https://ai4mi.epotentia.com

AI FOR MATERIALS INDUSTRY

ARTIFICIAL INTELLIGENCE

A MASSIVE OPEN ONLINE COURSE

Hands-on session 1

Steel defect classification with machine learning

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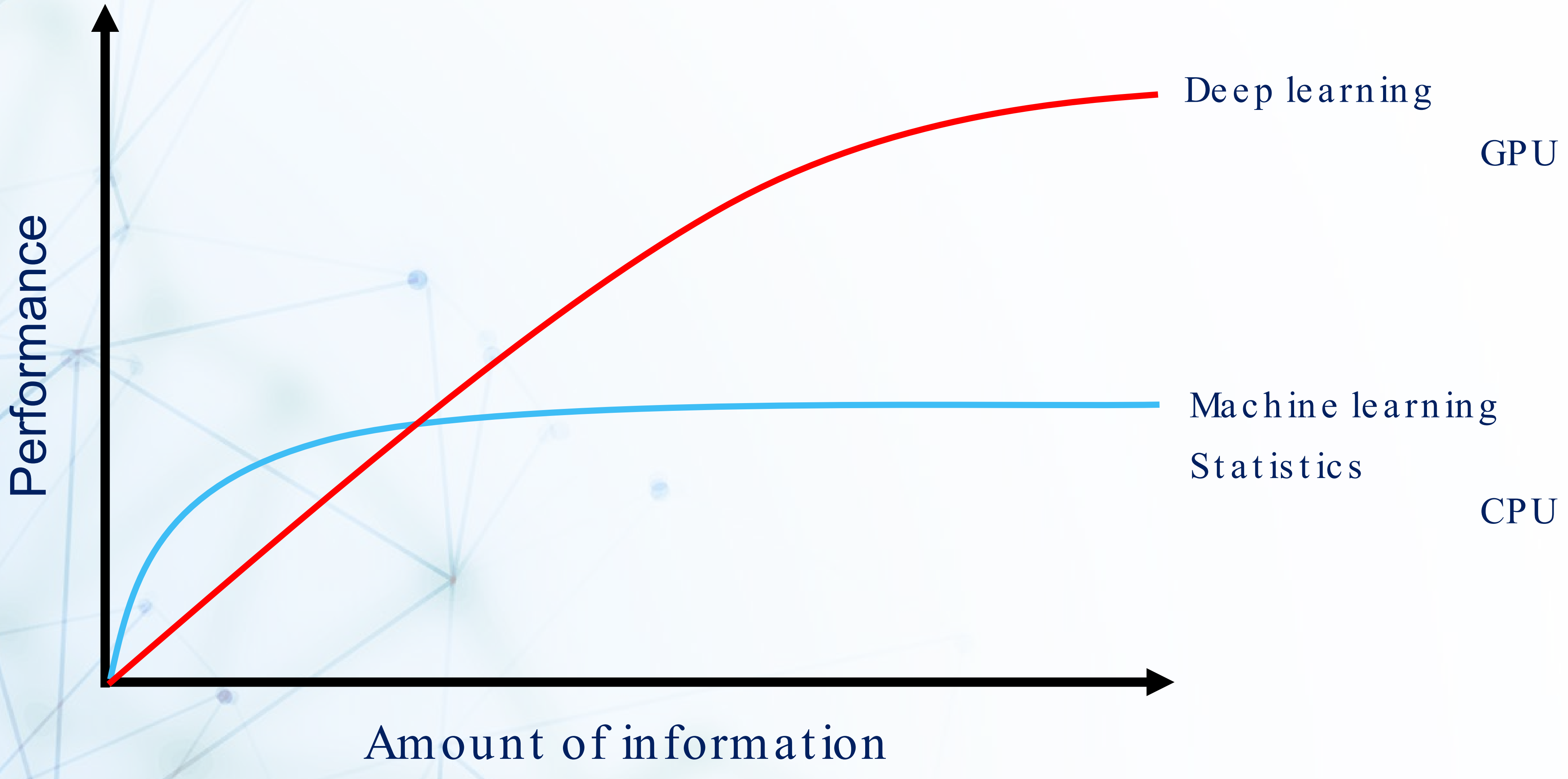
What is AI?

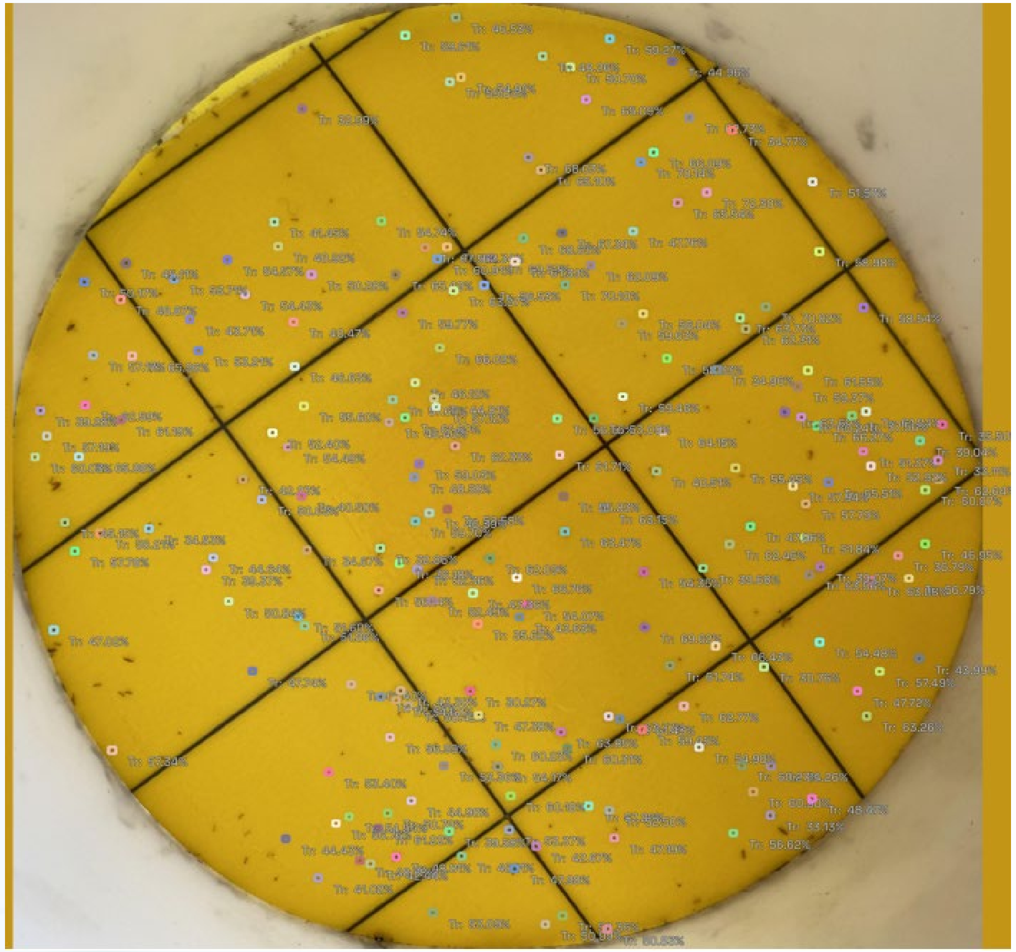
Series of techniques to extract **information** from data

Types of AI



The more data we have, the more we trade insight for predictive power

Example application: BioBest



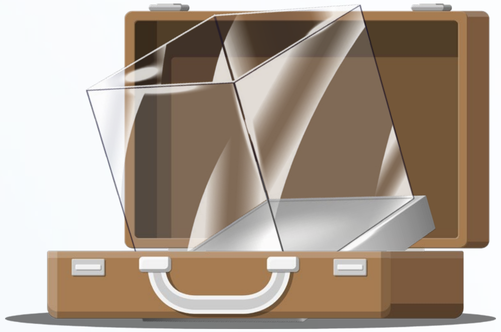
Case studies

Spreadsheet data

Steel

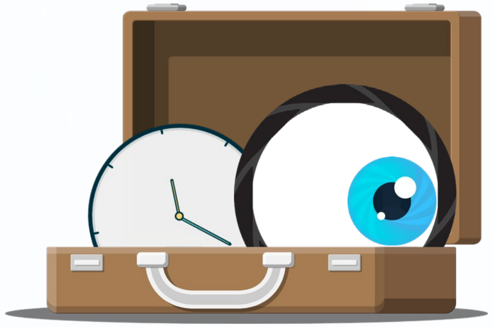
Computer vision

Glass



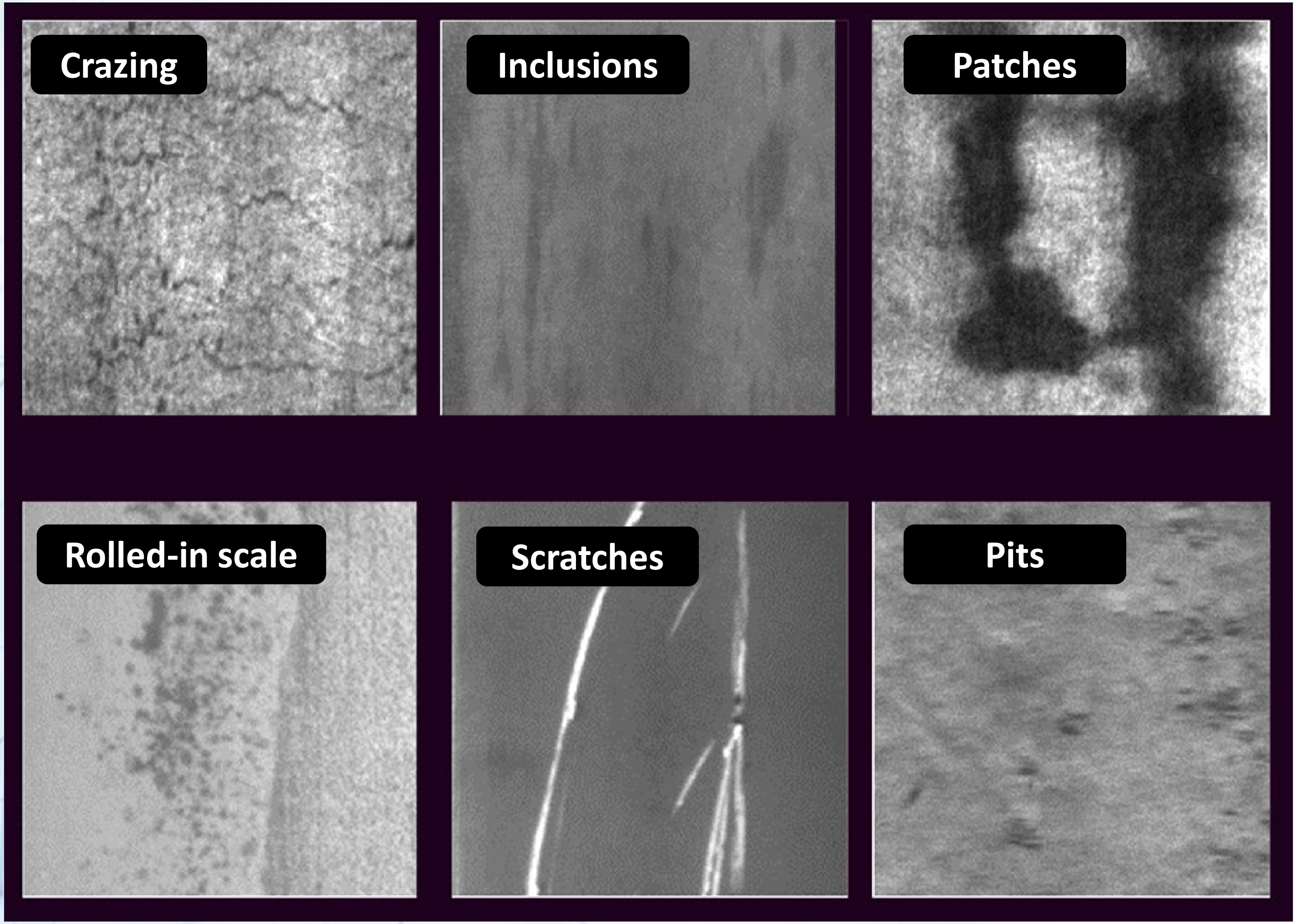
Materials discovery

Manufacturing

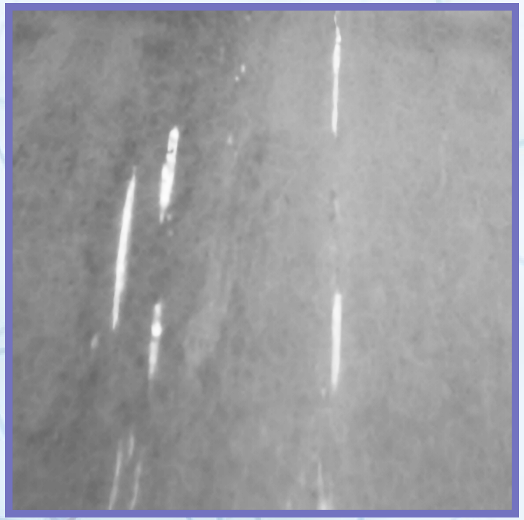


Sensor data

Steelplate defects



Multi-step pipeline



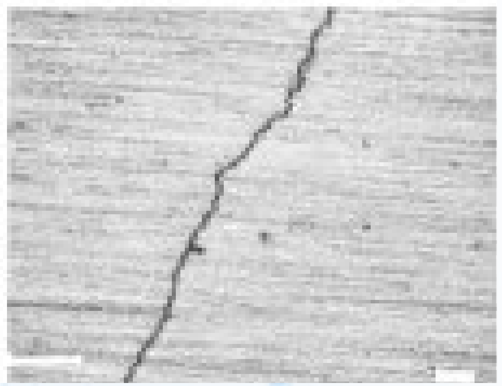
Detector → Featurizer → Classifier

Part of the pipeline needs to run in production

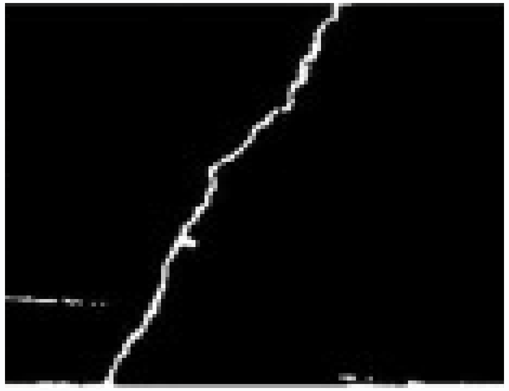
Detector

Original

Grayscale



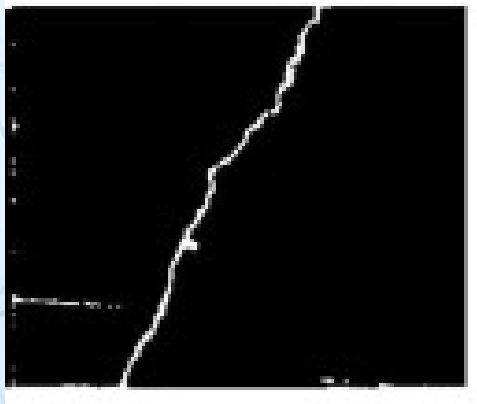
Threshold



Source: https://doi.org/10.1016/j.aej.2019.10.001

Simple and effective, but can be fickle

Featurizer



- Size and shape
- Brightness and contrast
- Materials properties
- Processing information

Features are numerical representation of the data created using our knowledge

This session

1. Analyze the features
2. (optional) Add more
3. Choose a model
4. Optimize the model
5. Evaluate the results
6. Interpret with explainable AI

Part of the pipeline needs to run in production

Requesting a job

Jupyter Lab

This app will launch a Jupyter Lab server on one or more nodes.

Cluster

dodrio cpu_rome

Time (hours)

12

Number of nodes

1

Number of cores per node

32 (quarter)

Mode

JupyterLab version

3.1.6 GCCcore 11.2.0

Custom code

```
source /dodrio/scratch/projects/explor_2022_008/init.sh
```

This code is executed before the JupyterLab is started. Primarily used for extra modules you want to load or swap.

Extra Jupyter Arguments

```
--notebook-dir=$PDIR/$USER
```

Project account

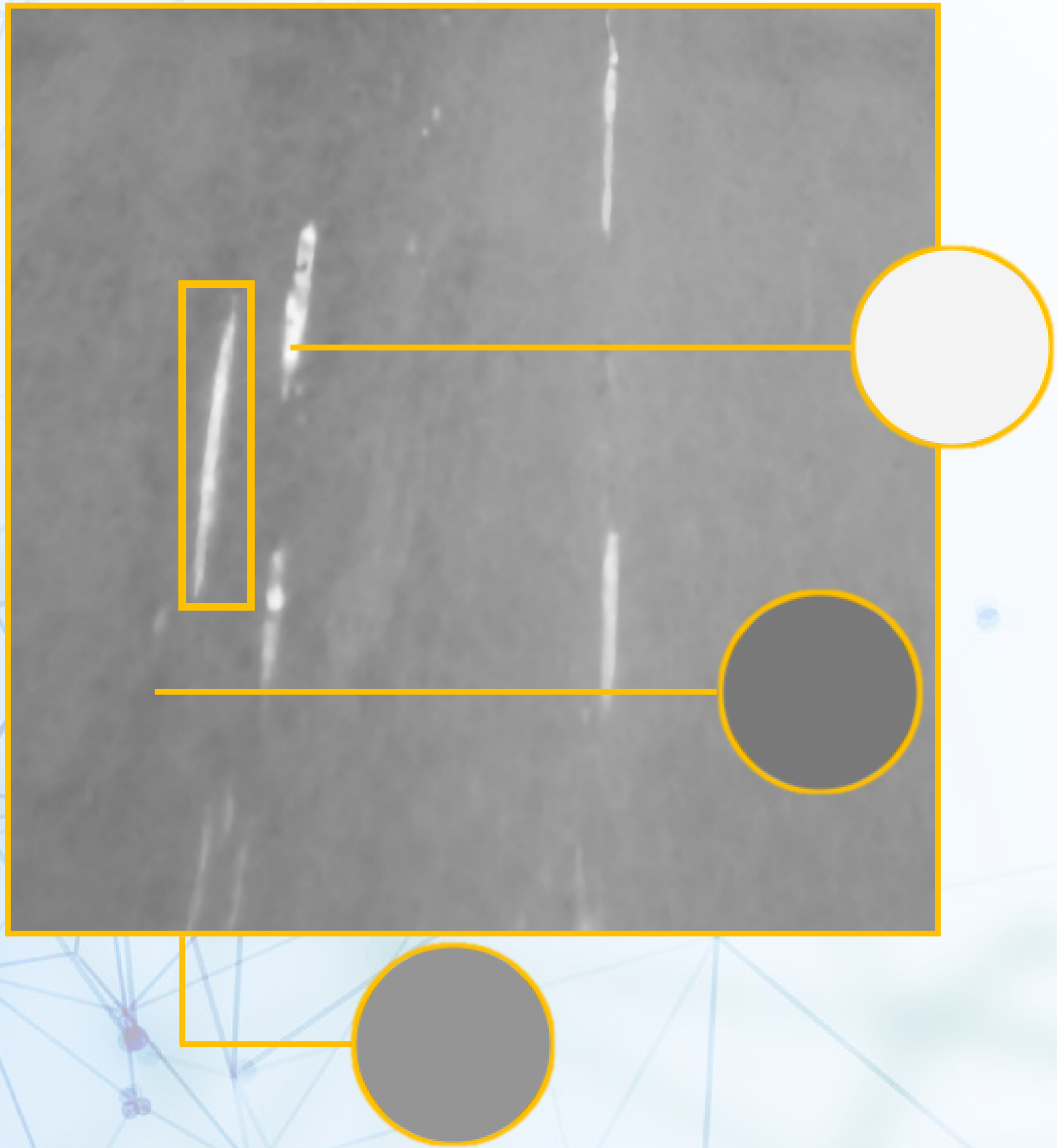
explor_2022_008

Extra sbatch arguments

```
--reservation=MaterialsAI-CPU
```

Log in at https://tier1.hpc.ugent.be

Dataset



- What is the dataset?
- Where did it come from?
- Who made it?
- What are the inputs?
- What are the outputs?

Tabular data

		Feature		
Datapoint		Value		

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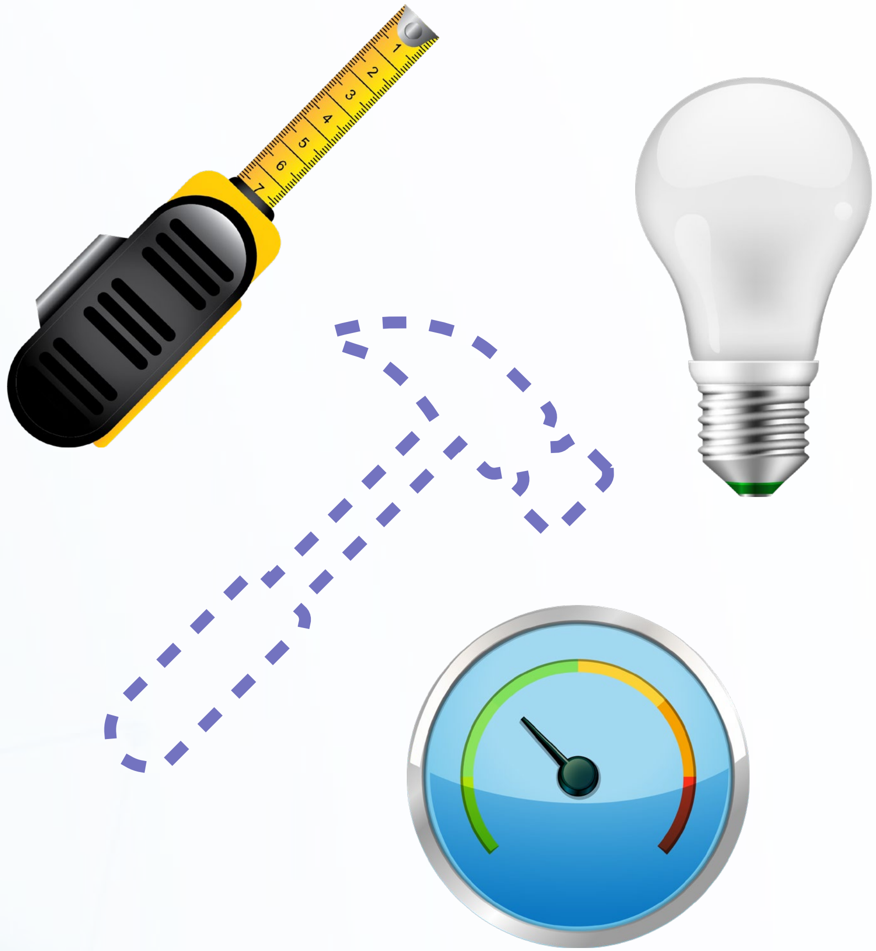
Python Pandas

pandas

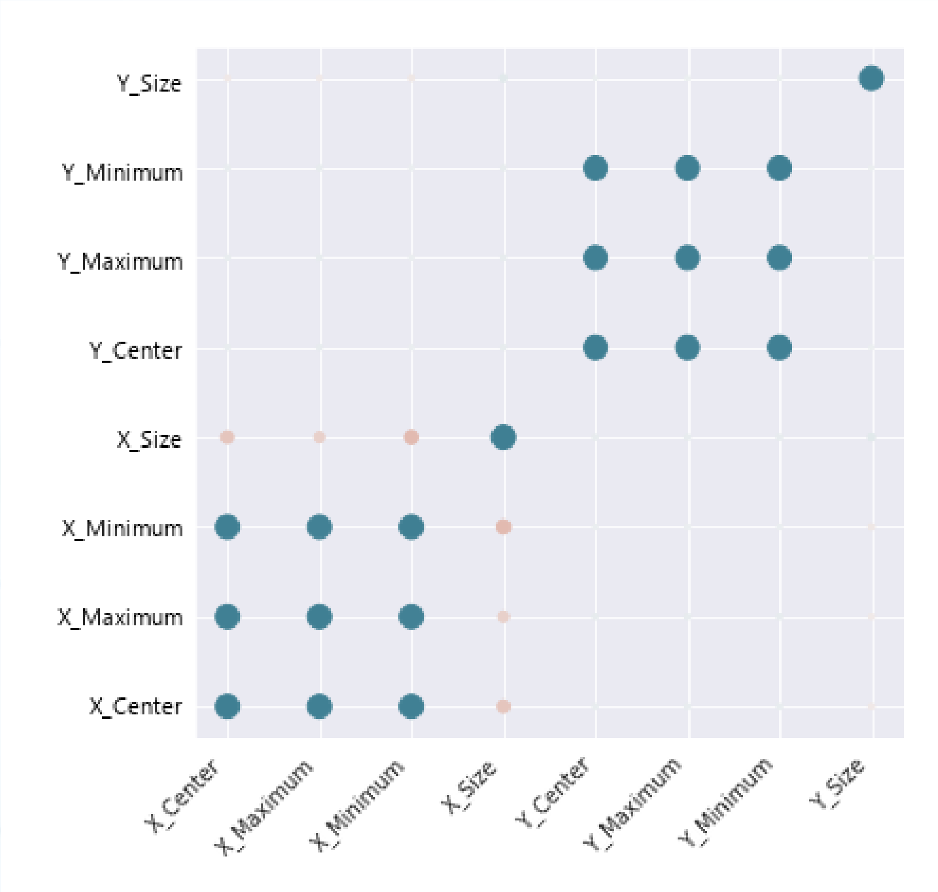
```
pip install pandas
```

Exploratory Data Analysis

- What kind of features are in the dataset?
- What is the range of the values?
- What do the features represent?
- Are they independent?
- Is there missing data?
- Are certain outputs rare or abundant?



Example: feature independence

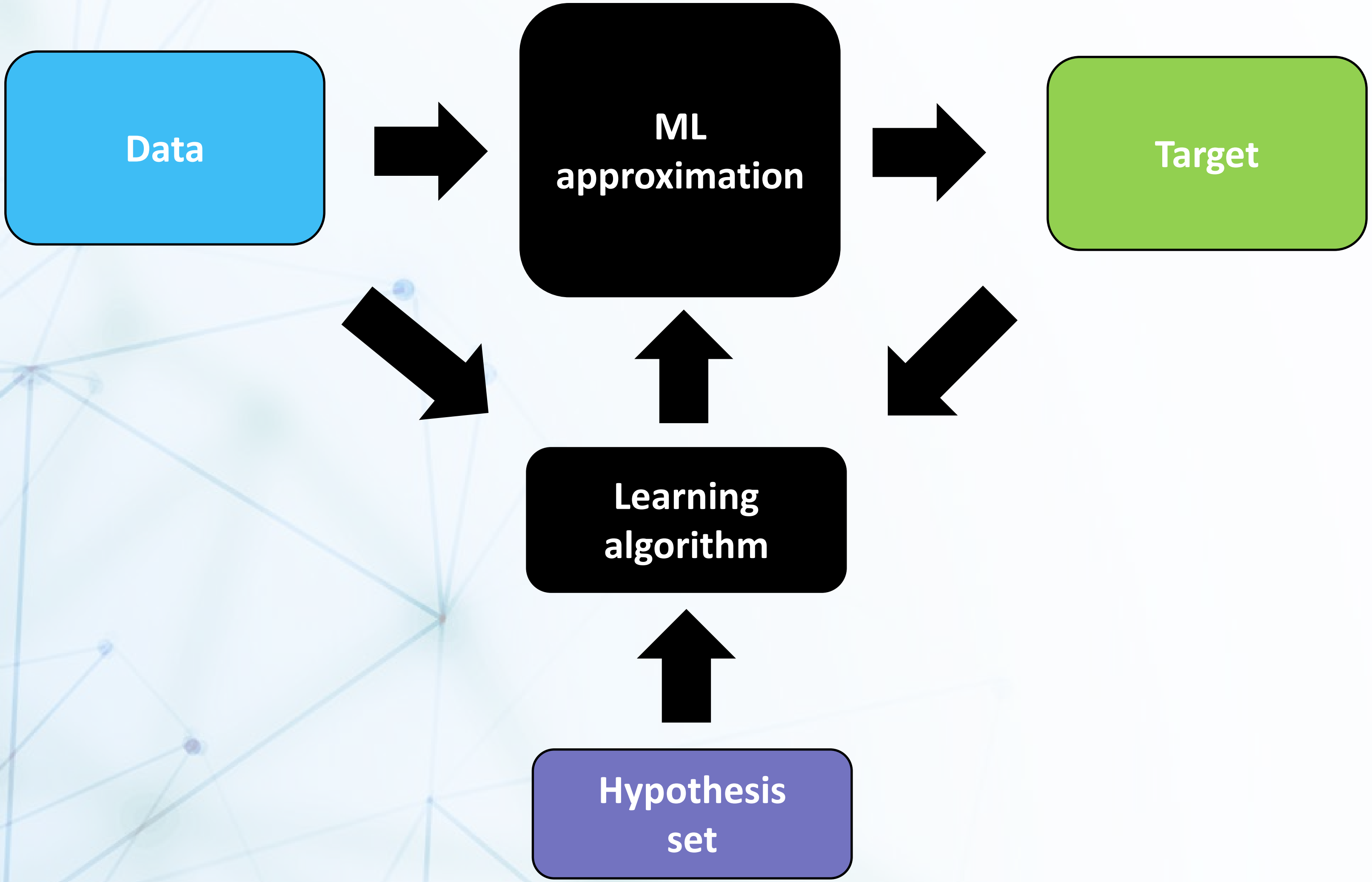


Strongly correlated features are opportunities for optimization

Machine learning ingredients

We must find the function that connects the inputs to the target

Machine learning ingredients



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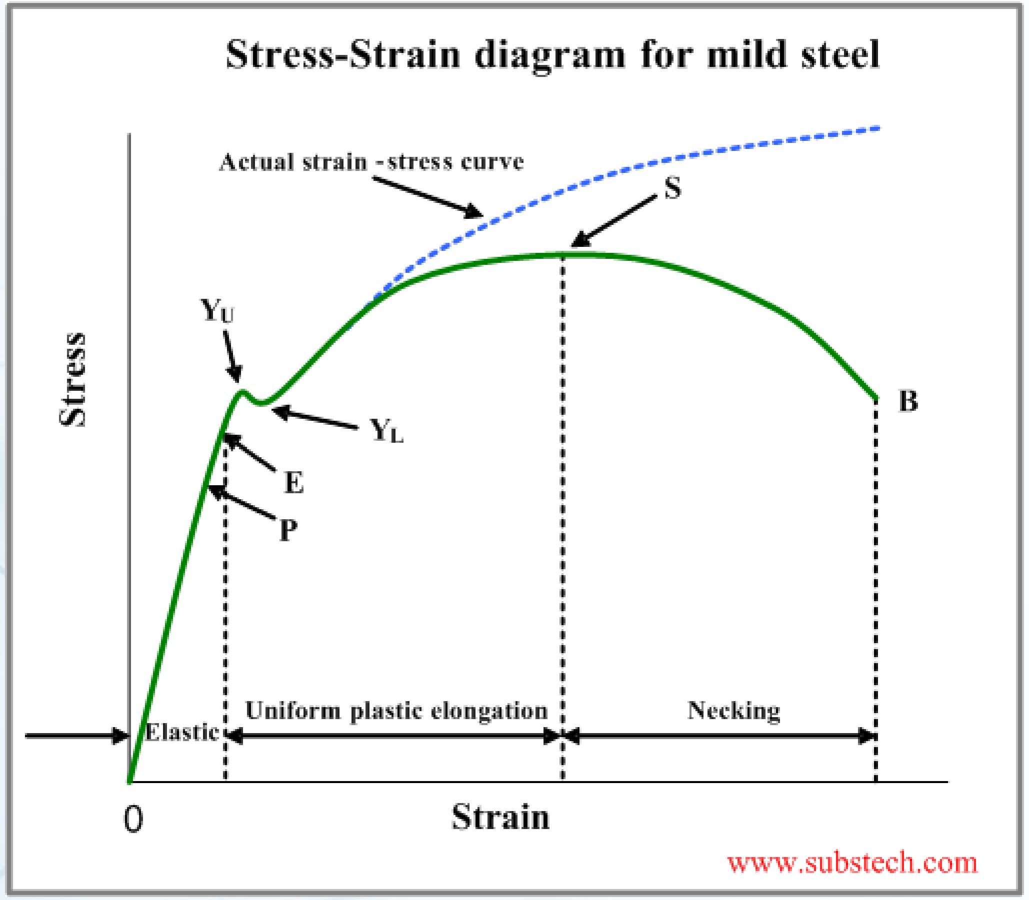
Example: tensile curve



Type of representation can greatly affect the performance

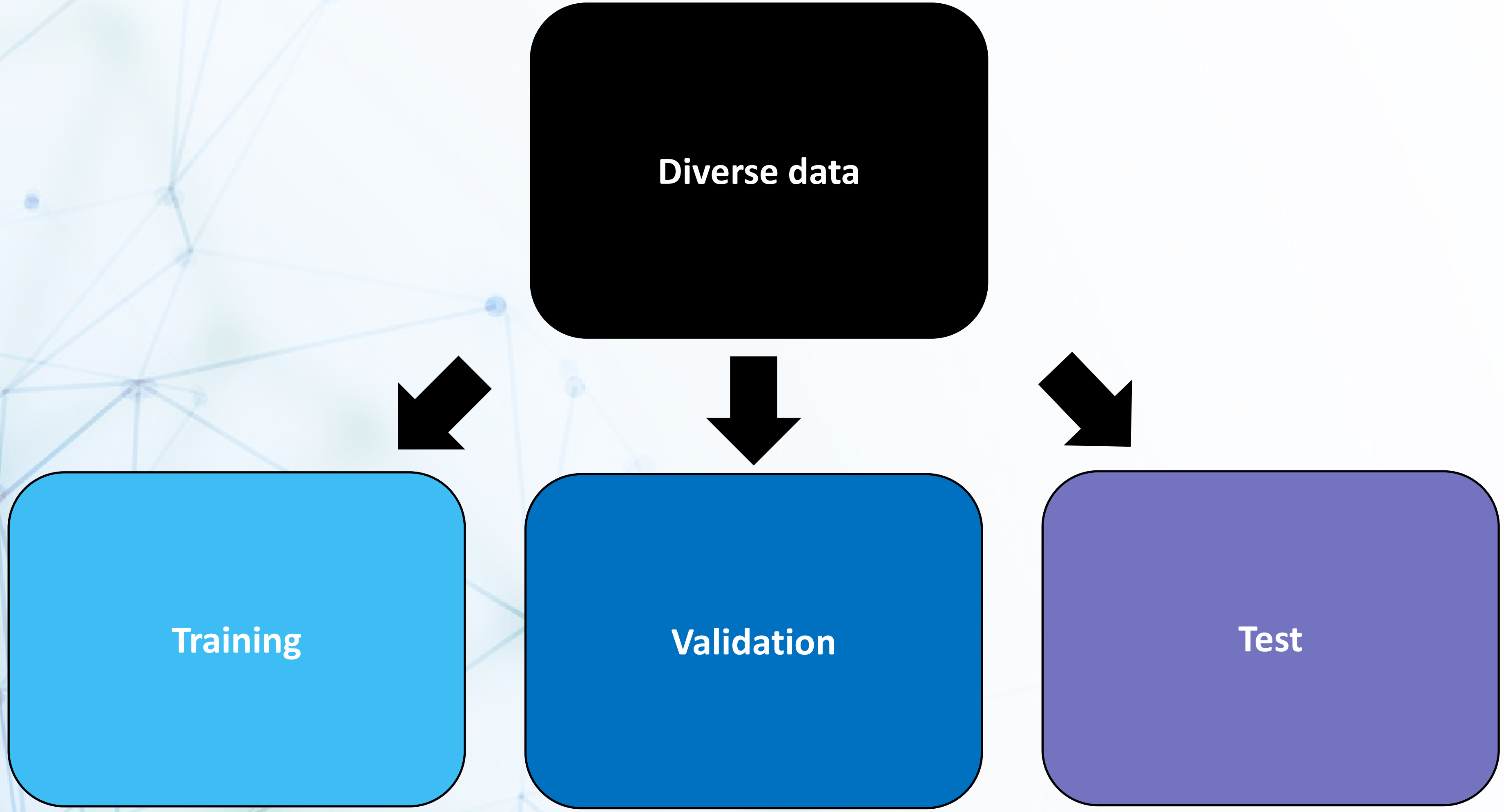
Constructing a dataset

Diverse dataset

- Materials
- Etchings
- Machines
- People

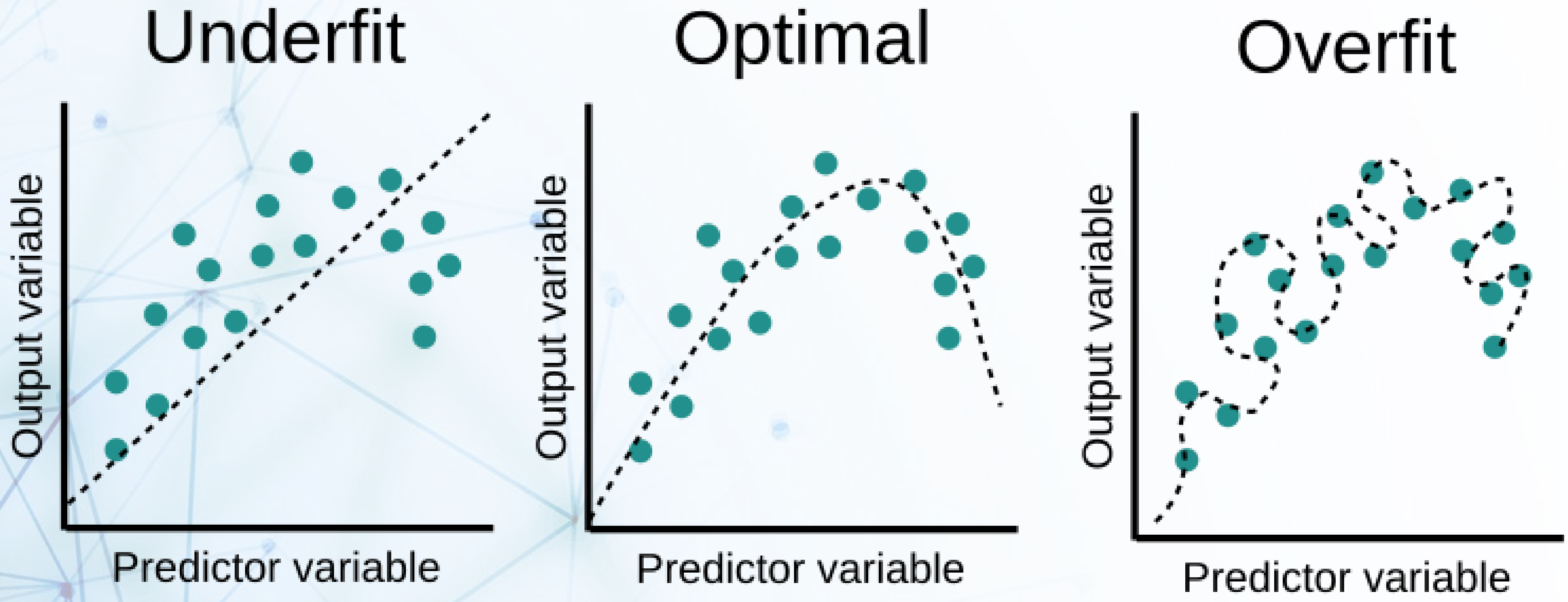
Collecting a good dataset takes time

Generalization



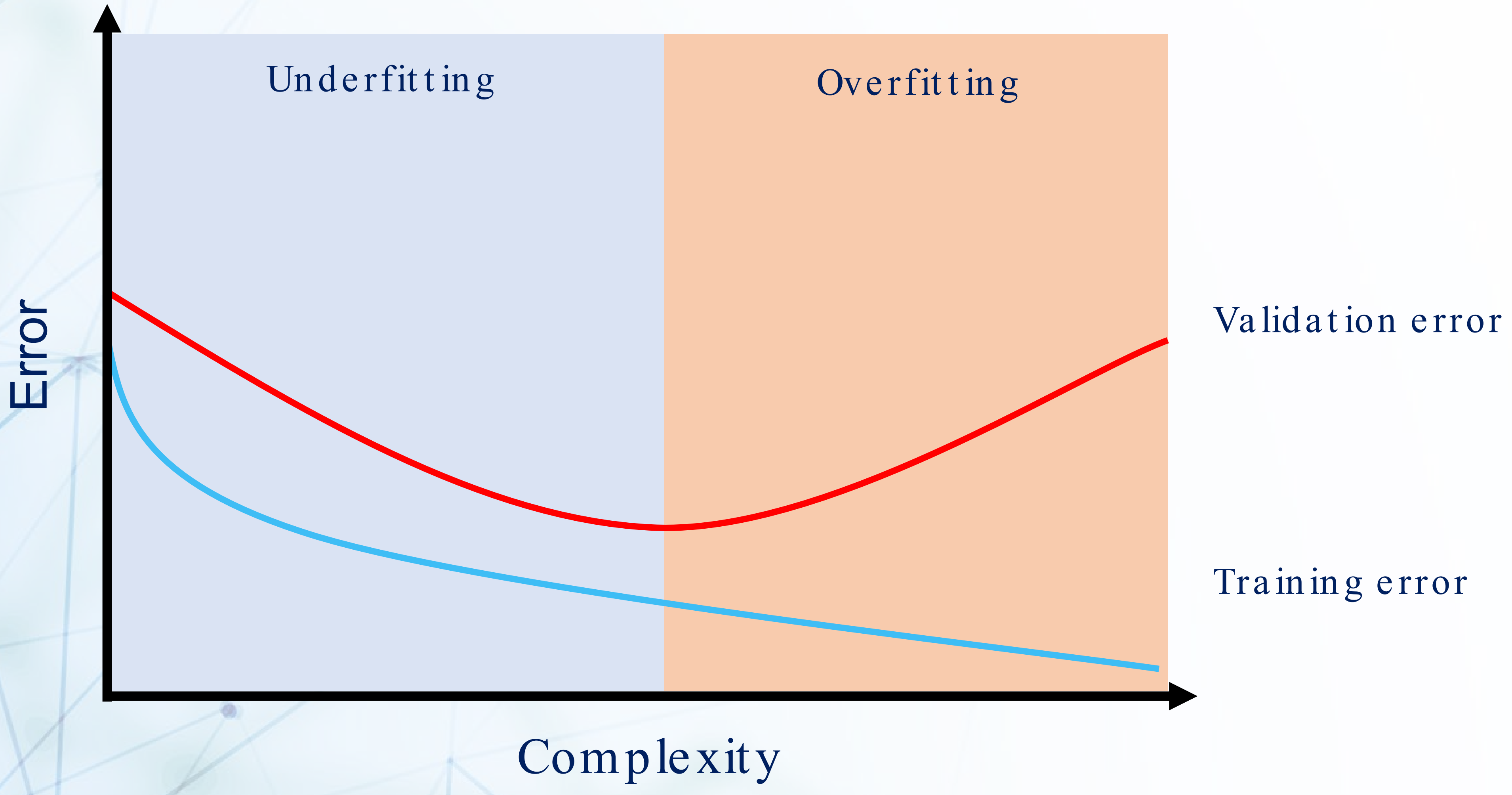
Be very careful for data leakage

Fitting your model



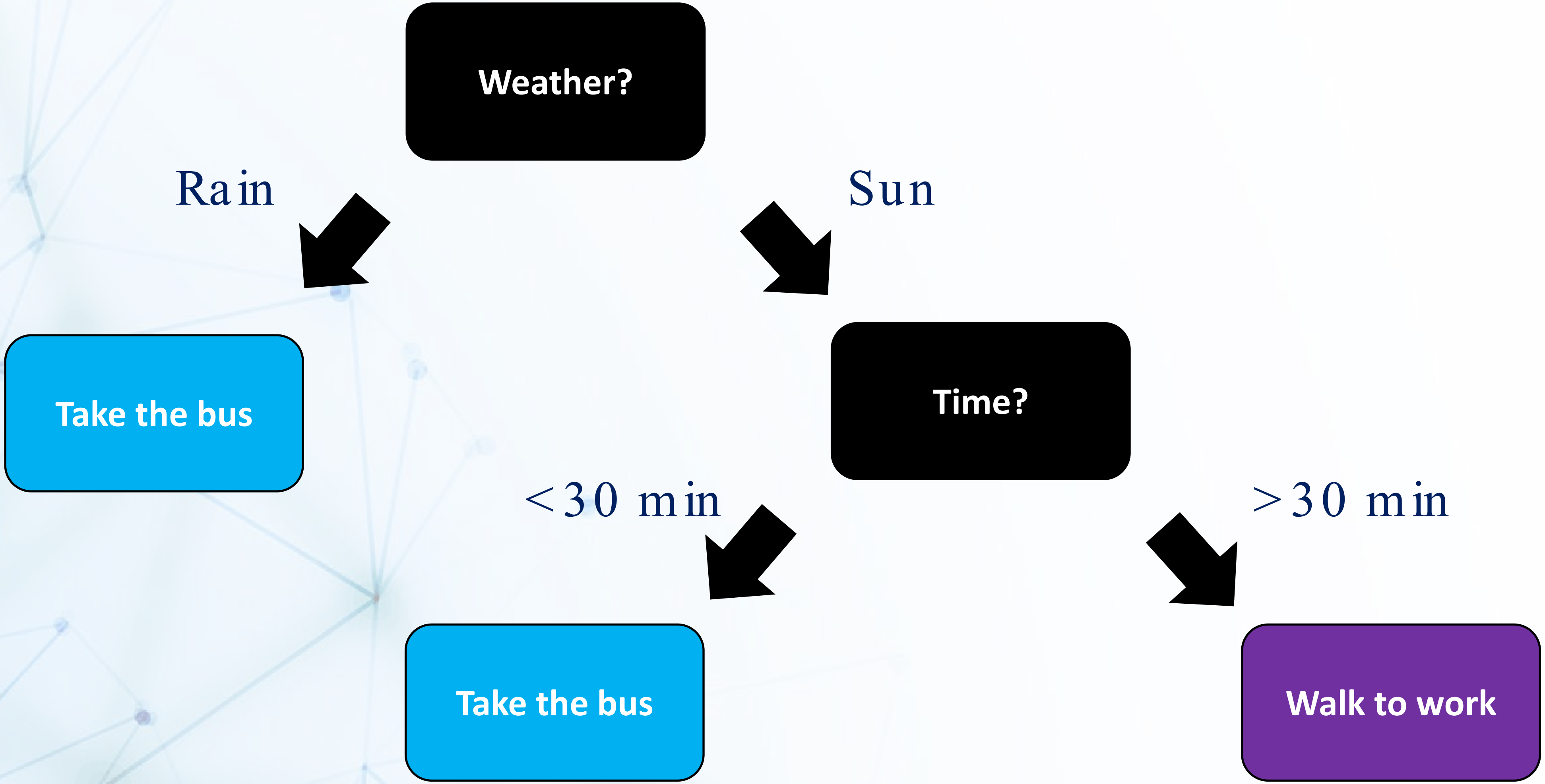
Choose a model of the right complexity and regularize where needed

Generalization



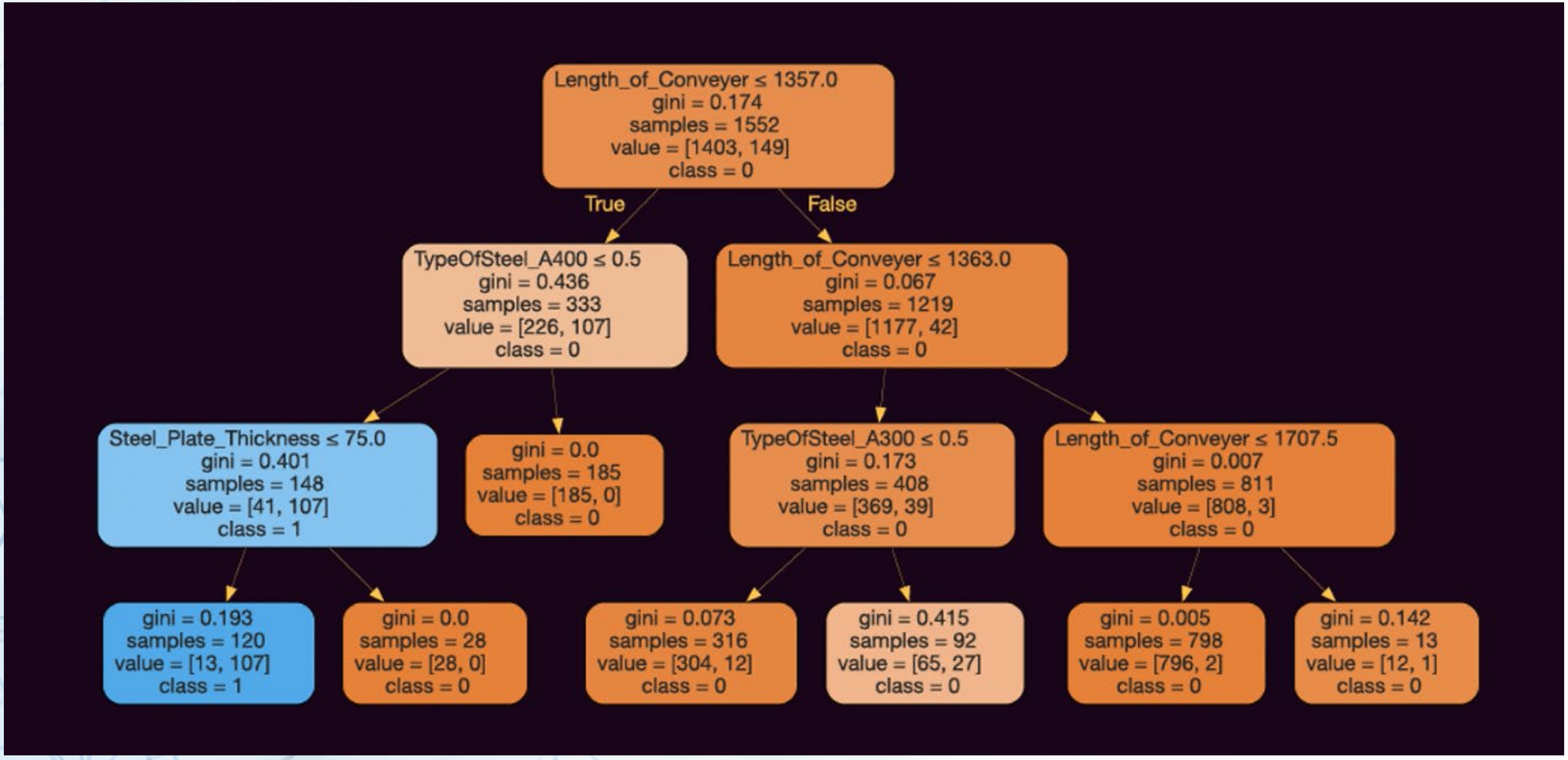
Regularization techniques can prevent overfitting

Decision trees



Robust, flexible in amount of data, controllable speed (CPU)

Bump decision tree



A single tree greatly risks overfitting

Random forests

By taking many simple trees, we average out the error and prevent overfitting

Out-of-bag score

N samples are chosen for each tree with repetition (bagging)

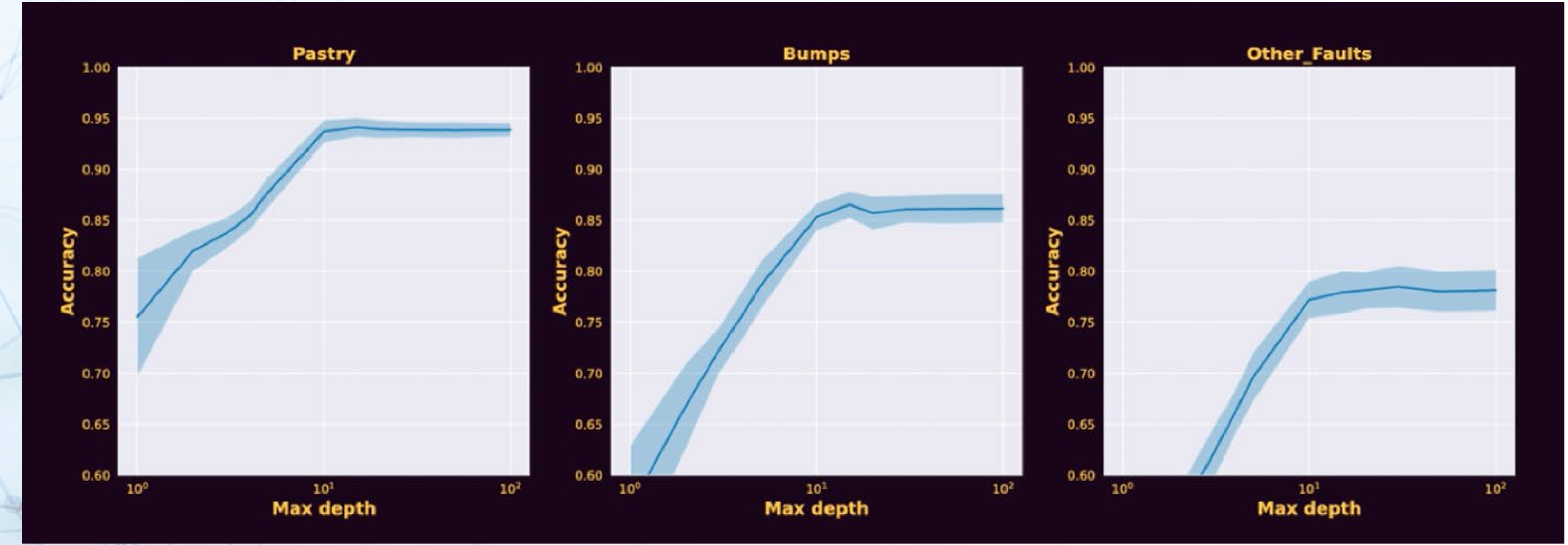
36,2% of the data is unseen by each tree which can be used for OOB validation

Hyperparameters

• Number of trees	`n_estimators`
• Depth of the trees	`max_depth`
• Amount of data per tree	`max_samples`
• Number of features per tree	`max_features`
• Samples per split	`min_samples_split`
• Samples per leaf	`min_samples_split`

Perfect for high-throughput screening

Example: tree depth



Deeper trees are better, but slower and risk overfitting

Accuracy

- **Decision trees** can split the dataset down to **individual samples**
- 100% accuracy on training is easy, almost trivial
- This doesn't mean good performance "in the wild", the model might have just learned to recognize distinct noise patterns that don't generalize
- This is why we need a validation and test set: a fair assessment

Metrics

- **Accuracy:** How often did we get it right? Gives no information about what type of mistakes are being made
- **Confusion matrix** : Very useful tool to understand what's going on, showing true positive (TP), false positive (FP), false negative (FN) and true negative (TN)

		Real data	
		+	-
Predicted data	+	TP	FP
	-	FN	TN

Metrics

		Real data	
		+	-
Predicted data	+	TP	FP
	-	FN	TN

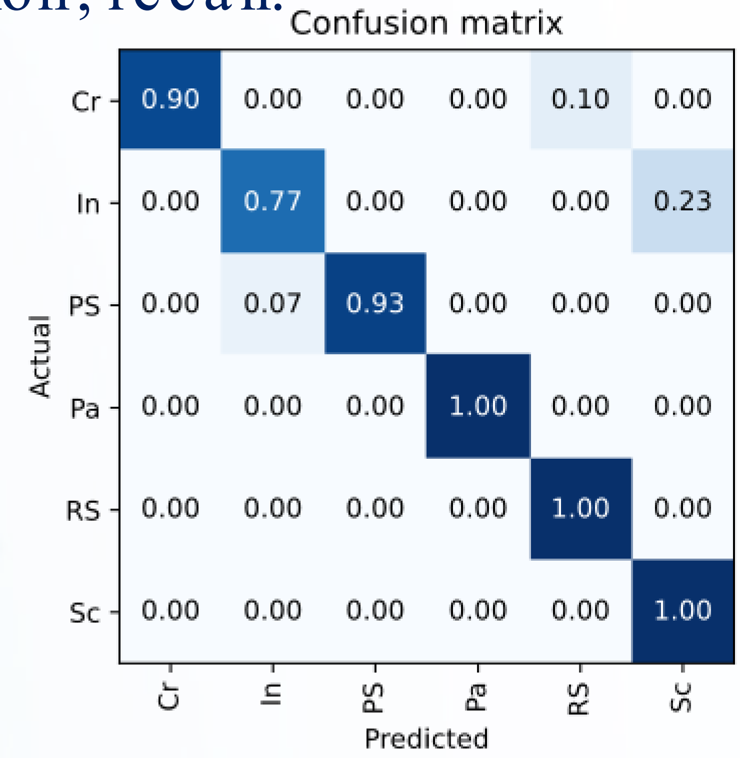
- **Accracy** : How often did we get it right? (TP and TN)
- **Precision** : Quality, how many of the positive samples are real? (FP)
- **Recall** : Quantity, How many of the positive samples did we find? (FN)

Choosing the right metric for your goal is important

Metrics

- The **confusion matrix** is more general than just true/false, can give insight in whether certain classes get confused for each other

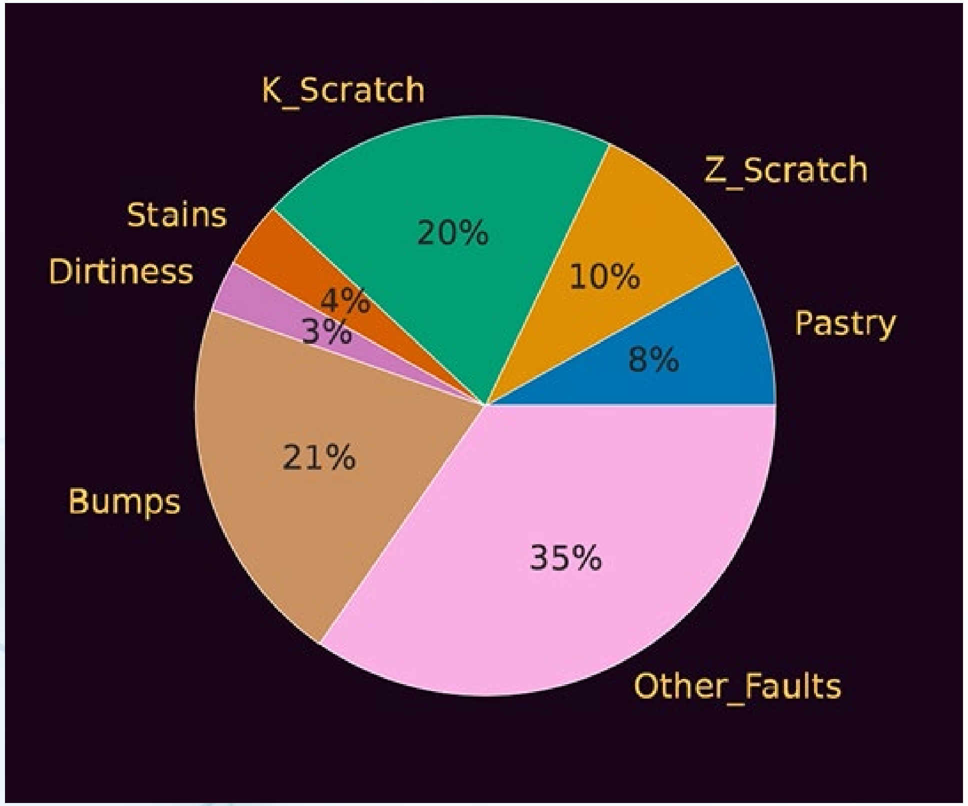
- **Other metrics** exist beyond accuracy, precision, recall.



- **F1-score:** geometric mean between precision and recall, good middle ground

- **Matthews Correlation Coefficient (MCC):** Cross-correlation between the real data and predicted data, ranges from -1 (anticorrelated) to +1 (correlated)

Results



Optimized	Pastry	Z Scratch	K Scratch	Stains	Dirtiness	Bumps	Other Faults
Accuracy	94%	98%	99%	100%	99%	88%	80%

Choosing the right metric for an application is important

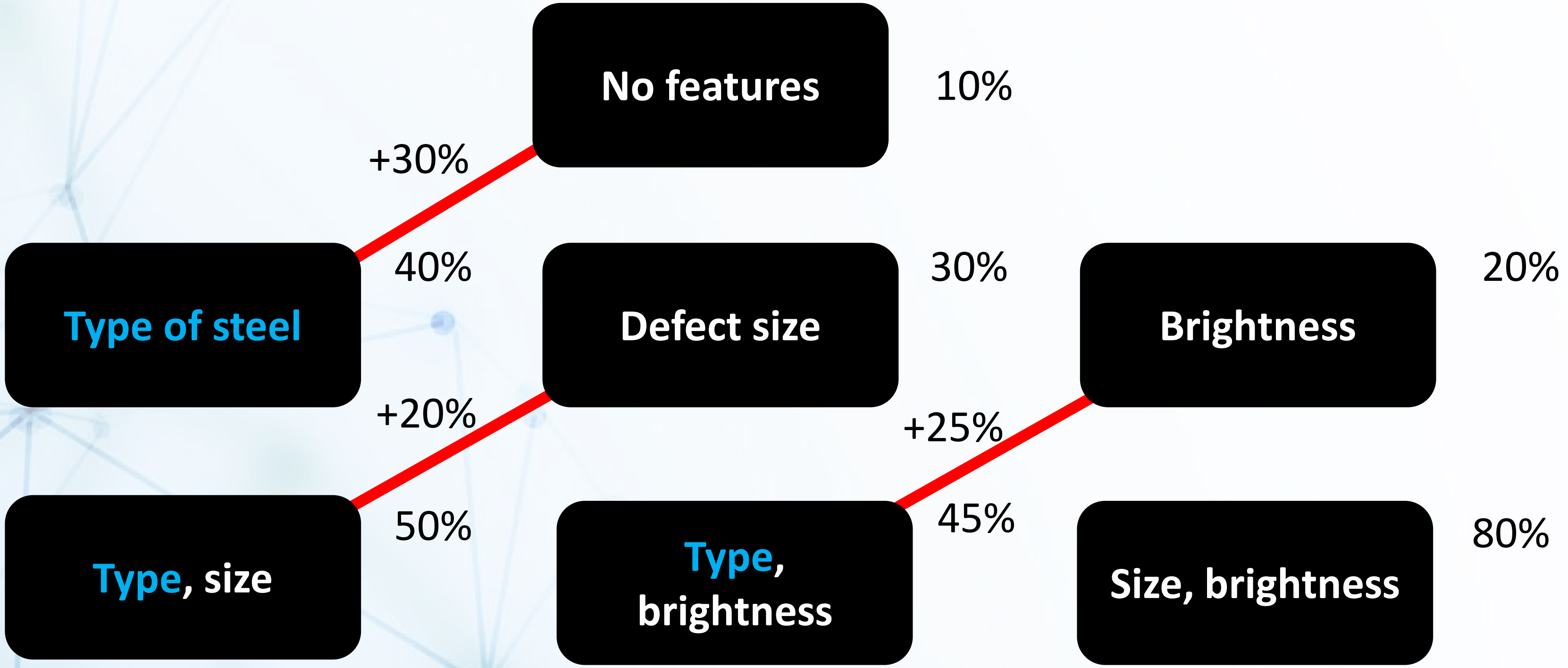
Explainable AI

- The model uses **features** to make predictions
- How **important** is a feature? Remove it and find out!
- **Drop-column feature importance:**
  1. Remove feature
  2. Retrain model
  3. Compare
- **Permutation feature importance:**
  1. Shuffle feature
  2. Make prediction with same model
  3. Compare

Explainable AI

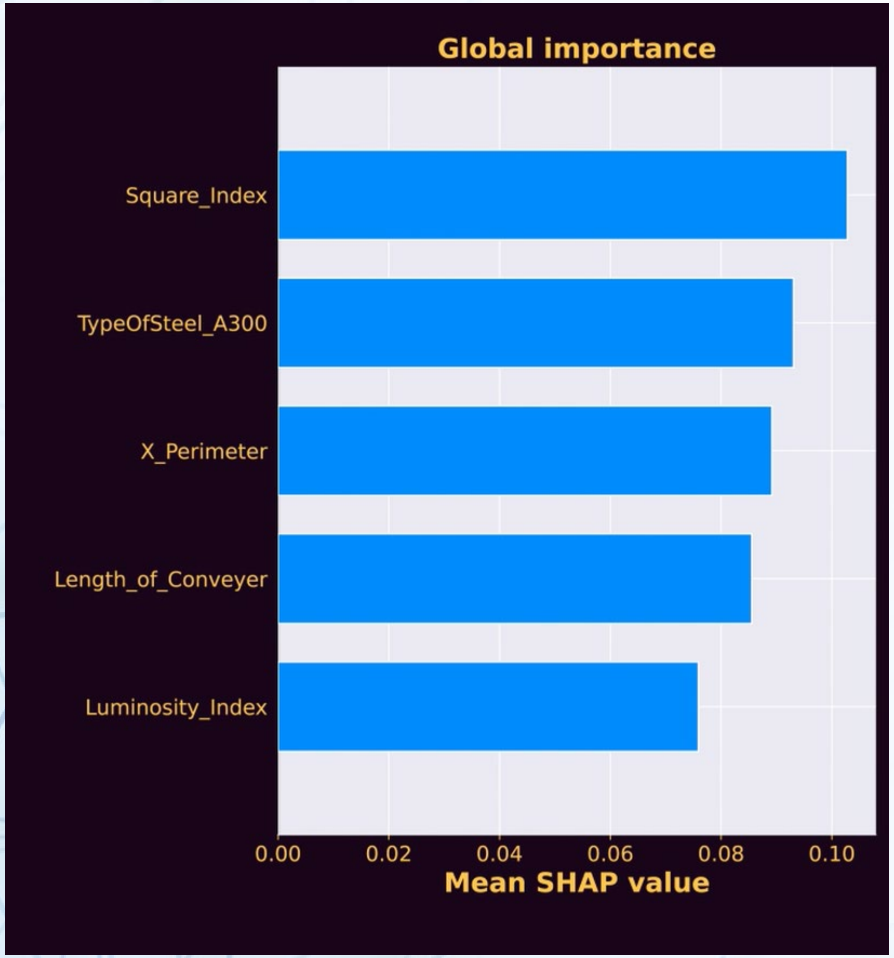
Features	Accuracy
No features	10%
Type of steel	40%
Defect size	30%
Brightness	20%
Type, size	50%
Type, brightness	45%
Size, brightness	80%

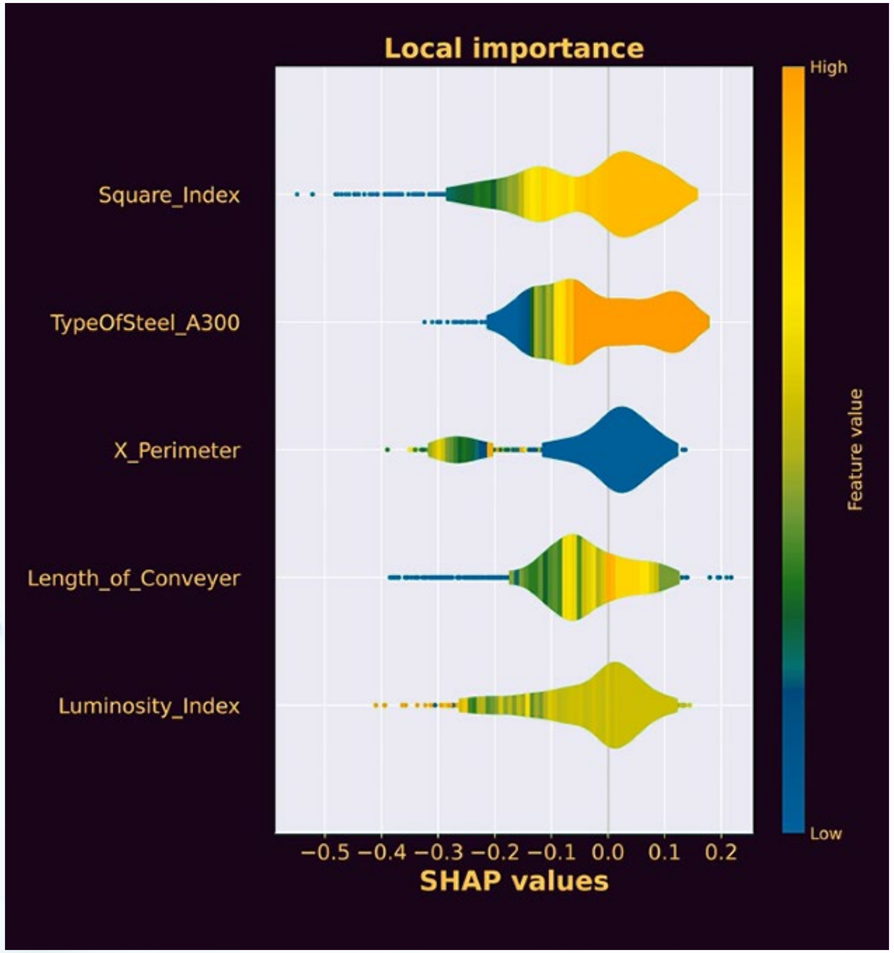
Explainable AI



If we could simulate all possible models we could evaluate the impact -> SHAP

Practical SHAP for bumps





https://github.com/slundberg/shap

SHAP helps us understand how a decision is reached

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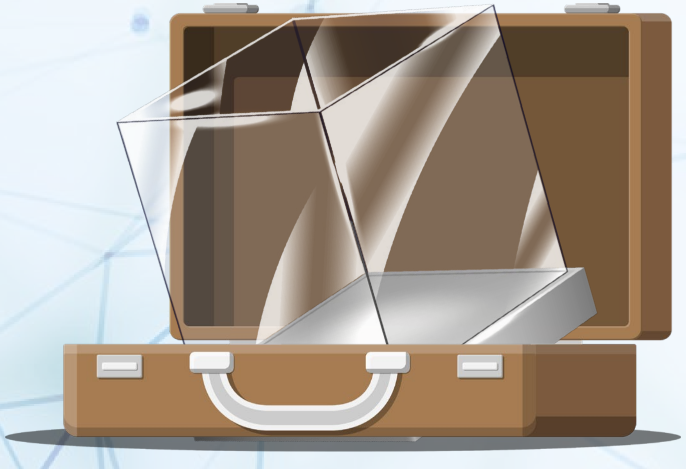
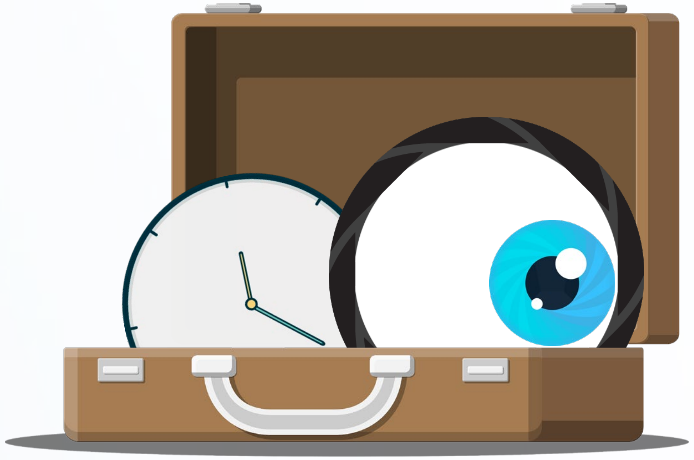
Glass



Materials discovery

Manufacturing



Sensor data

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