Applied Machine Learning

Brooks Paige

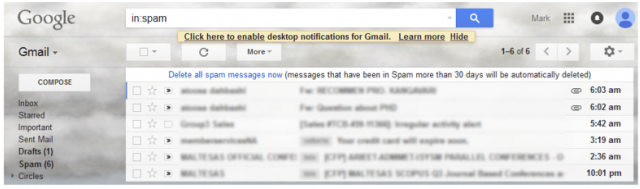
Week 1

What is applied machine learning?

- Not "theory" — asymptotic behavior, PAC bounds, ...
- Often:
  - how can we apply existing methods to new problems?
  - how can we scale existing (simple) methods to large data?
- How is ML used in industry? (When is ML not used?)
- What happens after a ML model is deployed in the "real world"?

What are machine learning applications?

- Spam filtering:



- Product recommendations:

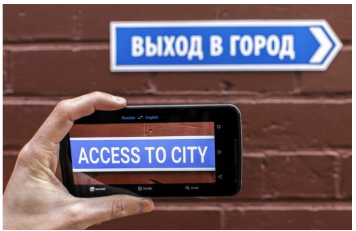
- Credit card fraud detection

Examples from https://www.cs.ubc.ca/~fwood/CS340/

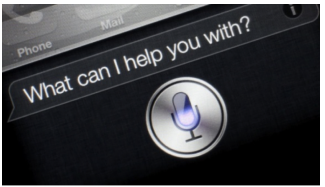
What are machine learning applications?

Motion capture:

Character recognition and machine translation:

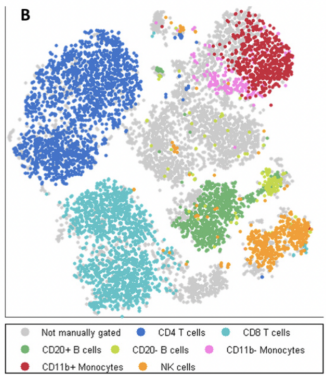


Voice recognition:

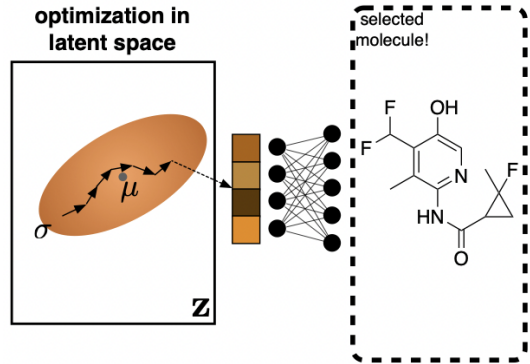


What are machine learning applications?

Identifying new cancer subtypes:



Developing new drugs:



Images: Amir et al. 2013; Bradshaw et al. 2019

Applied machine learning, bird's eye view

1. Collect data.
2. Fancy machine learning!
3. Profit?

Applied machine learning in practice

1. Learn about the domain / application
2. Identify an appropriate task
3. **Collect data**
4. Clean and preprocess data
5. Transform data or select useful features
6. Choose an appropriate method
7. **Fancy machine learning!**
8. Evaluate, visualize, and interpret results
9. **Profit?**

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Also, typically you'll go through **repeated cycles of these steps** ...

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9. **Profit?** (. . . and **monitor performance after deployment**)

Learn about the domain and identify a task

. . . Lots of work to do before collecting any data!

- For all of those example applications, the first step was to **identify a problem** that can be **solved with data**.

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- **This is hard.** (MSc students will experience this challenge a bit in narrowing down a thesis project!)

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- For all of those example applications, the first step was to **identify a problem** that can be **solved with data**.
- **This is hard.** (MSc students will experience this challenge a bit in narrowing down a thesis project!)
- In this module, we typically assume that the data already exists, in some form, and that we have a clearly defined task.
  - In real world or industry settings, this might actually be a lot of the work!

What is data?

What is data?

Most data comes in a **data frame** like the one on the right.

- Columns are per-instance attributes:
  - e.g. age, height, eye color, column ID, ...
  - Also called: feature, variable, field, ...
- Rows are instances
  - Also called: object, data point, sample, ...

Several steps before $\mathbf{X} \in \mathbb{R}^{N \times P}$...!

Attributes

Objects

Tid	Refund	Marital Status	Taxable Income	Cheat
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Table from Tan, Steinbach, Kumar, "Introduction to Data Mining"

Data types

- Numerical (real-valued)
- Categorical
- Ordinal
- Dates and times
- Coordinates (geospatial...)
- Text
- Unique identifiers
- Images, video, audio, ...

Numerical feature pre-processing

Pre-processing

- Scaling and centering (whitening)
- Rank tranformation
- Clipping
- Non-linear transformations (e.g. $\log$ or $\sqrt{\ldots}$)

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To consider: What machine learning models are sensitive to scaling? (What ones are not?)

Numerical feature pre-processing

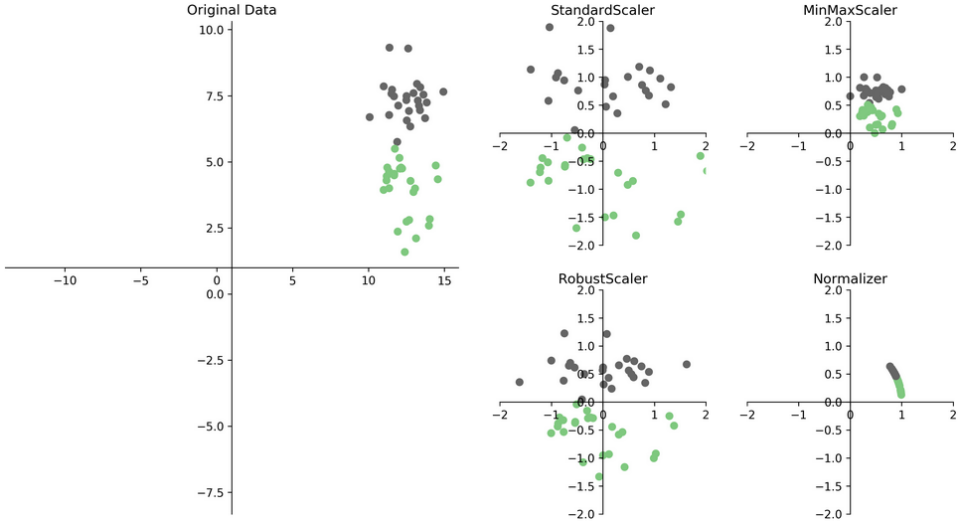
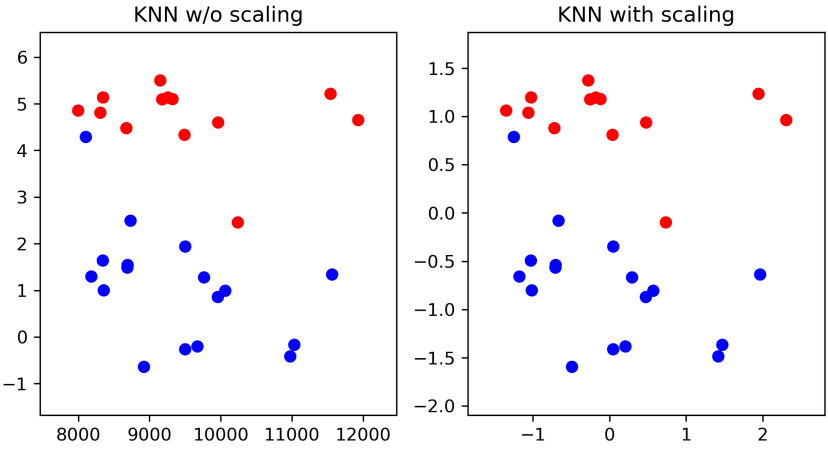


Figure: Andreas Müeller

Numerical feature pre-processing



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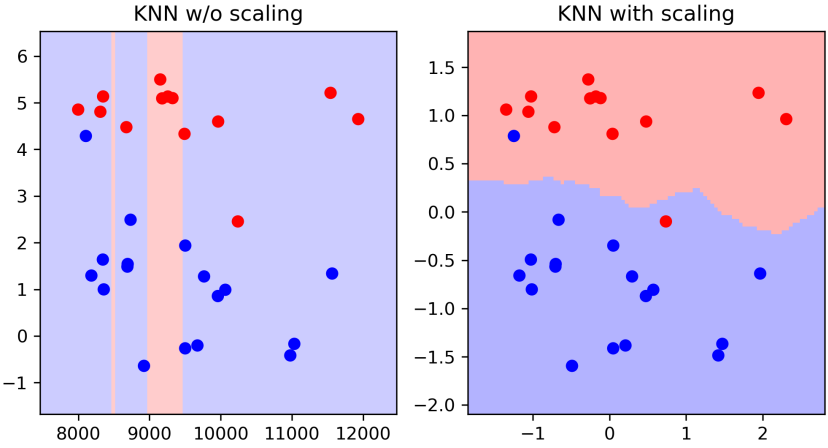

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Numerical feature pre-processing

Other thoughts:

- Be careful if scaling or centering **sparse** data!
- Fixed transforms are useful for addressing assumptions about domains, e.g.

$$\log(x) : \mathbb{R}^+ \to \mathbb{R}$$

$$\text{logit}(x) : [0, 1] \to \mathbb{R} \qquad \left(\text{logit}(x) \equiv \log \frac{x}{1 - x} \right)$$

- Sometimes helps with normality assumptions as well ...

Categorical feature pre-processing

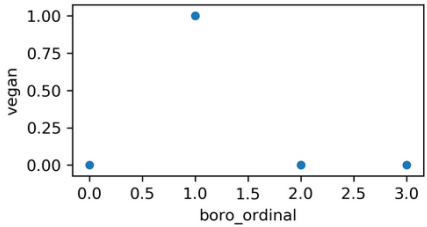
- One-hot encoding
- Label encoding
- Frequency encoding
- Target encoding
- Learn embeddings

	boro	salary	vegan
0	Manhattan	103	No
1	Queens	89	No
2	Manhattan	142	No
3	Brooklyn	54	Yes
4	Brooklyn	63	Yes
5	Bronx	219	No

Example: Andreas Müller

Categorical feature pre-processing

	boro	salary	vegan
0	2	103	No
1	3	89	No
2	2	142	No
3	1	54	Yes
4	1	63	Yes
5	0	219	No



Label or **ordinal** encoding — makes sense if there really is a natural order...

Categorical feature pre-processing

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	salary	vegan	boro_Bronx	boro_Brooklyn	boro_Manhattan	boro_Queens
0	103	No	0	0	1	0
1	89	No	0	0	0	1
2	142	No	0	0	1	0
3	54	Yes	0	1	0	0
4	63	Yes	0	1	0	0
5	219	No	1	0	0	0

One-hot or **dummy variable** encoding

Categorical feature pre-processing

Other ideas:

- **mean** encodings replace the categorical variable with some other statistic, e.g. the mean of the target variable
  - ...many potential pitfalls
- **Frequency** (or count) encodings record how often a particular value occurs
  - ...e.g. "Bag-of-words" representations for text
  - We'll come back to this later in the module
- Learned encodings / **embedding layers** in neural networks map each discrete value onto a vector in $\mathbb{R}^D$
  - ...a good option if trained end-to-end with the rest of the model
  - common in NLP (e.g. word or character embeddings)

How do we learn from data?

The combination of some data and an aching desire for an answer does not ensure that a reasonable answer can be extracted from a given body of data.

– John Tukey

Central goal of machine learning

In machine learning, we care about the error on test data!

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In machine learning, we care about the error on test data!

This is different than the error on our **training** data.
Analogy to sitting an exam:

- Training error is the score on a practice exam
- Test error is the score on the real exam
- We want to do well on the **real** exam, not the practice one.

Memorizing the practice exam will produce a low training error.
Learning is necessary to also have a low test error!

Fitting a polynomial

8 data points,
M parameters:

$$f(x) = \sum_{i=1}^{M} \beta_i x^i$$

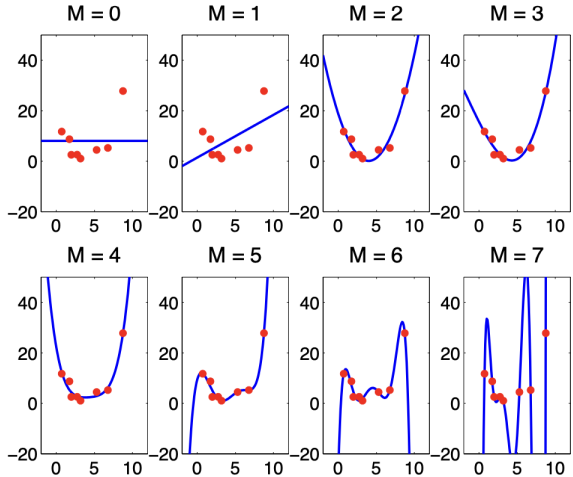

Figure: Zoubin Ghahramani

Why does machine learning work?

Fundamental assumption: **Test data is similar to training data**

- If the training data and test data are unrelated, then we can't learn anything
- Generalization requires assumptions!

Training error and generalization

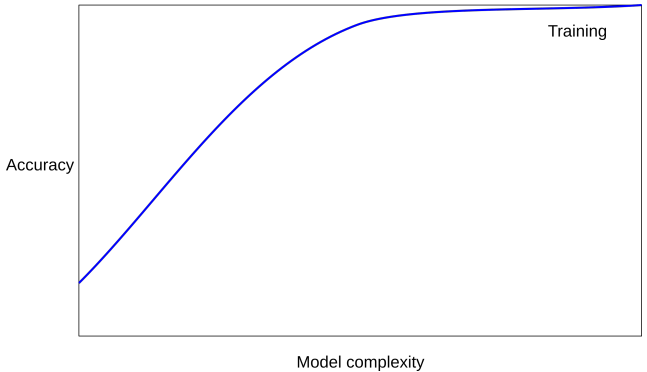

Figure: Andreas Müller

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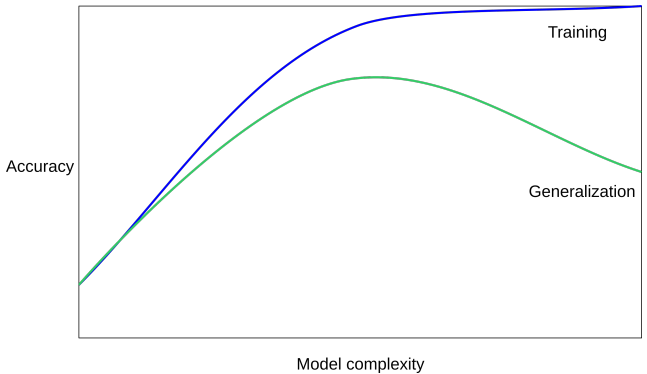

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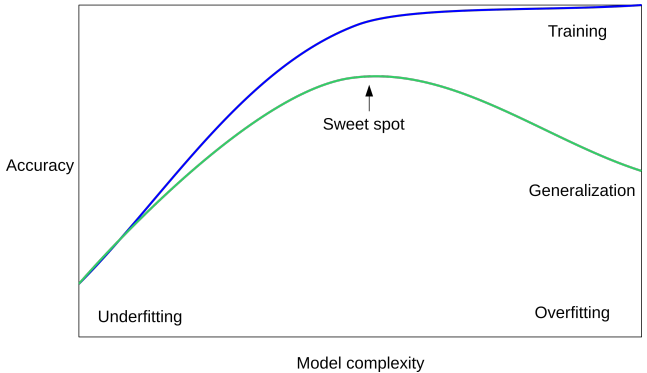
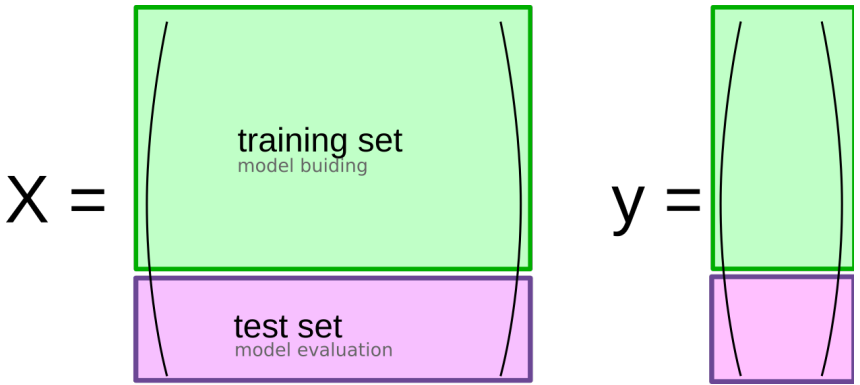


Figure: Andreas Müller

Don't overfit to the test set!



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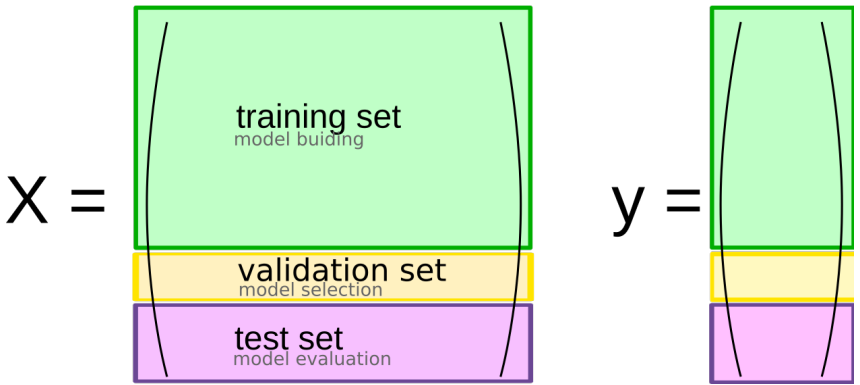

Figure: Andreas Müller

Cross-validation

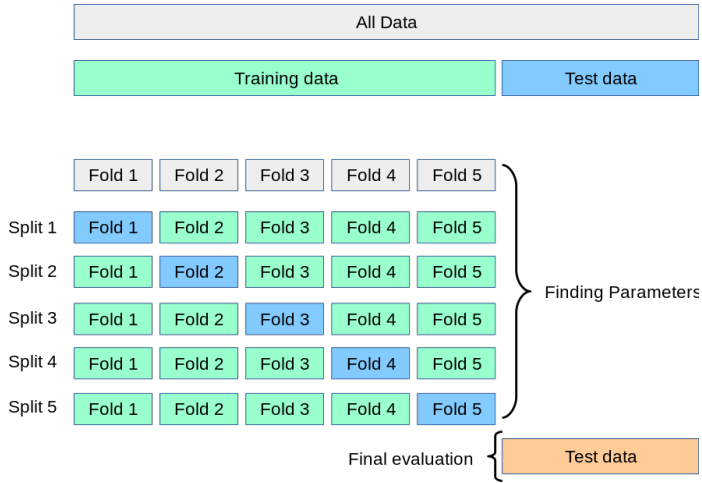

Figure: scikit-learn

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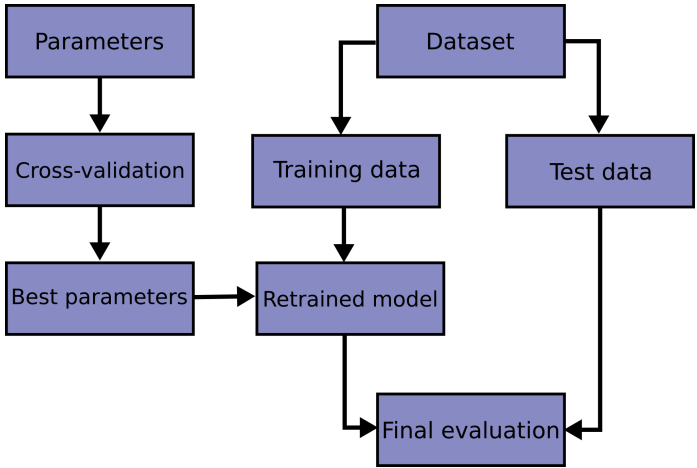

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Validation sets for non-iid data

Data is often not independent and identically distributed (*iid*)! A **random split** might not be appropriate.

- **Grouped data**: e.g. data collected from different cities, classrooms, etc, where we expect to see higher correlation within-group than between groups
  - **Stratified sampling** of cross-validation sets
- **Time-series data**: in a random split, you are effectively testing interpolation between points, instead of extrapolation into the future
  - Temporal splits ensure validation / testing only on held-out future data
  - **Careful:** more data than you think is actually time series data! Data is typically collected sequentially over a long period of time (even if you don't know it)

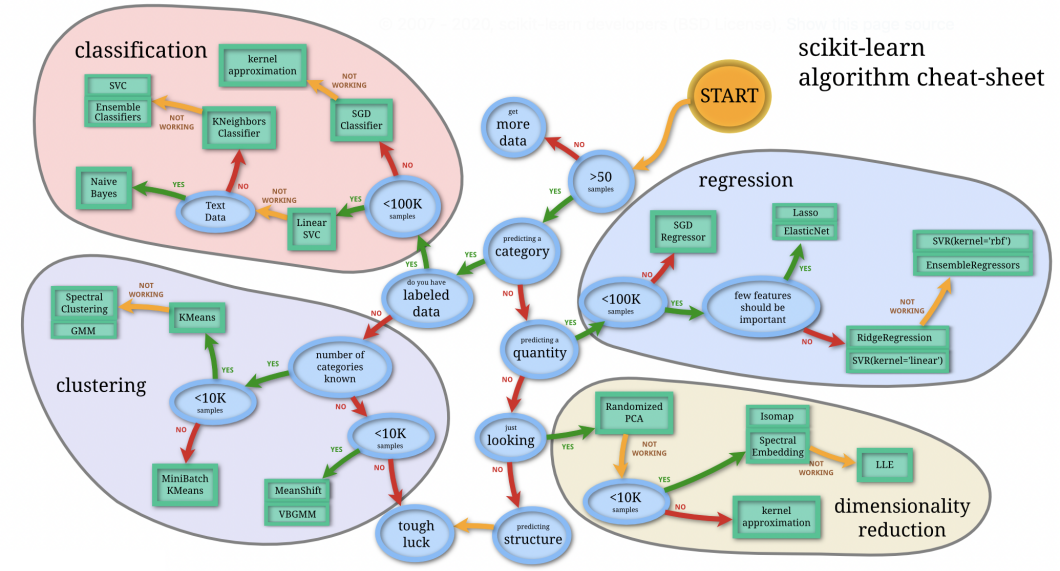
Pitfalls

Don't look at the test set!

- It's easy to accidentally look at the test set! Don't do it — you won't be able to trust your results
- Example: computing statistics for scaling transforms
- Example: visualizations and exploratory data analysis

Choosing a model

Machine learning as a bag of tricks



How much data do I need?

Two types of data sources

Cheap (infinite) data

Predict observable events

- Ad clicks
- Product recommendations
- Stock market
- House numbers
- Transcription autocorrect
- ...

Expensive data

Automate complex processes

- Medical diagnosis
- Drug trial
- Microchip design
- ...

Big data headaches

More data is not always better

- Is dealing with the large size worth the hassle? Data scientist / analyst time is expensive!
  - (can you get away with just using a subset that will fit in RAM?)

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- Is dealing with the large size worth the hassle? Data scientist / analyst time is expensive!
  - (can you get away with just using a subset that will fit in RAM?)
- Where did the data come from? Is it representative of future data?
- Would a smaller dataset of higher-quality data be more useful, or less useful?
  - (this can be situation dependent!)

Evaluation and metrics

Evaluation and metrics

(“did it work?”)

Metrics for classification

Accuracy: what fraction of examples are classified correctly?

$$\frac{1}{N}\sum_{i=1}^{N}\mathbb{I}[f(x_i) = y_i]$$

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- Hard predictions! Does not take into account uncertainty
- Can't be optimized with gradient-based methods
- Misleading for imbalanced classes

Metrics for classification

How do we choose a threshold value for "soft" classifiers?

- Suppose $f(x_i)$ returns some real-value (as opposed to a label $\hat{y}_i \in \{0, 1\}$).

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$$\hat{y}_i = \begin{cases} 1 & f(x_i) \geq c \\ 0 & f(x_i) < c \end{cases}$$

where c is a threshold or cutoff parameter.

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  where c is a threshold or cutoff parameter.
- Different values lead to different trade-offs between **false positives** and **false negatives**!

Understanding classifier performance

Two classes: positive and negative.

- **Precision**: "How many of those predicted positive are actually positive?"

$$\frac{\text{true positives}}{\text{true positives} + \text{false positives}}$$

- **Recall** or **sensitivity**: "How many of those which are actually positive are correctly predicted as positive?"

$$\frac{\text{true positives}}{\text{true positives} + \text{false negatives}}$$

- **Specificity**: "How many of those which are actually negative are correctly predicted as negative?"

$$\frac{\text{true negatives}}{\text{true negatives} + \text{false positives}}$$

Considering classifier trade-offs

Solution: look at the area under the curve (**AUC**)

- True positive vs false positive
- Precision vs recall
- ...

Exercise: think about how this is affected by class imbalance

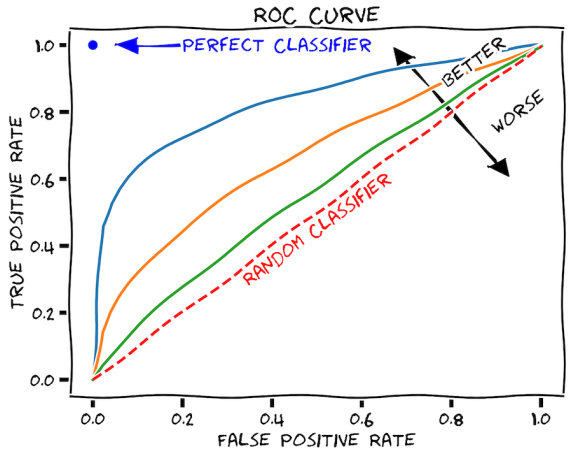

Figure: Martin Thoma

Classifier performance: log-loss

Maximum likelihood estimation:

- Define $f_\theta(x_i)$ which returns a value in the range $[0, 1]$
- Interpret this output as a probability $p(y_i = 1|x_i; \theta)$
- Optimize the parameters θ by maximizing the (log-)probability of the labels given the data:

$$\begin{aligned}\hat{\theta} &= \arg\max_\theta \sum_{i=1}^{N} \log p(y_i = 1|x_i; \theta) \\ &= \arg\max_\theta \sum_{i=1}^{N} y_i \log f_\theta(x_i) + (1 - y_i) \log(1 - f_\theta(x_i))\end{aligned}$$

This (with flipped sign) is also called **binary cross-entropy** loss.

Metrics for regression

Mean squared error (MSE):

$$\frac{1}{N}\sum_{i=1}^{N}(f(x_i) - y_i)^2$$

- Easy to optimize directly! (gradients, second-order methods)
- RMSE $= \sqrt{\text{MSE}}$
- Analogous to assuming normal-distributed errors
- Exercise: what is the best constant predictor?

Metrics for regression

Mean absolute error (MAE):

$$\frac{1}{N}\sum_{i=1}^{N}|f(x_i)-y_i|$$

- Also easy to optimize directly (though not by second-order methods)
- Less sensitive to outliers
- Analogous to assuming Laplace-distributed errors
- Exercise: what is the best constant predictor?

Also this week:

Mathematics refresher

Mathematics refresher

David Barber, *Bayesian Reasoning and Machine Learning* (BRML)

Online at `http://www.cs.ucl.ac.uk/staff/d.barber/brml/`

- Chapter 1 (Probabilistic reasoning)
- Appendix A (Background mathematics)
- Slides (from David) on Moodle

How (not) to do data science

1. there's no need to look at the data before running a model (the AI will handle it)
2. pick a model based on hype or social media mentions
3. don't worry about downstream tasks, users of the model, or what happens after deployment — just maximize "accuracy"
4. don't bother comparing performance against simple baselines