Data Ingestion and Data Preparation for Gaussian Processes

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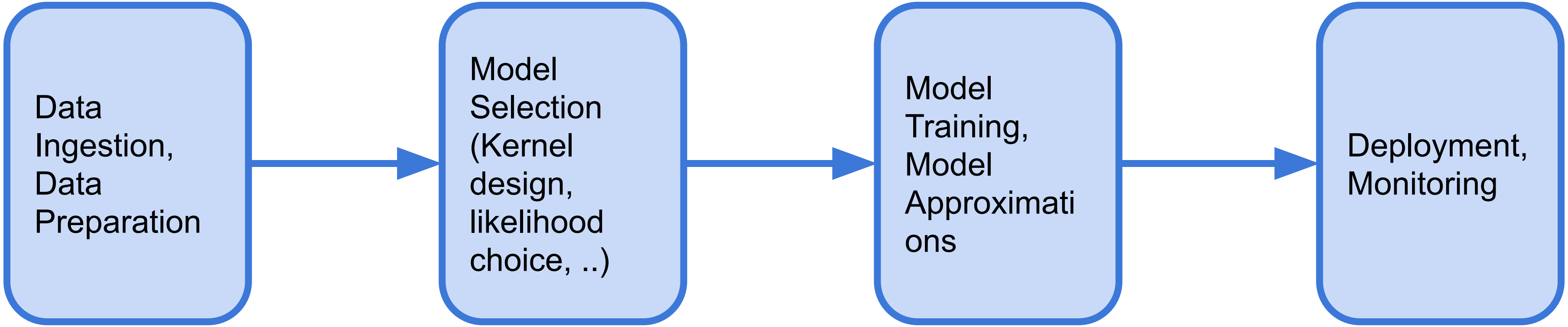
16 Jan 2020 - Gaussian Processes Meetup @Prowler.io

mind foundry

Working with Gaussian Processes



Data Ingestion, Data Preparation

Model Selection (Kernel design, likelihood choice, ..)

Model Training, Model Approximati ons

Deployment, Monitoring

Outline

- Data science pipeline
- Data ingestion
- Data Preparation for GPs
    - Standardization
    - Handling missing values
    - Data Types
- Conclusion

Data Science Pipeline

Data Science Pipeline

Collecting and manipulating data is the first step of the data science pipeline.

Many concepts:

Data Ingestion

Data Wrangling

Data Preparation

Data Cleaning

Data Cleansing

Data Pre- Processing

Data Science Pipeline

When working with Gaussian Processes, a good data preparation routine can:

- Improve the model selection routine
- Help to make simpler kernel choices and likelihood choices
- Improve training speed

⚠ Caution: you can make mistakes!

If you want to perform a data science task in a scientifically sounded way, you need to acknowledge that each action on your data means that you add some assumptions to your problem.

NEW ACTION == NEW ASSUMPTIONS

Data Ingestion

Data Ingestion

- Assume we ingest data in a reasonable **tabular format**
- Good practice: to record some relevant properties of the data which we know we will use to take action during the next steps (e.g. size and type)
- We record (but not impute) **missing data**

Data Preparation for GPs

Standardization

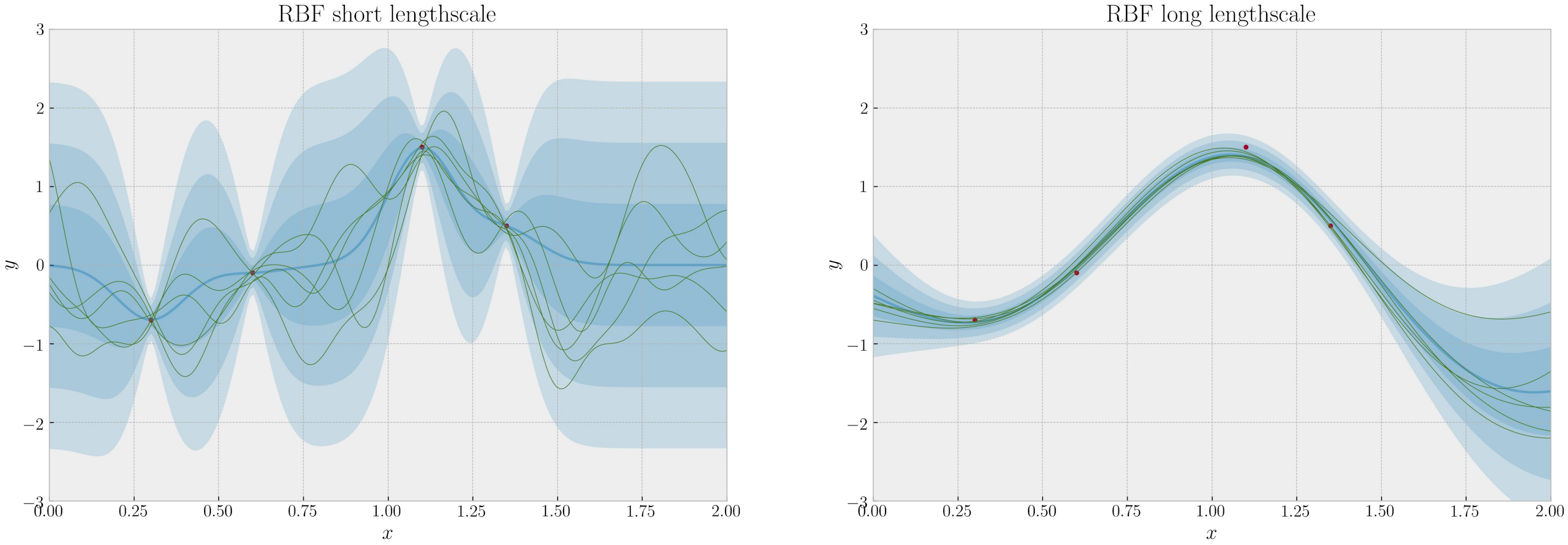
It is common practice to transform the data to have **zero mean** and **unit variance**.

One problem of GPs is to find the local minimum of the objective. Parameter initialization can be problematic; one could overcome this problem with many restarts, but it is time consuming.

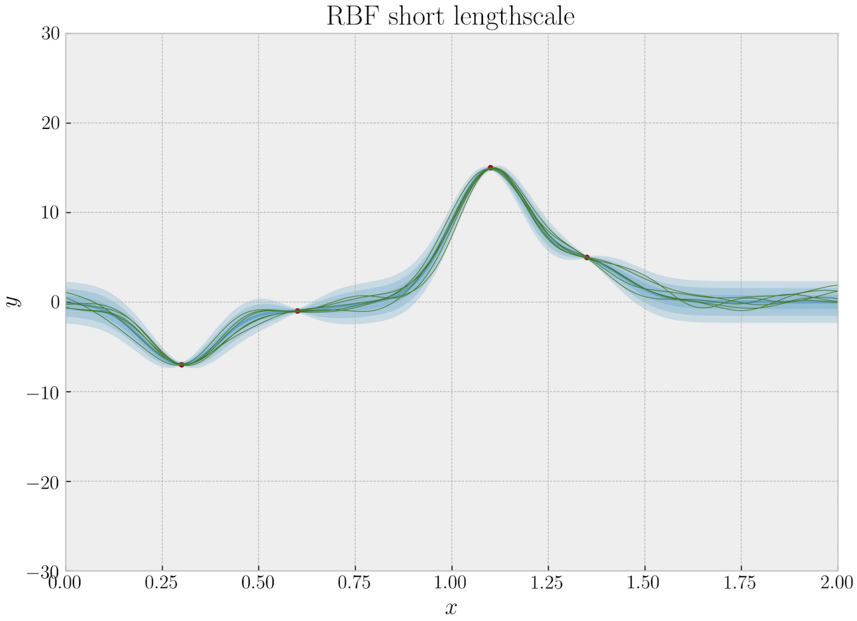
Therefore it is useful to initialize kernel parameters reasonably.

Caution: need to store the original mean and variance if you plan to manipulate new test points (this is one problem of data processing at training time: you need to do the same again at test time)

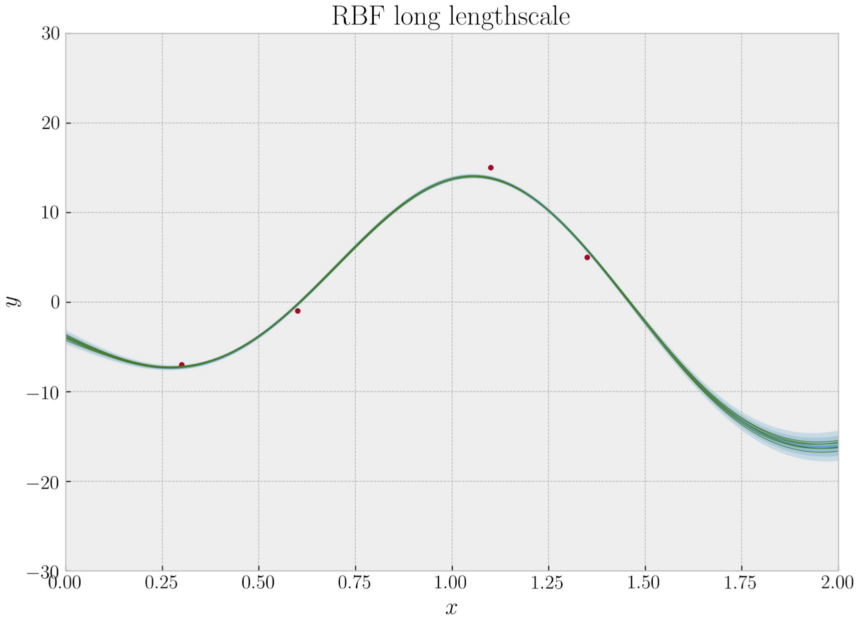
Standardization



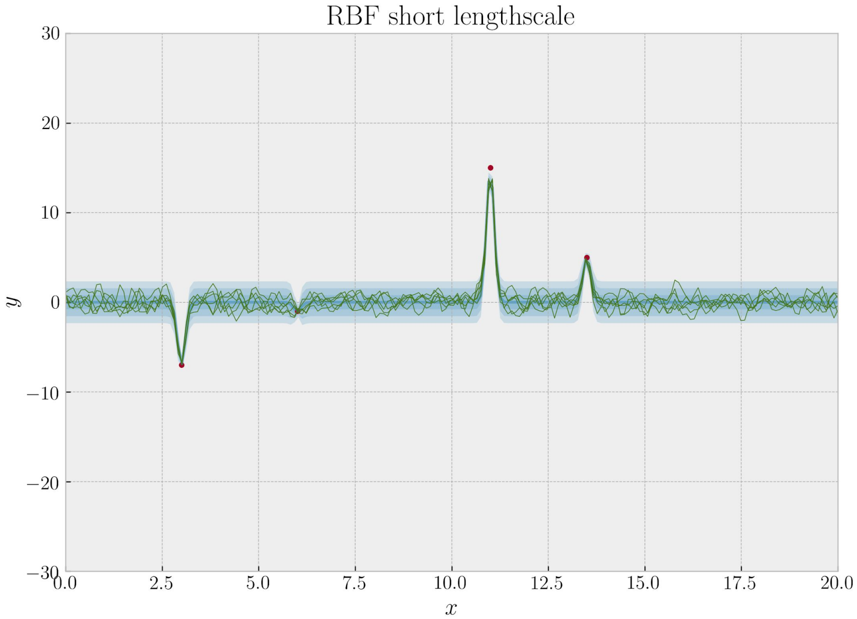
Standardization

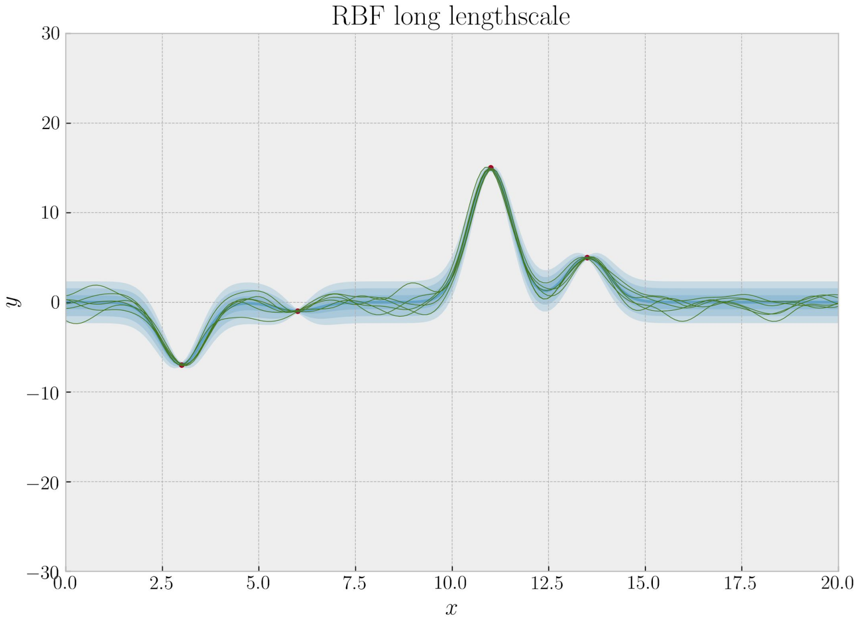


RBF short lengthscale



RBF long lengthscale


RBF short lengthscale


RBF long lengthscale

Standardization

References:

Nicolas Durrande. **Kernel Design**. Presentation at the Gaussian Processes Summer School 2019 (http://gpss.cc/gpss19/program). Slides here.

The automatic statistician project [https://www.automaticstatistician.com/index/].

Missing Values

Data imputation (different methods: mean, median, most frequent, previous value, etc).

⚠ Missing values can contain important information about your problem, if you impute them you might lose this information.

Always take into account model assumptions when doing imputation.

Data imputation can be used together with the model. [Quiñonero-Candela, Joaquin, and Sam T. Roweis. "Data imputation and robust training with Gaussian processes." (2003)]

Time Index

It is common practice to **identify a time index** (e.g. date time) and transform it to float.

References to time series modelling and dynamical systems

- Roberts, S., Osborne, M., Ebden, M., Reece, S., Gibson, N., & Aigrain, S. (2013). **Gaussian processes for time-series modelling**. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, *371*(1984), 20110550.
- Thomas Schön. **GP-based probabilistic modelling of dynamical systems**. Presentation at the Gaussian Processes Summer School 2018 (http://gpss.cc/gpss18/program). Slides here.

Oddball data and outliers

It is common practice to delete “oddball” data.

⚠ Outliers can contain important information about your problem, you might want to include them into your model.

You can also include these data into your model (heteroscedastic noise)

- Kersting, Plagemann, Pfaff, Burgard. (2007). **Most Likely Heteroscedastic Gaussian Process Regression**

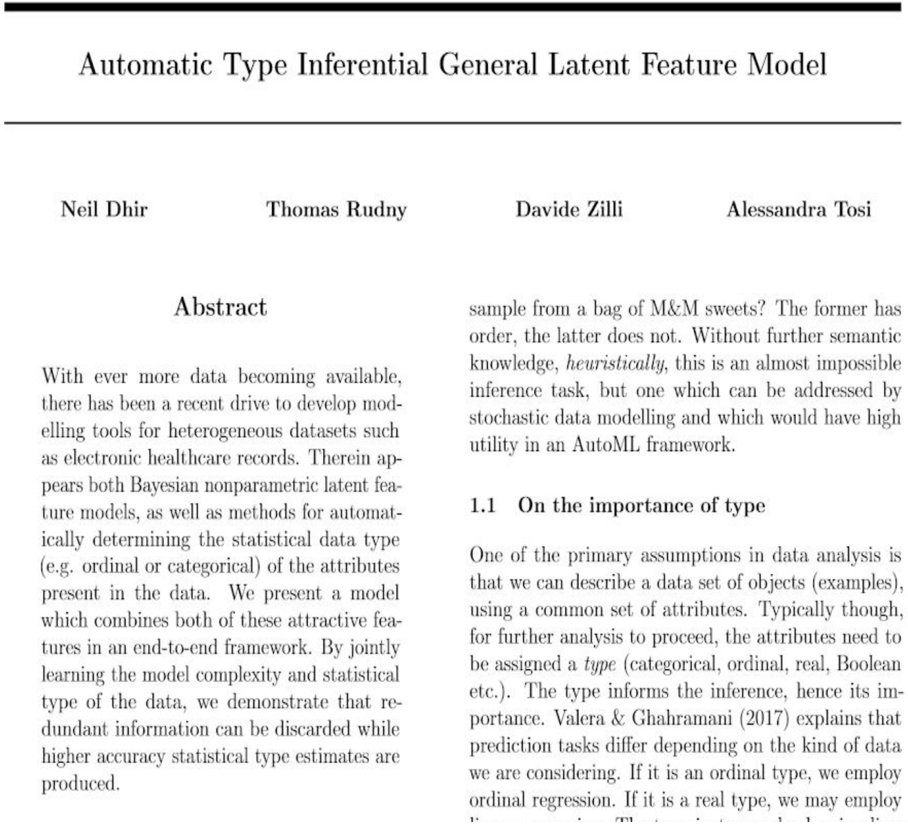
Data Types

GPs do not off-the-shelf work with all data types.

If we need to work with a variety of data type, we identify two common practices:

1. To **transform** your data
   - E.g. use one-hot encoding
2. To **choose** an appropriate kernel / combination of kernels
   - E.g. use string kernels

Automatic type inference



Automatic Type Inferential General Latent Feature Model

Neil Dhir   Thomas Rudny   Davide Zilli   Alessandra Tosi

Abstract

With ever more data becoming available, there has been a recent drive to develop modelling tools for heterogeneous datasets such as electronic healthcare records. Therein appears both Bayesian nonparametric latent feature models, as well as methods for automatically determining the statistical data type (e.g. ordinal or categorical) of the attributes present in the data. We present a model which combines both of these attractive features in an end-to-end framework. By jointly learning the model complexity and statistical type of the data, we demonstrate that redundant information can be discarded while higher accuracy statistical type estimates are produced.

sample from a bag of M&M sweets? The former has order, the latter does not. Without further semantic knowledge, *heuristically*, this is an almost impossible inference task, but one which can be addressed by stochastic data modelling and which would have high utility in an AutoML framework.

1.1 On the importance of type

One of the primary assumptions in data analysis is that we can describe a data set of objects (examples), using a common set of attributes. Typically though, for further analysis to proceed, the attributes need to be assigned a *type* (categorical, ordinal, real, Boolean etc.). The type informs the inference, hence its importance. Valera & Ghahramani (2017) explains that prediction tasks differ depending on the kind of data we are considering. If it is an ordinal type, we employ ordinal regression. If it is a real type, we may employ

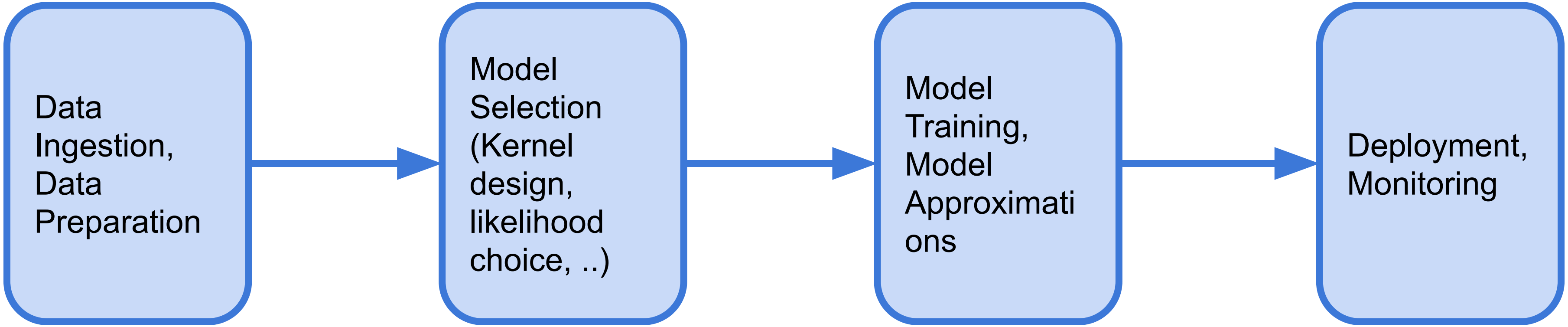
Conclusion

Summary

1) We have discussed Data ingestion and Data preparation for GPs, with a focus on: standardization, handling missing values and data types.

Summary

2) We have discussed the relationship between the Data Preparation step with the other steps of the data science pipeline.



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Take home message

Each **action** we take at each step of the Gaussian Process Modelling Pipeline has an impact on the other steps of the Pipeline because we are adding **new assumptions** to our problem.

Questions?