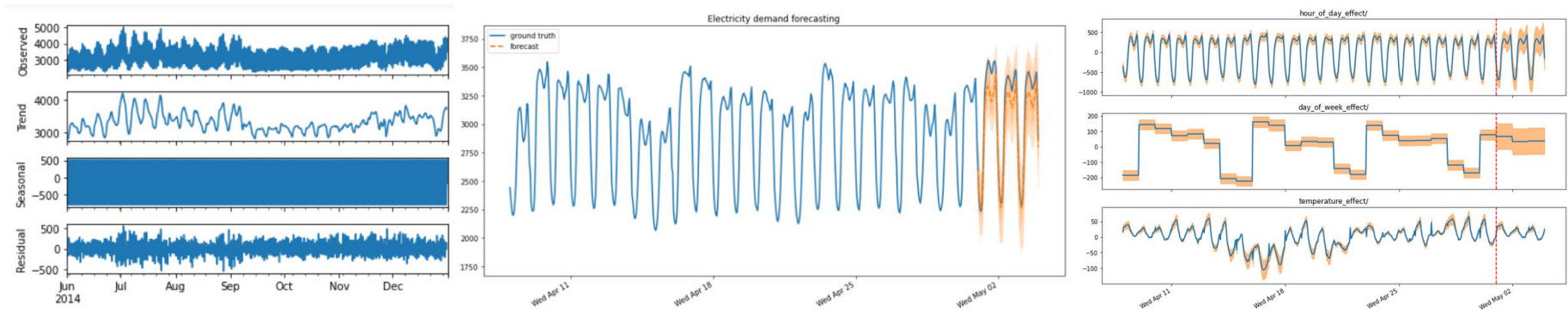


Data Driven Engineering II: Advanced Topics

State Space Models II

Institute of Thermal Turbomachinery
Prof. Dr.-Ing. Hans-Jörg Bauer



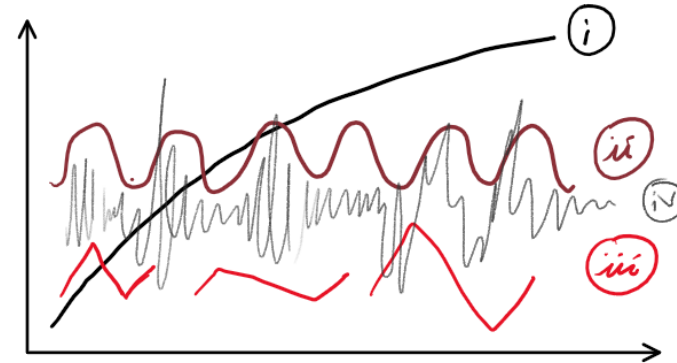
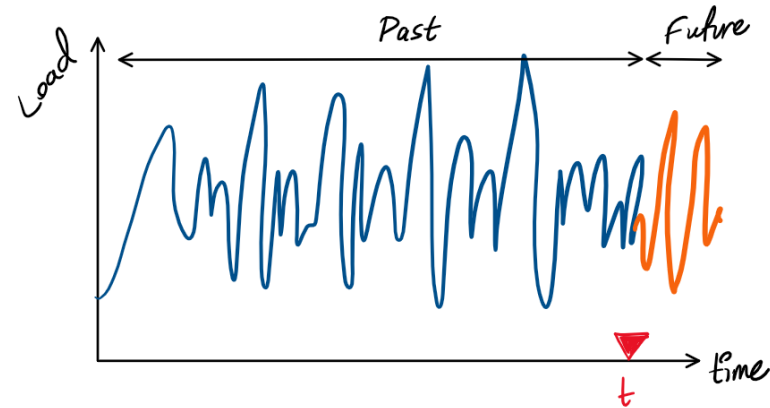
Dynamical Datasets: Time Series

Outline

- * Time Series = Overview
- * Statistical Models for time series
- * State space models \Rightarrow DDE II
- * Machine Learning Part I
- * Machine Learning Part II

Time Series Analysis

* Components of time series



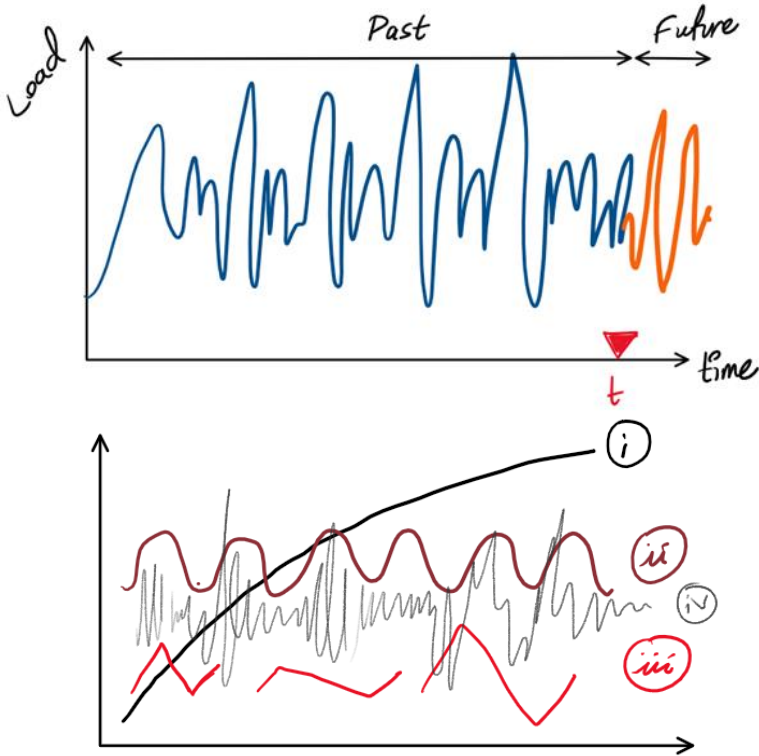
i) Long term trends

iii) Cyclic variations

ii) ST seasonal variations

iv) Random fluctuations

Time Series Analysis



* Components analysis



"Stationarity"

$$[\bar{X} \text{ \& } \sigma \neq f(t)]$$

~ Strong ~

$$[\bar{X} \text{ \& } \text{auto covariance} \neq f(t)]$$

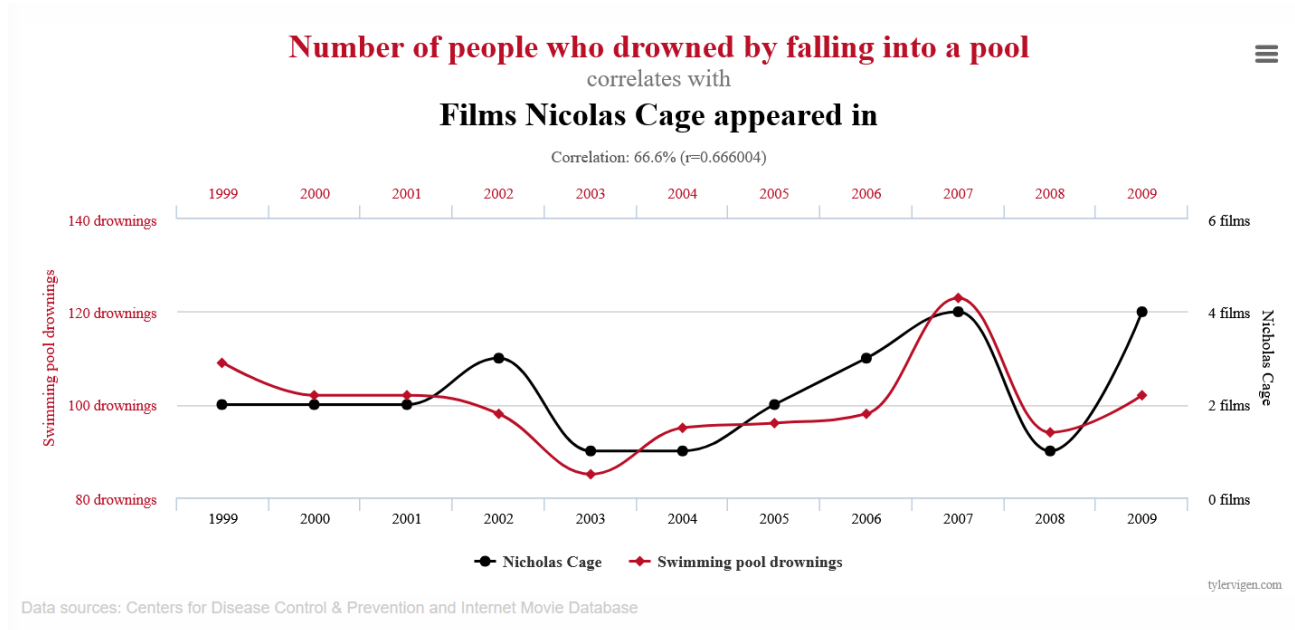
~ weak ~

* Forecasting:

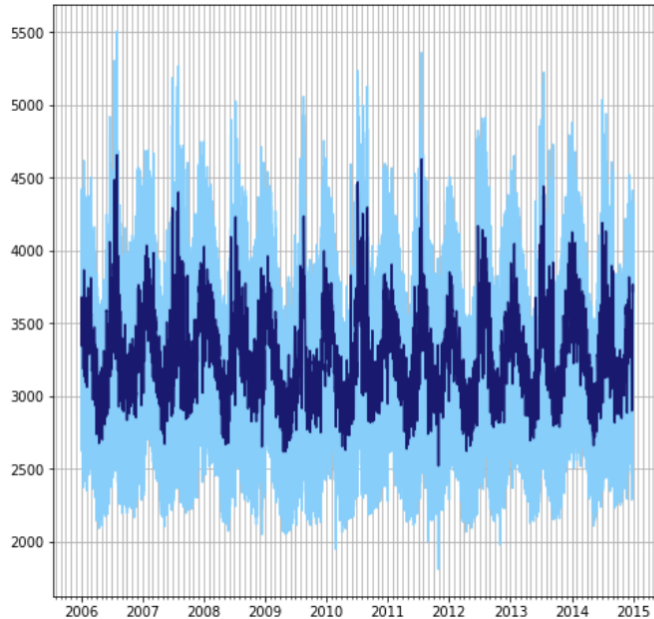
☑ There is an ordered relationship between observations

$$t_{i-j} \rightarrow t_i$$

Spurious Correlations

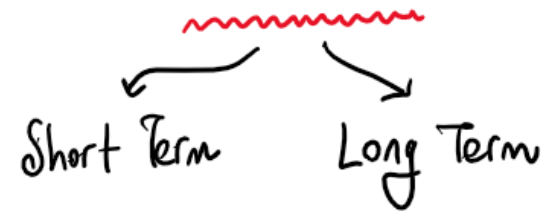


Case: Energy Demand Forecasting



* 8 years data of Temp & Load ($\Delta t = \text{hr}$)

? Power Demand forecasting



Case: Energy Demand Forecasting

* Short term load forecasting : ~ 1 hr to 24 hr
 \sim demand / supply

← near past is used

← Temperature is an important feature

* Long term LF : ~ 1 week to months
 \sim years

} Planning & investment

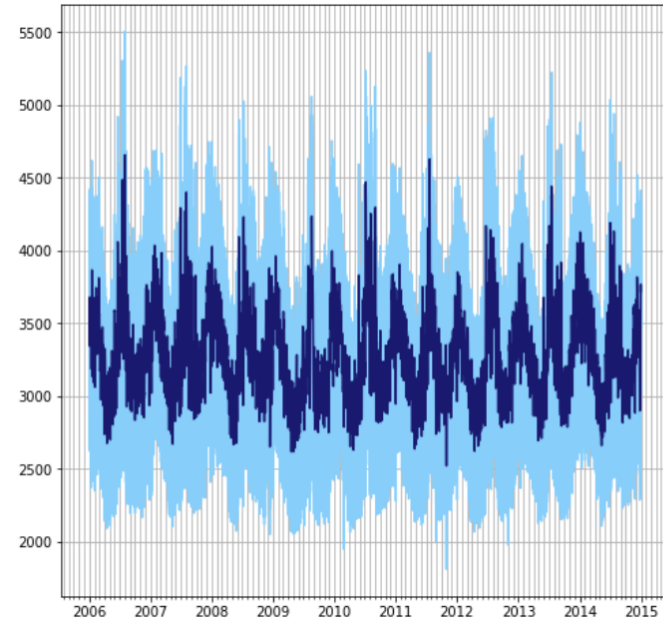
← Seasonal patterns

← Long term trends

← Climate Models

Case: Energy Demand Forecasting

Typical	STLF	LTLF
Horizon	1 hr - 2 days	≥ 1 months
Granularity	\sim hr	\sim hr - day
History Range	~ 2 years	$\sim \geq 5$ years
Accuracy	$\leq 5\%$ error	$\leq 25\%$ error
Forecasting freq.	\sim hr to day	\geq month



Data Exploration: Temporal Nature of data

① How to handle "time stamps",

	Date	Hour	load	T
0	01/01/2004	1	NaN	37.33
1	01/01/2004	2	NaN	37.67
2	01/01/2004	3	NaN	37.00
3	01/01/2004	4	NaN	36.33
4	01/01/2004	5	NaN	36.00



	load	T
2012-01-05 00:00:00	3167.0	19.00
2012-01-05 01:00:00	3014.0	22.33
2012-01-05 02:00:00	2921.0	22.33
2012-01-05 03:00:00	2874.0	22.00
2012-01-05 04:00:00	2876.0	21.67

Data Exploration: Temporal Nature of data

② Temporal data decomposition

Stationarity



how 'stable' your system ☒ Intuition



how much we should expect

the past reflects itself on future ?



"Self Correlations"



Bayesian Structural Time Series

* BSTS \Leftrightarrow linear Gaussian Model \ll Kalman F.

* Idea:  } $f_i := \text{Hypothesis library}$

$X = [\dots]$  \Rightarrow Describes & predicts system behavior

... Fitting ...

Bayesian Structural Time Series

* General pseudo-algorithm:

- (1) Define a structural model
- (2) Specify priors.
- (3) Update estimates of states based on / observation data
- (4) Perform variable selection (eg. spike & slab method)
- (5) Apply Bayesian model averaging
- (6) Forecasting



How fitting works?

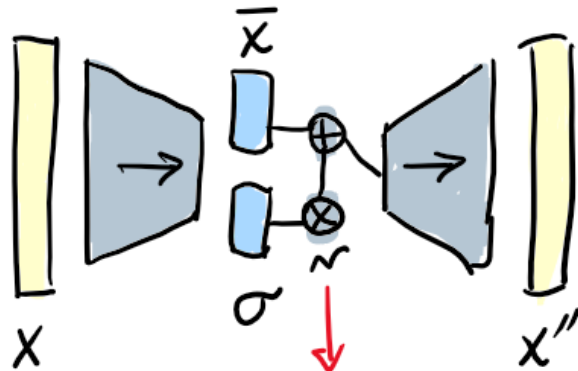
* Minimize Kullback-Leibler divergence (see VAE, DDE-I)

Variational Encoders:

* Gaussian Sampling



[enforced via cost-function]

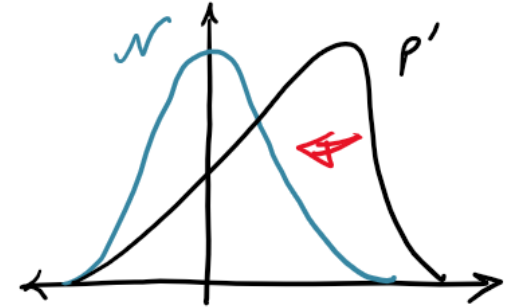


Sampled Randomly (ω)

Kullback - Leibler
(KL) Divergence
(\mathcal{N} & \mathcal{P}')

$$D_{KL}[\mathcal{P}'(\bar{x}, \sigma) || \mathcal{N}(0, 1)]$$

- $\mathcal{L}_{KL} = -\frac{1}{2} \sum_i 1 + \gamma_i - \exp(\gamma_i) - \bar{x}_i^2$
- $\gamma_i = \ln(\sigma_i^2)$



How fitting works?

* Minimize Kullback-Leibler divergence (see VAE, DDE-I)

• $x := \text{observable}$; $z := \text{'latent, variables'}$

• $p(z|x) = \frac{p(x|z)}{p(x)} \Rightarrow p(x) = \int \underbrace{p(x,z)}_{\text{red wavy line}} dz ?$

• Variational Inference $:= q^*(z) = \min_{\underbrace{q \in \mathcal{D}}_{\text{candidate approximations}}} \text{KL}(q(z) \parallel p(z|x))$

How fitting works?

$$\textcircled{1} \quad \text{KL} \left(q(z) \parallel p(z|x) \right) = \underbrace{\mathbb{E} \left[\log(q(z)) \right] - \mathbb{E} \left[\log(p(z|x)) \right]}_{(-\text{ELBO}): \text{evidence lower bound}} + \log(p(x)) \quad \text{!}$$

$$\begin{aligned} \text{ELBO}(q) &= \mathbb{E} \left[\log(p(z, x)) \right] - \mathbb{E} \left[\log(q(z)) \right] \\ &= \mathbb{E} \left[\log(p(x|z)) \right] - \text{KL} \left(q(z) \parallel p(z) \right) \end{aligned}$$

\sim balance btw. $\underbrace{\text{expected}}_{\text{likelihood}} \quad \sim \text{prior}$

How fitting works ?

② Variational Inference $:= q^*(z) = \min_{\underbrace{q \in \mathcal{Q}}_{\text{candidate approximations}}} \text{ELBO}(q)$

Tensorflow

* Create variational posteriors;

- Sample prior distributions
- Select an optimizer
- Fit posteriors by min. ELBO

```
# Building the variational surrogate posteriors `qs`:  
#https://www.tensorflow.org/probability/api\_docs/python/tfp/sts/build\_factored\_surrogate\_posterior  
variational_posteriors = tfp.sts.build_factored_surrogate_posterior(  
    model=load_model)
```

```
num_variational_steps = 120  
optimizer = tf.optimizers.Adam(learning_rate=.1)  
  
elbo_loss_curve = tfp.vi.fit_surrogate_posterior(  
    target_log_prob_fn=load_model.joint_log_prob(  
        observed_time_series=train),  
    surrogate_posterior=variational_posteriors,  
    optimizer=optimizer,  
    num_steps=num_variational_steps)
```



colab

Markov Chain Monte Carlo (MCMC)

* Invented after MC @ Los Alamos (1953)

↳ liq. phase eq. with its vapor (Eq. Thermodynamics)

↳ Metropolis Algorithm

↳ M-Hasting

↳ Gibbs Sampler

} Simulates
posterior dist.


Enables full Bayesian interface

Markov Chain Monte Carlo (MCMC)

* Markov Chains \Rightarrow early 20th cent; alternations of letters in a poem;
"Onegin" by Pushkin

• Characterization of
Sequence of random variables;

• $X_1, X_2, X_3, X_4, \dots, X_n, X_{n+1} \left\{ \begin{array}{l} (n+1) \text{ depends only} \\ (n) \end{array} \right.$



Markov Chain Monte Carlo (MCMC)

* Hidden Markov Models \Leftrightarrow Kalman Filter

② variables we observe may not be the most descriptive

③ "unsupervised learning"

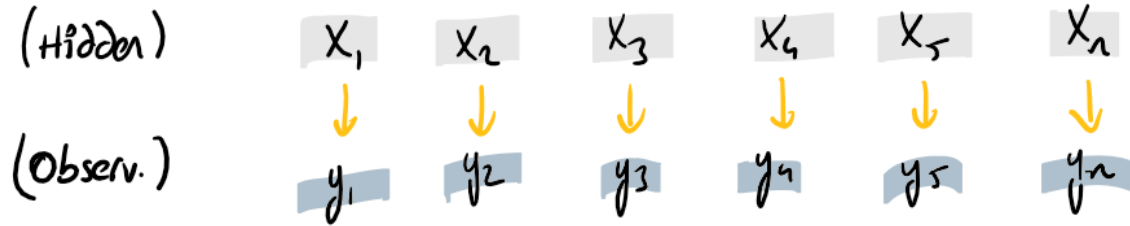
→ we have an idea about how system works.

~~Eg~~

State	L	G
L	0.6	0.4
G	0.2	0.8

? {
(0) state \rightarrow L
(1) 60% \Rightarrow L
40% \Rightarrow G

Markov Chain Monte Carlo (MCMC)



* We can describe a system if we know:

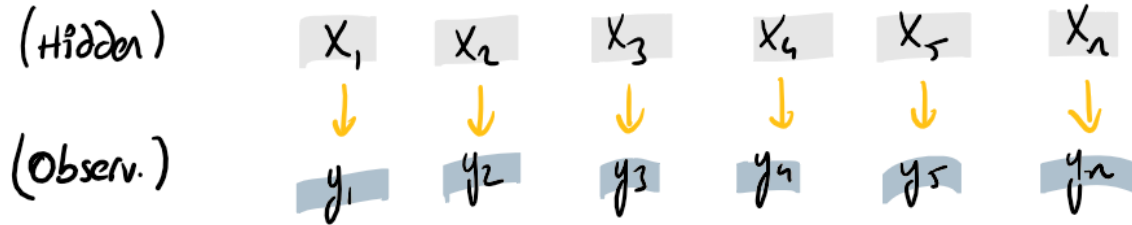
- initial state of the system (π_{ij})
- emission probability; prob. of observing y_i given x_i (b_{ij})
- Transition probability; $x_i \rightarrow x_{i+n}$ (a_{ij})

$$\lambda (\pi_{ij}, b_{ij}, a_{ij})$$


 y_i

iterative solution
for λ

Markov Chain Monte Carlo (MCMC)



$$\lambda (\pi_{ij}, b_{ij}, a_{ij})$$

λ — Frequentist inference

"with enough sampling,
we can find it"

Expectation Maximization (EM)
...
Baum-Welch Algorithm

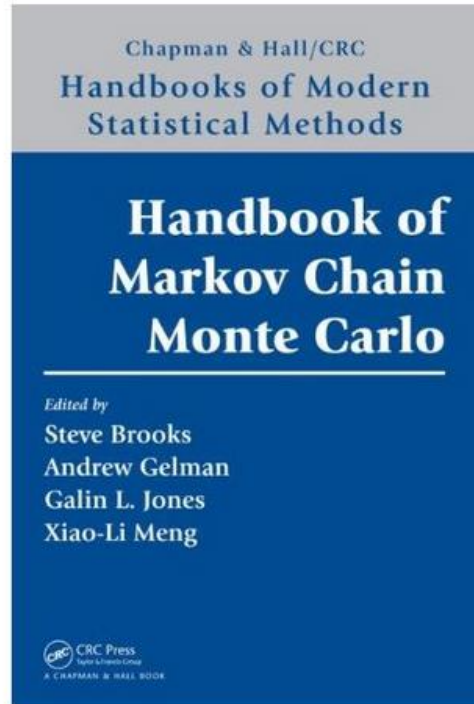
Bayesian inference

"continuously update the
posterior for best λ "

MCMC
Gibbs Sampling
VT Algorithm



colab



Variational Inference: A Review for Statisticians

David M. Blei
Department of Computer Science and Statistics
Columbia University

Alp Kucukelbir
Department of Computer Science
Columbia University

Jon D. McAuliffe
Department of Statistics
University of California, Berkeley

May 11, 2018

Additional Notes