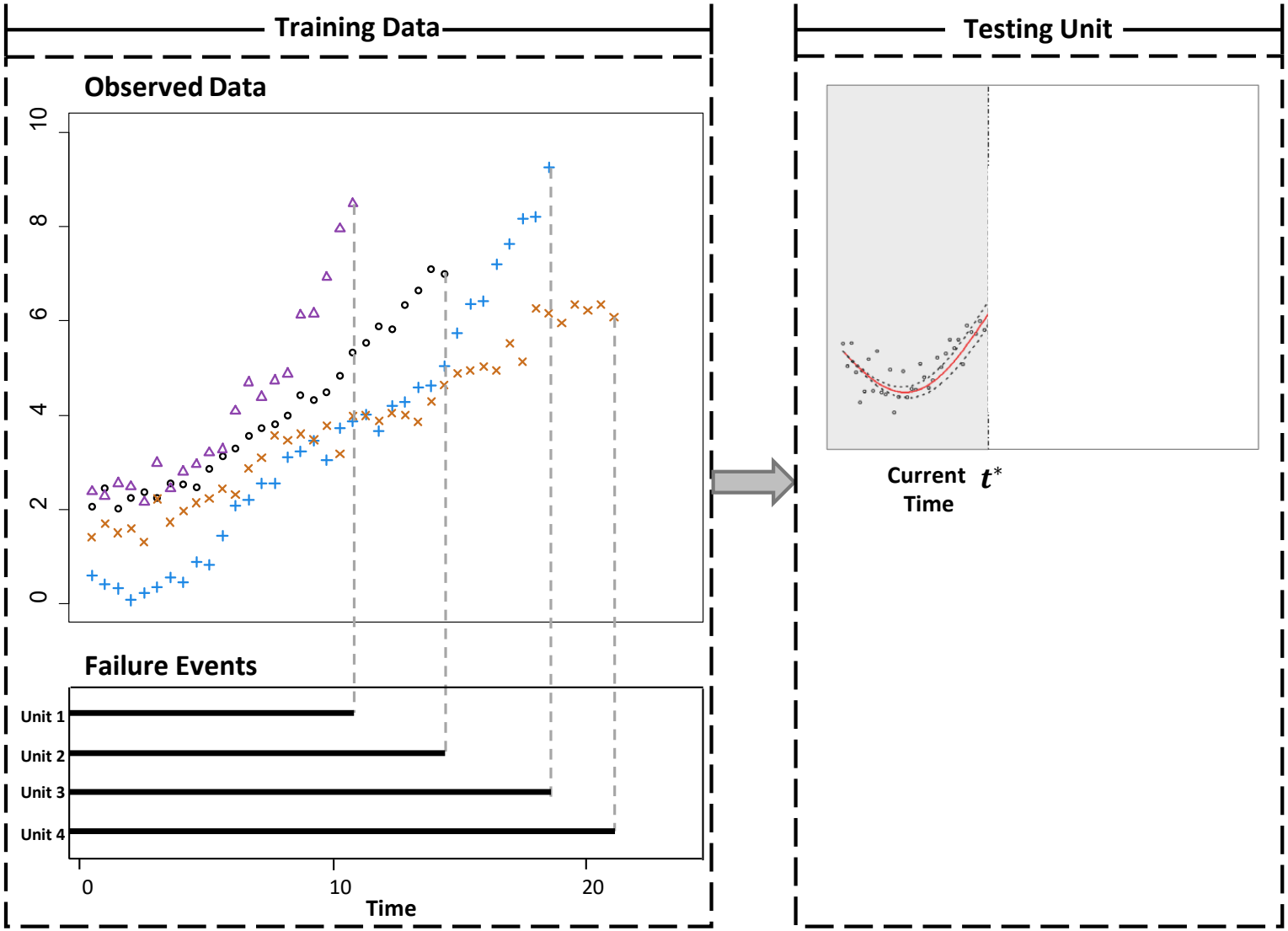
Time-series Data + Survival Data



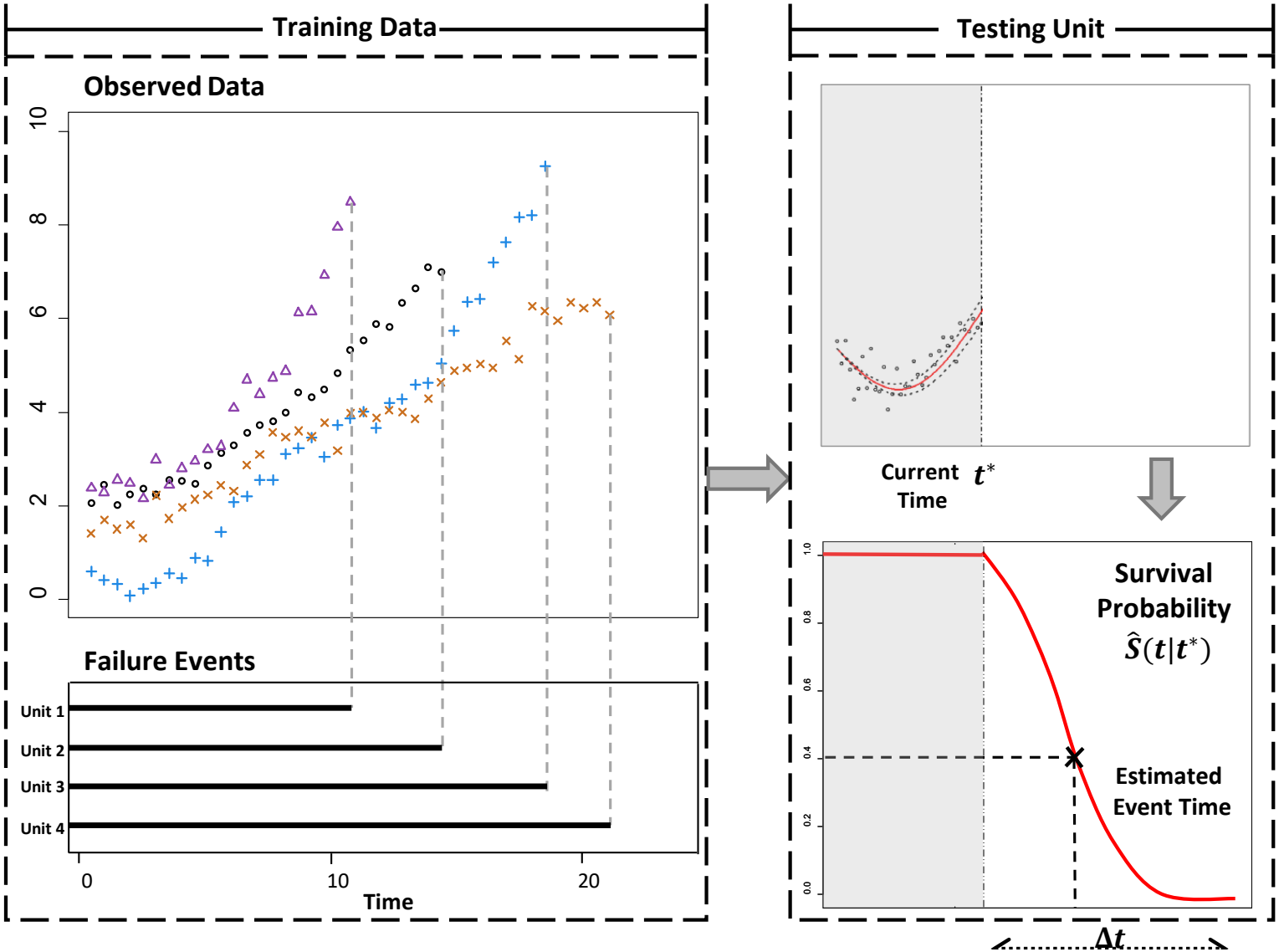


https://www.sentiance.com/2017/09/25/passenger-and-driver/
https://labblog.uofmhealth.org/industry-dx/for-optimizing-patient-data-track-and-share-every-moment

Framework


Training Data
Observed Data
0
2
4
6
8
10
Failure Events
Unit 1
Unit 2
Unit 3
Unit 4
0
10
20
Time
Testing Unit
Current Time
t^*

Framework


Training Data
Observed Data
Failure Events
Unit 1
Unit 2
Unit 3
Unit 4
Time
Testing Unit
Current Time t^*
Survival Probability $\hat{S}(t|t^*)$
Estimated Event Time
Δt

Data Structure

Data: $\{\boldsymbol{\mathcal{D}}_i\}_{i=1}^N = \{(V_i, \delta_i, \boldsymbol{w}_i, \boldsymbol{Y}_i)\}_{i=1}^N$.

- Outcome: occurrence of an event or losing information (censored).
- Event time $V_i = \min\{C_i, T_i\} \in \mathbb{R}_+$.
- Event indicator $\delta_i \in \{0, 1\}$.
- Fixed features $\boldsymbol{w}_i$ (e.g., gender).
- Observed longitudinal data $\boldsymbol{Y}_i$.

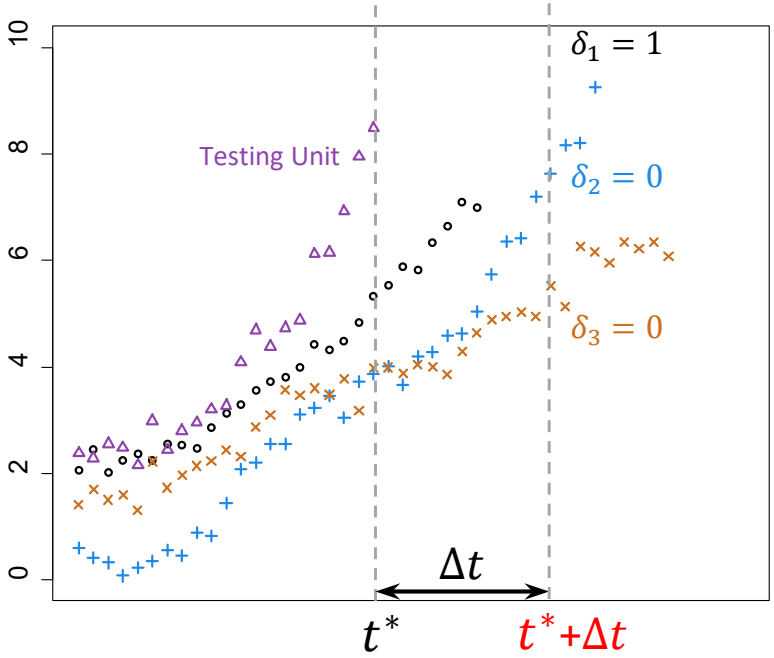
How?

- What is the most intuitive approach to analyze these data?

Survival Data - Logistic Regression/SVM

Time-series Classification

- Event data is transformed into binary labels $\delta_i = 1/0$ denoting whether units failed or not within the time interval $[t^*, \Delta t + t^*]$.
- The time-fixed covariate w_i and the last observed signal measurement at t^* are used as the model predictors.



Unit	Event Indicator δ at $t^* + \Delta t$	Longitudinal Signal Y at t^*
1	1	5.00
2	0	3.80
3	0	3.85

Problems?

- Fail to consider the functional form of longitudinal data: only use summary statistics.
- Unable to impute missing data.
- Fortunately, we have joint model (2008)!

Statistical Model

Joint Model

$$h_i(t) = h_0(t)\exp[\boldsymbol{\gamma}^T \boldsymbol{w}_i + \beta f_i(t)].$$

- $h_i(t)$: hazard; instantaneous failure rate at t.
- Data: $\boldsymbol{\mathcal{D}}_i = (V_i, \delta_i, \boldsymbol{w}_i, \boldsymbol{Y}_i)$.
- $\boldsymbol{\gamma}, \beta$: regression coefficient.
- $f_i(t)$: underlying latent values. Modeled as mixed-effect model.

$$y_i(t) = f_i(t) + \epsilon_i(t).$$

- $h_0(t)$: baseline hazard.

Parametric Model

Parametric Joint Model

- Linear mixed-effect model:

$$y_i(t) = f_i(t) + \epsilon_i(t) = \boldsymbol{z}^T(t)\boldsymbol{b}_i + \epsilon_i(t).$$

- e.g., $y_i(t) = b_{i0} + b_{1t} + b_{i2}t^2$.

Parametric Model

Parametric Joint Model

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- Likelihood function is intractable.
- Plug estimated parameters into the survival model (two-stage inference).

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Remark

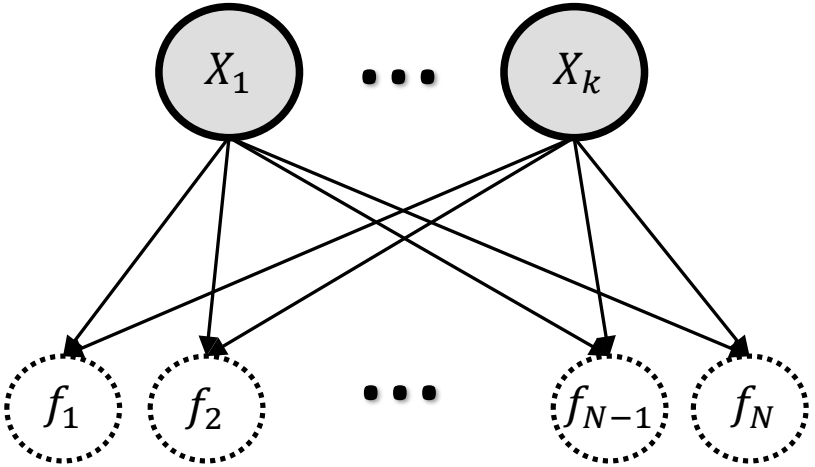
- Strong parametric assumption.
- Fail to propagate the uncertainty from time-series data to the survival component.

First Contribution

Contribution 1

- Introduce a flexible non-parametric mixed-effect model.
- Flexible: ability to handle heterogeneous data.
- Scalable: efficient for big data.

Multivariate Gaussian Convolution Process (MGCP)

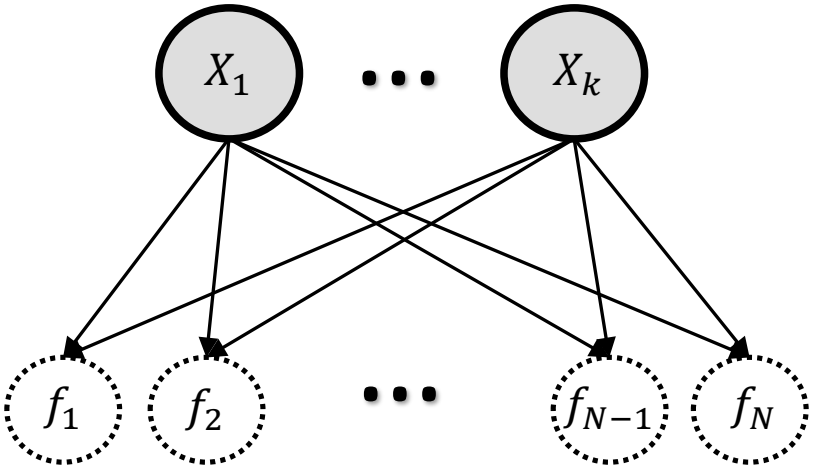


Model

- MGP:

$$\begin{bmatrix} y_1(t) \\ y_2(t) \\ \vdots \\ y_N(t) \end{bmatrix} = \begin{bmatrix} f_1(t) \\ f_2(t) \\ \vdots \\ f_N(t) \end{bmatrix} + \begin{bmatrix} \epsilon_1(t) \\ \epsilon_2(t) \\ \vdots \\ \epsilon_N(t) \end{bmatrix}$$

Multivariate Gaussian Convolution Process (MGCP)



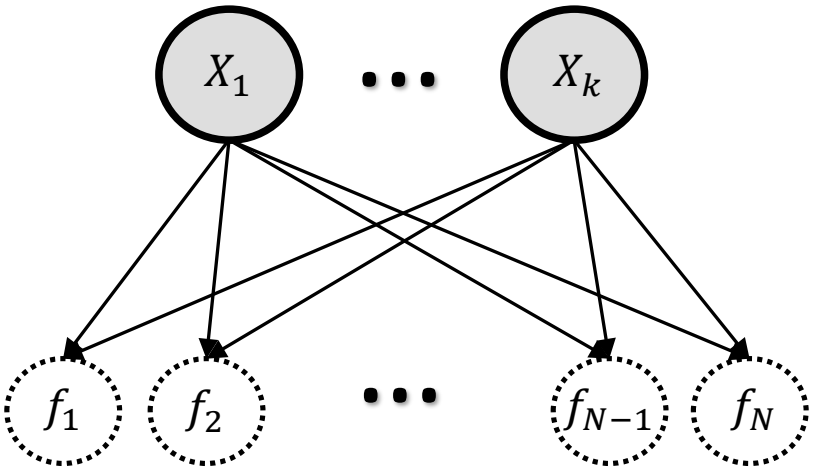
Convolution and Smoothing Kernels

- Each signal is expressed as a convolution of latent functions drawn from a GP. The Convolution of GP is GP.

$$f_i(t) = \sum_{k=1}^{K} \int_{\mathbb{R}} G_{i,k}(t-u) X_k(u) du.$$

- Bayesian interpretation. Alternative to neural network, etc.

Multivariate Gaussian Convolution Process (MGCP)



Contribution 1 (Recap)

- Introduce a flexible and scalable non-parametric mixed-effect model.
- Flexible: ability to handle heterogeneous data by shared latent functions.
- Scalable: efficient for big data.

MGCP - Sparse

Complexity

- Time complexity $\mathcal{O}(n^3)$, n is number of data points for all individuals.
- Take several hours even for small data.

$$\boldsymbol{\Sigma} = \begin{bmatrix} \Sigma_{1,1} & \cdots & \Sigma_{1,n} \\ \vdots & \ddots & \vdots \\ \Sigma_{n,1} & \cdots & \Sigma_{n,n} \end{bmatrix} \Longrightarrow \boldsymbol{\Sigma}^{-1} = \begin{bmatrix} \Sigma_{1,1} & \cdots & \Sigma_{1,n} \\ \vdots & \ddots & \vdots \\ \Sigma_{n,1} & \cdots & \Sigma_{n,n} \end{bmatrix}^{-1}$$

100 units with 300 observations:

N= 30,000

MGCP - Sparse

Contribution 1 (Recap)

- Introduce a flexible and scalable non-parametric mixed-effect model.
- Flexible: ability to handle heterogeneous data.
- Scalable: efficient for big data.

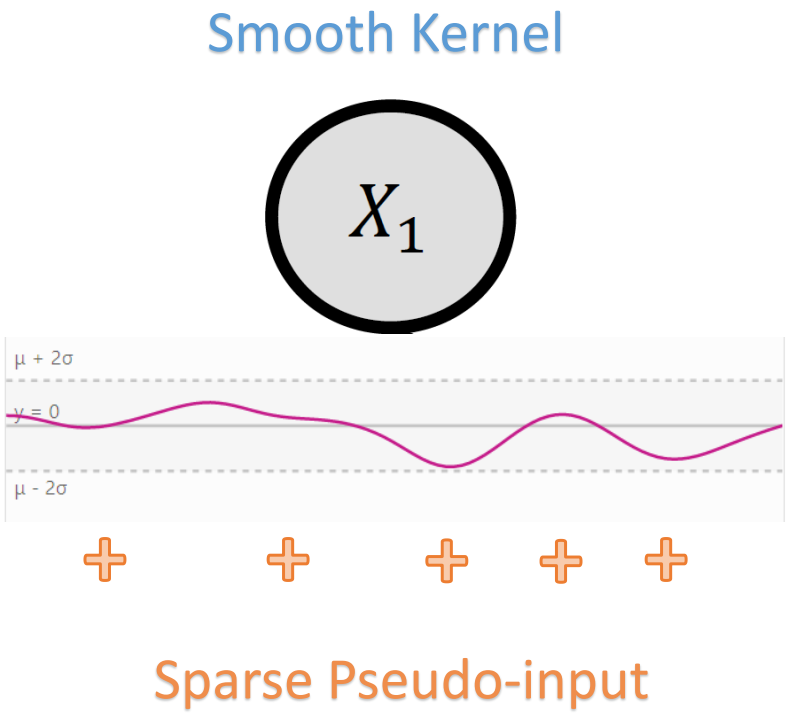
Pseudo-inputs

- Introduce $M(\ll n)$ pseudo-inputs from the latent functions denoted as $\boldsymbol{X}_k(\mathcal{Z}) = [X_k(z_1), \ldots, X_k(z_M)]^T$ where $\mathcal{Z} = \{z_i\}_{i=1}^M$.
- Time complexity $\mathcal{O}(n^3) \rightarrow \mathcal{O}(nM^2)$ (by the Woodbury formula).

MGCP - Sparse

Pseudo-inputs

- M pseudo-inputs to the latent functions.
- Use finite samples from latent functions.



Short Summary

MGCP+Survival Model→ Joint Model!

- Apply the sparse MGCP to the mixed-effect model.
- Joint Model:

$$h_i(t) = h_0(t) \exp\left[\boldsymbol{\gamma}^T \boldsymbol{w}_i + \beta \sum_{k=1}^{K} \int_{\mathbb{R}} G_{i,k}(t-u) X_k(u) du\right].$$

- Likelihood function is intractable.

Short Summary

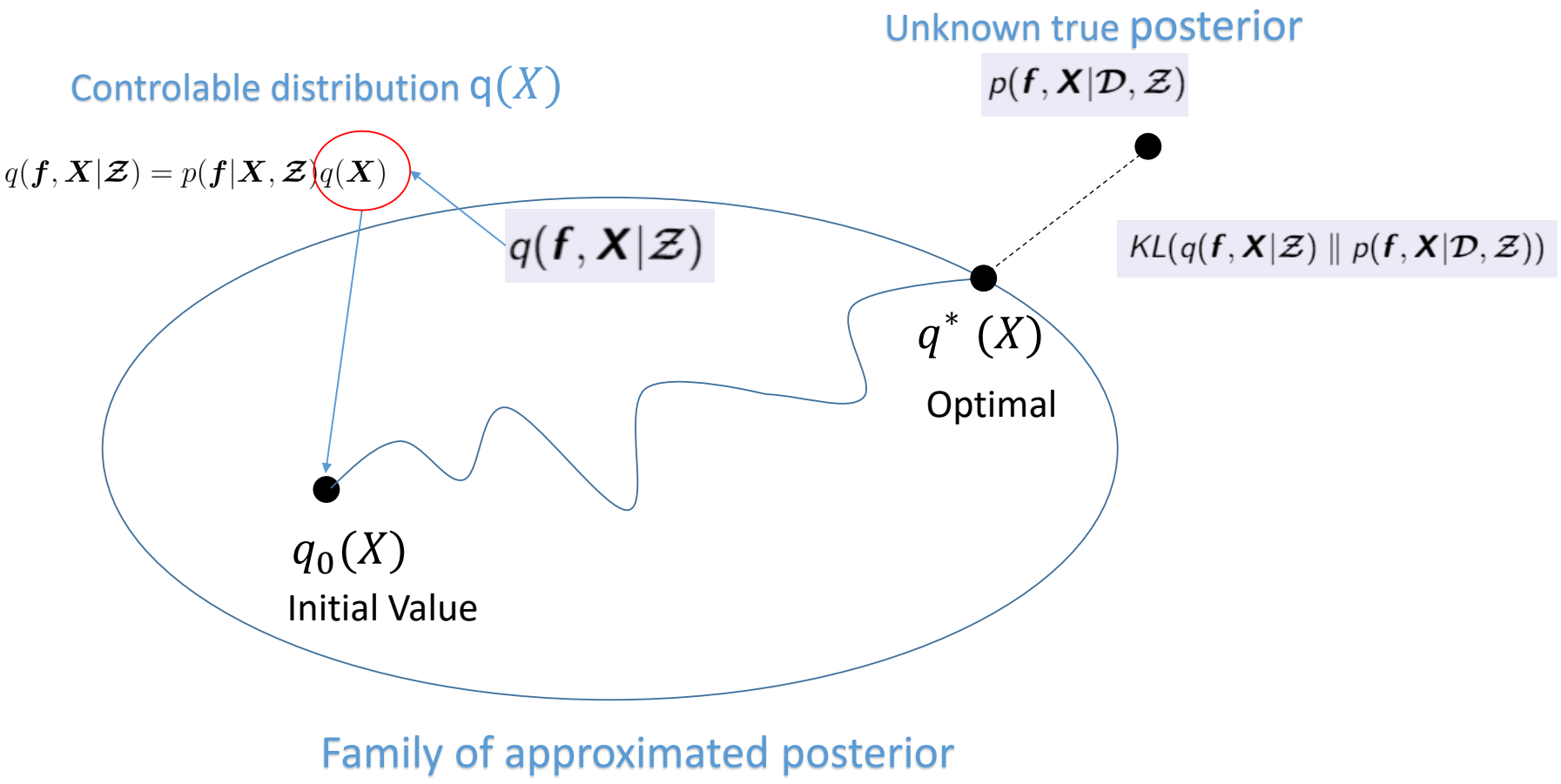
Contribution 1 (Recap)

- Introduce a flexible and scalable non-parametric mixed-effect model.
- Flexible: ability to handle heterogeneous data.
- Scalable: efficient for big data.

Contribution 2

- Introduce a variational inference framework to jointly estimate all parameters simultaneously.
- Big pic: find the lower bound of the likelihood function.
- VI provides a penalized likelihood function and a sparse approximation to the covariance matrix.

Joint Model and Variational Inference - 1



https://nips.cc/Conferences/2016/Schedule?showEvent=6199

Joint Model and Variational Inference - 2

Variational Inference

- Variational distribution $q(\boldsymbol{f}, \boldsymbol{X}|\mathcal{Z}) = p(\boldsymbol{f}|\boldsymbol{X}, \mathcal{Z})q(\boldsymbol{X})$.

$$
\begin{aligned}
& KL(q(\boldsymbol{f}, \boldsymbol{X}|\mathcal{Z}) \parallel p(\boldsymbol{f}, \boldsymbol{X}|\mathcal{D}, \mathcal{Z})) \\
&= \log p(\mathcal{D}) - \int q(\boldsymbol{f}, \boldsymbol{X}|\mathcal{Z}) \log \frac{p(\boldsymbol{f}, \boldsymbol{X}, \mathcal{D}|\mathcal{Z})}{q(\boldsymbol{f}, \boldsymbol{X}|\mathcal{Z})} d\boldsymbol{X} d\boldsymbol{f} \\
&= \log p(\mathcal{D}) - \mathcal{L} \geq 0.
\end{aligned}
$$

- Select the optimal distribution $q(\boldsymbol{X})$ to maximize $\mathcal{L}$.

Joint Model and Variational Inference - 2

Variational Inference

- Variational distribution $q(\boldsymbol{f}, \boldsymbol{X}|\mathcal{Z}) = p(\boldsymbol{f}|\boldsymbol{X}, \mathcal{Z})q(\boldsymbol{X})$.

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\end{aligned}
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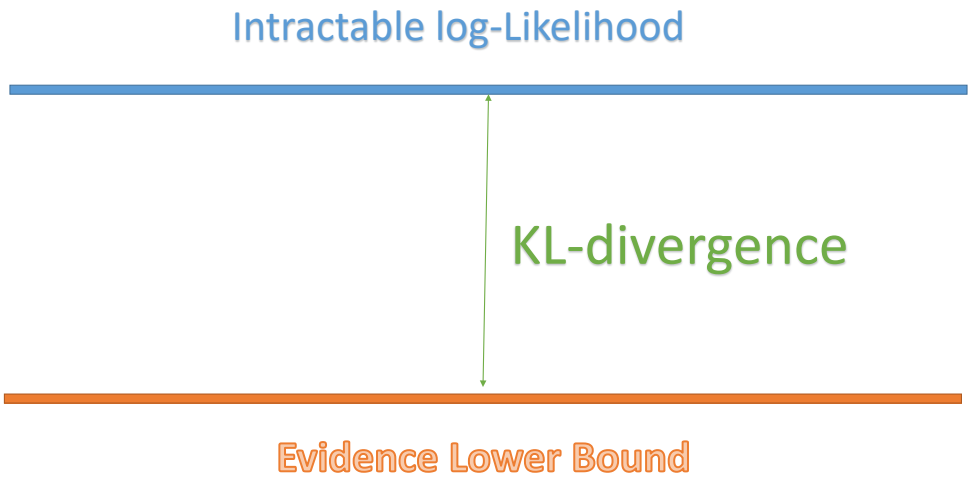


Evidence Lower Bound

Lemma

$$\mathcal{L}^* = \log[\mathcal{N}(\mathbf{0}, \sigma_\epsilon^2 \boldsymbol{I} + \boldsymbol{Q})] + \zeta + \sum_{i=1}^{N} \Big\{\delta_i \big\{ \log h_0(V_i) + \boldsymbol{\gamma}^T \boldsymbol{w}_i + \beta \mu_i(V_i) \big\}$$
$$- \int_0^{V_i} h_0(u) \exp[\boldsymbol{\gamma}^T \boldsymbol{w}_i] \exp\big[\beta[\mu_i(u) + \frac{1}{2}\sigma_i^2(u)]\big] du \Big\}.$$

- $\boldsymbol{Q} = \boldsymbol{K}_{\boldsymbol{f},\boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{f}}$ and $\zeta = -\frac{1}{2\sigma_\epsilon^2} \mathrm{Tr}(\boldsymbol{K}_{\boldsymbol{f},\boldsymbol{f}} - \boldsymbol{Q})$.
- $\mu_i(u) = \boldsymbol{K}_{f_i(u),\boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}}^{-1} \sigma_\epsilon^{-2} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}} (\boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}} + \sigma_\epsilon^{-2} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{f}} \boldsymbol{K}_{\boldsymbol{f},\boldsymbol{X}})^{-1} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{f}} \boldsymbol{Y}$.
- $\sigma_i^2(u) = \boldsymbol{K}_{f_i(u),f_i(u)} - \boldsymbol{K}_{f_i(u),\boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}}^{-1} (\boldsymbol{I} - \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}} (\boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}} + \sigma_\epsilon^{-2} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{f}} \boldsymbol{K}_{\boldsymbol{f},\boldsymbol{X}})^{-1} \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}}) \boldsymbol{K}_{\boldsymbol{X},\boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{X},f_i(u)}$.

Sparse

Pseudo-inputs

- M (e.g., 5-10) pseudo-inputs to the latent functions.

Large Matrix

$$\mathbf{\Sigma} = \begin{bmatrix} \Sigma_{1,1} & \cdots & \Sigma_{1,n} \\ \vdots & \ddots & \vdots \\ \Sigma_{n,1} & \cdots & \Sigma_{n,n} \end{bmatrix}$$

Approximation

$$(\sigma_\epsilon^2 I + K_{f,X} K_{X,X}^{-1} K_{X,f})^{-1}$$
$$= \sigma_\epsilon^{-2} I - \sigma_\epsilon^{-4} K_{f,X} (K_{X,X} + \sigma_\epsilon^{-2} K_{X,f} K_{f,X})^{-1} K_{X,f}$$

$\mathcal{O}(n^3) \rightarrow \mathcal{O}(nM^2)$

$$\Sigma = K_{f,X} K_{X,X}^{-1} \; K_{X,f}$$

$$(A + UCV)^{-1} = A^{-1} - A^{-1}U(C^{-1} + VA^{-1}U)^{-1}VA^{-1}.$$

Sparse Low-rank Matrix

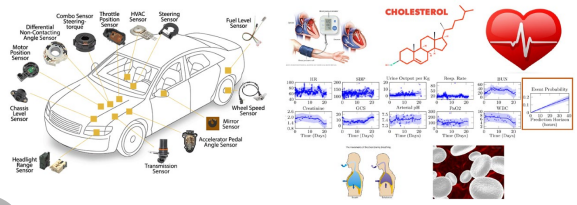
Woodbury Formula

Short Summary

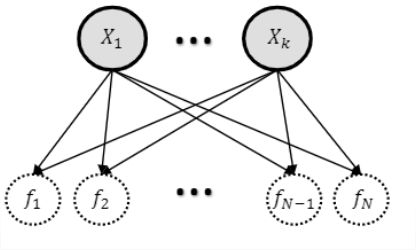
Joint Model

$$h_i(t) = h_0(t)\exp[\gamma^T w_i + \beta f_i(t)].$$

Application



Map

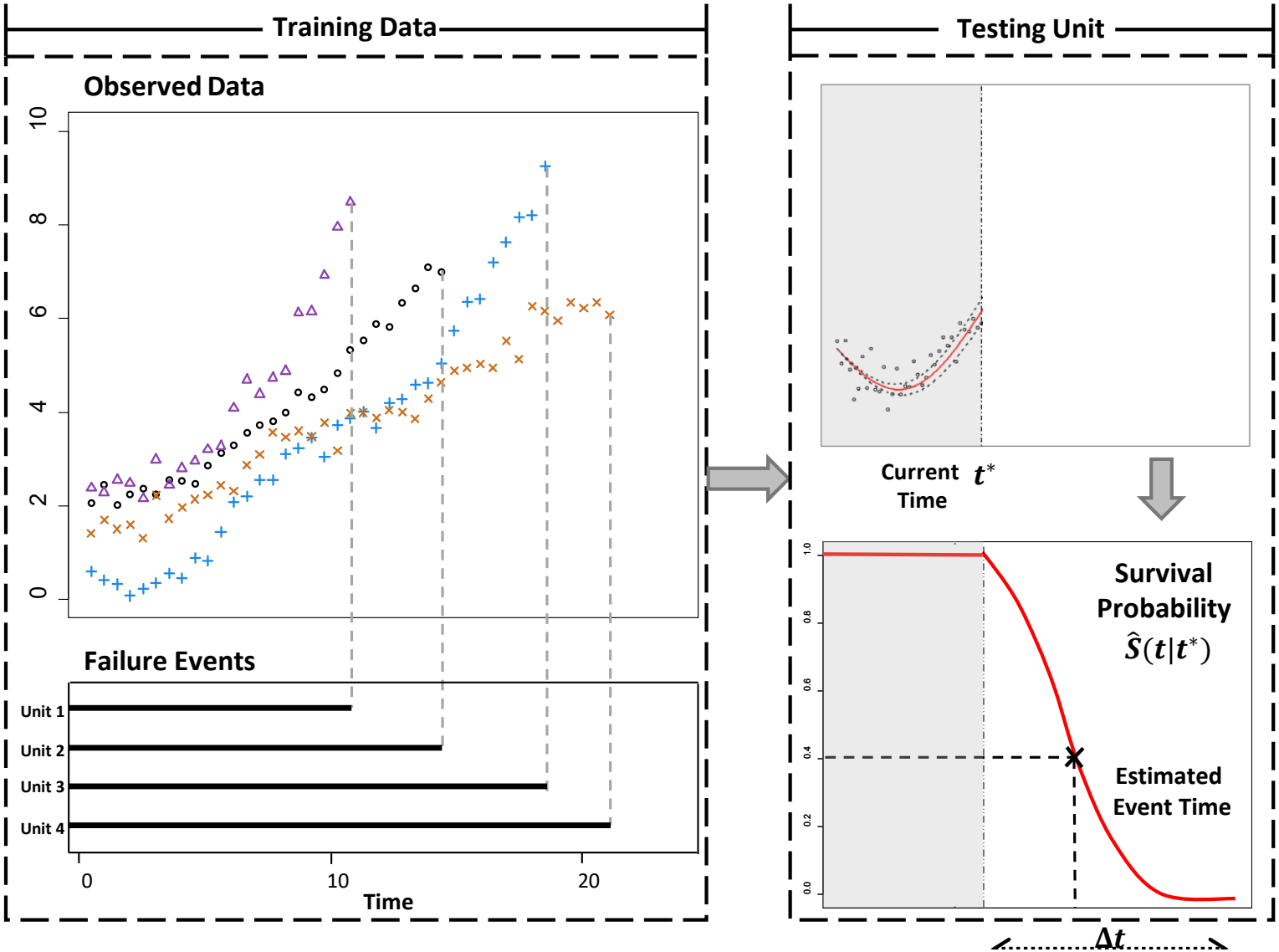


MGCP

$$\mathcal{L}^* = \log[\mathcal{N}(\mathbf{0}, \sigma_\epsilon^2 \boldsymbol{I} + \boldsymbol{Q})] + \zeta + \sum_{i=1}^{N} \{\delta_i \{ \log h_0(V_i) + \gamma^T \boldsymbol{w}_i + \beta \mu_i(V_i)\}$$
$$- \int_0^{V_i} h_0(u) \exp[\gamma^T \boldsymbol{w}_i] \exp\left[\beta[\mu_i(u) + \frac{1}{2}\sigma_i^2(u)]\right] du\}.$$

Inference

Short Summary



Event Prediction

Survival Probability Prediction

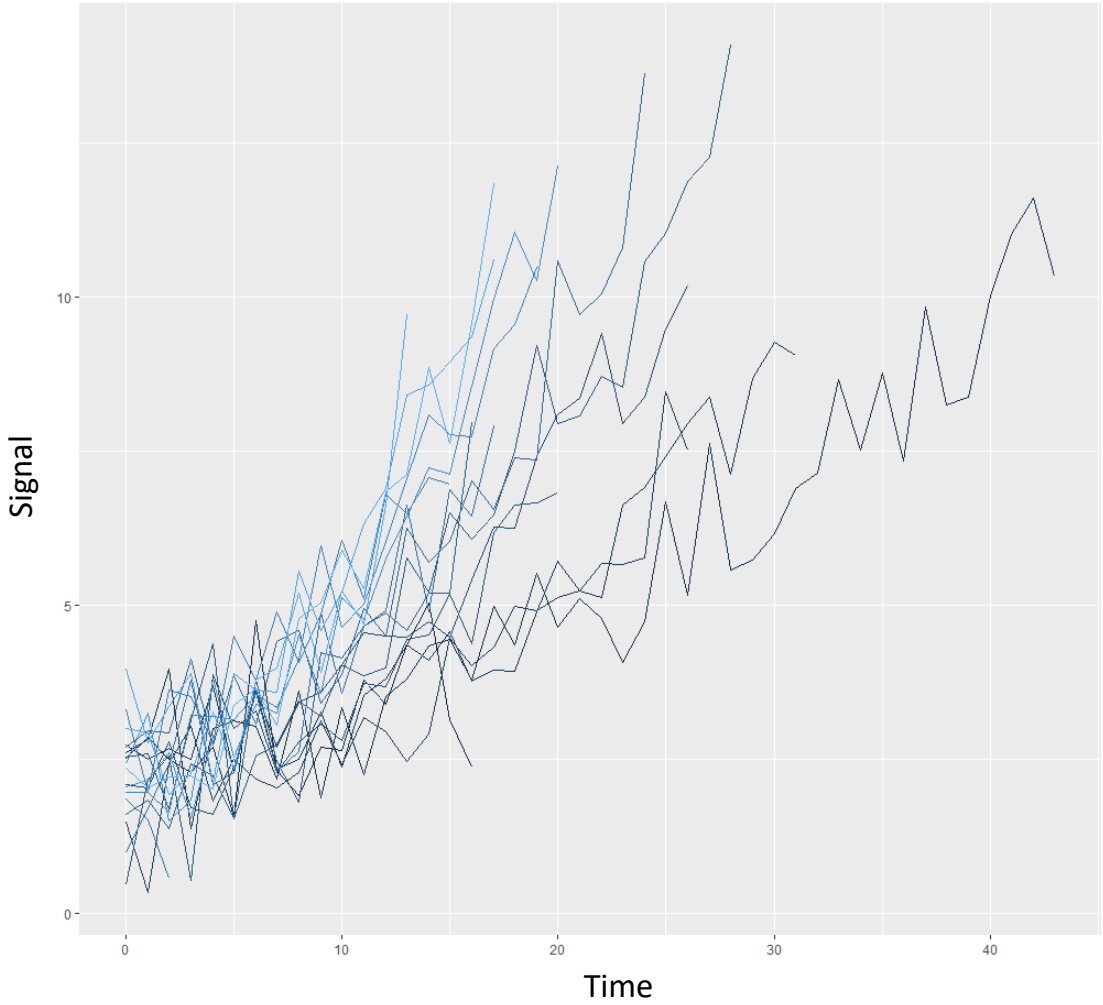
$$\hat{P}_{\Delta t} = \hat{S}(t^* + \Delta t | t^*, \boldsymbol{w}_N, \boldsymbol{f}_N) = \frac{\hat{S}(t^* + \Delta t | \boldsymbol{w}_N, \boldsymbol{f}_N)}{\hat{S}(t^* | \boldsymbol{w}_N, \boldsymbol{f}_N)}$$
$$= \exp\{-\int_{t^*}^{t^*+\Delta t} \hat{h}_0(u) \exp\left[\hat{\gamma}^T \boldsymbol{w}_N + \hat{\beta} \boldsymbol{A} \boldsymbol{D}^{-1} \boldsymbol{Y}\right] du\}.$$

Prediction of f

$$p(f_N(T^*)|\boldsymbol{Y}) = \int p(f_N(T^*)|\boldsymbol{X}) p(\boldsymbol{X}|\boldsymbol{Y}) d\boldsymbol{X}$$
$$= \mathcal{N}(\boldsymbol{A}\boldsymbol{D}^{-1}\boldsymbol{Y}, \boldsymbol{K}_{f_N(T^*), f_N(T^*)} - \boldsymbol{A}\boldsymbol{D}^{-1}\boldsymbol{A}^T),$$

- $\boldsymbol{A} = \boldsymbol{K}_{f_N(T^*), \boldsymbol{X}} \boldsymbol{K}_{\boldsymbol{X}, \boldsymbol{X}}^{-1} \boldsymbol{K}_{\boldsymbol{X}, \boldsymbol{f}}$ and $\boldsymbol{D} = \boldsymbol{Q} + \sigma_\epsilon^2 \boldsymbol{I}$.

Simulation - Training Units (Parametric)

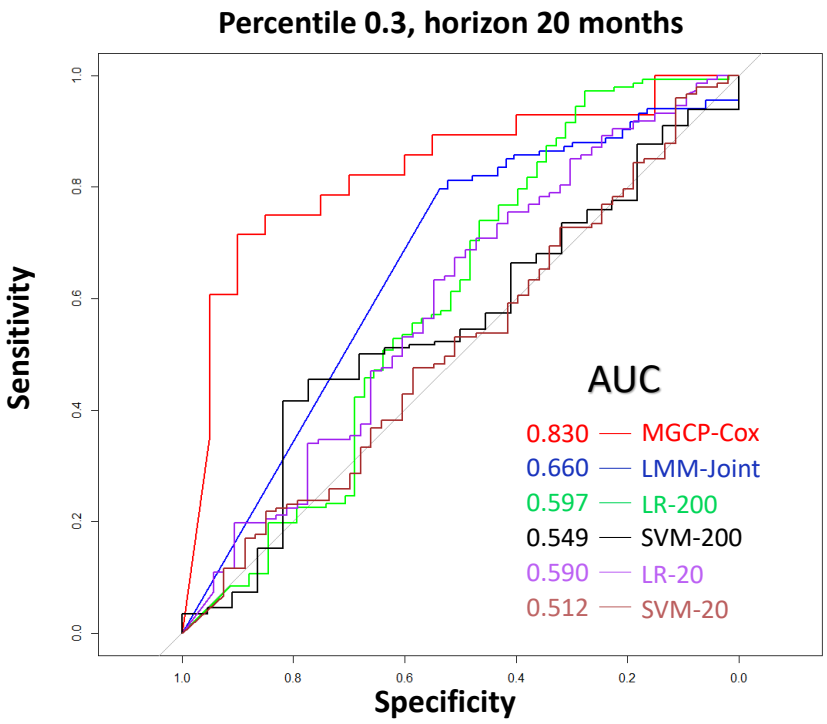


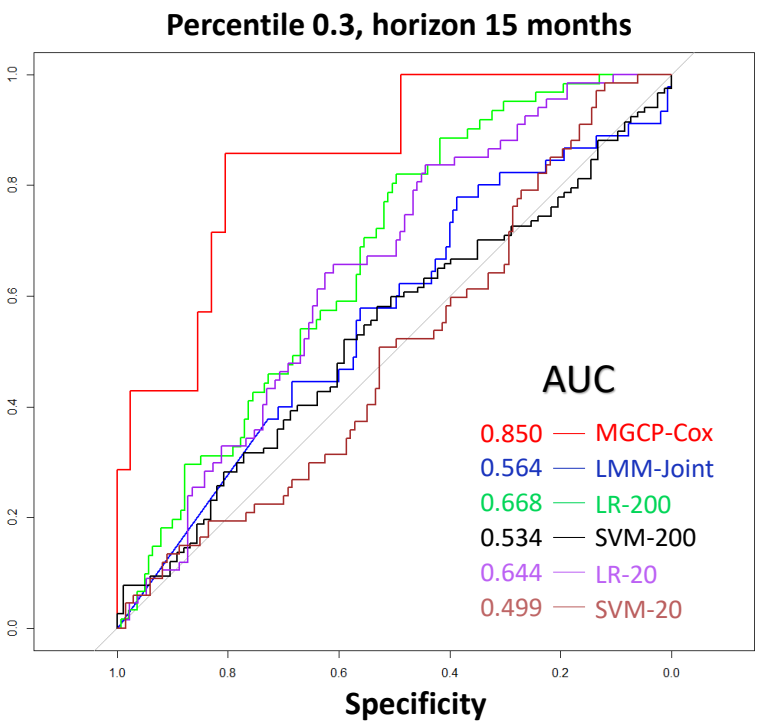
$$y = b_{i0} + b_{i1}t^{1.2} + b_{i2}t^{1.7} + \epsilon_i(t).$$

Simulation - Classification Problem

- Sample size $N = 20$.
- Predict survival probability within a future time interval Δt.
- Transform probabilities into binary variables by a certain classification threshold.
- Performance is evaluated the the Receiver Operating Characteristic (ROC) curve.
- Baseline methods: logistic regression ($N = 200$), SVM ($N = 200$), parametric joint model (LMM-Joint) ($N = 30$).

Early-stage (30% observation)

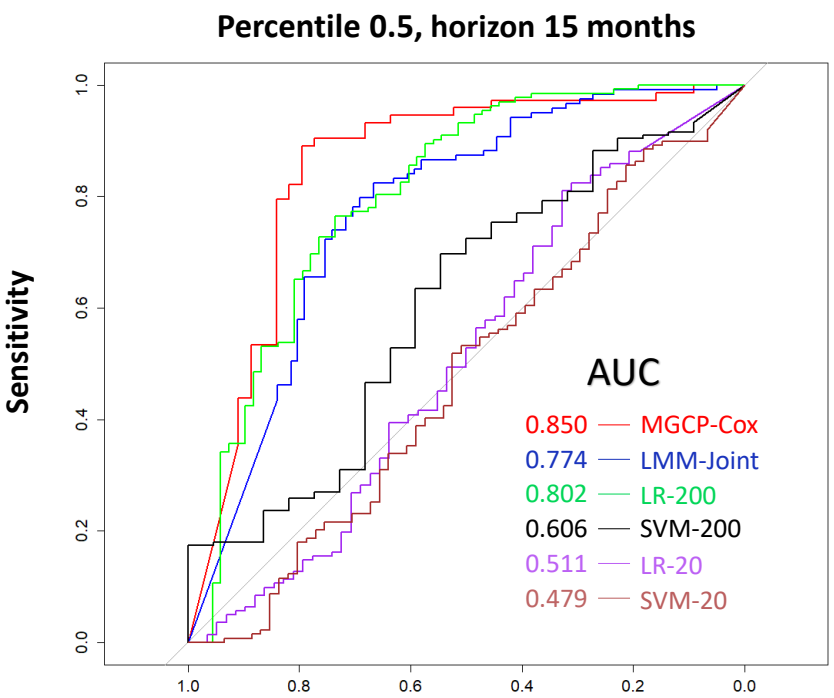


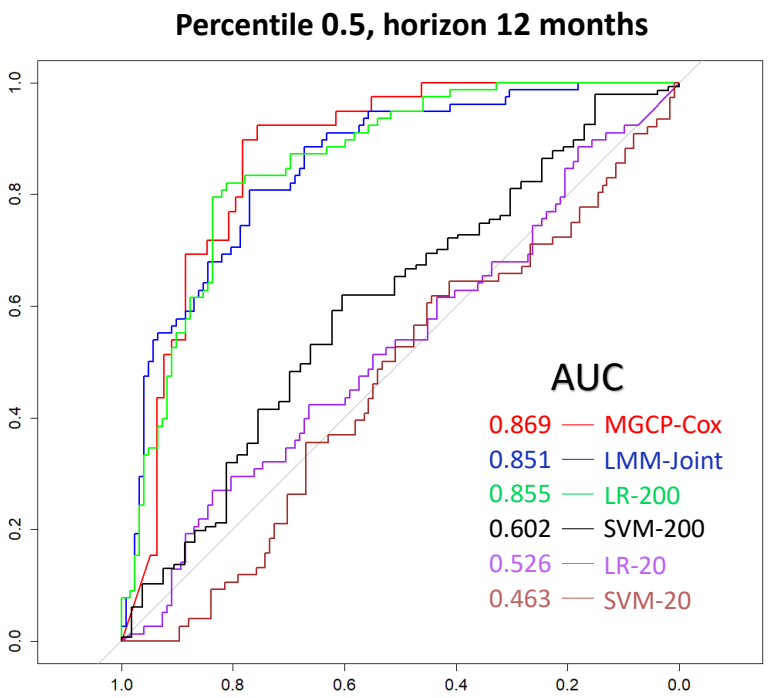


Discussion

- Accurately detect failure event at early stage.
- Important. Avoid economic loss!

Middle-stage (50% observation)

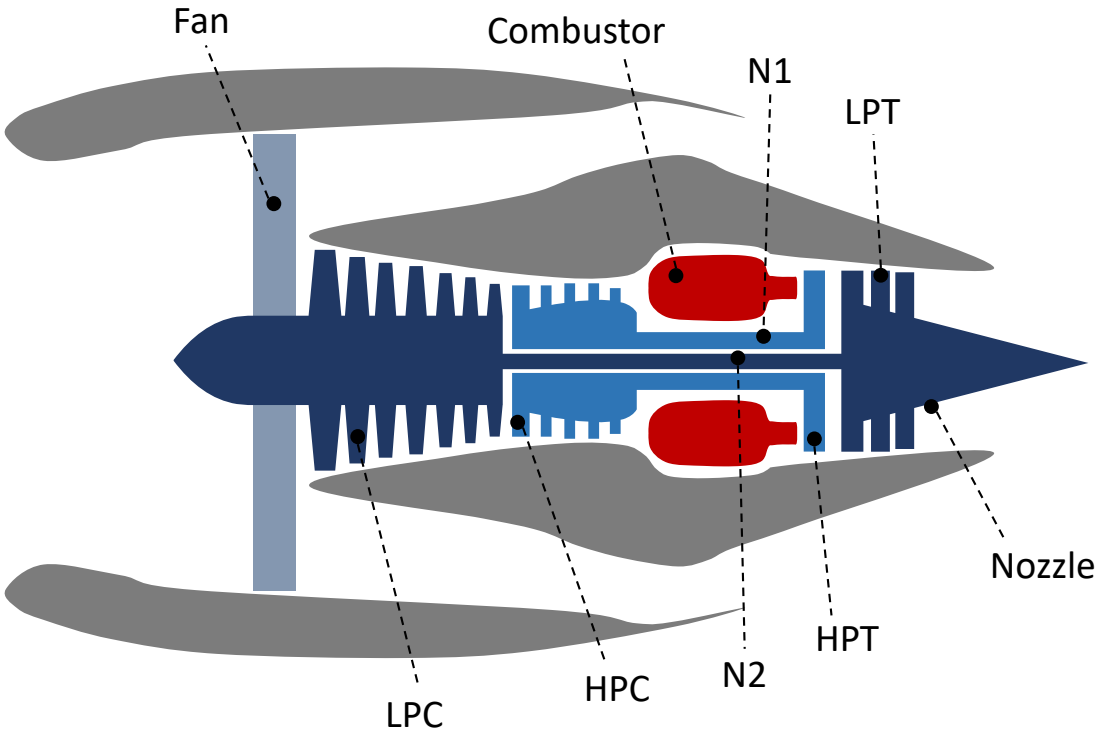




Discussion

- Require small sample size. Cost-effective.
- Outperform parametric model.

NASA Data - Description



Symbol	Description	Units
T2	Total temperature at fan inlet	°R
T24	Total temperature at LPC outlet	°R
T30	Total temperature at HPC outlet	°R
T50	Total temperature at LPT outlet	°R
P2	Pressure at fan inlet	psia

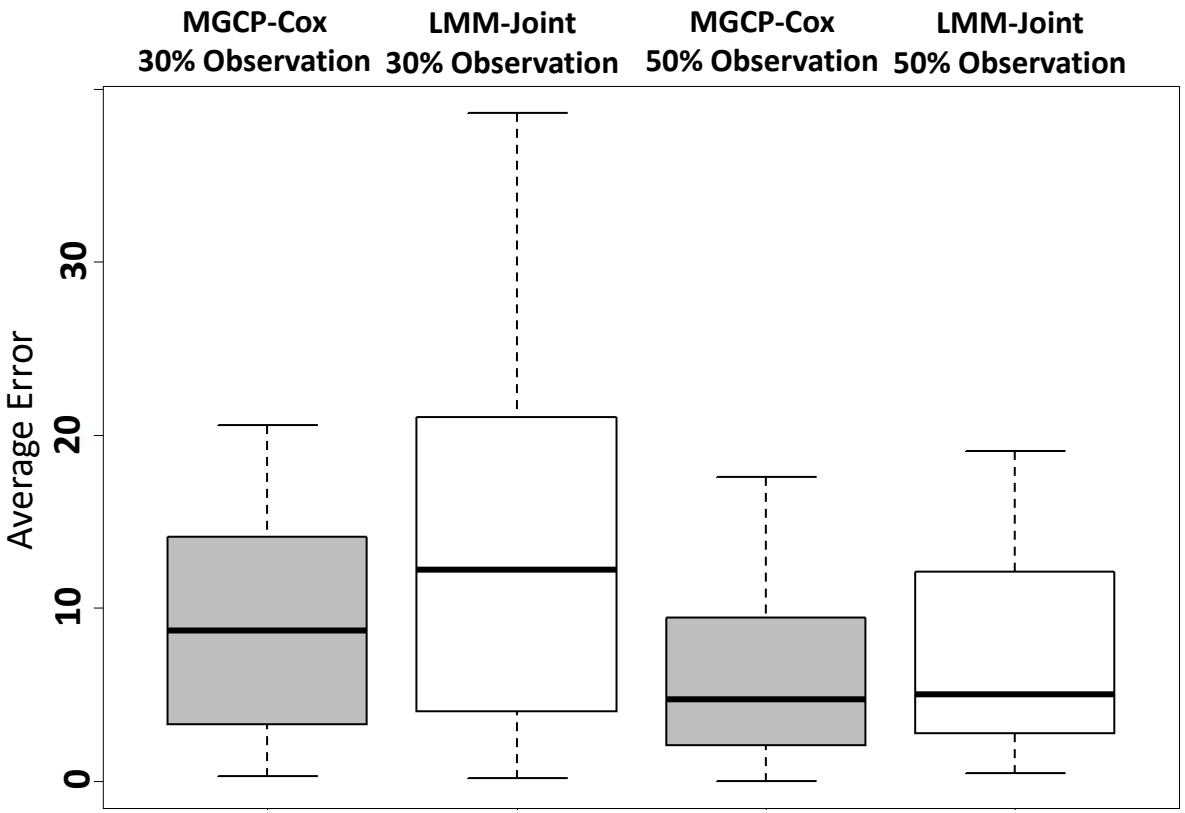
NASA Data - Description

- Failure time data of aircraft turbofan engines and degradation signals from sensors mounted on these engines.
- Time domain: 0-300.
- The mean remaining lifetime

$$\widehat{mrl}(t^*) = \int_{t^*}^{\infty} \hat{S}(u|t^*, \boldsymbol{w}_{test}, \boldsymbol{f}_{test})du.$$

- Evaluation: absolute error $AE = |rl_j - \widehat{mrl}_j|$ where rl_j is the true remaining lifetime of the testing unit.

NASA Data - Result



Conclusion

Contribution

- Relieve parametric assumption: introduce a flexible and scalable non-parametric mixed-effect model.
- Introduce a variational inference framework to jointly estimate all parameters simultaneously.

Impact

- Accurate, requires small sample-size.
- Applicable to healthcare system, automobile system, or even large and complex connected system.