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# Bridging the chasm between Research and Software Development

By Linda Stougaard Nielsen At goto copenhagen, 4 October 2022



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## Agenda

Context – company & products The problem – two examples Possible solutions Remaining challenges Q&A

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## ava – a femtec health company

Swiss company, 2014, awards in startup, medtec Acquired by femtec health 2022 Female reproductive health

Wearable device collecting signals:

- Heart rate, heart rate variability, temperature, breathing rate, perfusion, sleep state every 10 s
- 200'000 users each collecting 1 mio data points every night

Applications:

- Fertility app launched in 2016 (CE & FDA approved)
- Contraception app
- Covid early detection (research project)



#### How does it work



Wearable Sensors Reveal Menses-driven Changes in Physiology and Enable Prediction of the Fertile Window: an Observational Study, Goodale, B. M., Shilaih, M., Falco, L., Dammeier, F., Hamvas, G., & Leeners, B. (2019)

## $\mathcal{M}$

## Medical research

- Hormonal changes throughout cycle, pregnancy, infections, menopause
- Influence on physiological signals

## Clinical trials

- Cooperation with research institutes
- Certification and postmarket surveillance
- Statistical analyses

## Machine learning

- Signal processing
- Classical statistics and machine-learning
- Neural Networks
- Constraints on noisy data and risk



# "One of the hardest parts of machine learning is effectively putting models in production."

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# $\mathcal{M}$

https://neptune.ai



The problem 2 examples

### Example 1: Re-process all raw data files



Parse, split, filter Extract nightly features Assess quality

	EXISTING
Production code	Python module for data processing
Scaling solution	Spark on AWS
Challenges	<ul> <li>Spark own language</li> <li>Re-implement solution</li> <li>Maintain 2 parallel implementations</li> </ul>

## $\mathcal{M}$

#### Example 1: Re-process all raw data files



Parse, split, filter Extract nightly features Assess quality Production c Scaling solut Challenges

## $\mathcal{M}$

	OLD	NEW
ode	Python module for data processing	
tion	Spark on AWS	Parallel on AWS
	<ul> <li>Spark own language</li> <li>Re-implement solution</li> <li>Maintain 2 parallel implementations</li> </ul>	- Additional implementation of infrastructure to run parallelisation



#### Example 2: Re-train a tensorflow model

Tensorflow model – not the issue (ok packaged)

Data handling:

- Input data into tensor
- Normalisation
- Filtering of data (outlier detection)
- Model output into app input

#### Scattered all over the code

- Impossible to follow and to maintain / extend

Different code than used in training

- Impossible to prove consistency between eg. outlier handling in training code vs. production code

## $\mathcal{M}$

#### Well-known issue a.k.a "glue code"

- supporting code for getting data in and out of generic ML packages
- ~95% of code
- anti-pattern

#### Re-implementation of code

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## $\mathcal{M}$

## Issues identified

- "Glue code"

Re-implementation of code



# Solutions Just a question of writing good code, right?

#### Re-use of code

- But some-one has to write the code that can be re-used
- And it may require additional infrastructure (eg. batch processing)
- And what about experimentation: modifying code slightly in various ways





#### Experimentation / research

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<pre>     In [143]:</pre>	
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<pre>In [143]: for phase in ['follicular', 'luteal']:     user_stats[phase + " length"].hist(histtype="step")</pre>	
<pre>fig = plt.gcf() fig.set_size_inches(11, 6) median = np.round(np.median(np.abs(user_stats[phase + ' length'])), 3) mean = np.round(np.mean(np.abs(user_stats[phase + ' length'])), 3) std = np.round (np.std (np.abs(user_stats[phase + ' length'])), 3) plt.title(phase + " length ({} cycles, median = {}, mean = {}, std = {})".format(len(user_s # plt.legend() # plt.savefig('histogram_error_' + phase, dpi=250) plt.savefig() plt.show()</pre>	
follicular length (278 cycles, median = 17.0, mean = 17.547, std = 5.141)	
120	
100	
80	
60	
40	
20	

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#### Research code

Scientific tools are different

- Ex Jupyter Notebook
- Line-by-line execution

Iterative approach

- Experimentation requires trial & error
- Lot of alternative code for different approaches
- Often incorporates with external tools (ex tensorboard for training)

Scientists are generalists

- "One solution to fits all" -> End up with long scripts that can do EVERYTHING
- Not specific to single problem (many trials)



Research code	Production code	Consequences / differences
Flexibility (can do everything)	Specialised (one purpose / fixed final version)	Full of redundant code
Manual usage	Automated repeated usage	No focus on stability, exception handling, and unit testing
Used by 1 person	Maintained by many people	Not following best practices
Row by row execution	Script execution	Not object oriented / pattern
Stand-alone	Interacting with system	No clear interfaces
Data from large data sets	One data point from stream	Data handling is different
Need parallelising within	Need parallelising around	Need restructuring and optimising





### Machine learning code into production (bridging the chasm)



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### Required infrastructure surrounding lifecycle of ML code



Source: "Hidden Technical Debt in Machine Learning Systems", NIPS 28 (2015) by Google



	Data collection Testing and debugging		d g	Resource management			
on	Data	ML code		Model analysis			Serving infrastructure
	vermoution			Process			
					management		
on	Feature engineerir	Ig	Metadata management				Monitoring





### Who should implement all this glue code

Educate researchers to be good SW devs

NO!

- No interest / no skills in this area
- Focus on research / modelling / data processing

## $\mathcal{M}$

Let SW devs build the code

Depends... SW glue: yes! ML glue: no!

- Parallel implementations
- Inconsistency problems
- Time to market

#### High level architecture



#### devops: infrastructure, integration, code versioning, automation, scaling, monitoring

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## M



#### ML modules as microservices



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#### Modularise the DS modules

#### Algorithm module

Kafka connector Input/output handling Logging and monitoring Unit testing Docker, Jenkins integration Setup. dependencies **Business logic** Load and execute a trained model

Infrastructure utilities

![](_page_19_Picture_8.jpeg)

#### Microservices and modularising the common code

![](_page_20_Figure_1.jpeg)

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## $\mathcal{M}$

#### Inject trained models

#### Algorithm module

Kafka connector Input/output handling Logging and monitoring Unit testing Docker, Jenkins integration Setup. dependencies Business logic

Load and execute a trained model +

config

## $\mathcal{M}$

Platform / framework for experimentation and evaluation

Trained model # n

![](_page_21_Picture_10.jpeg)

#### Most popular ml-ops tools for managing ML life cycle

<b>Kubeflow</b>	mlflow
Google	Databricks
Tensorflow (TFX)	Python
Pipeline based	Experimentation
Deploy and manage complex ML systems	Tracking of exper
Kubernetes infrastructure (more complex)	Local or cloud, eg locally and track

![](_page_22_Figure_5.jpeg)

![](_page_22_Picture_7.jpeg)

### ML lifecycle Architecture

![](_page_23_Figure_1.jpeg)

## $\mathcal{N}$

#### Data handling

#### Algorithm module

Predict using selected model

Run-id: 0edd84ca89b9435eb8773cd712070145

![](_page_23_Picture_9.jpeg)

# mlflow

#### mlflow Experiments Models

Experiments	+
Search Experiments	
Default	// 而
my_exp	⊻ ₪
pipeline1	_ ₪
prepare_data	_ ₪
train_pipe_0613	2

#### train\_pipe\_0613 🧻

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![](_page_24_Picture_6.jpeg)

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## Experimentation

Try out different models and data sets Track: parameters, metrics, and artifacts Comparison between experiments

## Model registry

Store trained models for later use Load selected trained model by ID

## Advantages

Tracking of experiments Reproducibility (models, params, data sets) Easy deployment of trained models

![](_page_24_Picture_15.jpeg)

#### Everything needed for serving model is automatically saved

Project 👻 😤 🏹		EADM
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> evaluate_algoworker	3	
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artifacts	8	
Closing-model	9	
conda.yaml	10	
🖆 MLmodel	11	
model.pkl	12	m
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> 1c84b30255de476b9ab8b5b44369e4d6		
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## $\mathcal{M}$

train.py × 📶 mlruns/.../conda.yaml × 🖆 False × 🖆  $E.md \times$ artifact\_path: closing-model lavors: python\_function: env: conda.yaml loader\_module: mlflow.sklearn model\_path: model.pkl python\_version: 3.7.11 sklearn: pickled\_model: model.pkl serialization\_format: cloudpickle sklearn\_version: 1.0.2 nodel\_uuid: 2552f3fc84d14f9fbd3c7df4f198adea oun\_id: 0edd84ca89b9435eb8773cd712070145 tc\_time\_created: '2022-03-22 17:17:04.702535'

![](_page_25_Picture_6.jpeg)

Follow pattern from scikit-learn (sklearn)

```
class FertilityModel(BaseEstimator, ClassifierMixin, metaclass=abc.ABCMeta):
   MODEL = "algo_model"
   MODEL_PARAMETERS = "algo_model_parameters"
```

```
def ___init__(self):...
@abc.abstractmethod
def fit(self, X=None, y=None, sample_weight=None, check_input=True):...
@abc.abstractmethod
def predict(self, cycle: CycleData, *args, **kwargs) -> (np.ndarray, np.ndarray):...
```

```
@classmethod
def get_model_name(cls):...
```

```
def serialise(self) -> dict:...
```

```
def score(
    self, cycle: CycleData, true_fertility_indications, sample_weight=None
) -> float:...
```

![](_page_26_Picture_12.jpeg)

### Available functionality from *scikit-learn* (*sklearn*)

#### **Standard classes eg:**

- RandomForestClassifier
- BaggingClassifier
- GridSearchCV
- StandardScaler
- Pipeline

```
search_grid = close_model.get_parameter_filter(random_grid=True, **extra_kwargs)
grid_search_classifier = RandomizedSearchCV(
    close_model, search_grid, scoring=model_scorer, n_iter=int(n_iter)
```

```
pipeline = Pipeline(
```

```
pipeline.fit(cycle_lists[TRAIN_SPLIT_NAME])
mlflow.log_metrics(grid_search_classifier.best_params_)
df = pd.DataFrame(grid_search_classifier.cv_results_)
store_artifact_local_dump(
   artifact_name="cv_results.csv", dump_function=df.to_csv, index=False
```

```
score = pipeline.score(cycle_lists[TRAIN_SPLIT_NAME])
```

```
("smoother", LowessSignalSmoother(lowess_look_back_period, lowess_frac)),
("grid_search_classifier", grid_search_classifier),
```

![](_page_27_Picture_15.jpeg)

### Mlflow for experimentation and model serving

![](_page_28_Figure_1.jpeg)

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## $\mathcal{M}$

devops: infrastructure, integration, code versioning, automation, scaling, monitoring

![](_page_28_Picture_7.jpeg)

Summary And challenges

Solution at ava

Separate data science modules as micro-services with clean interfaces to the rest of the system (most of the glue)

Separate parts of each data science module that is related to standard software tasks (some of the glue)

The core part is the models, the lifecyle is managed by a mlops tool and a trained model is stored in a blob

![](_page_30_Figure_4.jpeg)

### Remaining challenges

It is still possible to build a mess

- Follow best practices
- Recognize when code can be re-used
- Communication to prevent duplication

It is out of comfort zone for most researchers

- Different tools
- Outside core competences
- Need training and support
- Still some researchers will never go down this path...

ML engineer / SW developer is needed for parts

- To write the glue
- Use same libraries and language •
- Coordination and communication

Not solving all problems (eg. Example 1)

## $\mathcal{M}$

![](_page_31_Picture_17.jpeg)

conditions sperm

![](_page_31_Picture_20.jpeg)

- and the solution is agile?

 Cross-functional teams: researchers and data engineers / sw devs T-shaped skills
 Pairing up, code review

✓ Work on different projects

![](_page_32_Picture_4.jpeg)

![](_page_32_Picture_5.jpeg)

## Questions?

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## $\mathcal{M}$

# Thank you!

![](_page_33_Picture_4.jpeg)