Boosting Research with Machine Learning

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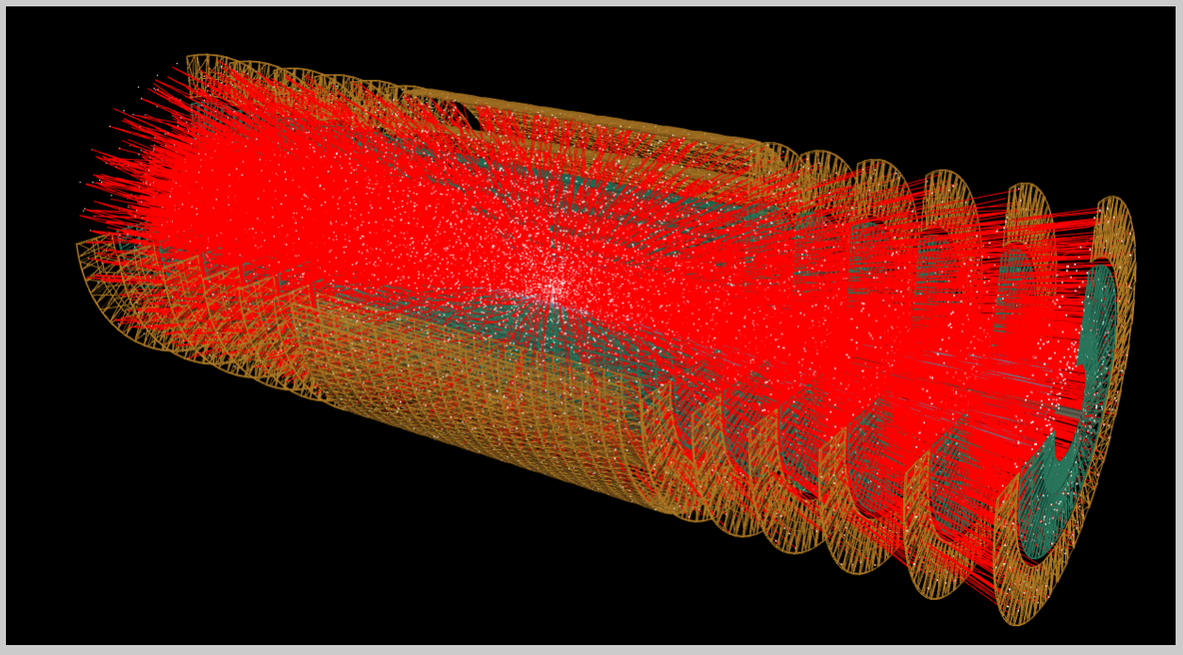
Informatikdienste

Scientific IT Services

Examples for ML in research

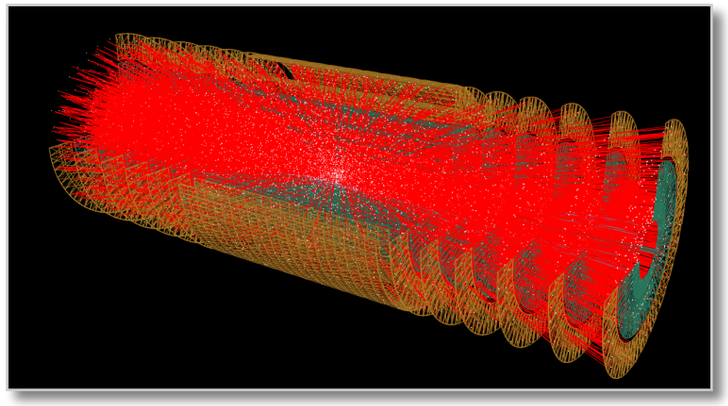
Examples for ML in research

Discovery and characterisation
of new particles

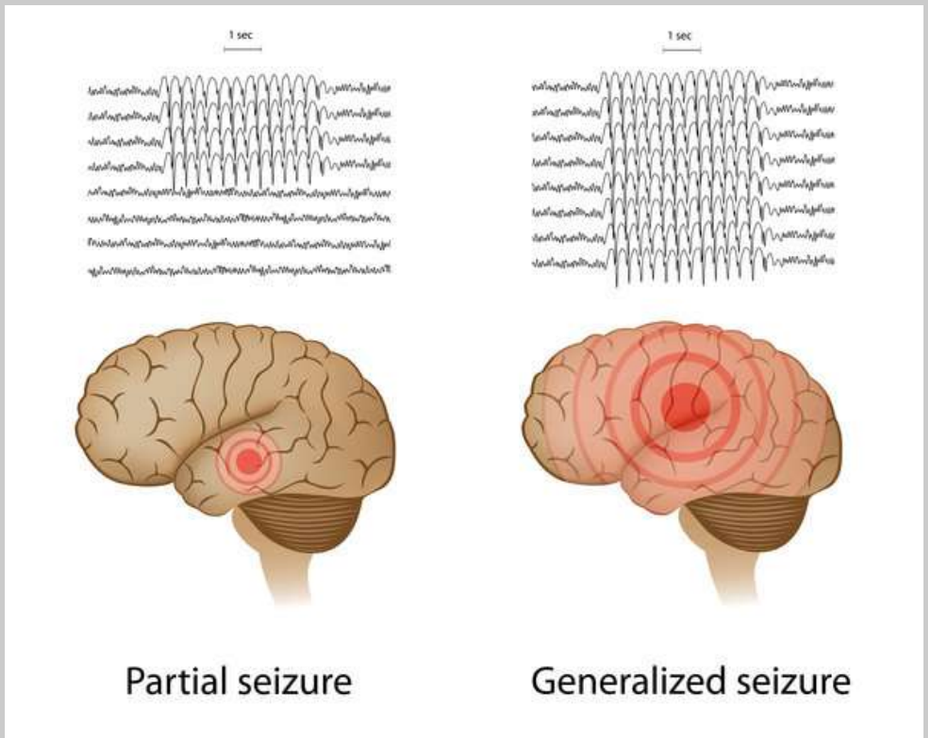


https://home.cern/

Examples for ML in research

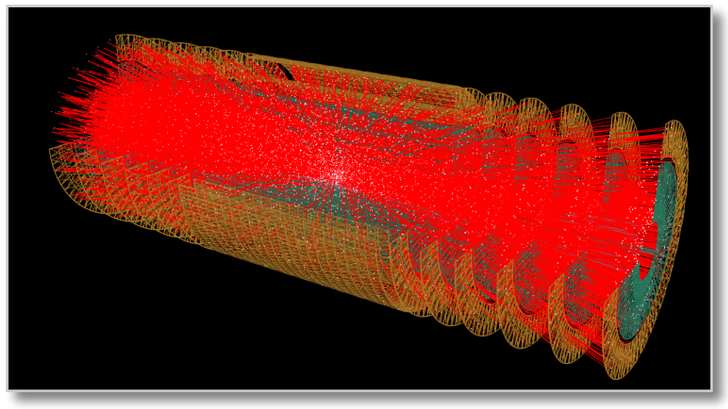


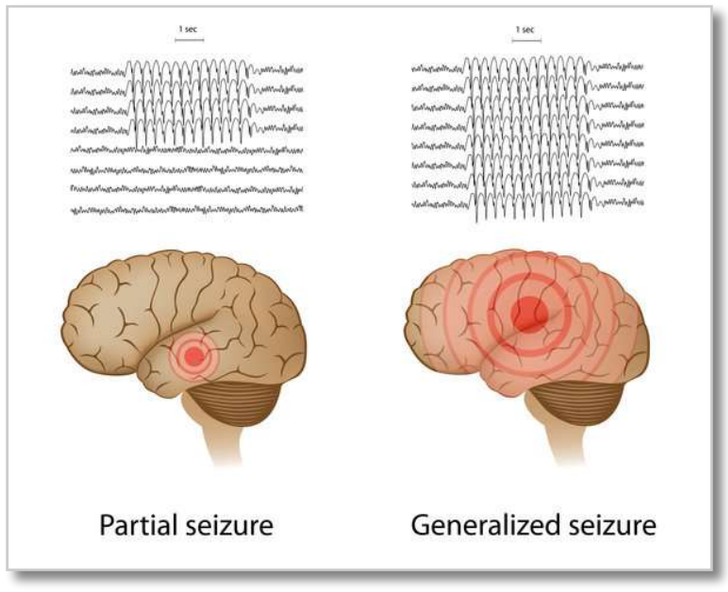
Prediction of
epileptic seizures



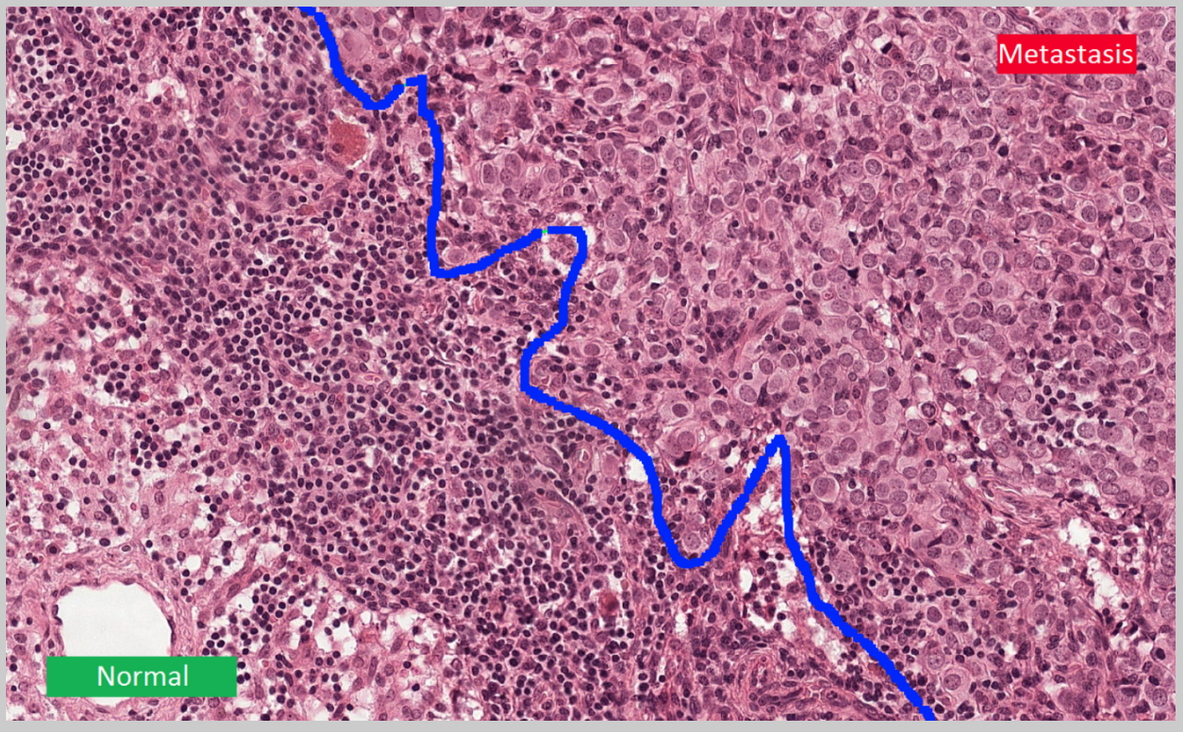
https://medicalxpress.com

Examples for ML in research



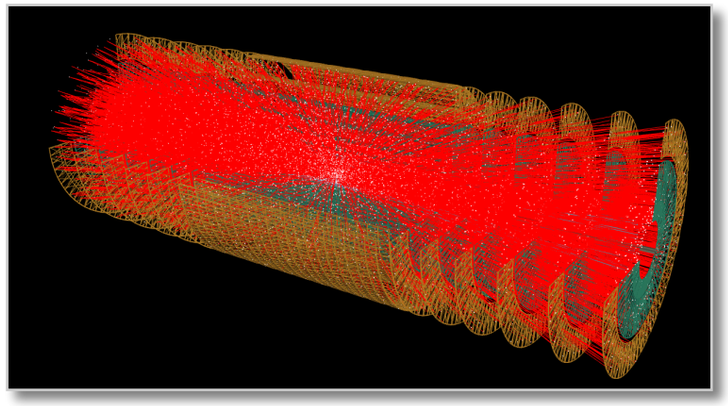


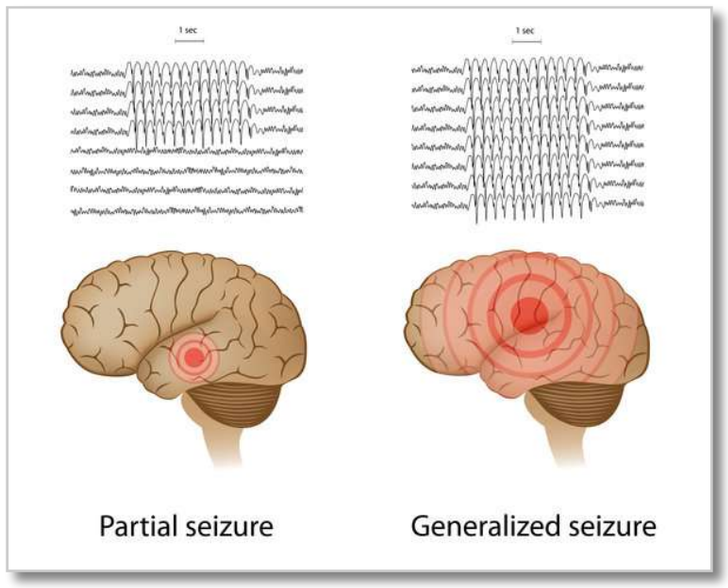
Characterisation
of cancer regions

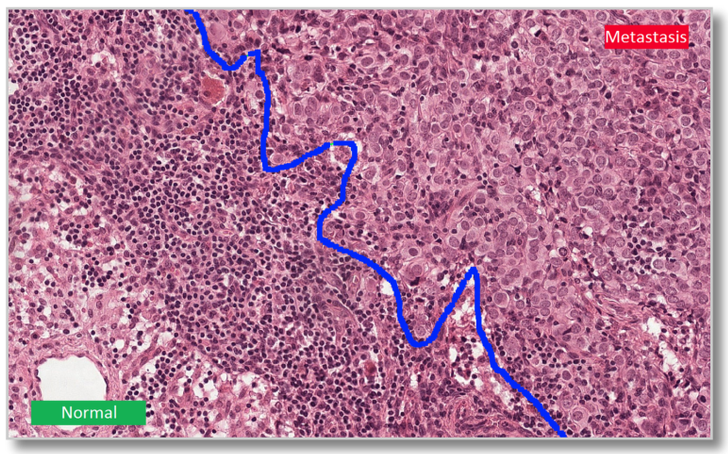


https://camelyon16.grand-challenge.org

Examples for ML in research







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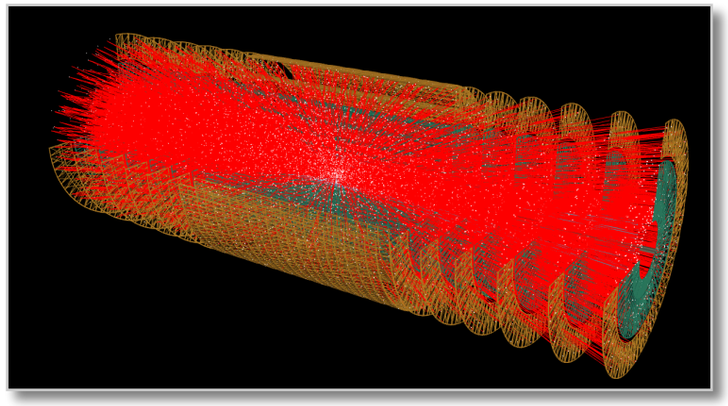
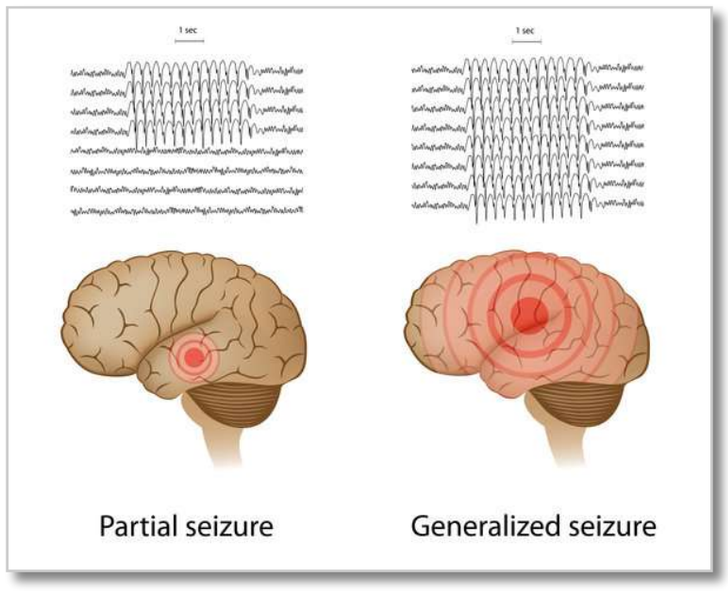
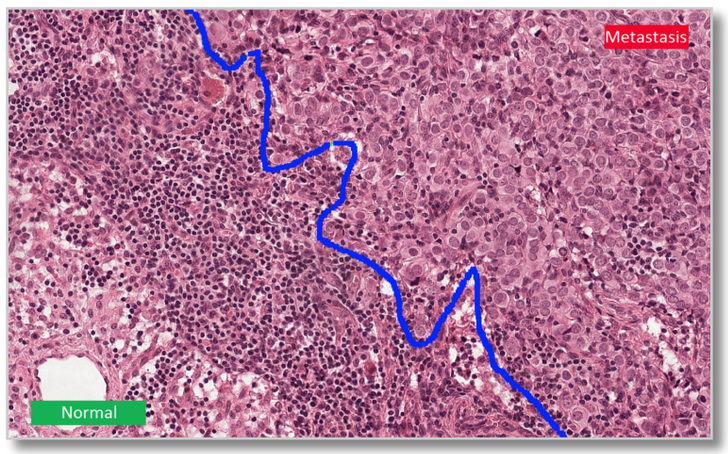




Applications of ML in research:

- Uncover hidden patterns in data
- Automatisation of time-consuming processes

Examples for ML in research



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- Automatisation of time-consuming processes

How to apply ML in research?

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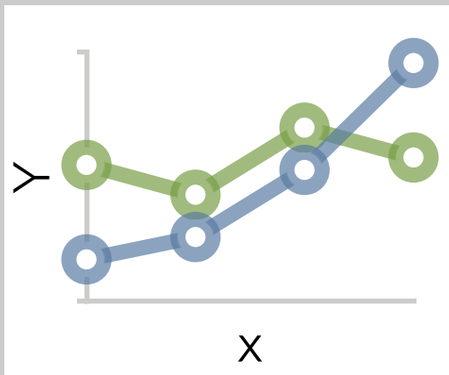
Data



Preprocessing

scipy

pandas

pandas

Model

scikit-learn

keras

Prediction

$$\begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \dots \end{pmatrix}$$

How to apply ML in research?

Data

```
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LogisticRegression
from sklearn.metrics import accuracy_score
from my_helper import data, preprocess

## Load data
X = data.data
y = data.target
```

Preprocessing

```
## Preprocessing of data
X_proc = preprocess(X)

## Split into training and validation set
X_train, X_val, y_train, y_val = train_test_split(
    X_stand, y, test_size=0.33)
```

Model

```
## Model
lr = LogisticRegression()
lr.fit(X_train, y_train)
```

Prediction

```
y_pred = lr.predict(X_val)
print(accuracy_score(y_val, y_pred))
```

Use case 1: EEG signal detection

Use case 1: Experimental setup

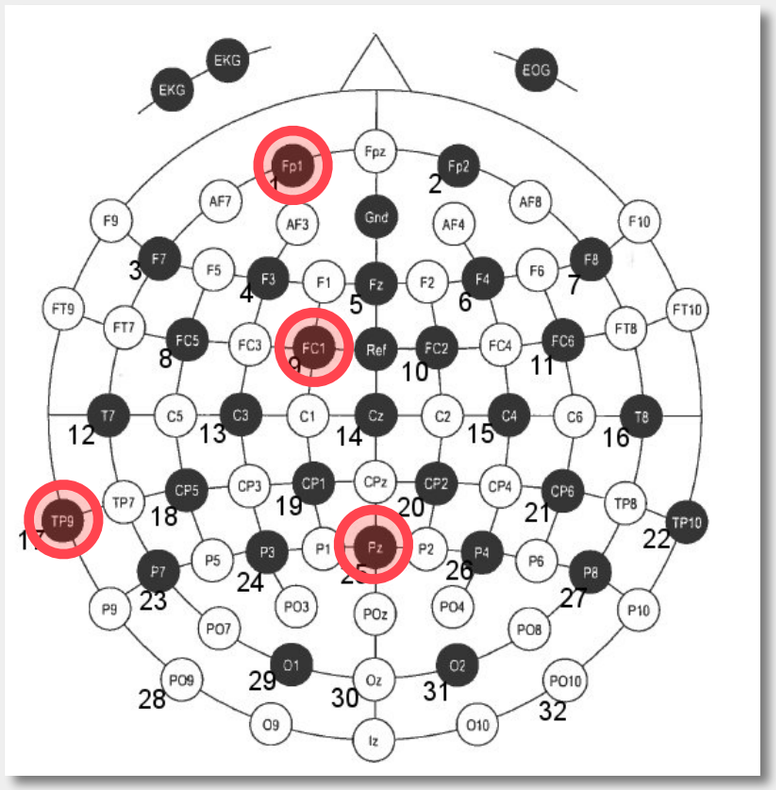
Experimental setup

Hand movement

Luciw et al., Nature, 2014

Use case 1: Preprocessing

Recording



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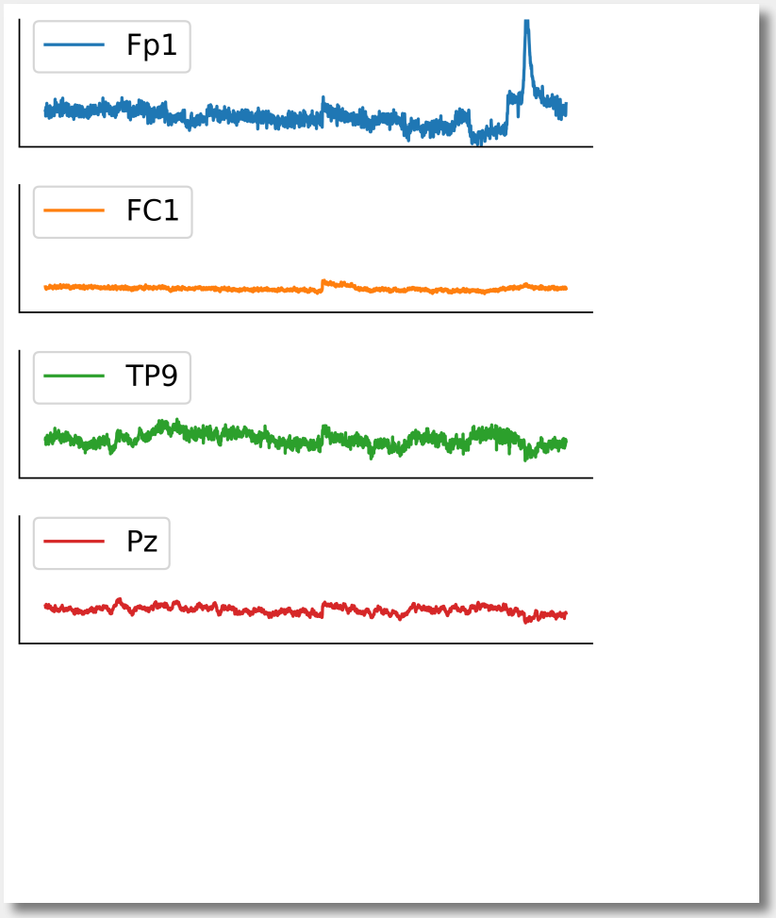
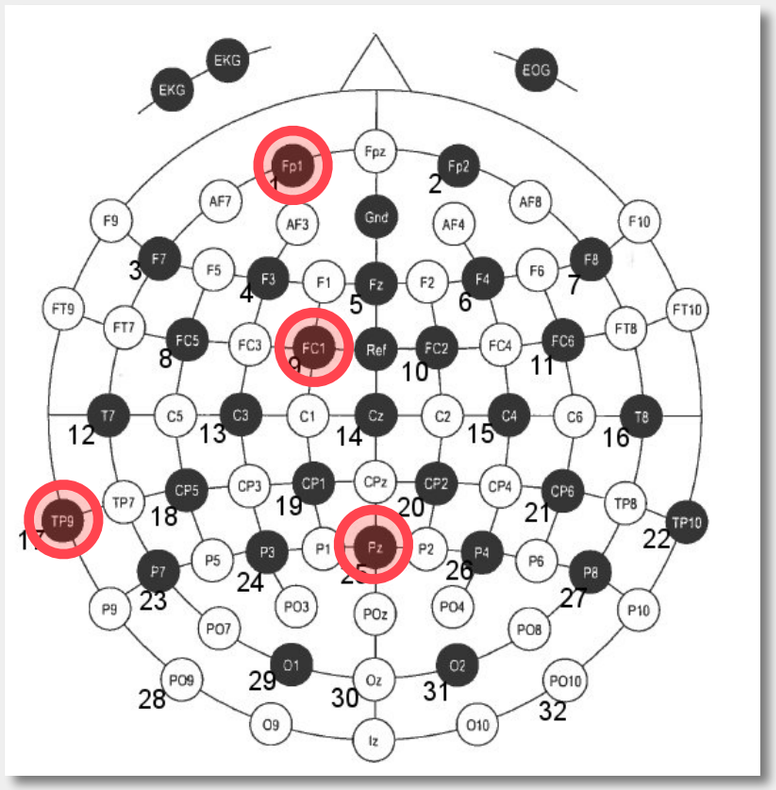


Use case 1: Preprocessing

Recording



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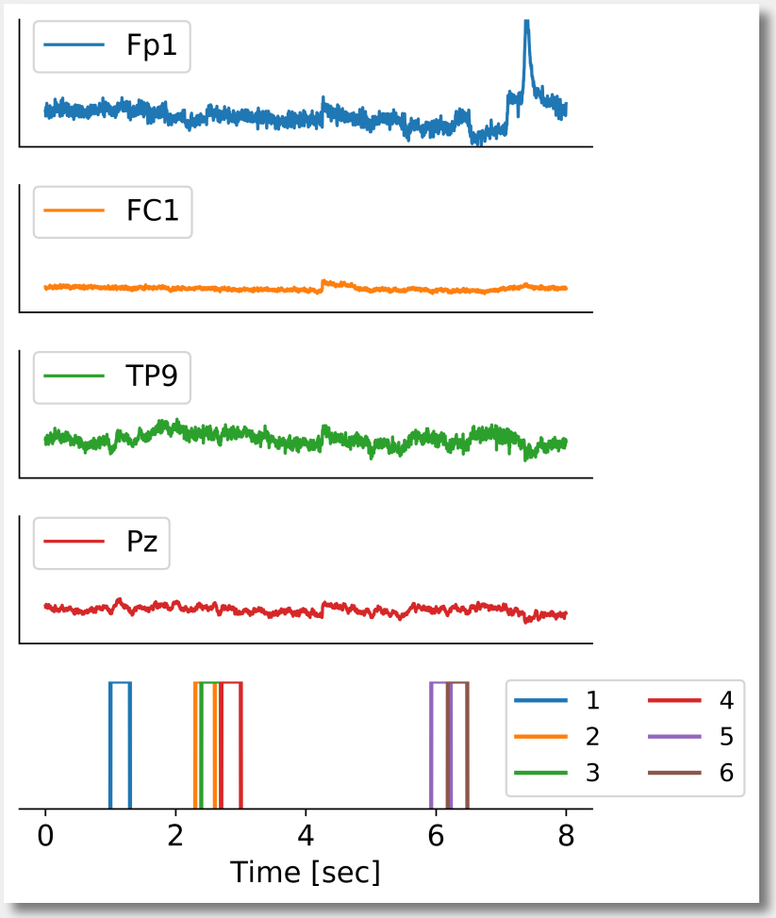

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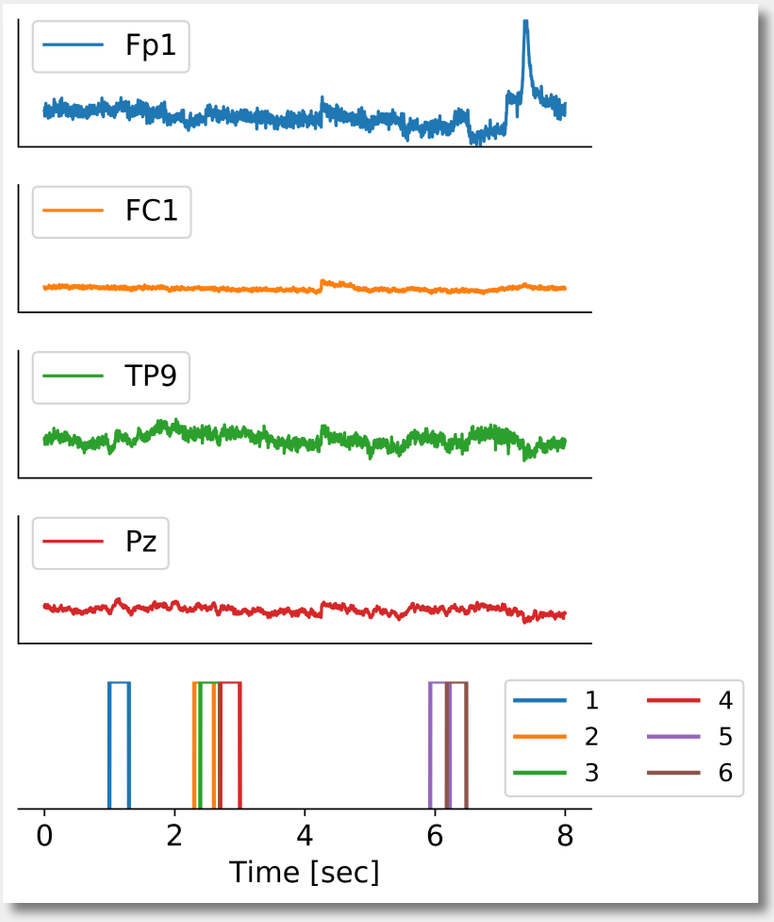
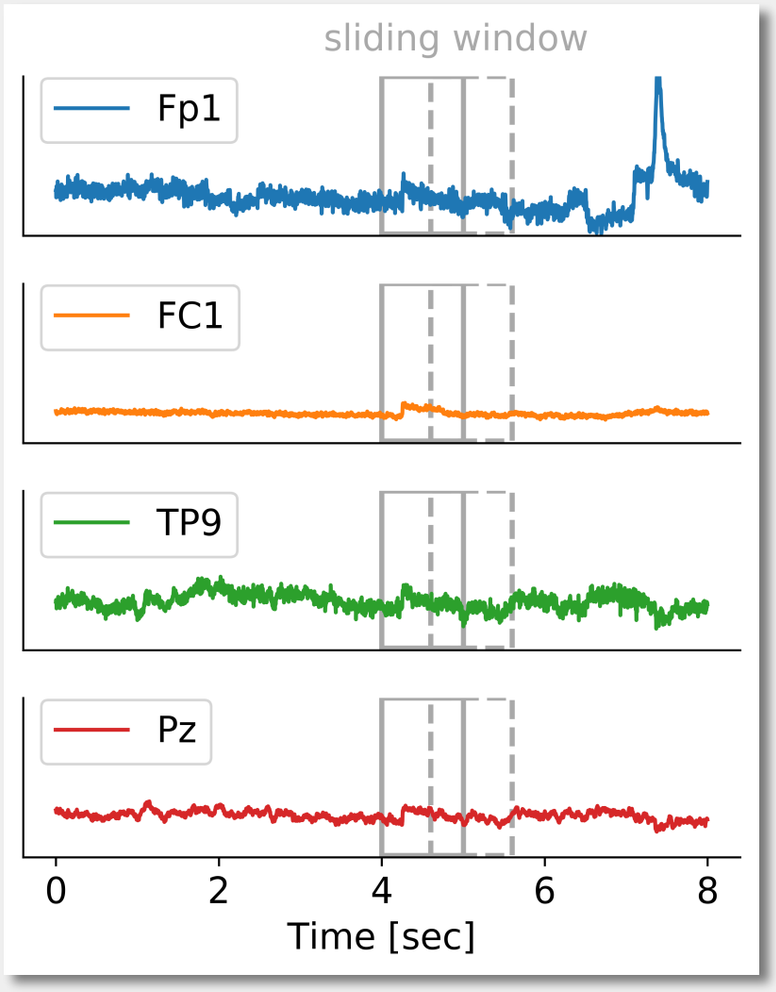


Sliding window



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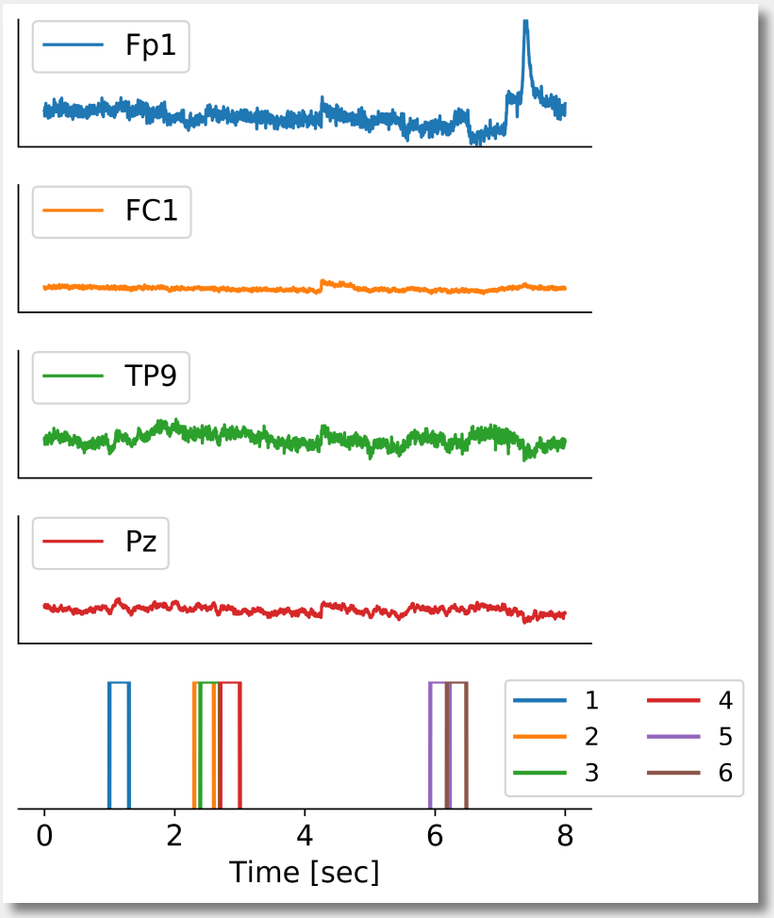

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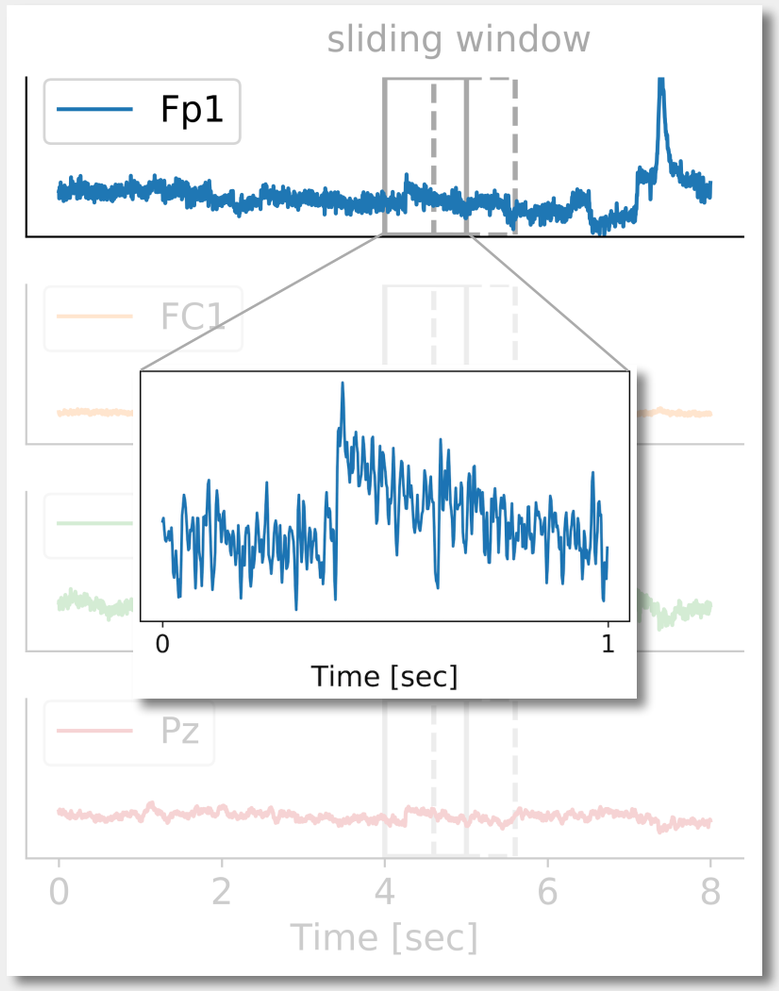
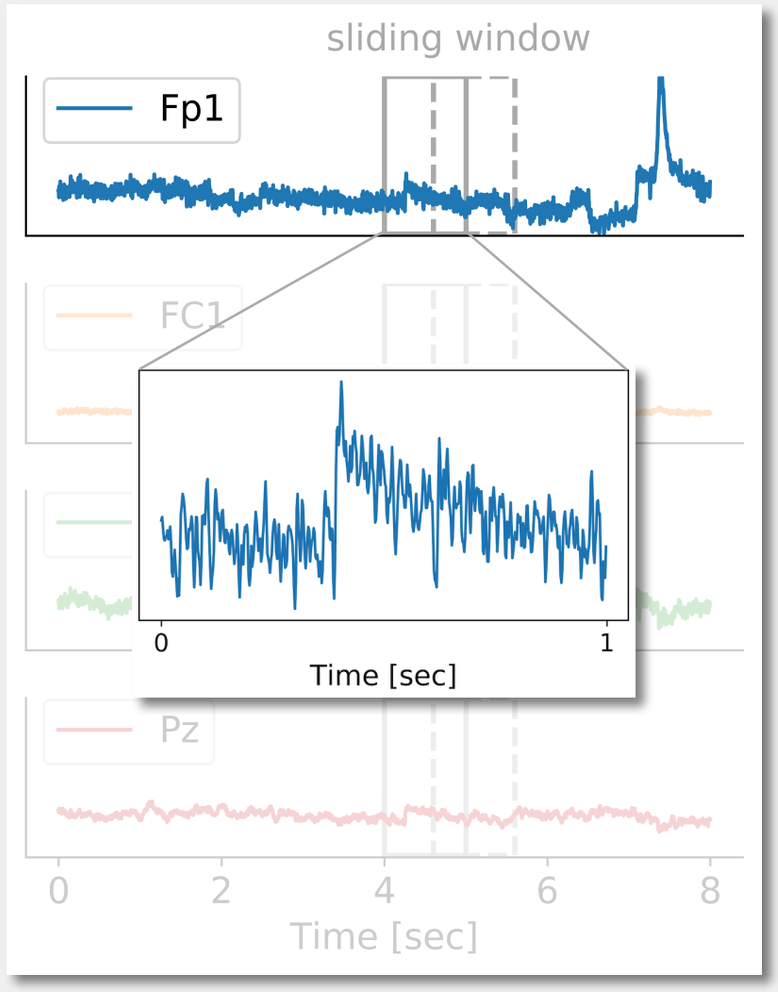
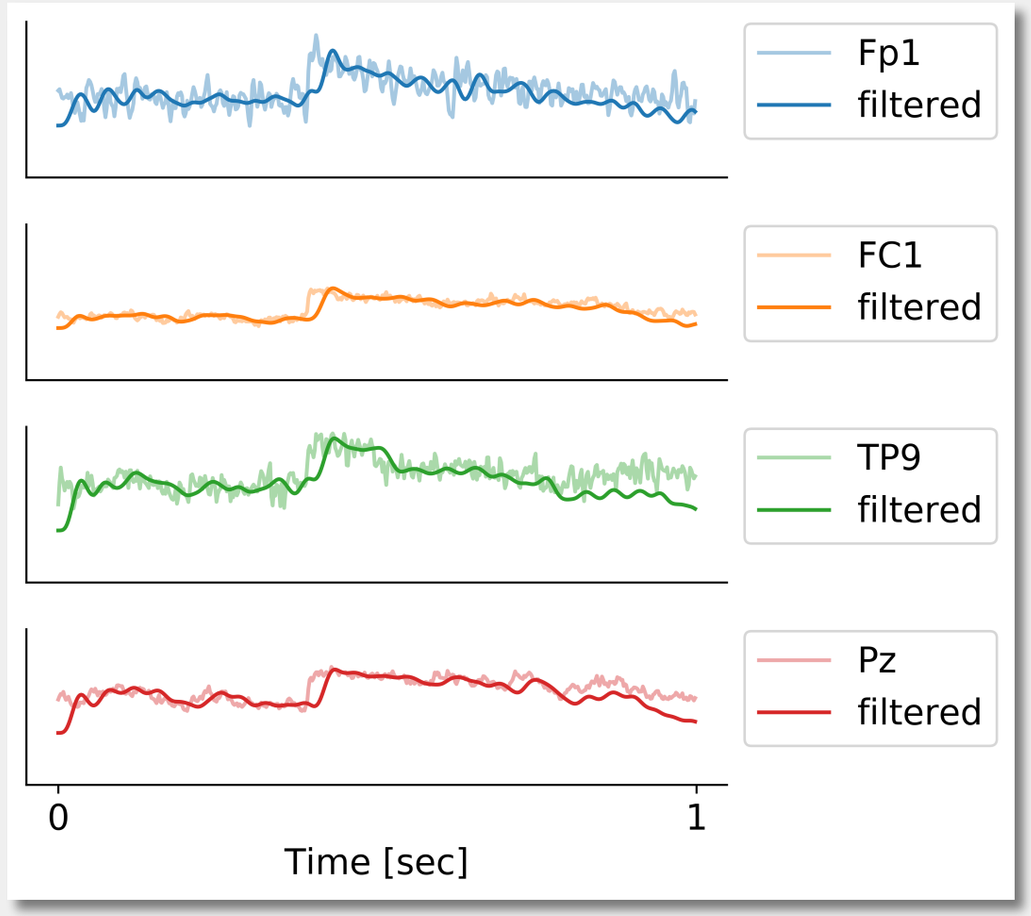


Use case 1: Preprocessing

Sliding window

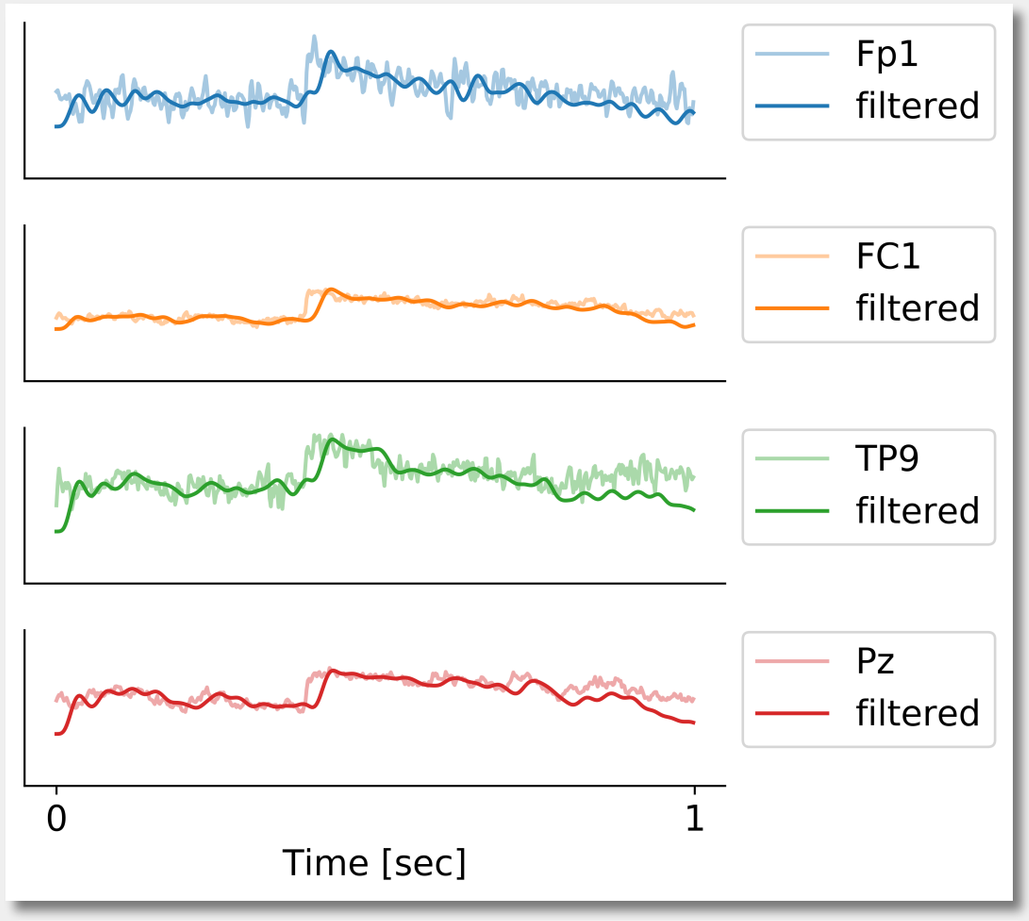


Low-pass filter

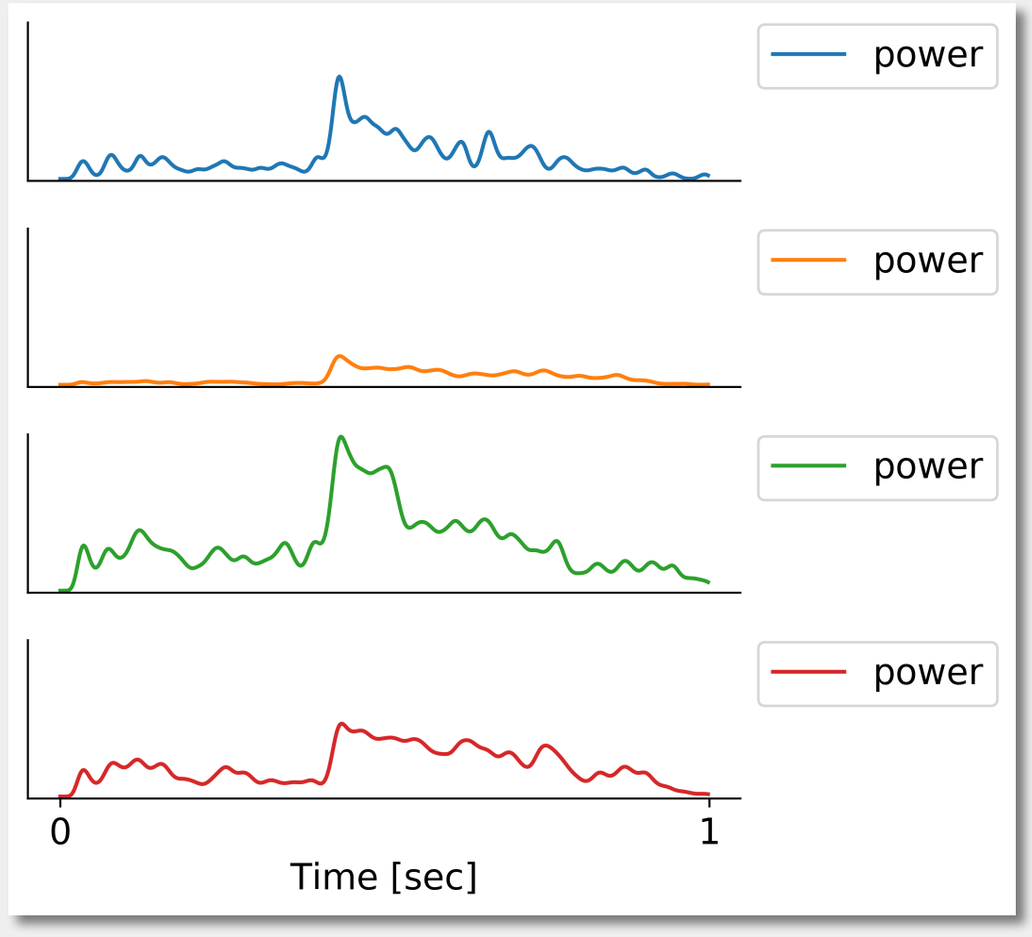


Use case 1: Preprocessing

Low-pass filter

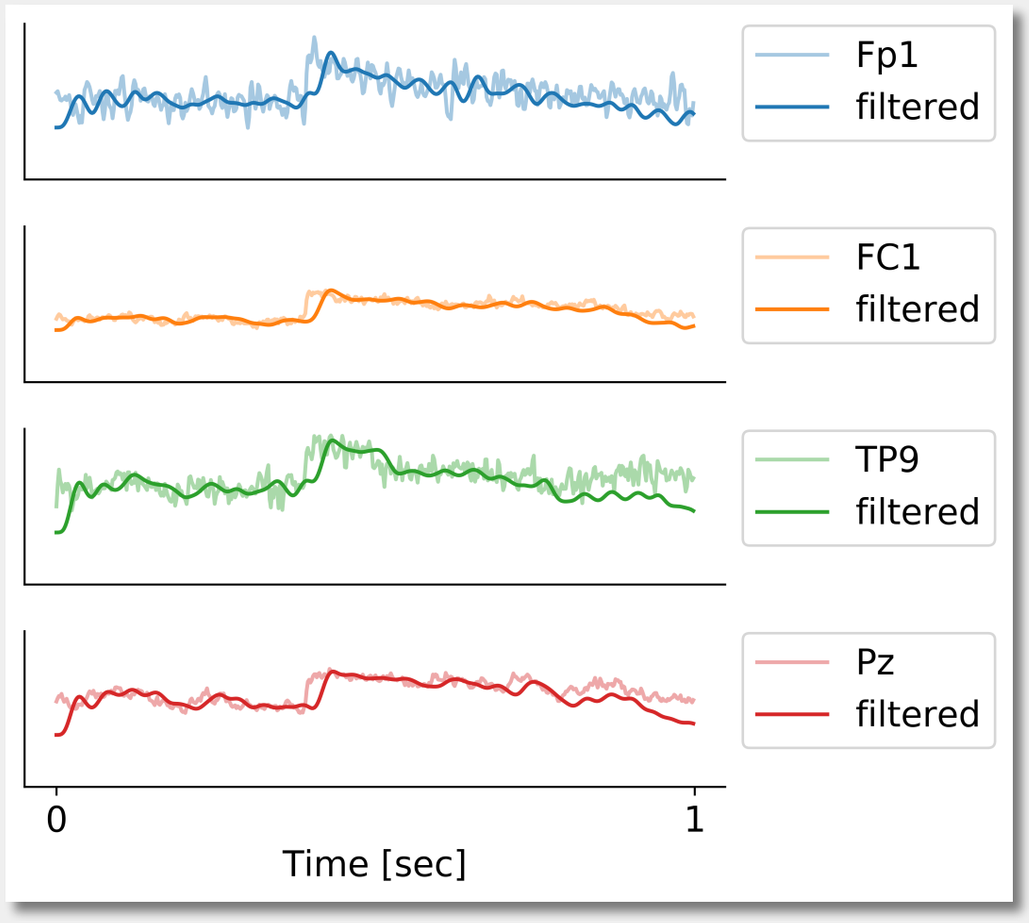


Power

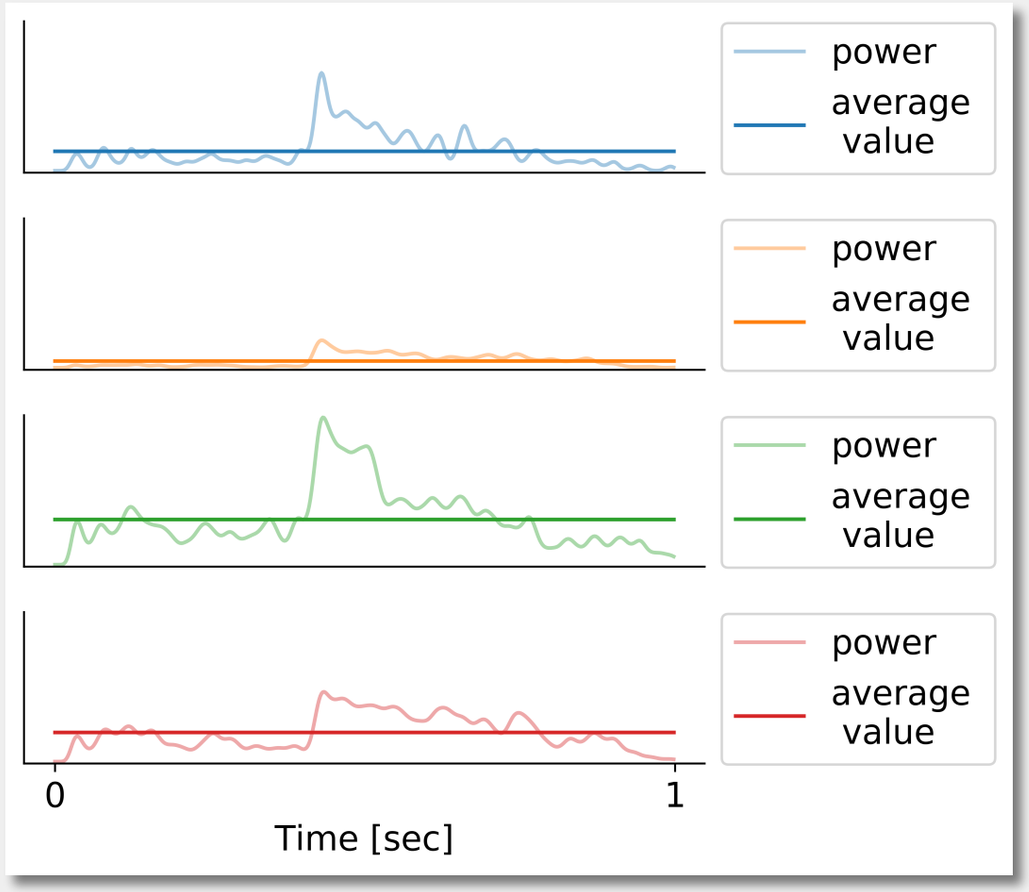


Use case 1: Preprocessing

Low-pass filter



Average Power



Use case 1: Model

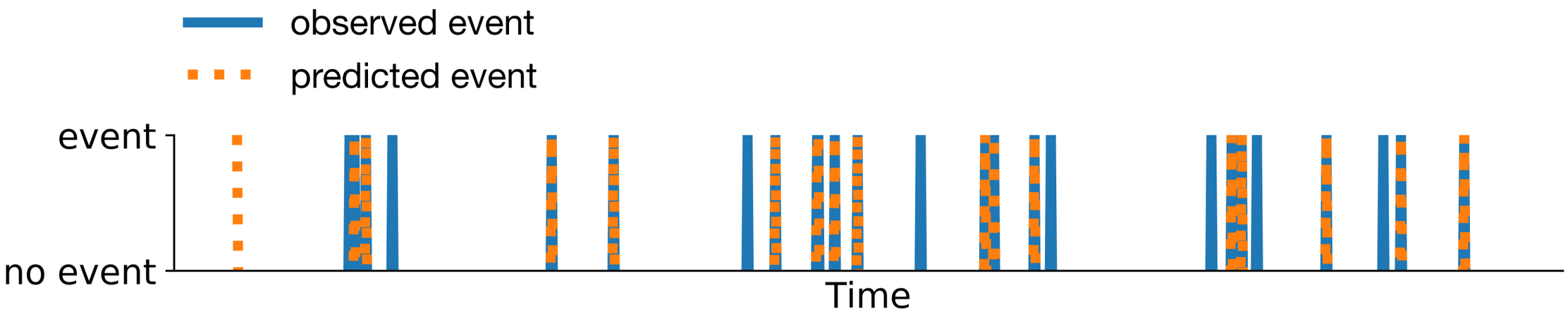
Model

```
lda = LDA()
rf = RandomForestClassifier(class_weight = 'balanced')
lr = LogisticRegression(class_weight = 'balanced')

eclf = VotingClassifier(estimators=[('lda', lda),
                                    ('rf', rf),
                                    ('lr', lr)],
                        voting = 'soft', weights=[1,1,1])
```

Prediction

```
eclf.fit(X_train, y_train)
y_pred = eclf.predict(X_test)
```

Use case 1: Prediction

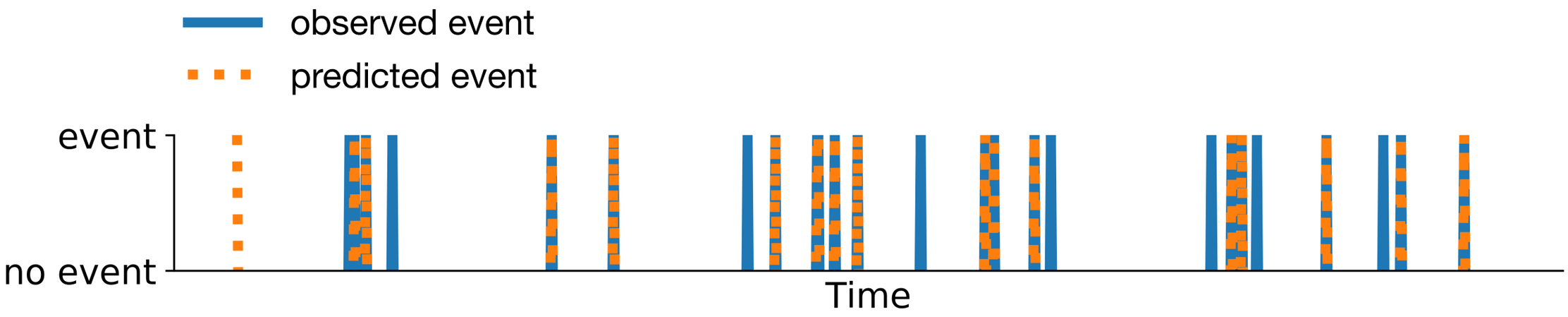


confusion matrix

	Predicted: No	Predicted: Yes
Actual: No	456263	113
Actual: Yes	3833	9016

- 70% of the events were correctly predicted

Use case 1: Prediction



confusion matrix

	Predicted: No	Predicted: Yes
Actual: No	456263	113
Actual: Yes	3833	9016

- 70% of the events were correctly predicted
- hardly any false alarm

Use case 1: Summary

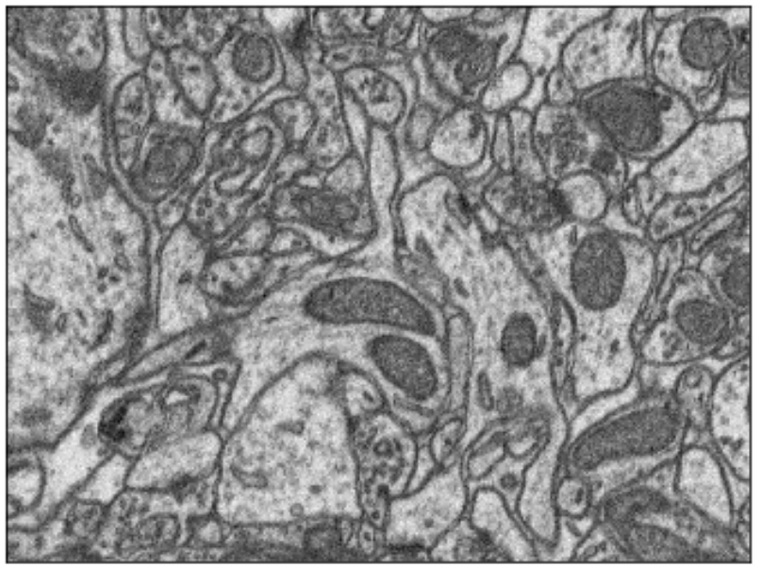
Classic ML model provides:

- a reasonably good prediction
- deeper insight into data due to interpretable models
- computational low costs (training: ~30m on single CPU)

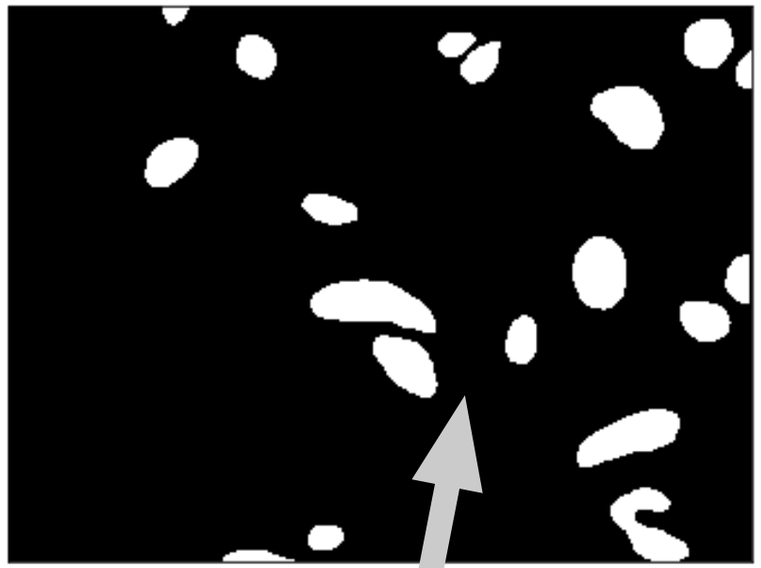
Use case 2: Segmentation

Use case 2: Data

Raw image

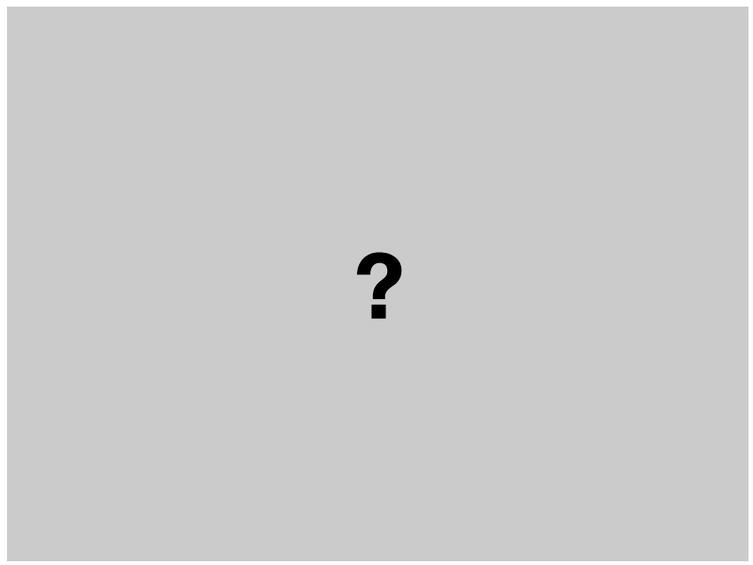


Segmentation



done by hand

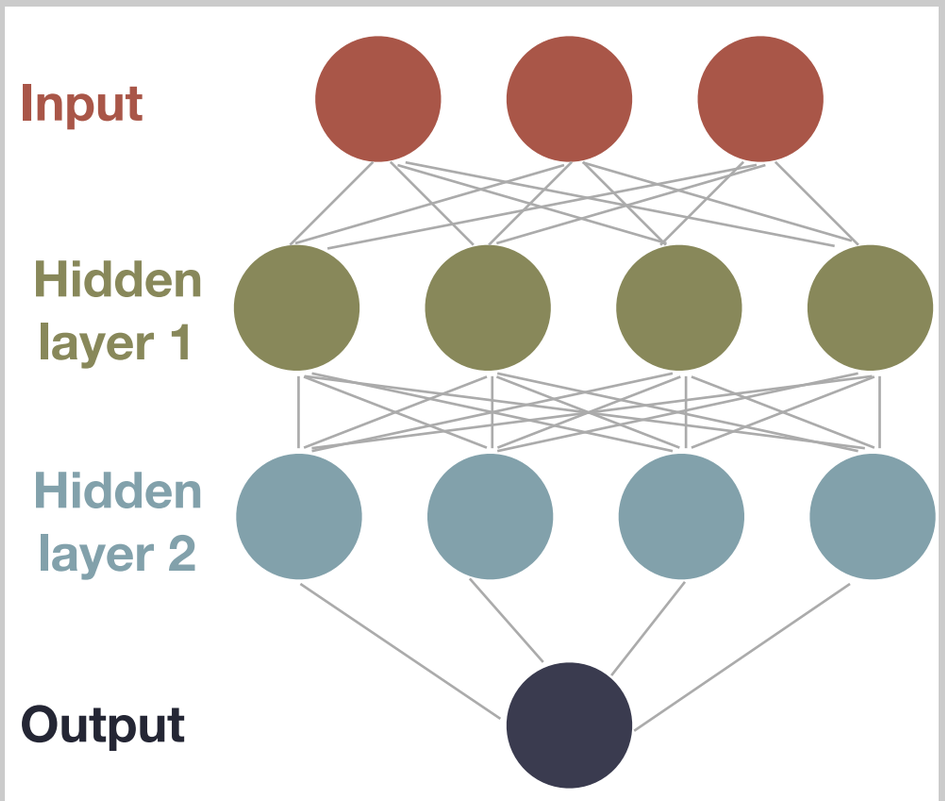
Automatic detection



Data acquired by: Graham Knott and Marco Cantoni at EPFL

Use case 2: Model

Neural Network

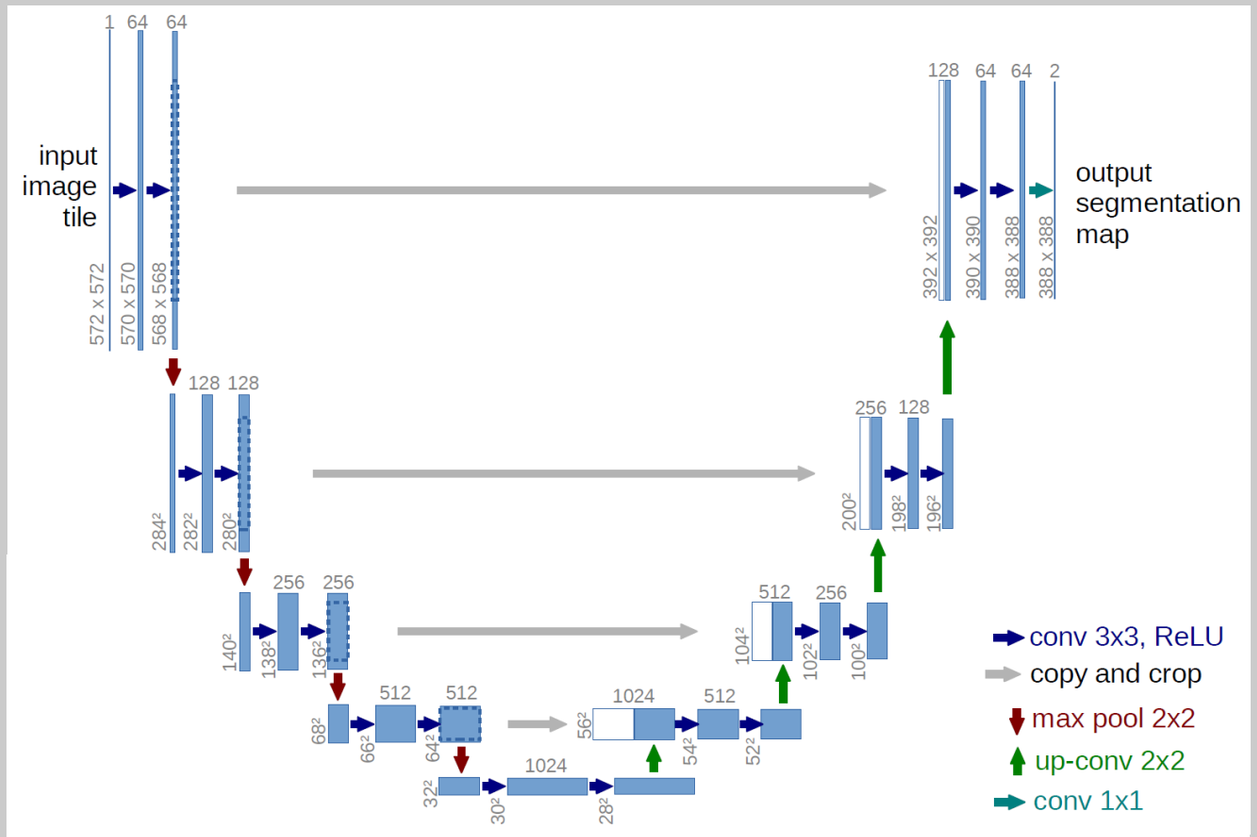


Implementation

```
from keras.models import Model
from keras.layers import Input, Dense

inp = Input(shape=(3,))


hidden_1 = Dense(4)(inp)


hidden_2 = Dense(4)(hidden_1)


outp = Dense(1)(hidden_2)

model = Model(inputs=inp, outputs=outp)
```

Use case 2: Model

U-Net



- **Downstream branch**: ‘what’-information
- **Upstream branch**: ‘where’-information

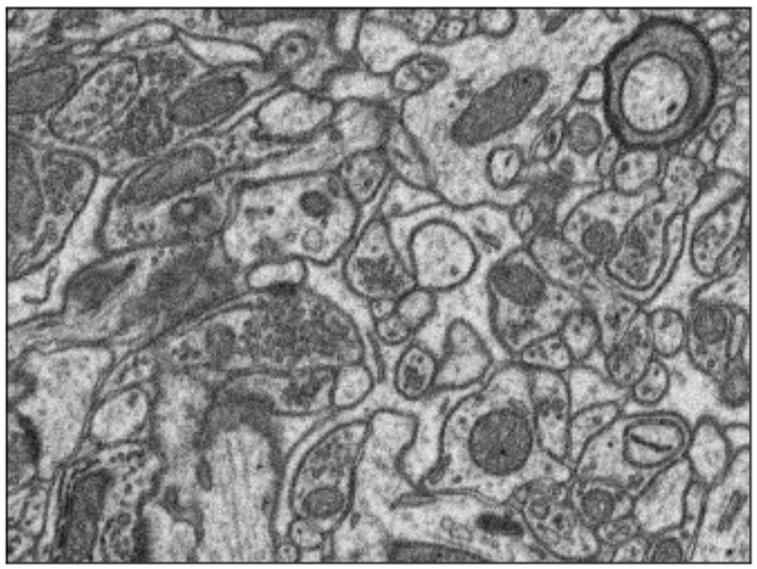
Implementation

```
from my_models import unet

model = unet()

model.fit(X_train, y_train)

results = model.predict(X_test)
```

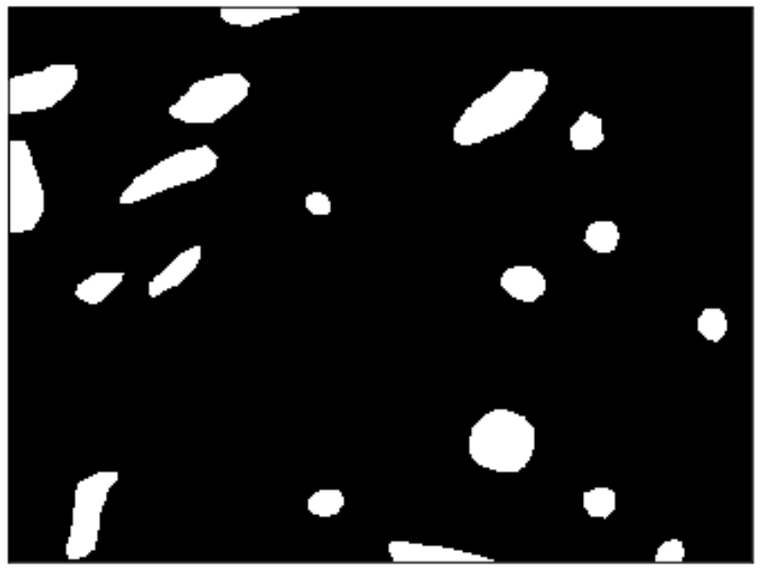
Ronneberger et al, MICCAI 2015

Use case 2: Prediction

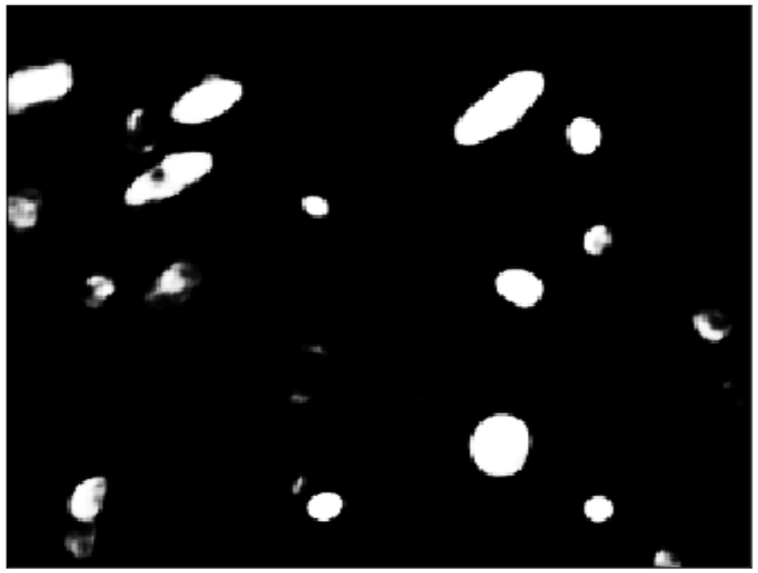
Raw image



Ground truth



Prediction



Use case 2: Summary

Deep learning model provides:

- automatisation of time-consuming process
- recognition of patterns in complex dataset
- no interpretability of model
- computationally heavy solution

  (Training: ~2h runtime on single GPU/~2d on single CPU)

Summary

Machine Learning in research:

- uncover hidden patterns in data
- interpretable models allow further insight
- automatisation of time-consuming processes

Thank you for your attention!