Aalto University
School of Chemical
Engineering

Parameter Prediction for Stochastic Job Shop Scheduling Using probabilistic Machine Learning

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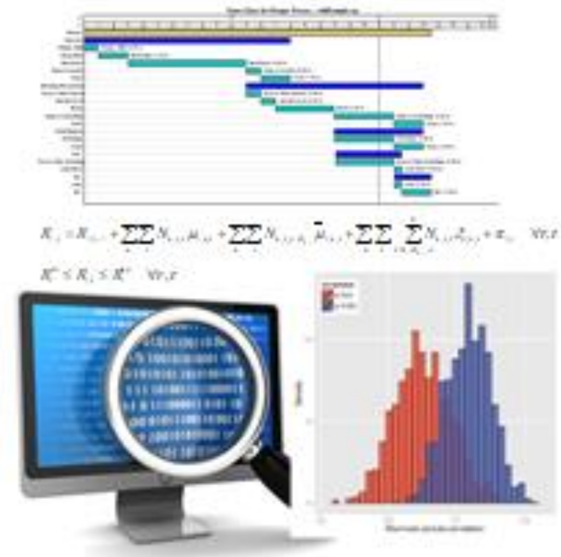
2nd November 2018
AIChE Annual Meeting 2018
Aalto University

SINGPRO Project (2018-2019)
Synergistic and intelligent process optimization

- **Earlier in AIChE:**
  - 530h Scheduling and Analytics – Towards better planning (Iiro Harjunkoski)
- **In brief**
  - PI: Adj. Professor Iiro Harjunkoski (Aalto University / ABB)
  - Partner: Professor Keijo Heljanko (University of Helsinki)
  - The goal is to use data analytics with mathematical optimization models collaboratively, in order to create adaptive data-driven online scheduling models

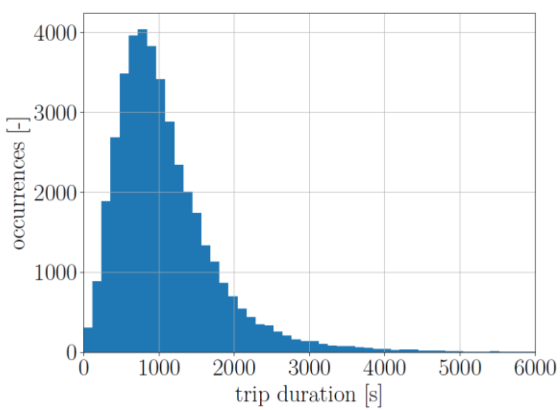


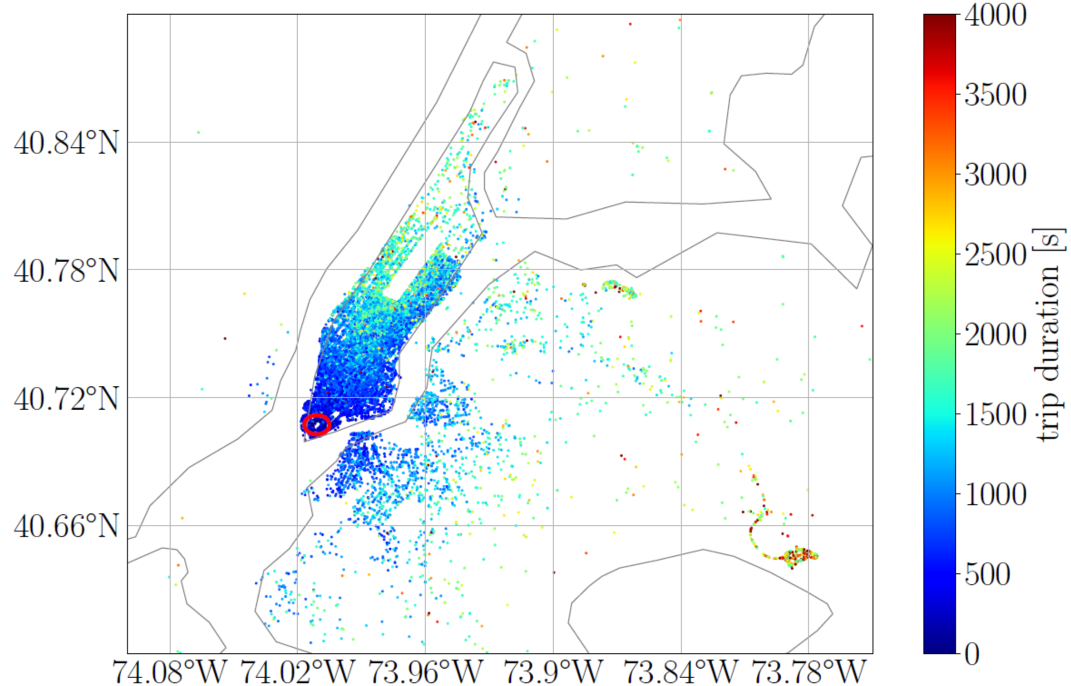
Outline

- **New York City taxi duration dataset**
- **Scheduling problem**
- **Methods**
  - Prediction models
  - Scheduling model
- **Results**
  - Example problem
  - Statistical experiment
- **Conclusions and future work**

New York City (NYC) taxi duration dataset

- Openly available dataset at https://www.kaggle.com/c/nyc-taxi-trip-duration
- Data of over 1.4 million taxi tips in NYC
- The ground truth is the trip duration
- Examples of features
  - Passenger count, pick-up and drop-off date, time and coordinates





Scheduling problem

- A company, head quartered at Wall street, performs surveys at remote sites in NYC
- Objective: minimize the make span of performing surveying trips at six different sites (Fig. 1)
- Surveying trip consists of outbound taxi trip, survey and inbound taxi trip (Fig. 2)
- Constraints:
  - Only two taxi trips can be performed at the same time
  - Only two surveys can be performed at the same time
- Durations of taxi trips are predicted, the surveys have a fixed duration of 1800 s

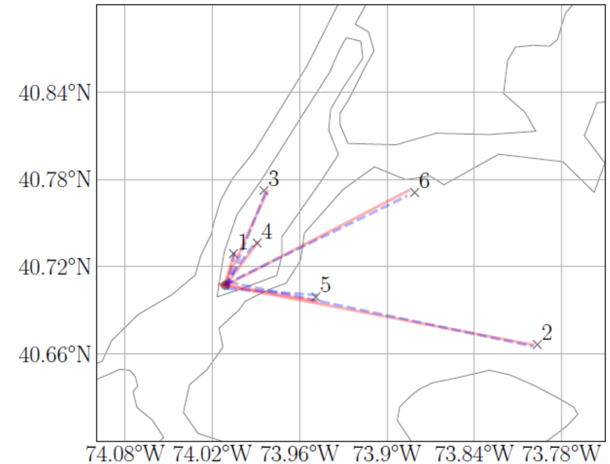


Fig. 1: An example set of surveying sites

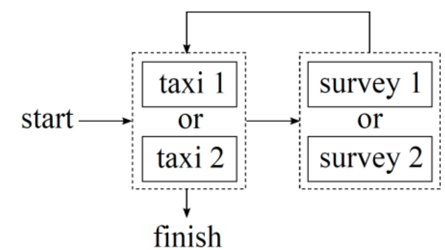
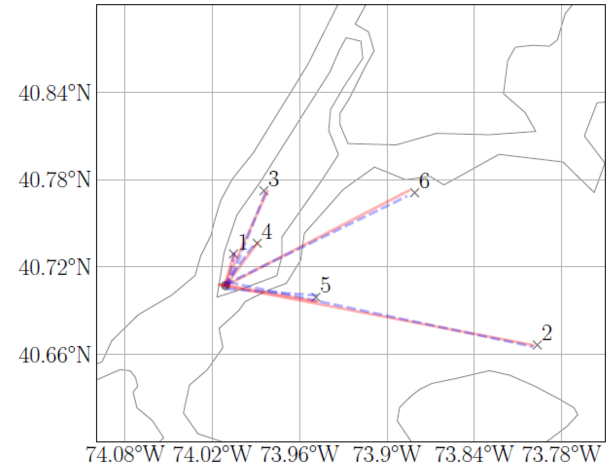


Fig. 2: Procedure of performing a surveying trip

Scheduling problem: industrial correspondence

Scheduling problem	Corresponding industrial examples
Outbound taxi trip	Preparation, heating
Survey	Chemical reaction, mechanical operation
Inbound taxi trip	Purification, cooling



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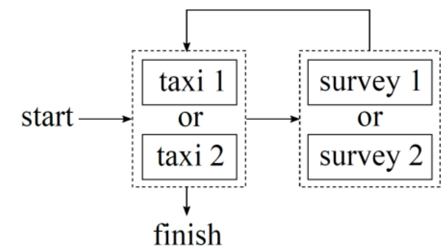
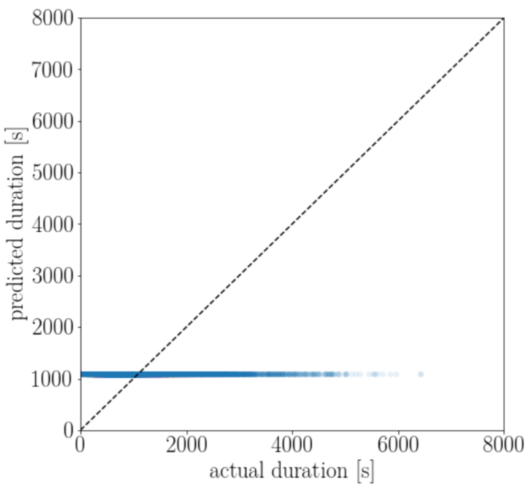


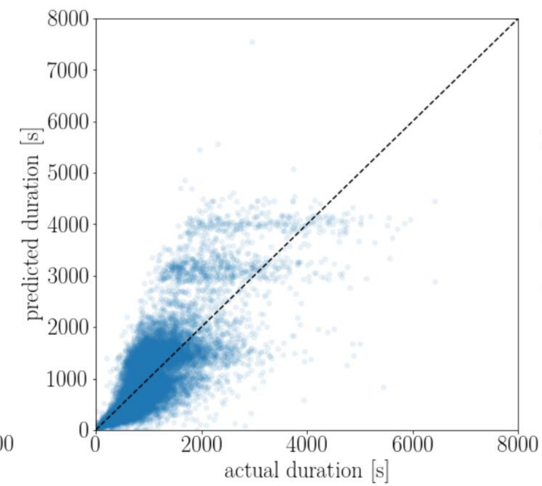
Fig. 2: Procedure of performing a surveying trip

Prediction models

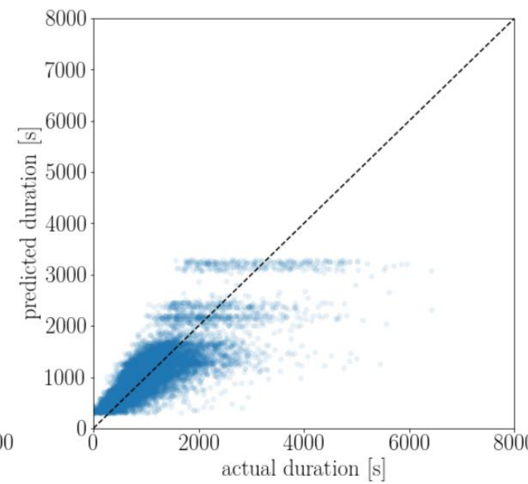
Prediction models, starting from the lowest fidelity



1) Average model



2) Rate model



3) Gaussian process (GP) model

prediction model	RMSE	r^2
average	701.8	-2.37e-4
rate	556.5	0.371
GP	438.4	0.610

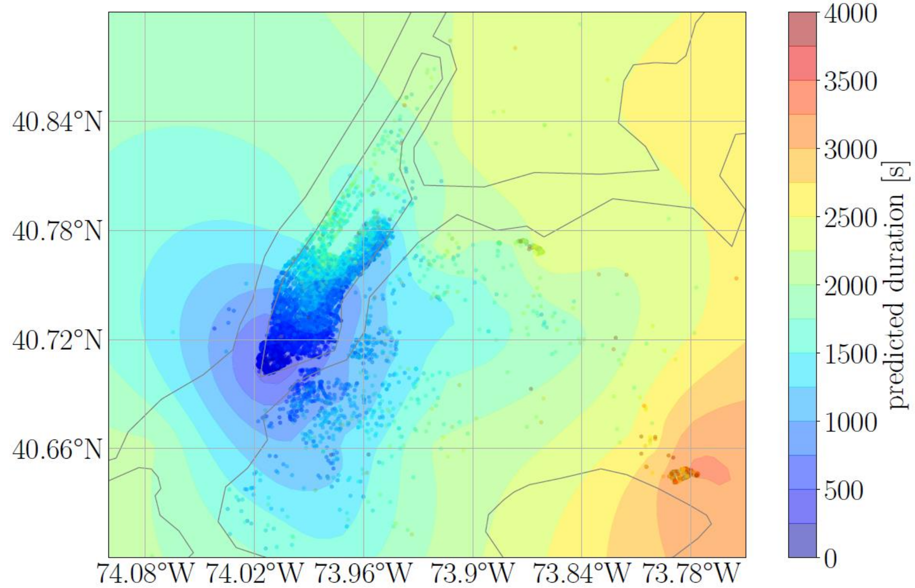
RMSE = the root mean square error
r^2 = the coefficient of determination

Prediction models: industrial correspondence

Prediction model	Industrial correspondence
Average	A static table value, which is determined as an average of historical values
Rate	A model which considers the task to have a constant processing rate (e.g. heating or purification of a volume of material)

Prediction models: Gaussian process regression

- **Kernel**
  - Exponential kernel
    $$\kappa(x, x') = \sigma_f^2 \exp\left(-\frac{\|x - x'\|}{2l^2}\right)$$
  - Noise term
- **Choosing the hyperparameters**
  - Tuned using the maximum a posteriori (MAP) estimate
- **3000 random samples from the training data**



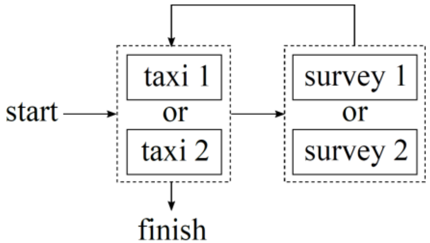
Scheduling model

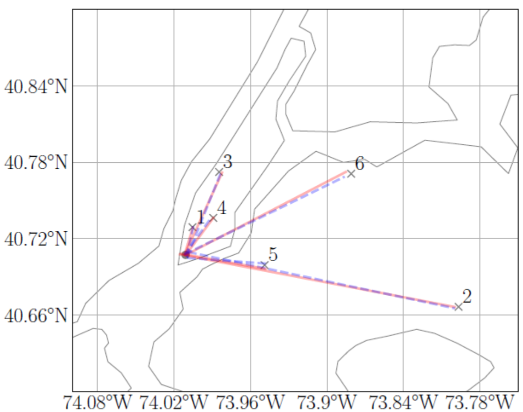
- **Unit-specific continuous-time scheduling model by Shaik and Floudas (2009)**
- **We use the value $\Delta n = 1$ (which defines the number of event points a job can span over)**
- **The number of total event points is determined by iteratively increasing n until the model has a feasible solution**

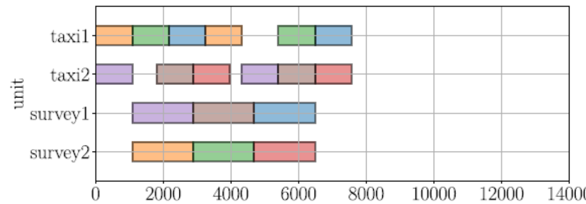
Shaik, M.A. and Floudas, C.A. (2009). Novel unified modeling approach for short-term scheduling. *Industrial & Engineering Chemistry Research*, 48(6), 2947-2964.

Results: a single scheduling problem

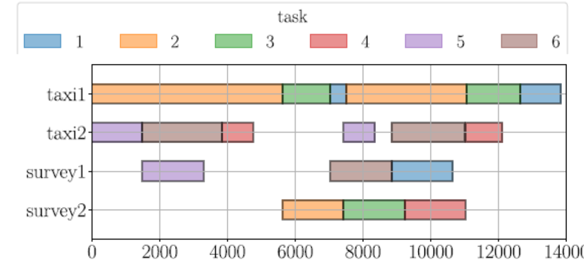
Optimized and realized schedules of six tasks, consisting of outbound taxi, survey, and inbound taxi



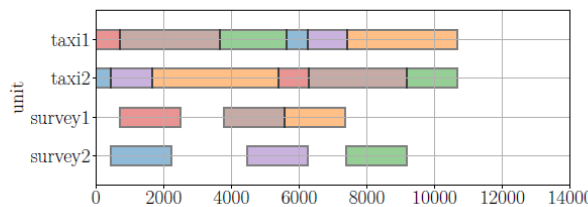




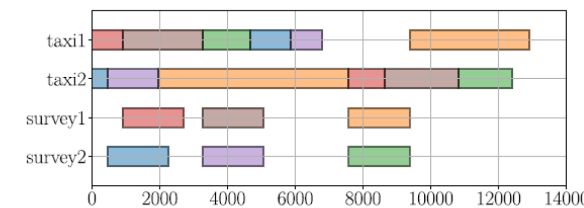
(a) Average prediction model: optimized schedule



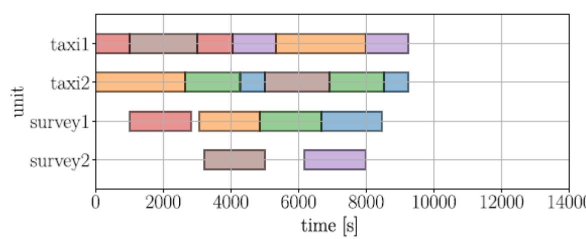
(b) Average prediction model: realized schedule (ms =13 830 s)



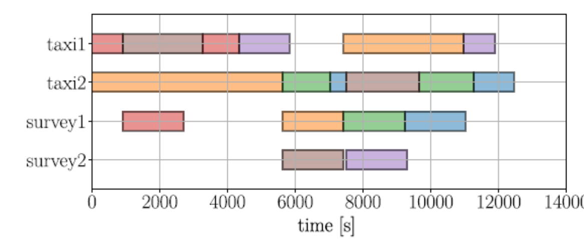
(c) Rate prediction model: optimized schedule



(d) Rate prediction model: realized schedule (ms =12 910 s)

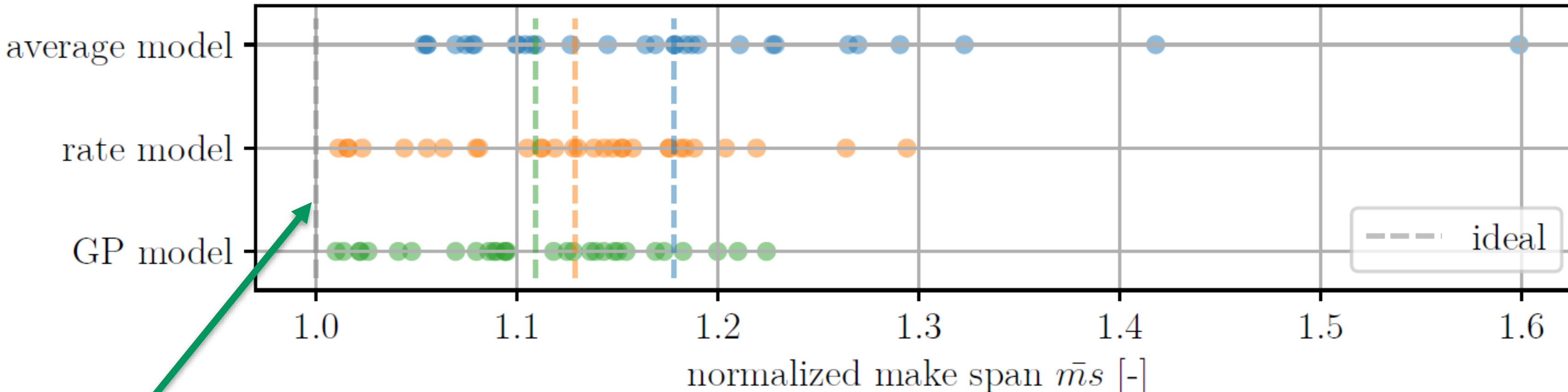


(e) GP prediction model: optimized schedule



(f) GP prediction model: realized schedule (ms =12 450 s)

Results: 30 different scheduling problems



The reference model is the *ideal predictor*, for which $r^2 = 1$ and RMSE = 0.

Results: 30 different scheduling problems

prediction model	$\bar{ms}$ [-]		solution time [s]		
	mean	sd	mean	min	max
average	1.178	0.119	4.45	4.25	5.74
rate	1.129	0.072	45.94	7.71	121.69
GP	1.109	0.061	79.66	16.44	344.82

- **Average prediction model requires an order of magnitude shorter solution time than the rate and GP prediction models**

Conclusions

- Job shop scheduling with data-driven duration prediction of three levels of fidelity is studied
- In the studied problem, the GP prediction model yields shorter make spans than average and rate prediction models by the margins of 5.8% and 1.8%, respectively
- However, the computational costs of GP and rate prediction models are an order of magnitude higher than that of the average prediction model

Future work

- Proactive scheduling (e.g. adjustable robust optimization) with the uncertainty predictions from Gaussian process regression
- Applications to industrial-scale scheduling problems
- Prediction of other scheduling parameters (e.g. customer demand, product yields)