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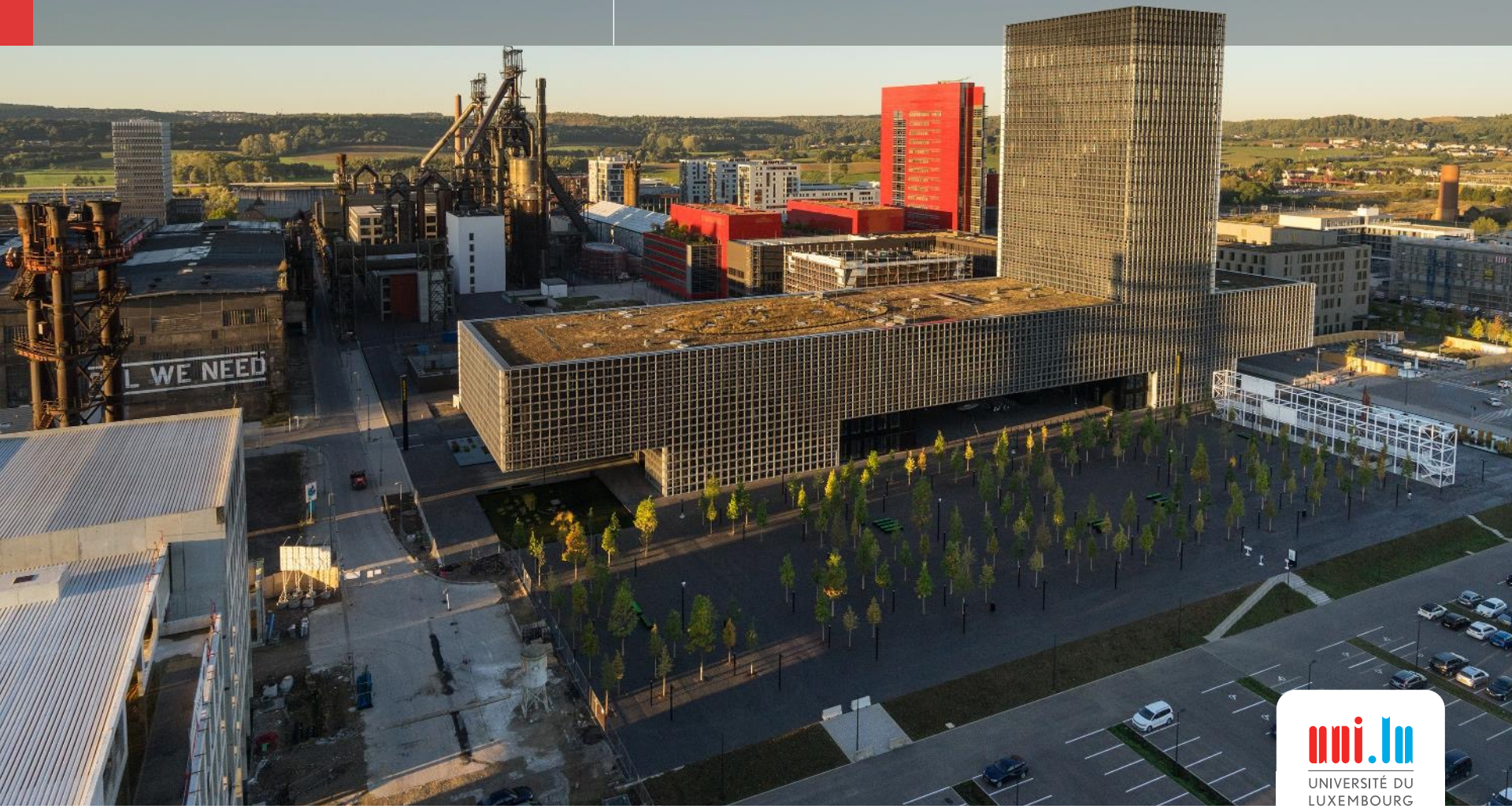
Machine Learning

Martin GUBRI, 04/11/2022



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Overfitting & Underfitting

Empirical risk minimization (ERM)

How to learn from data?

$f(x_i)$: the model's prediction for i-th example

Loss: a measure of how far a model's predictions are from its label

In binary classification: $L(y_i, f(x_i)) = \mathbb{I}(y_i \neq f(x_i))$

Empirical Risk: Average of the loss across the dataset's examples

$$R_{emp}((X, y), f) = \frac{1}{N} \sum_{i=1}^{N} L(y_i, f(x_i))$$

Empirical Risk Minimization: finding a model that minimize the empirical risk

$$\min_f R_{emp}((X, y), f)$$

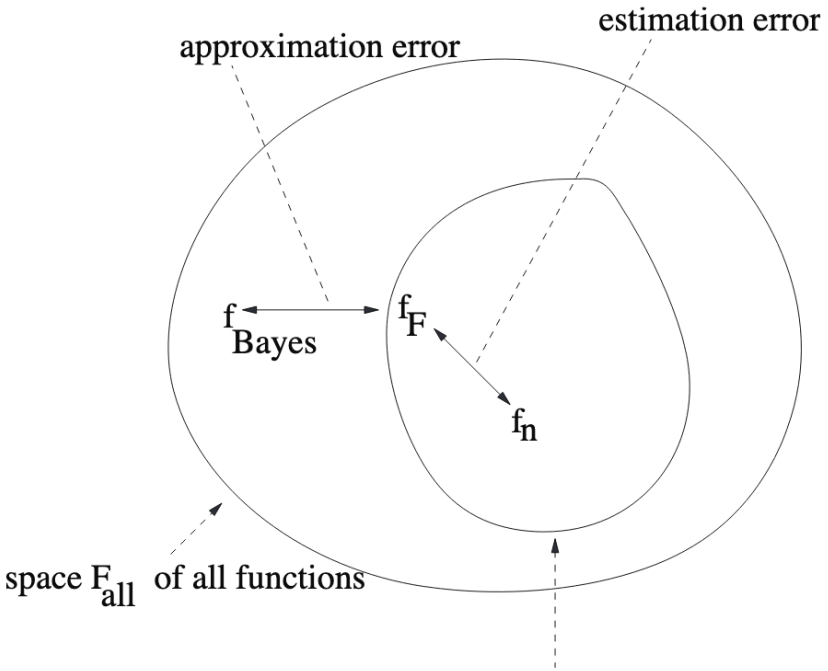
Decomposition of the error

$$R(f_n) - R(f_{Bayes}) = \underbrace{\left(R(f_n) - R(f_{\mathcal{F}})\right)}_{\text{estimation error}} + \underbrace{\left(R(f_{\mathcal{F}}) - R(f_{Bayes})\right)}_{\text{approximation error}}$$

your trained model

"best" unknown model
possible with the current set of features

best unknown model possible
with the chosen algorithm
(and the current set of features)



Source image:
U. von Luxburg and B. Scholkopf.
"Statistical Learning Theory: Models, Concepts, and Results",2011.

Decomposition of the error

$$R(f_n) - R(f_{Bayes}) = \underbrace{\left(R(f_n) - R(f_{\mathcal{F}})\right)}_{\text{estimation error}} + \underbrace{\left(R(f_{\mathcal{F}}) - R(f_{Bayes})\right)}_{\text{approximation error}}$$

VARIANCE ⟷ BIAS

Source image:
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“Statistical Learning Theory: Models, Concepts, and Results”,2011.

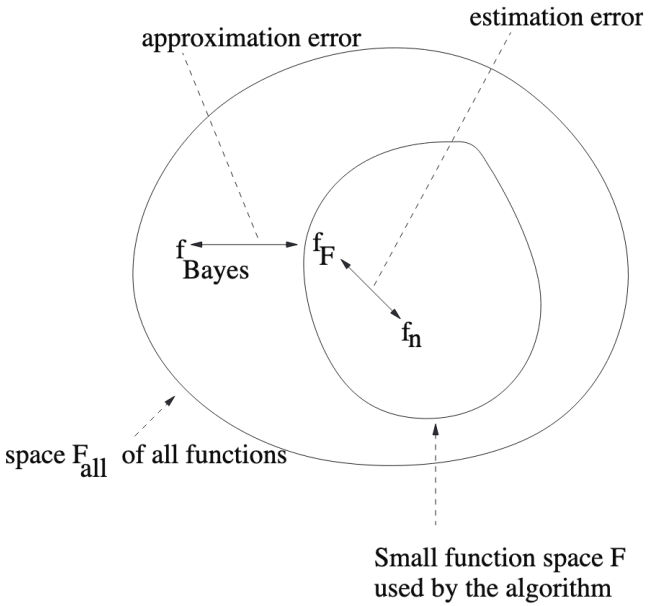
Bias-Variance tradeoff

Biais

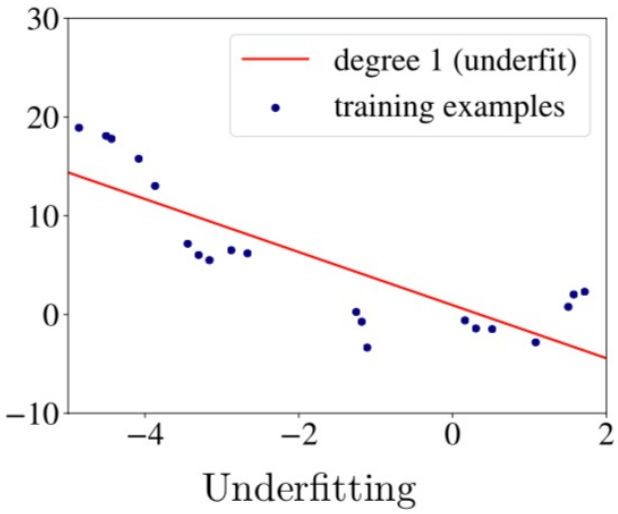
Large approximation error, small estimation error → **Underfit**

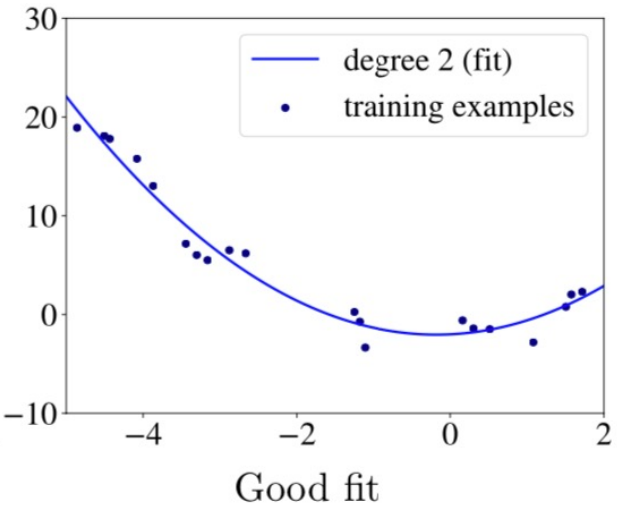
Variance

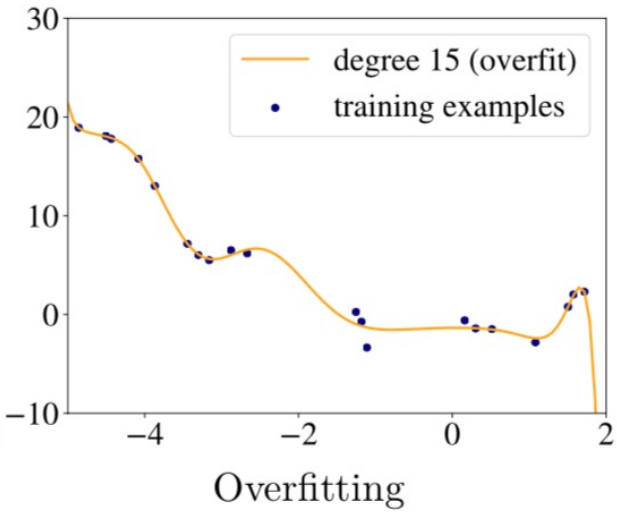
Large estimation error, small approximation error → **Overfit**



Bias-Variance tradeoff







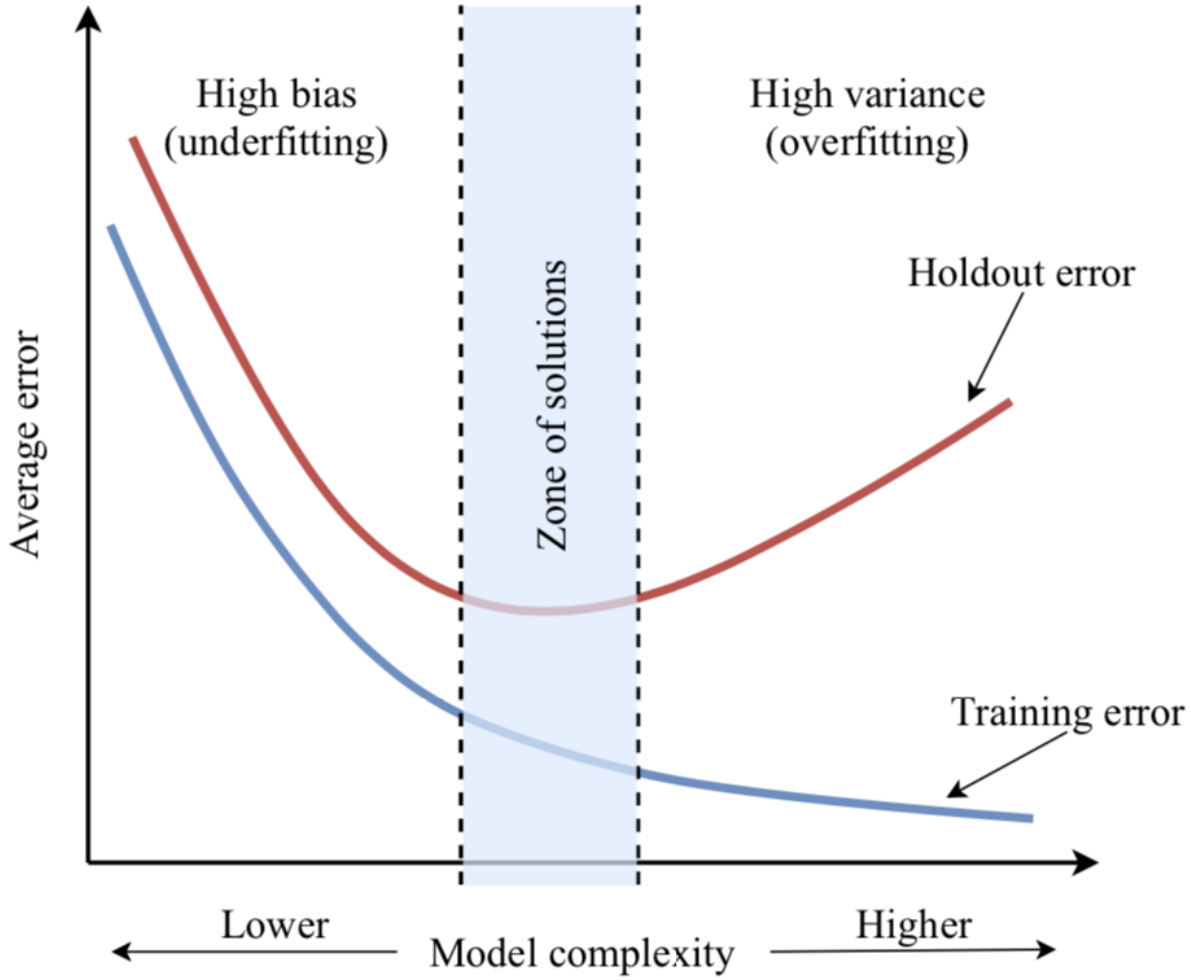
Oversimplification of the data

Learning the true signal

Fitting the noise of the data

Source image:
A. Burkov, “Machine Learning Engineering”.

Bias-Variance tradeoff



Source image:
A. Burkov, "Machine Learning Engineering".

Interactive quiz

Question 1

You trained a binary classifier (for example a spam filter) and you expect the same number of examples from both classes. You obtained the following accuracies:

- accuracy computed on the train set (the examples that were used to train the model): **99%**
- accuracy computed on the holdout set (the examples that where **not** used to train the model): **70%**

Do you think that the trained model is overfitting?

- True
- False

Question 2

Same context, but now you obtained the following accuracies:

- accuracy computed on the train set (the examples that were used to train the model): **88%**
- accuracy computed on the holdout set (the examples that where **not** used to train the model): **87%**

Do you think that the trained model is overfitting?

- True
- False

Question 3

Same context, but now you obtained the following accuracies:

- accuracy computed on the train set (the examples that were used to train the model): **61%**
- accuracy computed on the holdout set (the examples that where **not** used to train the model): **60%**

Do you think that the trained model is overfitting?

- True
- False

Question 4

You want to classify images of cats and dogs. Your model takes as inputs pixels values of images, and outputs if the image corresponds to a cat (0) or a dog (1).

For this task you choose a decision tree. You set up a maximum depth of the tree of 8 (which means that for each image to predict your model will use at most 8 conditions to recognize a cat or a dog).

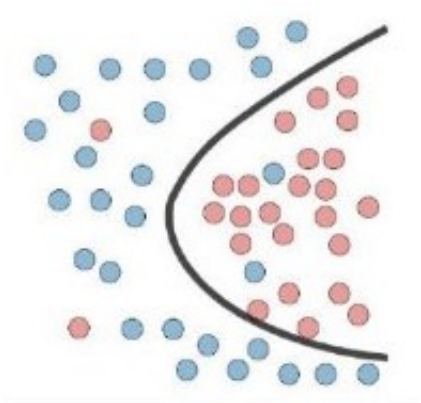
Is this model underfitting?

- True
- False

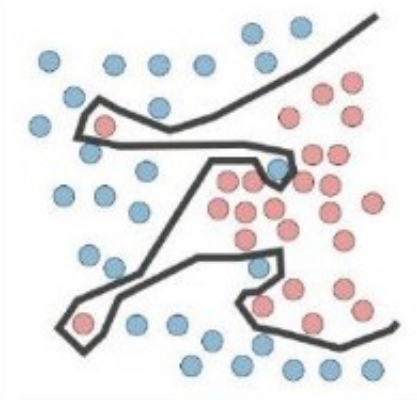
Question 5

Example of classification

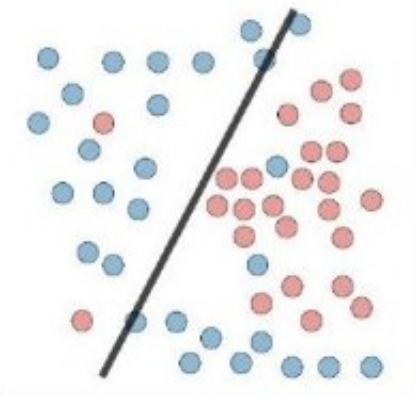
Which one is overfitting, underfitting, or just a good fit?



a)



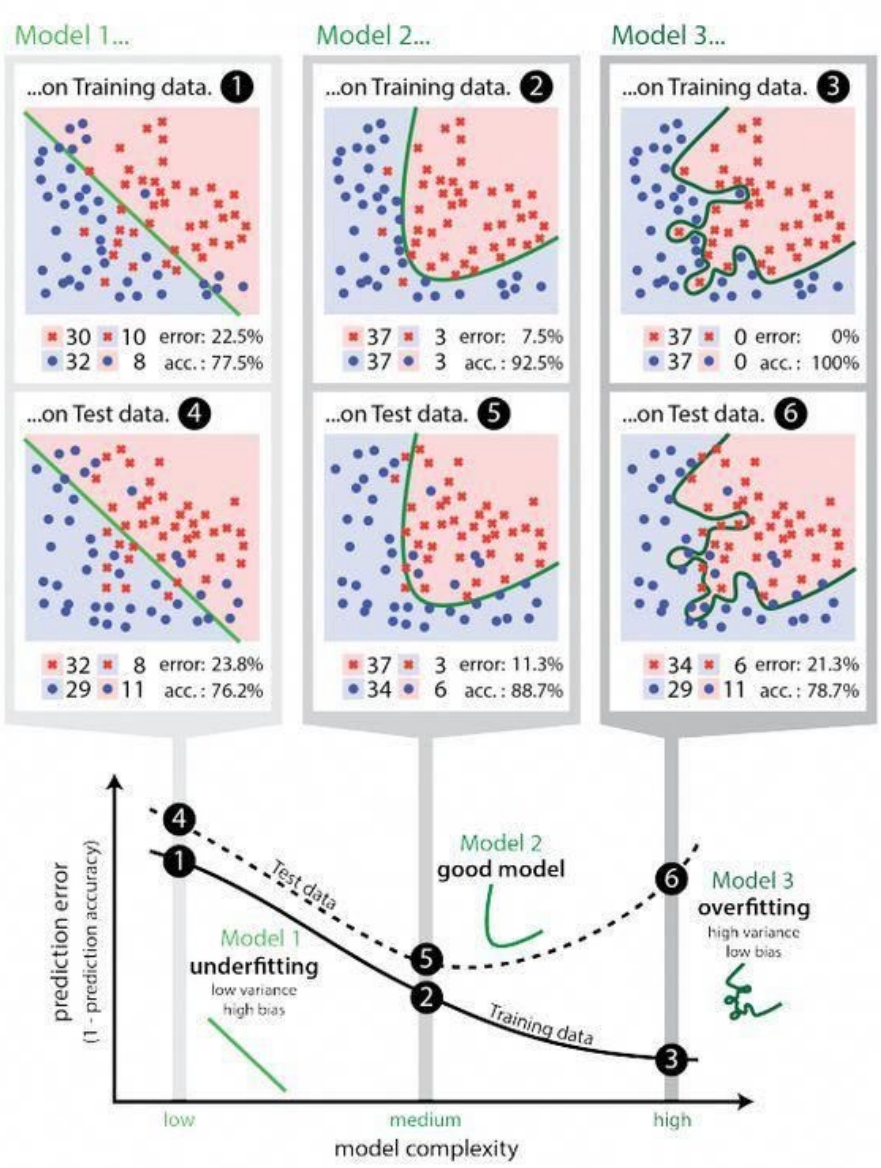
b)



c)

Source image.

Summary



Source image.

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Overview of the life cycle of ML project

ML project life cycle

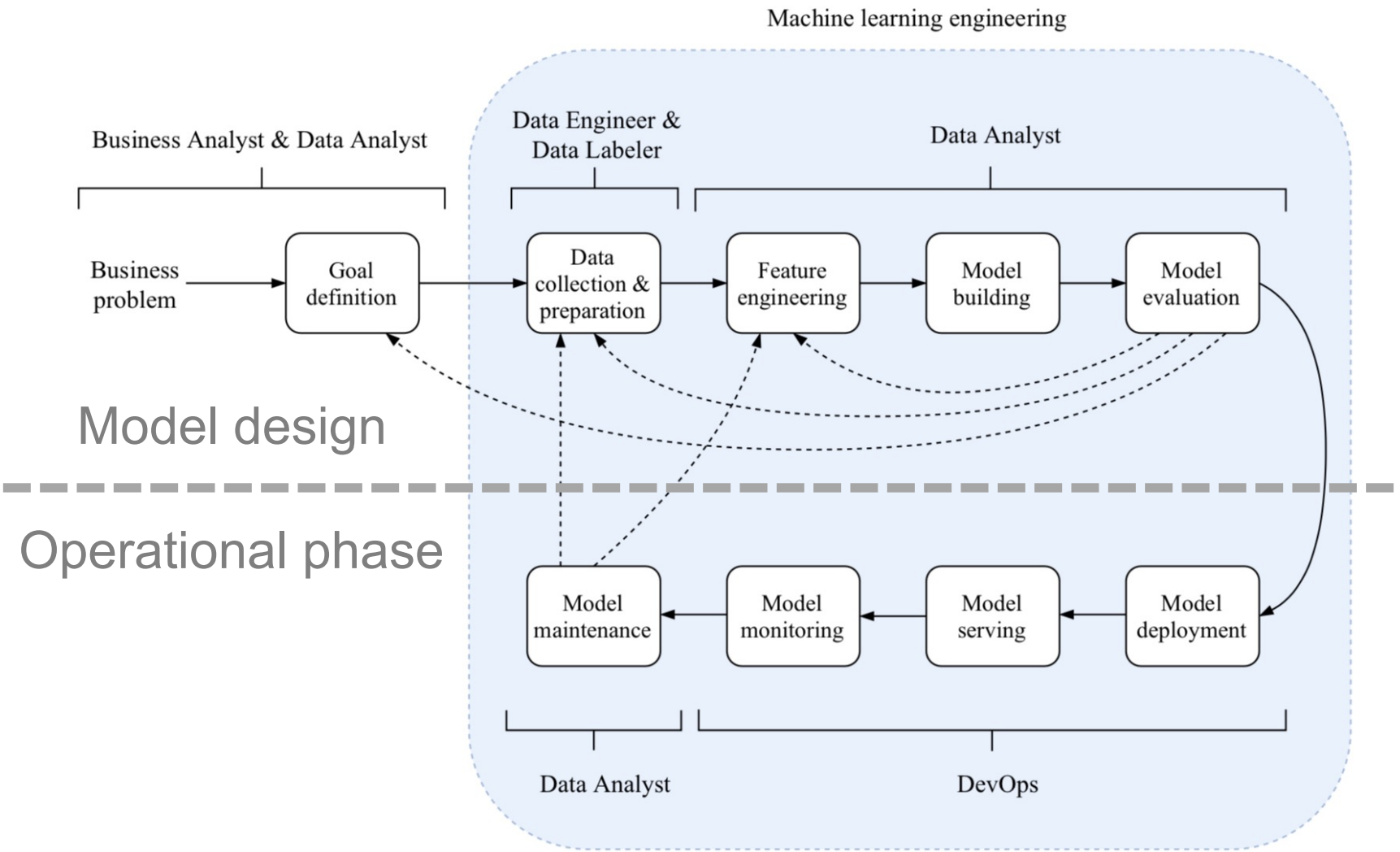


Figure 3: Machine learning project life cycle.

Source image:
A. Burkov, "Machine Learning Engineering".

ML project lifecycle

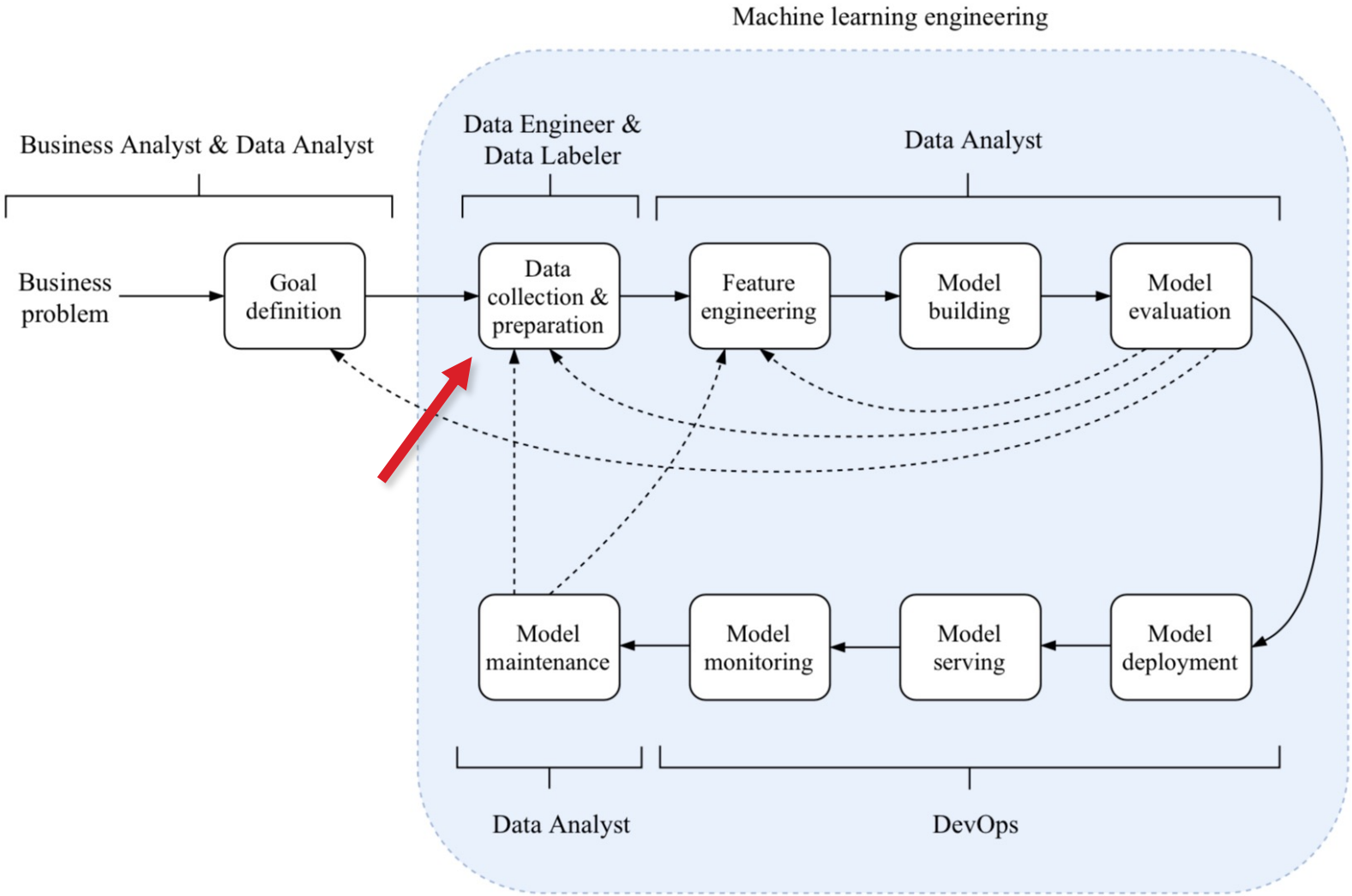


Figure 3: Machine learning project life cycle.

Source image:
A. Burkov, "Machine Learning Engineering".

Data collection & preparation

In industry: 80% building dataset, 20% playing with it

Steps:

- Existing data:
  - access to existing data (negotiation, paperwork, anonymization, etc.), database work, merging datasets, etc.
- Creating a dataset
  - ⚠ can be very long
  - collecting data, statistical sampling, scraping, survey, labelling data, etc.
- Data cleaning
  - Domain validity, outliers, errors, duplicates, expired data, etc.

Data collection & preparation

Advices

Think of **reproducibility** from the beginning

- you might have to extract the same data again in the future: bugs, adding features, update data, etc.
- avoid manual labor on data in Excel: error-prone & difficult to traceback

Always check raw data and processed data

- Don't trust your implementation
- Keep backups of both datasets

Don't assume that your data is valid

- Check domain validity (e.g. postal code, age)
- Properly encode missing values (e.g. "-1", "99999" → NaN)

ML project lifecycle

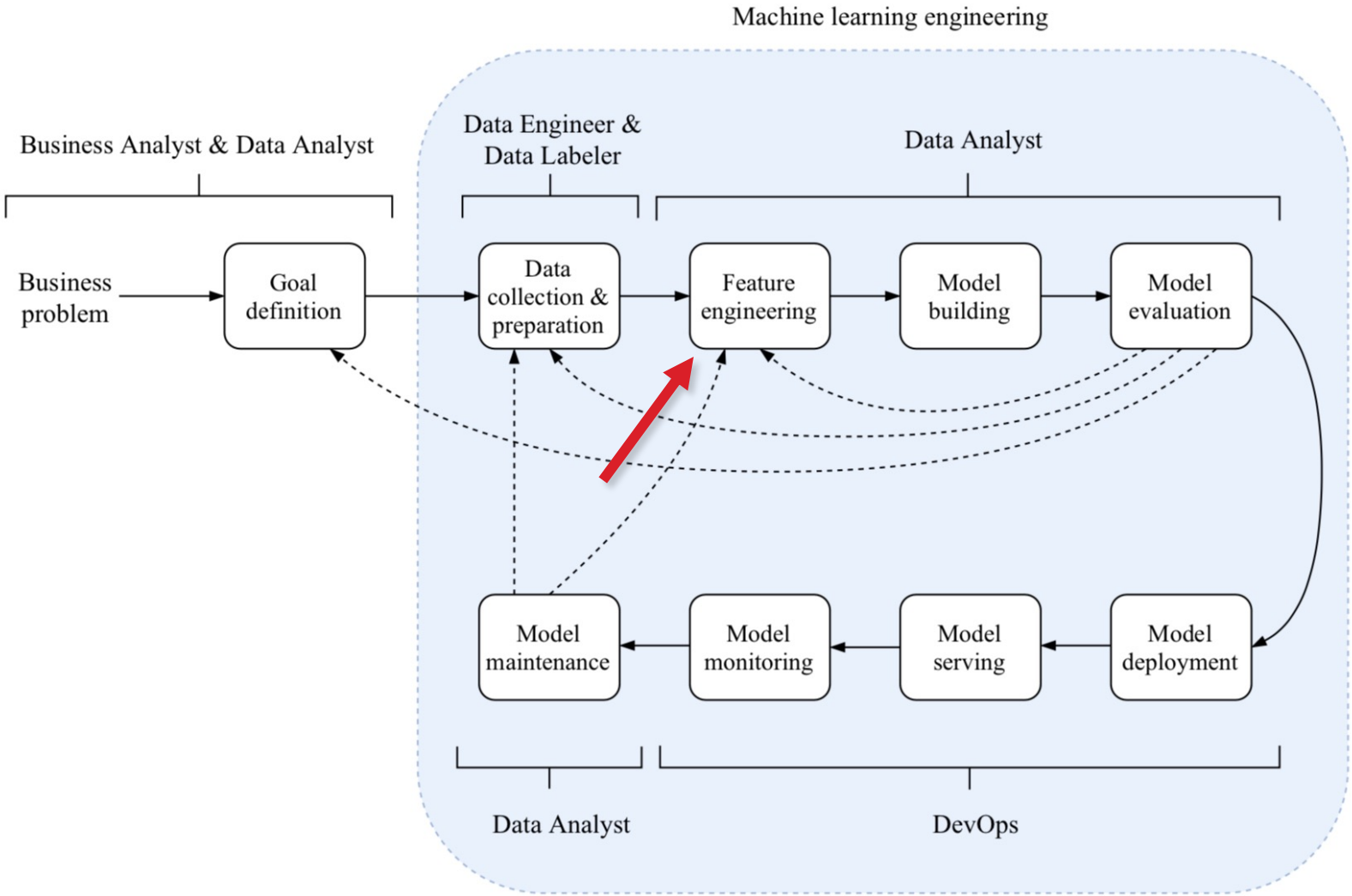


Figure 3: Machine learning project life cycle.

Source image:
A. Burkov, "Machine Learning Engineering".

Goal

Transform raw data into tidy data with numerical or categorical features

Example:

Plain text email → Frequencies of “$”, “!”, “#”, “viagra”, “buy”, “mail”, etc.
Average length of uninterrupted sequences of capital letters.
Etc.

Tidy data

Follow principles of **tidy data**

- 1 row ←→ 1 example
- 1 column ←→ 1 feature
- single dataset

Sources of messiness:

- Column headers are values, not variable names
- Multiple variables are stored in one column
- Variables are stored in both rows and columns
- Multiple types of experimental unit stored in the same table
- One type of experimental unit stored in multiple tables

Source content:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

Tidy data

	John Smith	Jane Doe	Mary Johnson
treatmenta	—	16	3
treatmentb	2	11	1

person	treatment	result
John Smith	a	—
Jane Doe	a	16
Mary Johnson	a	3
John Smith	b	2
Jane Doe	b	11
Mary Johnson	b	1

See more examples of bad practices:
https://www.jstatsoft.org/article/view/v059i10

Source images:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

Steps

1. Defining the features to represent well your examples
   - Usually involve domain experts
   - Document everything into a schema file (spreadsheet or Json with name, type, definition, missing values, source, etc.)

2. Implement their computation
   - reproducibility + checks
   - data manipulation: filter, transform, aggregate, sort

Summarizing data

You can compute **mean & standard deviation** for each feature to aggregate

Example of Churn Analysis

User

User ID	Gender	Age	...	Date Subscribed
1	M	18	...	2016-01-12
2	F	25	...	2017-08-23
3	F	28	...	2019-12-19
4	M	19	...	2019-12-18
5	F	21	...	2016-11-30

Order

Order ID	User ID	Amount	...	Order Date
1	2	23	...	2017-09-13
2	4	18	...	2018-11-23
3	2	7.5	...	2019-12-19
4	2	8.3	...	2016-11-30

Call

Call ID	User ID	Call Duration	...	Call Date
1	4	55	...	2016-01-12
2	2	235	...	2016-01-13
3	3	476	...	2016-12-17
4	4	334	...	2019-12-19
5	4	14	...	2016-11-30

Figure 24: Relational data for churn analysis.

User features

User ID	Gender	Age	Mean Order Amount	Std Dev Order Amount	Mean Call Duration	Std Dev Call Duration
2	F	25	12.9	7.1	235	0
4	M	19	18	0	134.3	142.7

Figure 25: Synthetic features based on sample mean and standard deviation.

Steps

3. Encoding categorical features
   - Models accept **only numerical** values
   - Categorial features should be encoded as integers (**one-hot encoded**):
     - “male”, “female”, “female” → 0, 1, 1
     - “bachelor”, “master”, “bachelor”, “high school”, “master” →

0	1	0
0	0	1
0	1	0
1	0	0
0	0	1

4. Discretization of continuous variable *(optional):*
   - Age: 8, 65, 42, 15 → “-18”, “50+”, “18-50”, “-18” →

1	0	0
0	0	1
0	1	0
1	0	0

Steps

4. **Missing data treatment**
   - Most models don't accept missing data
   - Solutions: imputation, categorization, etc.

5. **Data Normalization of continuous features**
   - I.e. mean removal and variance scaling
   - Almost all models performs better with normalized data

6. Other features transformation
   - E.g, polynomial features: (X_1, X_2) to $(1, X_1, X_2, X_1^2, X_1X_2, X_2^2)$

Practical advices

Informative features (high predictive power)

- Constant data are useless
- Totally unrelated features are not useful
- Duplicated features are not useful (e.g. weight in kg and in pounds)

Always check the presence of missing data

Use all data analysis tools to help you

- descriptive statistics (mean, standard deviation, min, max, quantiles, absolute and relative frequencies, etc.), data visualization, etc.

Use small sample to develop and debug

- Unit test for each data extractor

Quiz

ML or not ML

Cost to increase accuracy

In general, the cost to train a model (ie. developers' time + computational needs) grows linearly with its accuracy

- True
- False

Cross-validation

We want to predict the GDP of countries from its economics caracteristics.
We collect these variables for each year since 1900 and each countries.
We shuffle all the data, keep-out 20% for the test set, and train a time-series model on the 80%.

What are the issues with this model?

Is it tidy data?

country	year	m014	m1524	m2534	m3544	m4554	m5564	m65	mu	f014
AD	2000	0	0	1	0	0	0	0	—	—
AE	2000	2	4	4	6	5	12	10	—	3
AF	2000	52	228	183	149	129	94	80	—	93
AG	2000	0	0	0	0	0	0	1	—	1
AL	2000	2	19	21	14	24	19	16	—	3
AM	2000	2	152	130	131	63	26	21	—	1
AN	2000	0	0	1	2	0	0	0	—	0
AO	2000	186	999	1003	912	482	312	194	—	247
AR	2000	97	278	594	402	419	368	330	—	121
AS	2000	—	—	—	—	1	1	—	—	—

Table 9: Original TB dataset. Corresponding to each 'm' column for males, there is also an 'f' column for females, `f1524`, `f2534` and so on. These are not shown to conserve space. Note the mixture of 0s and missing values (—). This is due to the data collection process and the distinction is important for this dataset.

Source images:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

Is it tidy data?

country	year	column	cases
AD	2000	m014	0
AD	2000	m1524	0
AD	2000	m2534	1
AD	2000	m3544	0
AD	2000	m4554	0
AD	2000	m5564	0
AD	2000	m65	0
AE	2000	m014	2
AE	2000	m1524	4
AE	2000	m2534	4
AE	2000	m3544	6
AE	2000	m4554	5
AE	2000	m5564	12
AE	2000	m65	10
AE	2000	f014	3

Is it tidy data?

country	year	column	cases
AD	2000	m014	0
AD	2000	m1524	0
AD	2000	m2534	1
AD	2000	m3544	0
AD	2000	m4554	0
AD	2000	m5564	0
AD	2000	m65	0
AE	2000	m014	2
AE	2000	m1524	4
AE	2000	m2534	4
AE	2000	m3544	6
AE	2000	m4554	5
AE	2000	m5564	12
AE	2000	m65	10
AE	2000	f014	3

(a) Molten data

country	year	sex	age	cases
AD	2000	m	0–14	0
AD	2000	m	15–24	0
AD	2000	m	25–34	1
AD	2000	m	35–44	0
AD	2000	m	45–54	0
AD	2000	m	55–64	0
AD	2000	m	65+	0
AE	2000	m	0–14	2
AE	2000	m	15–24	4
AE	2000	m	25–34	4
AE	2000	m	35–44	6
AE	2000	m	45–54	5
AE	2000	m	55–64	12
AE	2000	m	65+	10
AE	2000	f	0-14	3

(b) Tidy data

Table 10: Tidying the TB dataset requires first melting, and then splitting the `column` column into two variables: `sex` and `age`.

Source images:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

Is it tidy data?

id	year	month	element	d1	d2	d3	d4	d5	d6	d7	d8
MX17004	2010	1	tmax	—	—	—	—	—	—	—	—
MX17004	2010	1	tmin	—	—	—	—	—	—	—	—
MX17004	2010	2	tmax	—	27.3	24.1	—	—	—	—	—
MX17004	2010	2	tmin	—	14.4	14.4	—	—	—	—	—
MX17004	2010	3	tmax	—	—	—	—	32.1	—	—	—
MX17004	2010	3	tmin	—	—	—	—	14.2	—	—	—
MX17004	2010	4	tmax	—	—	—	—	—	—	—	—
MX17004	2010	4	tmin	—	—	—	—	—	—	—	—
MX17004	2010	5	tmax	—	—	—	—	—	—	—	—
MX17004	2010	5	tmin	—	—	—	—	—	—	—	—

Table 11: Original weather dataset. There is a column for each possible day in the month. Columns d9 to d31 have been omitted to conserve space.

Source images:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

Is it tidy data?

id	date	element	value
MX17004	2010-01-30	tmax	27.8
MX17004	2010-01-30	tmin	14.5
MX17004	2010-02-02	tmax	27.3
MX17004	2010-02-02	tmin	14.4
MX17004	2010-02-03	tmax	24.1
MX17004	2010-02-03	tmin	14.4
MX17004	2010-02-11	tmax	29.7
MX17004	2010-02-11	tmin	13.4
MX17004	2010-02-23	tmax	29.9
MX17004	2010-02-23	tmin	10.7

Is it tidy data?

id	date	element	value
MX17004	2010-01-30	tmax	27.8
MX17004	2010-01-30	tmin	14.5
MX17004	2010-02-02	tmax	27.3
MX17004	2010-02-02	tmin	14.4
MX17004	2010-02-03	tmax	24.1
MX17004	2010-02-03	tmin	14.4
MX17004	2010-02-11	tmax	29.7
MX17004	2010-02-11	tmin	13.4
MX17004	2010-02-23	tmax	29.9
MX17004	2010-02-23	tmin	10.7

(a) Molten data

id	date	tmax	tmin
MX17004	2010-01-30	27.8	14.5
MX17004	2010-02-02	27.3	14.4
MX17004	2010-02-03	24.1	14.4
MX17004	2010-02-11	29.7	13.4
MX17004	2010-02-23	29.9	10.7
MX17004	2010-03-05	32.1	14.2
MX17004	2010-03-10	34.5	16.8
MX17004	2010-03-16	31.1	17.6
MX17004	2010-04-27	36.3	16.7
MX17004	2010-05-27	33.2	18.2

(b) Tidy data

Table 12: (a) Molten weather dataset. This is almost tidy, but instead of values, the `element` column contains names of variables. Missing values are dropped to conserve space. (b) Tidy weather dataset. Each row represents the meteorological measurements for a single day. There are two measured variables, minimum (`tmin`) and maximum (`tmax`) temperature; all other variables are fixed.

Source images:
Wickham, H. (2014). Tidy Data. Journal of Statistical Software, 59(10)

ML project lifecycle

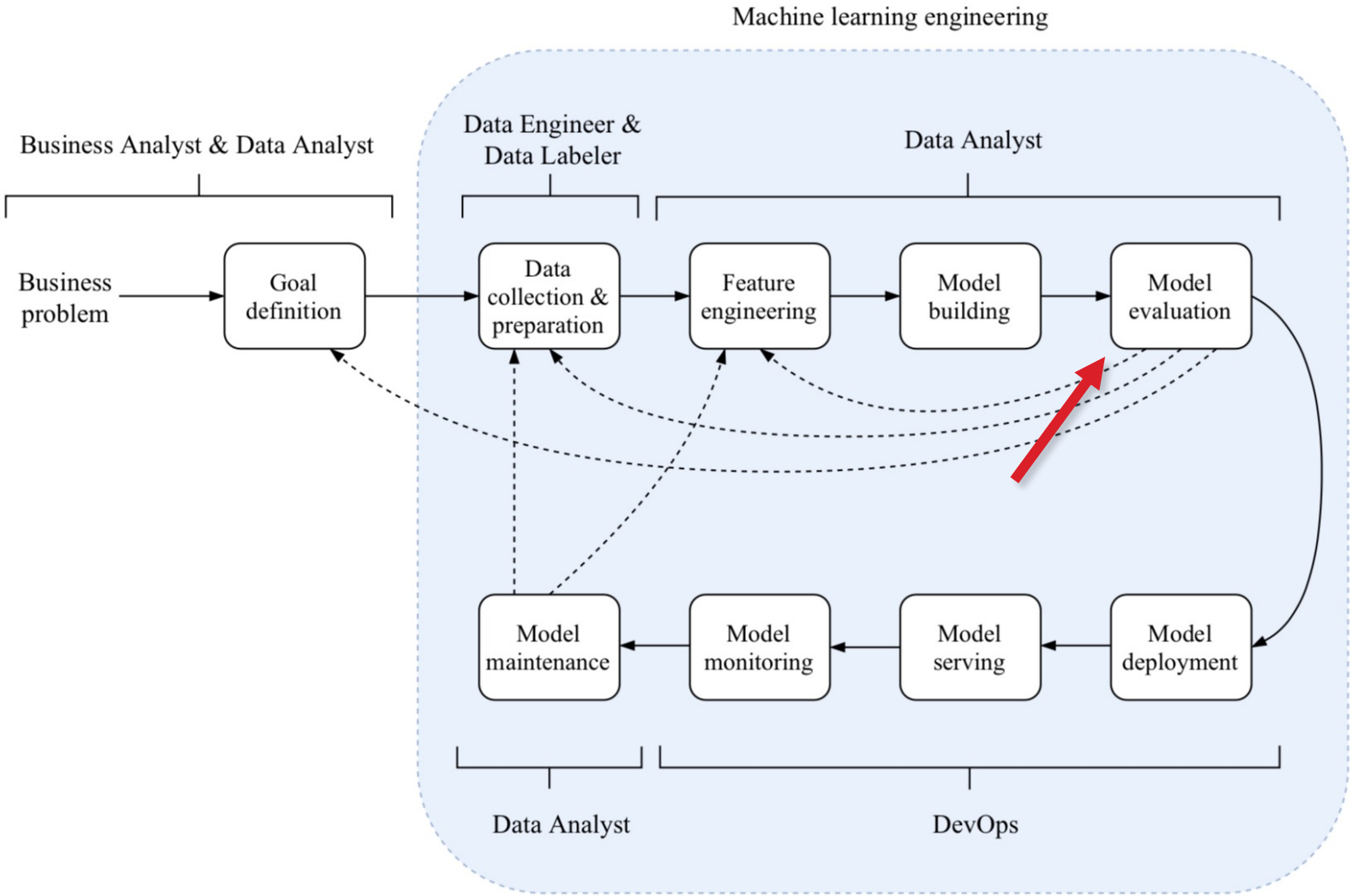


Figure 3: Machine learning project life cycle.

Source image:
A. Burkov, "Machine Learning Engineering".

Overfitting ⚠

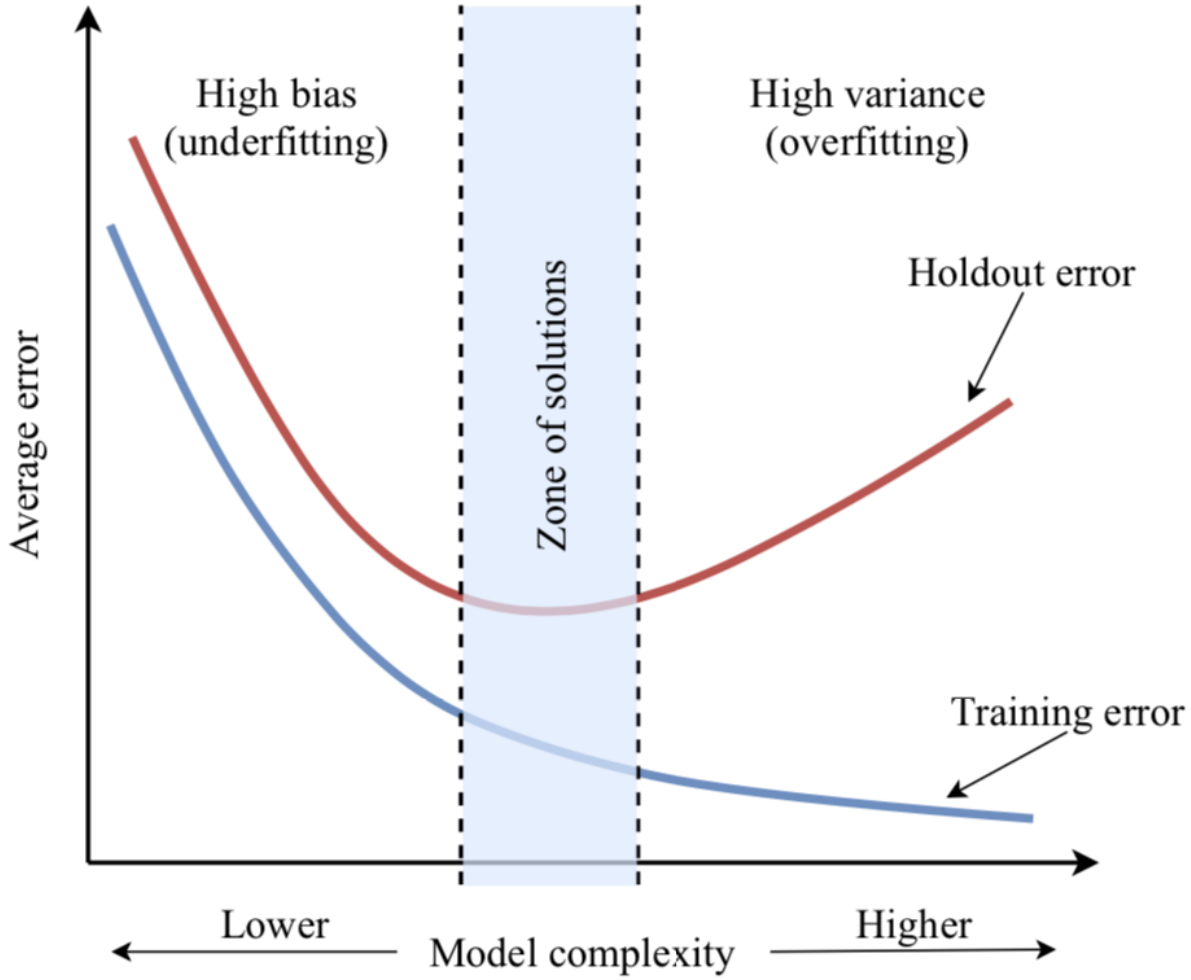
Always use **Cross-Validation!**

- Split them into 3 distinct sets:
  1. Training set → for model training
  2. Validation set → for tuning hyperparamers & choosing models
  3. Test set → for independent evaluation of your final model
- Good practice: split before at the beginning of data preparation step
- How to split?
  - Random subsets if examples are independent.
  - Use more complex splits if examples are dependent, e.g., time series

Extreme case:

- Your model simply memorizes its training examples but returns random labels for new examples.
- Need to evaluate on “unseen” examples.

Detecting Underfitting / Overfitting



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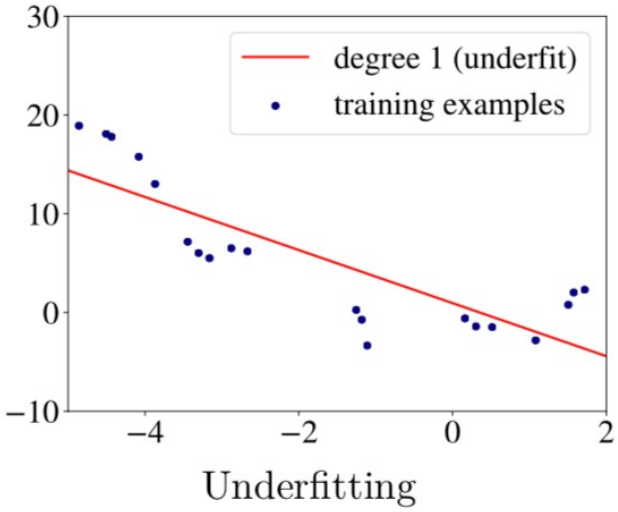
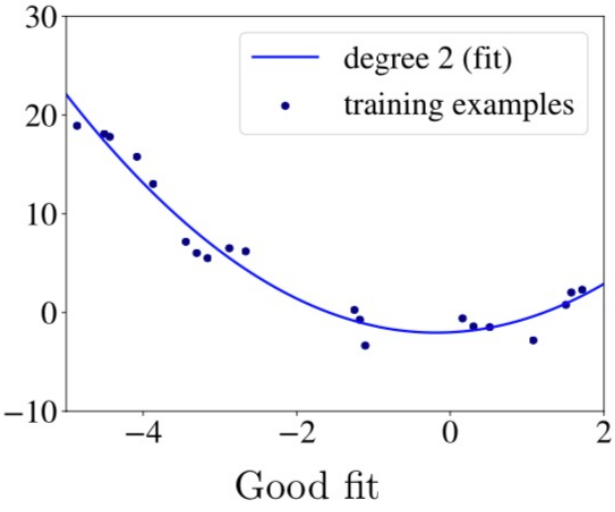
Detecting Underfitting / Overfitting

Example of Regression



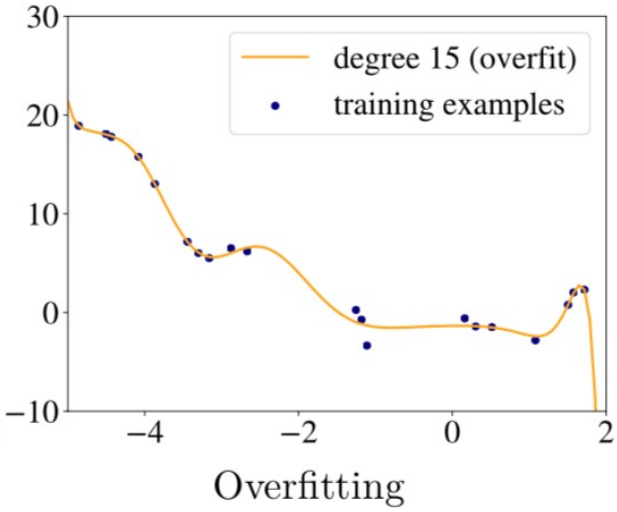
Underfitting

Oversimplification of the data



Good fit

Learning the true signal



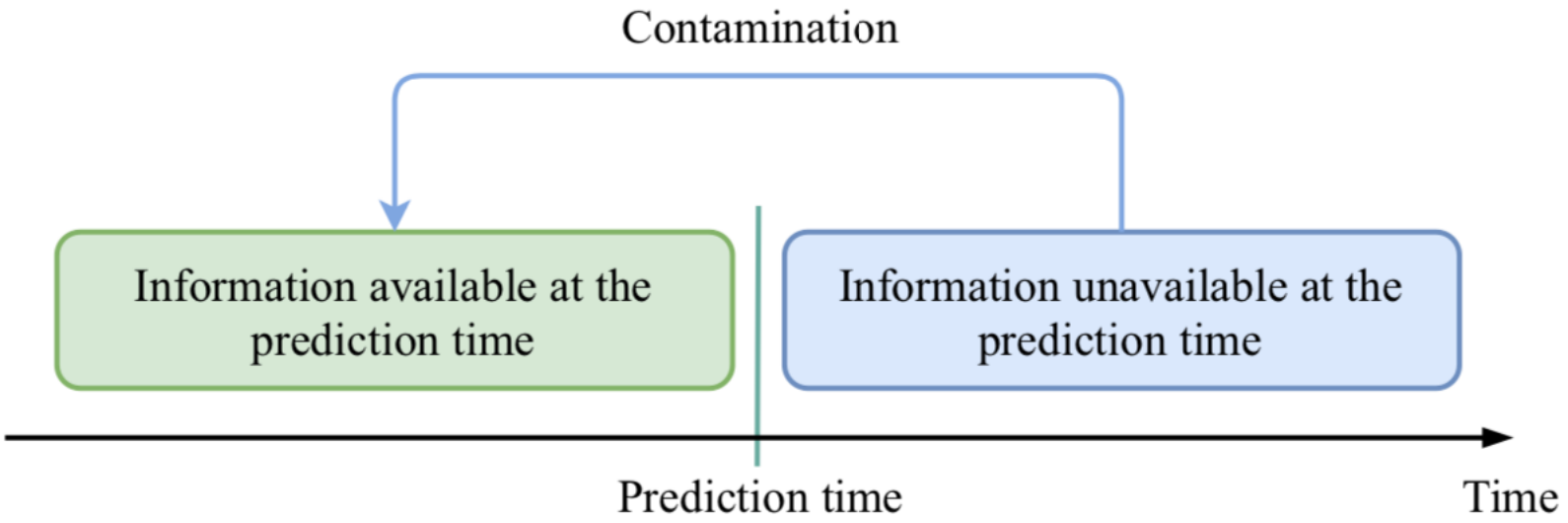
Overfitting

Fitting the noise of the data

Source image:
A. Burkov, “Machine Learning Engineering”.

Data Leakage

Be careful to **data leakage** if your examples are not independent



Source image:
A. Burkov, "Machine Learning Engineering".

Model evaluation

Choose an appropriate metric for your problem

- Report it computed on the test set
- Baseline:
  - performance of the simplest algorithm, usually random labelling
  - human performance

Be careful to class imbalance problem

- Consider credit card fraud detection
- Probably have 1% of fraud among all transactions
- Accuracy isn't appropriate metric here: you can achieve 99% accuracy, just by classifying all transactions as genuine, which has 0 practical use
- In that case, metrics