Lecture 1: Introduction

A few useful things to know about machine learning

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Why Machine Learning?

- Search engines (e.g. Google)
- Recommender systems (e.g. Netflix)
- Automatic translation (e.g. Google Translate)
- Speech understanding (e.g. Siri, Alexa)
- Game playing (e.g. AlphaGo)
- Self-driving cars
- Personalized medicine
- Progress in all sciences: Genetics, astronomy, chemistry, neurology, physics,...

What is Machine Learning?

- Learn to perform a task, based on experience (examples) X, minimizing error $\mathcal{E}$
  - E.g. recognizing a person in an image as accurately as possible
- Often, we want to learn a function (model) f with some model parameters θ that produces the right output y

$$f_{\theta}(X) = y$$

$$\underset{\theta}{\operatorname{argmin}} \mathcal{E}(f_{\theta}(X))$$

- Usually part of a *much* larger system that provides the data X in the right form
  - Data needs to be collected, cleaned, normalized, checked for data biases,...

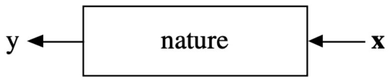
Inductive bias

- In practice, we have to put assumptions into the model: *inductive bias* b
    - What should the model look like?
        - Mimick human brain: Neural Networks
        - Logical combination of inputs: Decision trees, Linear models
        - Remember similar examples: Nearest Neighbors, SVMs
        - Probability distribution: Bayesian models
    - User-defined settings (hyperparameters)
        - E.g. depth of tree, network architecture
    - Assuptions about the data distribution, e.g. $X \sim N(\mu, \sigma)$
- We can *transfer* knowledge from previous tasks: $f_1, f_2, f_3, ... \Longrightarrow f_{new}$
    - Choose the right model, hyperparameters
    - Reuse previously learned values for model parameters θ
- In short:

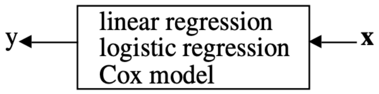
$$\underset{\theta,b}{\operatorname{argmin}} \mathcal{E}(f_{\theta,b}(X))$$

Machine learning vs Statistics

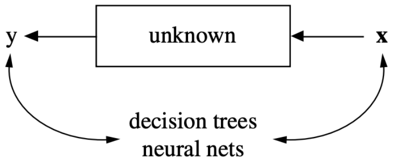
- See Breiman (2001): Statistical modelling: The two cultures
- Both aim to make predictions of natural phenomena:



- Statistics:
  - Help humans understand the world
  - Assume data is generated according to an understandable model



- Machine learning:
  - Automate a task entirely (partially *replace* the human)
  - Assume that the data generation process is unknown
  - Engineering-oriented, less (too little?) mathematical theory



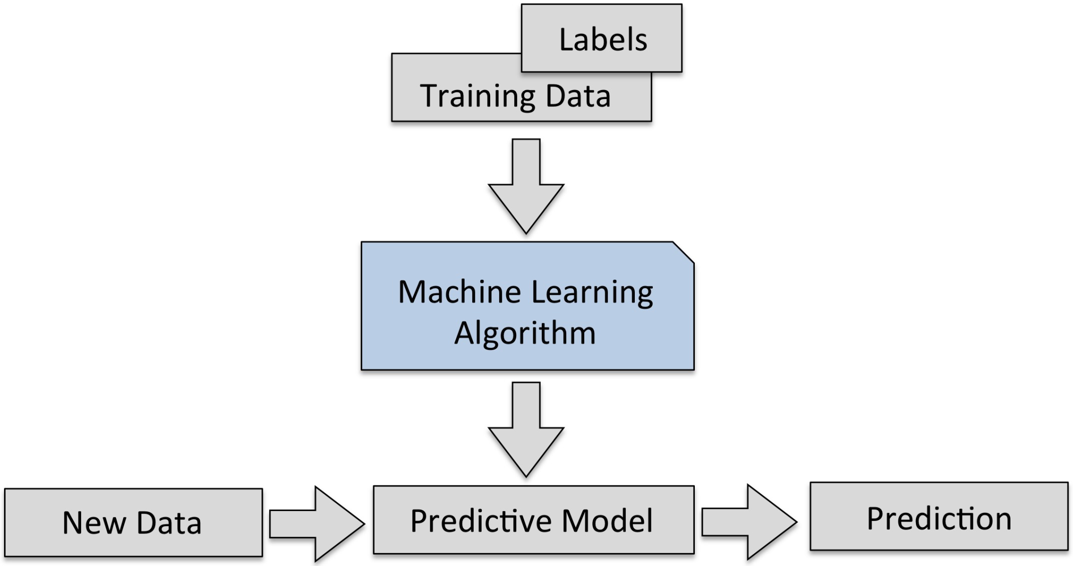
Types of machine learning

- **Supervised Learning**: learn a *model* f from *labeled data* (X, y) (ground truth)
    - Given a new input *X*, predict the right output *y*
    - Given examples of stars and galaxies, identify new objects in the sky
- **Unsupervised Learning**: explore the structure of the data (X) to extract meaningful information
    - Given inputs *X*, find which ones are special, similar, anomalous, ...
- **Semi-Supervised Learning**: learn a model from (few) labeled and (many) unlabeled examples
    - Unlabeled examples add information about which new examples are likely to occur
- **Reinforcement Learning**: develop an agent that improves its performance based on interactions with the environment

Note: Practical ML systems can combine many types in one system.

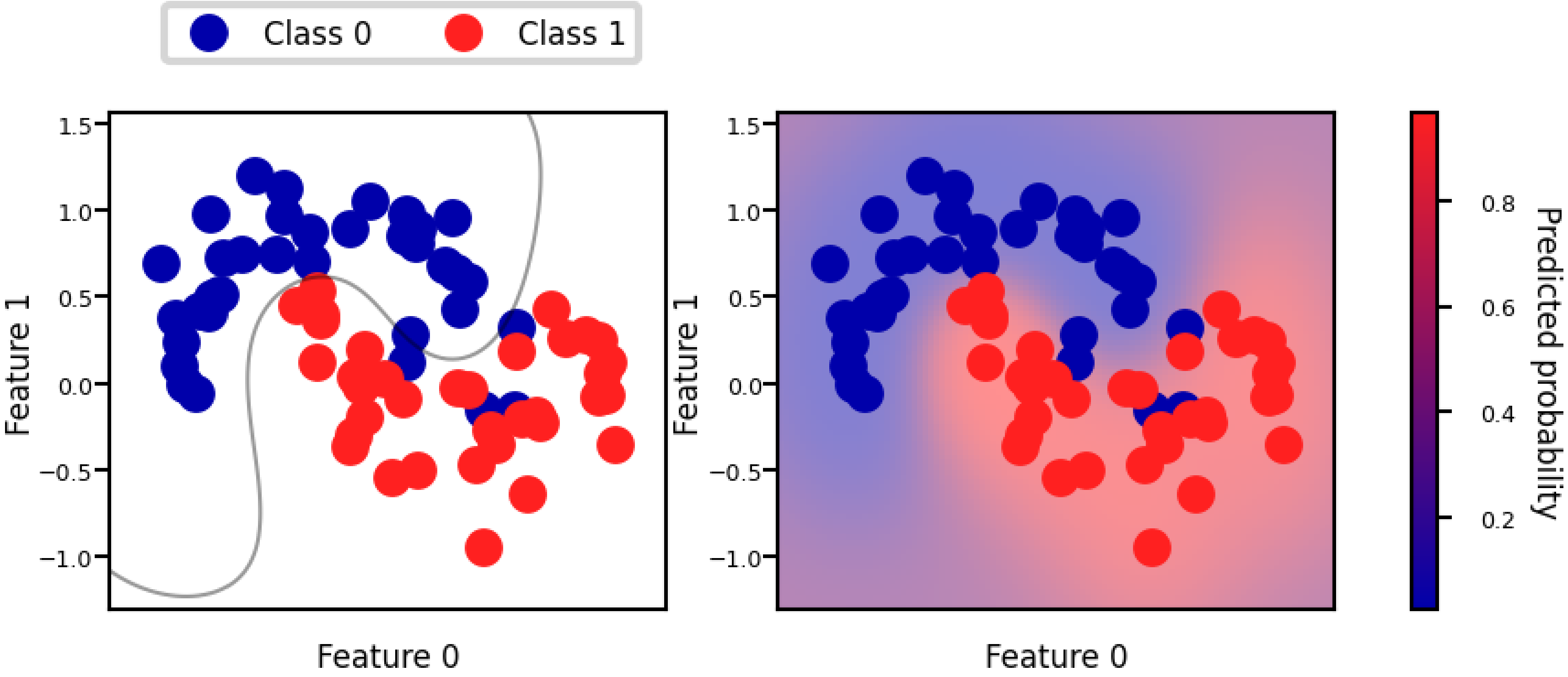
Supervised Machine Learning

- Learn a model from labeled training data, then make predictions
- Supervised: we know the correct/desired outcome (label)
- Subtypes: *classification* (predict a class) and *regression* (predict a numeric value)
- Most supervised algorithms that we will see can do both



Classification

- Predict a *class label* (category), discrete and unordered
    - Can be *binary* (e.g. spam/not spam) or *multi-class* (e.g. letter recognition)
    - Many classifiers can return a *confidence* per class
- The predictions of the model yield a *decision boundary* separating the classes

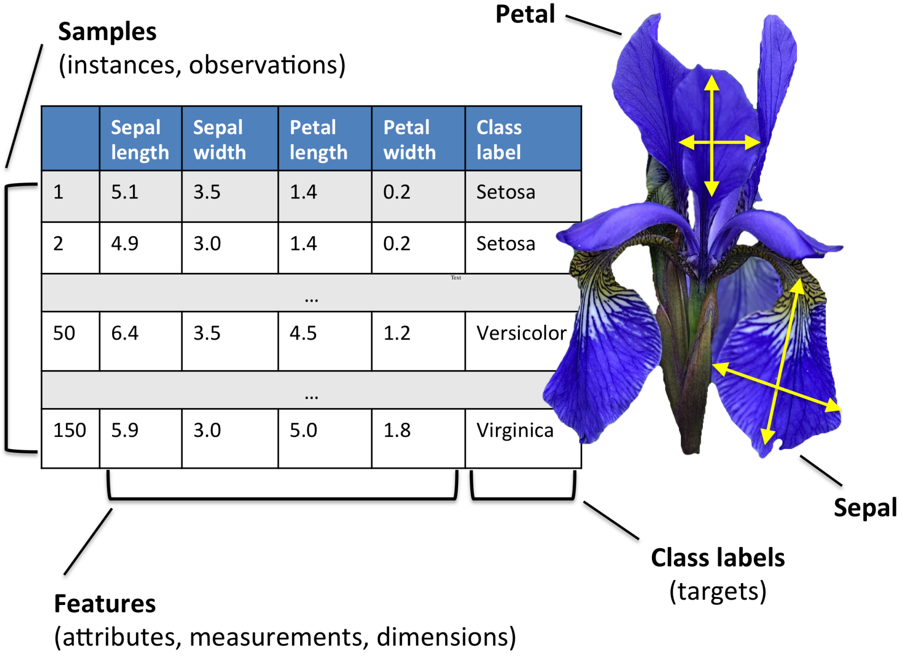


Example: Flower classification

Classify types of Iris flowers (setosa, versicolor, or virginica). How would you do it?

Representation: input features and labels

- We could take pictures and use them (pixel values) as inputs (-> Deep Learning)
- We can manually define a number of input features (variables), e.g. length and width of leaves
- Every `example' is a point in a (possibly high-dimensional) space



Samples
(instances, observations)

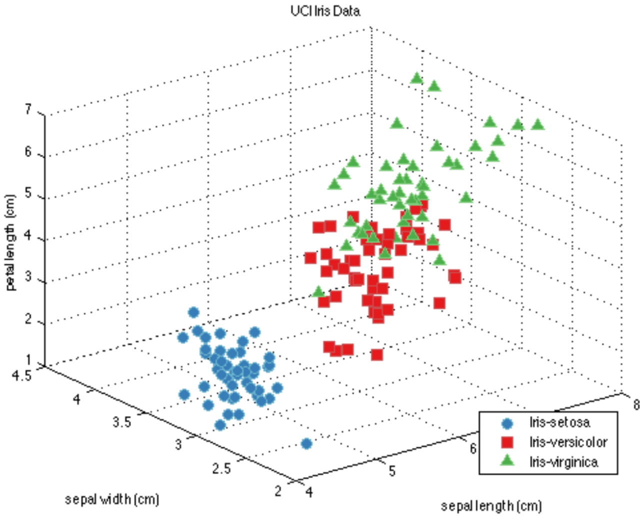
Petal

	Sepal length	Sepal width	Petal length	Petal width	Class label
1	5.1	3.5	1.4	0.2	Setosa
2	4.9	3.0	1.4	0.2	Setosa
			…		
50	6.4	3.5	4.5	1.2	Versicolor
			…		
150	5.9	3.0	5.0	1.8	Virginica

Sepal

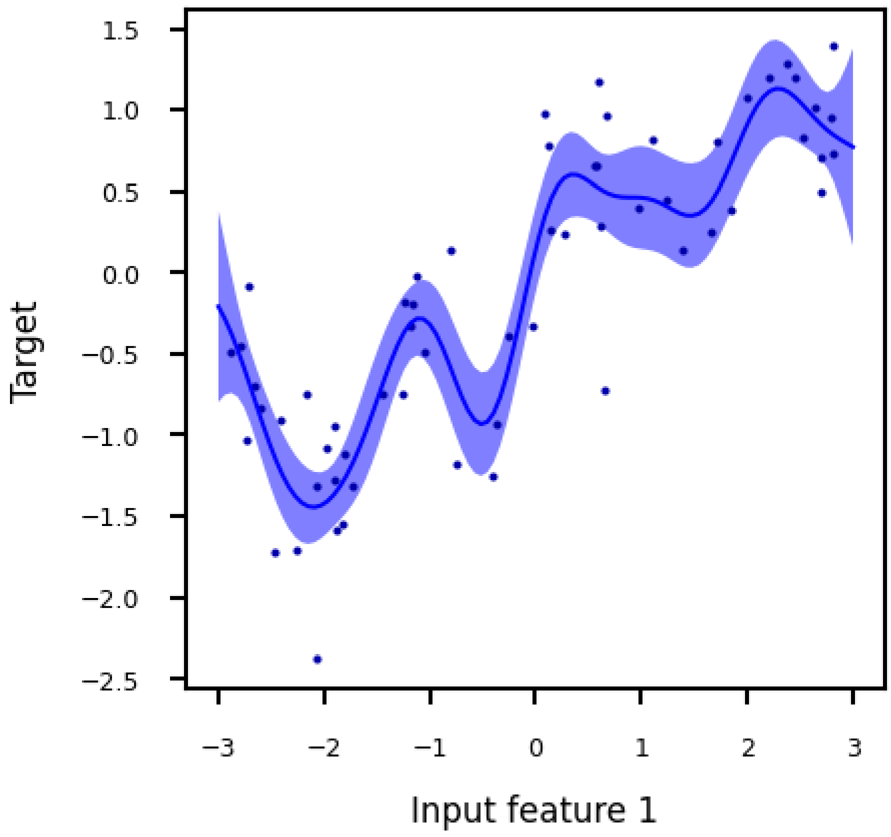
Features
(attributes, measurements, dimensions)

Class labels
(targets)



Regression

- Predict a continuous value, e.g. temperature
    - Target variable is numeric
    - Some algorithms can return a *confidence interval*
- Find the relationship between predictors and the target.

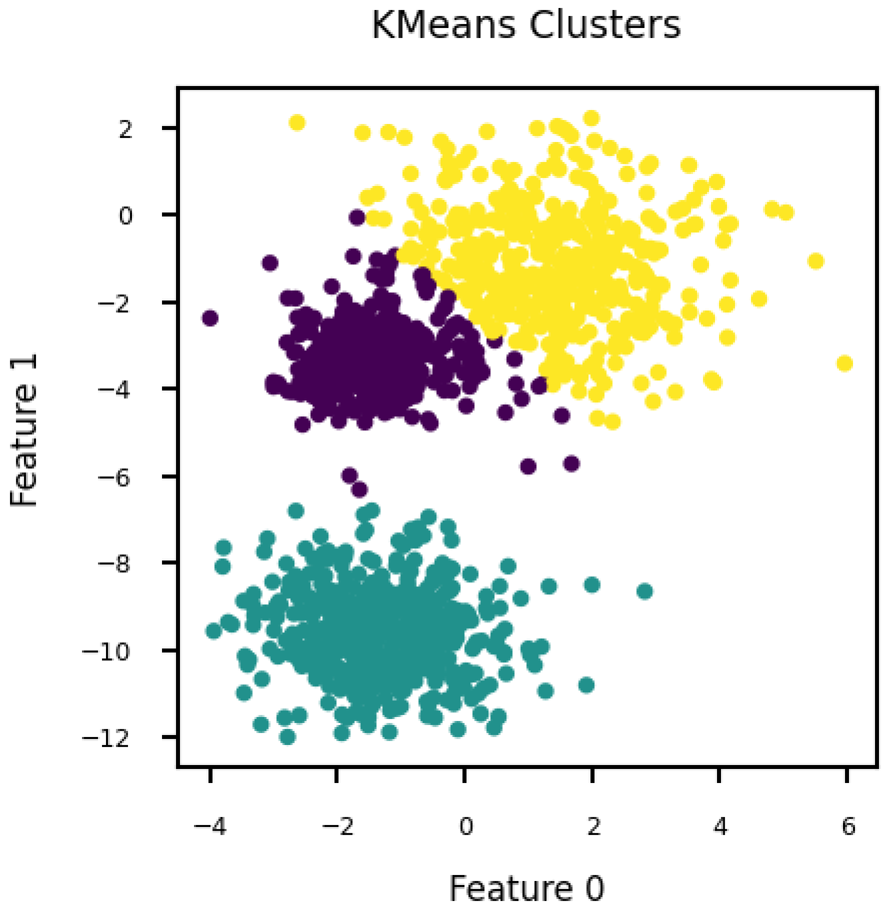


Unsupervised Machine Learning

- Unlabeled data, or data with unknown structure
- Explore the structure of the data to extract information
- Many types, we'll just discuss two.

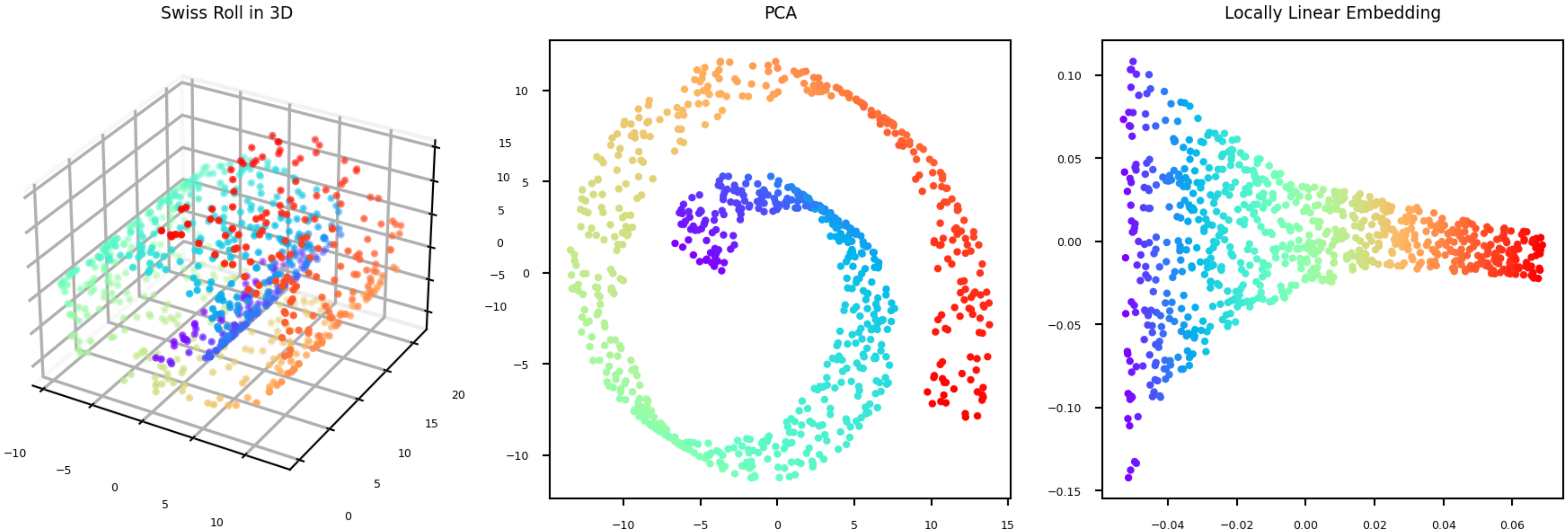
Clustering

- Organize information into meaningful subgroups (clusters)
- Objects in cluster share certain degree of similarity (and dissimilarity to other clusters)
- Example: distinguish different types of customers



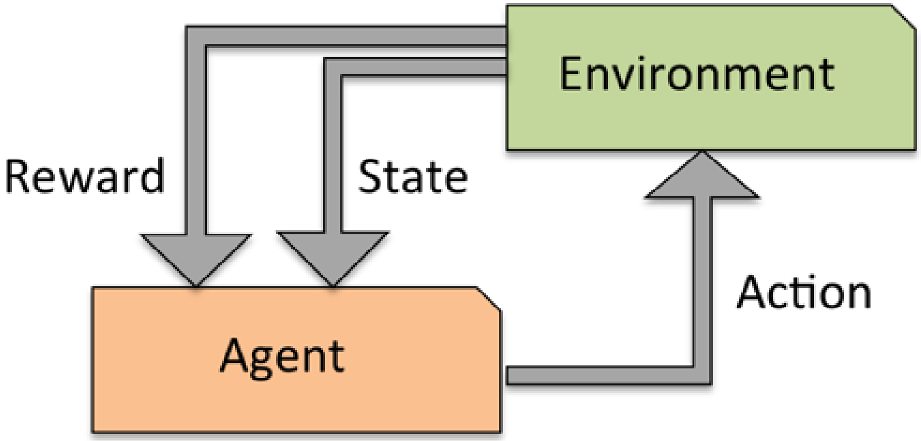
Dimensionality reduction

- Data can be very high-dimensional and difficult to understand, learn from, store,...
- Dimensionality reduction can compress the data into fewer dimensions, while retaining most of the information
- Contrary to feature selection, the new features lose their (original) meaning
- The new representation can be a lot easier to model (and visualize)



Reinforcement learning

- Develop an agent that improves its performance based on interactions with the environment
    - Example: games like Chess, Go,...
- Search a (large) space of actions and states
- *Reward function* defines how well a (series of) actions works
- Learn a series of actions (policy) that maximizes reward through exploration



Learning = Representation + evaluation + optimization

All machine learning algorithms consist of 3 components:

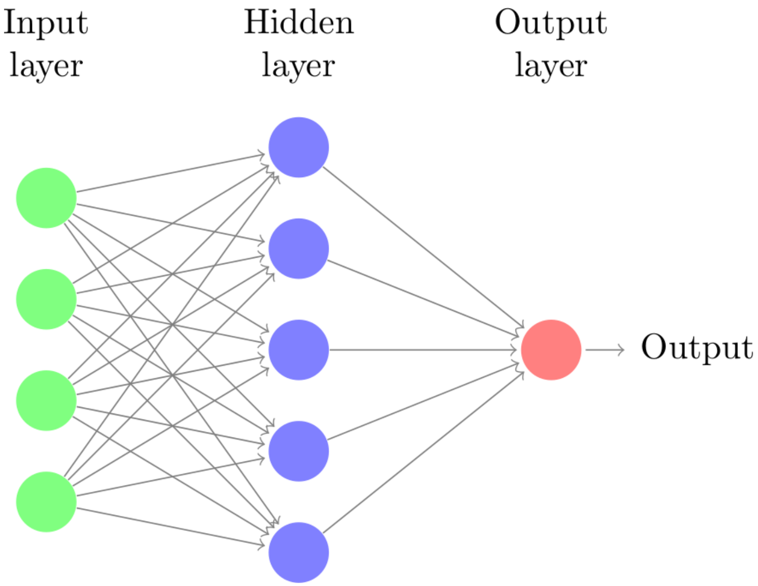
- **Representation**: A model f_θ must be represented in a formal language that the computer can handle
    - Defines the 'concepts' it can learn, the *hypothesis space*
    - E.g. a decision tree, neural network, set of annotated data points
- **Evaluation**: An *internal* way to choose one hypothesis over the other
    - Objective function, scoring function, loss function $\mathcal{L}(f_\theta)$
    - E.g. Difference between correct output and predictions
- **Optimization**: An *efficient* way to search the hypothesis space
    - Start from simple hypothesis, extend (relax) if it doesn't fit the data
    - Start with initial set of model parameters, gradually refine them
    - Many methods, differing in speed of learning, number of optima,...

A powerful/flexible model is only useful if it can also be optimized efficiently

Neural networks: representation

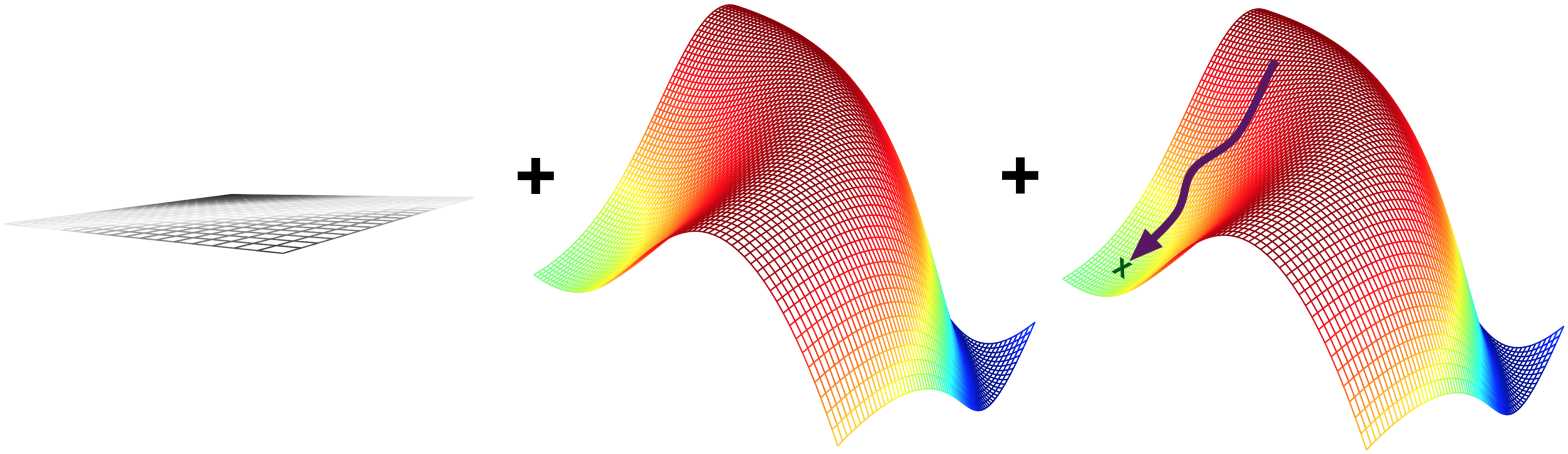
Let's take neural networks as an example

- Representation: (layered) neural network
  - Each connection has a *weight* θ_i (a.k.a. model parameters)
  - Each node receives weighted inputs, emits new value
  - Model f returns the output of the last layer
- The architecture, number/type of neurons, etc. are fixed
  - We call these *hyperparameters* (set by user, fixed during training)



Neural networks: evaluation and optimization

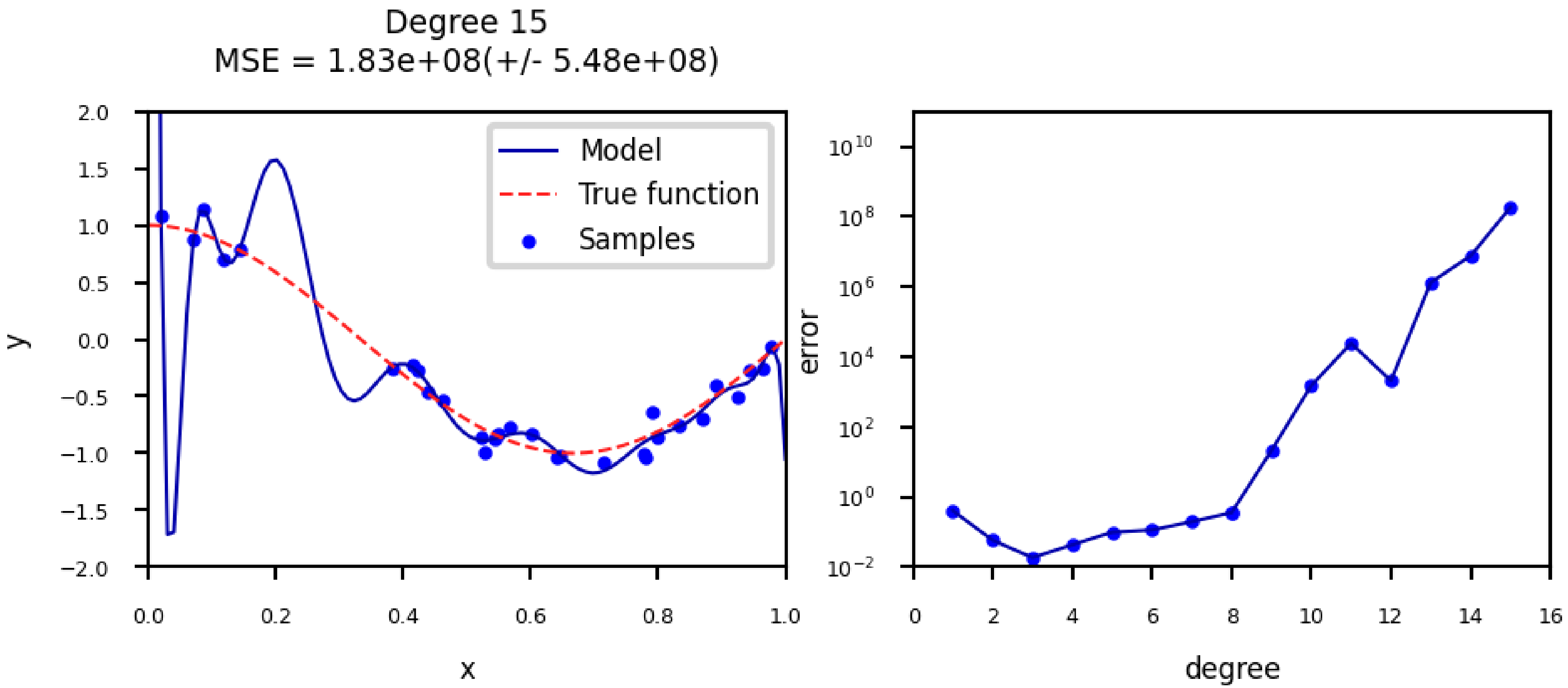
- Representation: Given the structure, the model is represented by its parameters
  - Imagine a mini-net with two weights (θ_0, θ_1): a 2-dimensional search space
- Evaluation: A *loss function* $\mathcal{L}(f_\theta)$ computes how good the predictions are
  - *Estimated* on a set of training data with the 'correct' predictions
  - We can't see the full surface, only evaluate specific sets of parameters
- Optimization: Find the optimal set of parameters
  - Usually a type of *search* in the hypothesis space
  - E.g. Gradient descent: $\theta_i^{new} = \theta_i + \frac{\mathcal{L}(f_\theta)}{\partial \theta_i}$



Overfitting and Underfitting

- It's easy to build a complex model that is 100% accurate on the training data, but very bad on new data
- Overfitting: building a model that is *too complex for the amount of data* you have
    - You model peculiarities in your training data (noise, biases,...)
    - Solve by making model simpler (regularization), or getting more data
    - **Most algorithms have hyperparameters that allow regularization**
- Underfitting: building a model that is *too simple given the complexity of the data*
    - Use a more complex model
- There are techniques for detecting overfitting (e.g. bias-variance analysis). More about that later
- You can build *ensembles* of many models to overcome both underfitting and overfitting

- There is often a sweet spot that you need to find by optimizing the choice of algorithms and hyperparameters, or using more data.
- Example: regression using polynomial functions



Model selection

- Next to the (internal) loss function, we need an (external) evaluation function
    - Feedback signal: are we actually learning the right thing?
        - Are we under/overfitting?
    - Carefully choose to fit the application.
    - Needed to select between models (and hyperparameter settings)

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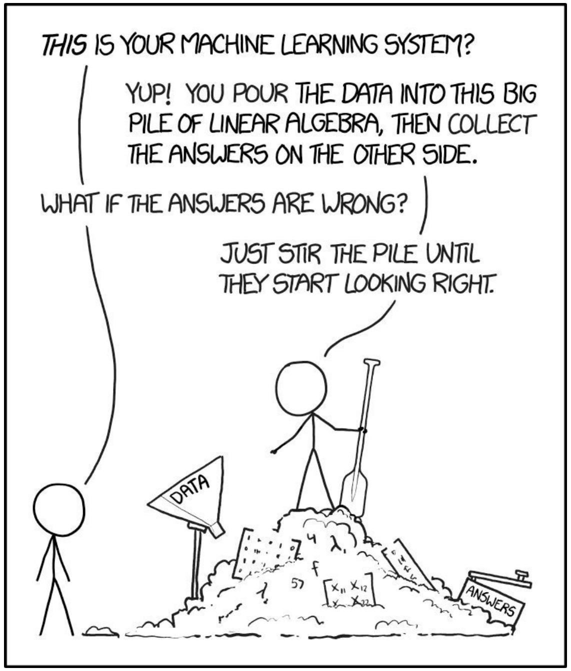
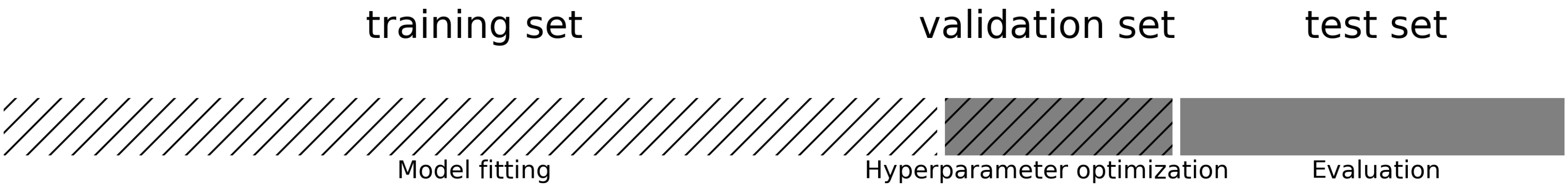
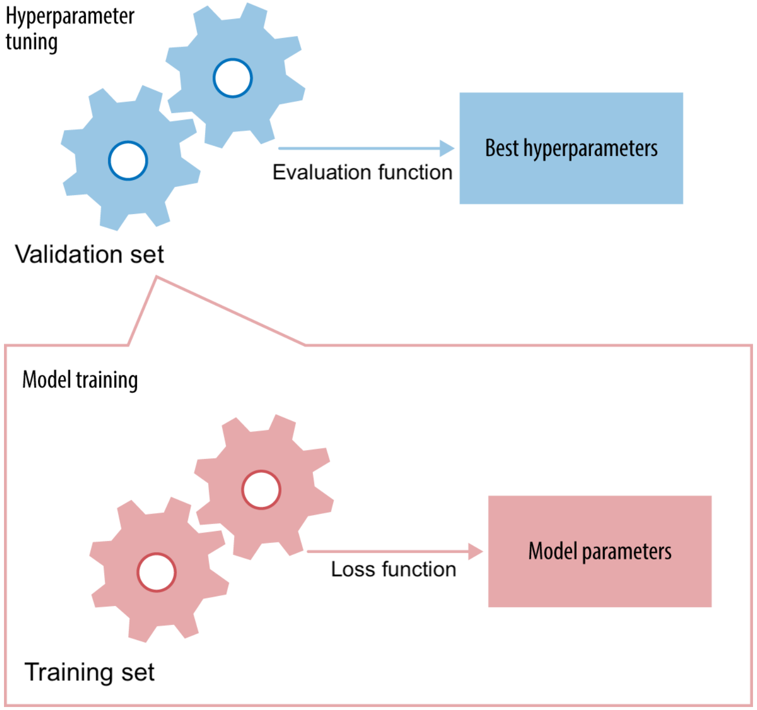

THIS IS YOUR MACHINE LEARNING SYSTEM?
YUP! YOU POUR THE DATA INTO THIS BIG PILE OF LINEAR ALGEBRA, THEN COLLECT THE ANSWERS ON THE OTHER SIDE.
WHAT IF THE ANSWERS ARE WRONG?
JUST STIR THE PILE UNTIL THEY START LOOKING RIGHT.
DATA
ANSWERS

- Data needs to be split into *training* and *test* sets
    - Optimize model parameters on the training set, evaluate on independent test set
- Avoid *data leakage*:
    - Never optimize hyperparameter settings on the test data
    - Never choose preprocessing techniques based on the test data
- To optimize hyperparameters and preprocessing as well, set aside part of training set as a *validation* set
    - Keep test set hidden during *all* training



- For a given hyperparameter setting, learn the model parameters on training set
  - Minize the loss
- Evaluate the trained model on the validation set
  - Tune the hyperparameters to maximize a certain metric (e.g. accuracy)

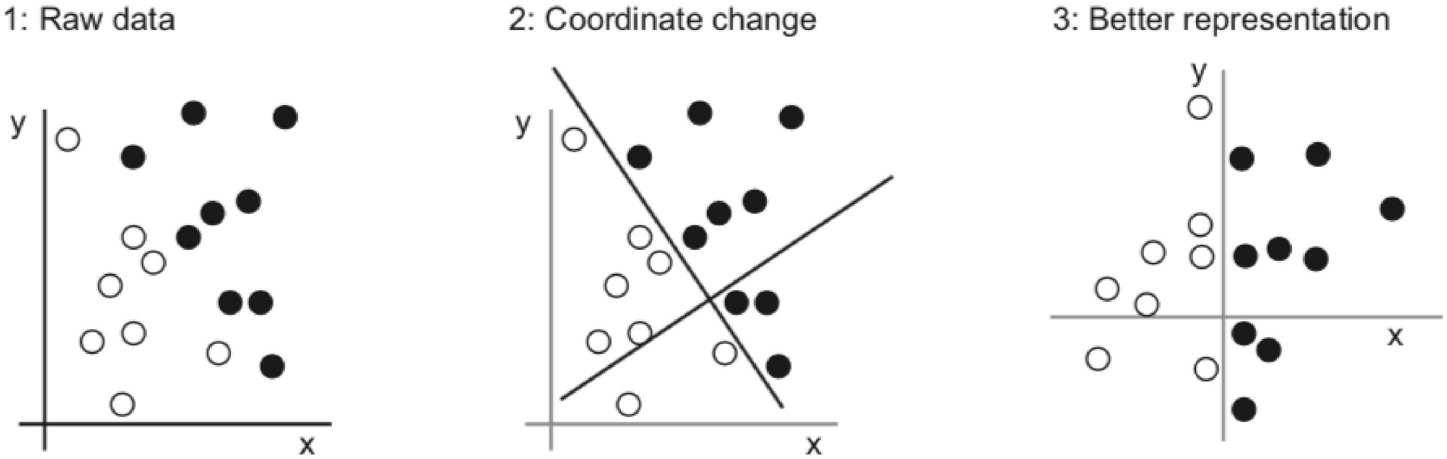


Only generalization counts!

- Never evaluate your final models on the training data, except for:
    - Tracking whether the optimizer converges (learning curves)
    - Diagnosing under/overfitting:
        - Low training and test score: underfitting
        - High training score, low test score: overfitting
- Always keep a completely independent test set
- On small datasets, use multiple train-test splits to avoid sampling bias
    - You could sample an 'easy' test set by accident
    - E.g. Use cross-validation (see later)

Better data representations, better models

- Algorithm needs to correctly transform the inputs to the right outputs
- A lot depends on how we present the data to the algorithm
  - Transform data to better representation (a.k.a. *encoding* or *embedding*)
  - Can be done end-to-end (e.g. deep learning) or by first 'preprocessing' the data (e.g. feature selection/generation)



1: Raw data

2: Coordinate change

3: Better representation

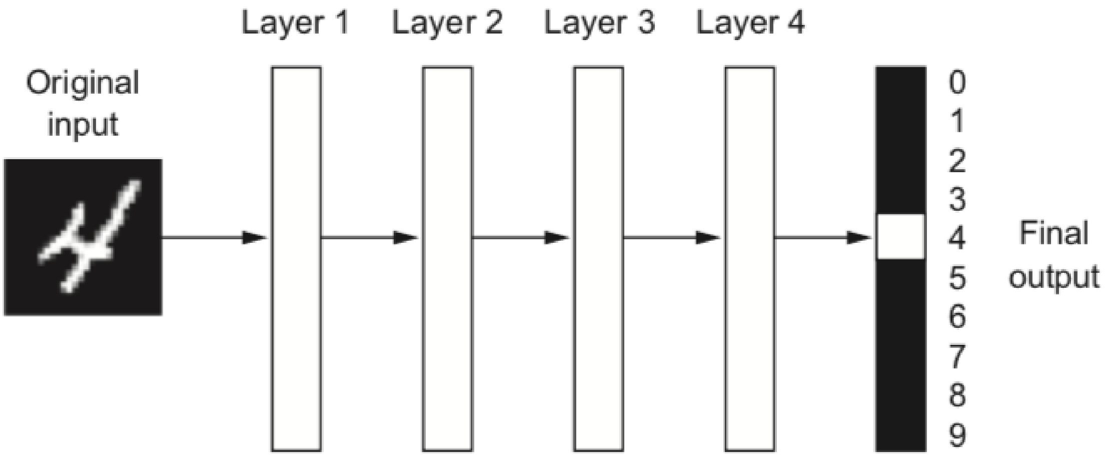
Feature engineering

- Most machine learning techniques require humans to build a good representation of the data
- Especially when data is naturally structured (e.g. table with meaningful columns)
- Feature engineering is often still necessary to get the best results
    - Feature selection, dimensionality reduction, scaling, ...
    - *Applied machine learning is basically feature engineering (Andrew Ng)*
- Nothing beats domain knowledge (when available) to get a good representation
    - E.g. Iris data: leaf length/width separate the classes well

Build prototypes early-on

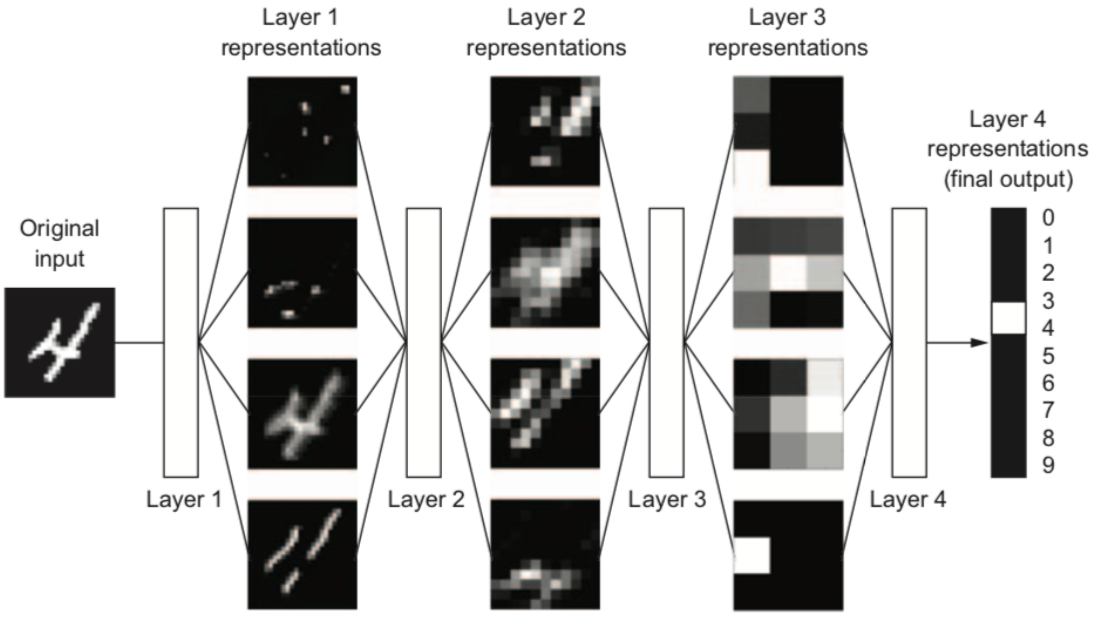
Learning data transformations end-to-end

- For unstructured data (e.g. images, text), it's hard to extract good features
- Deep learning: learn your own representation (embedding) of the data
    - Through multiple layers of representation (e.g. layers of neurons)
    - Each layer transforms the data a bit, based on what reduces the error



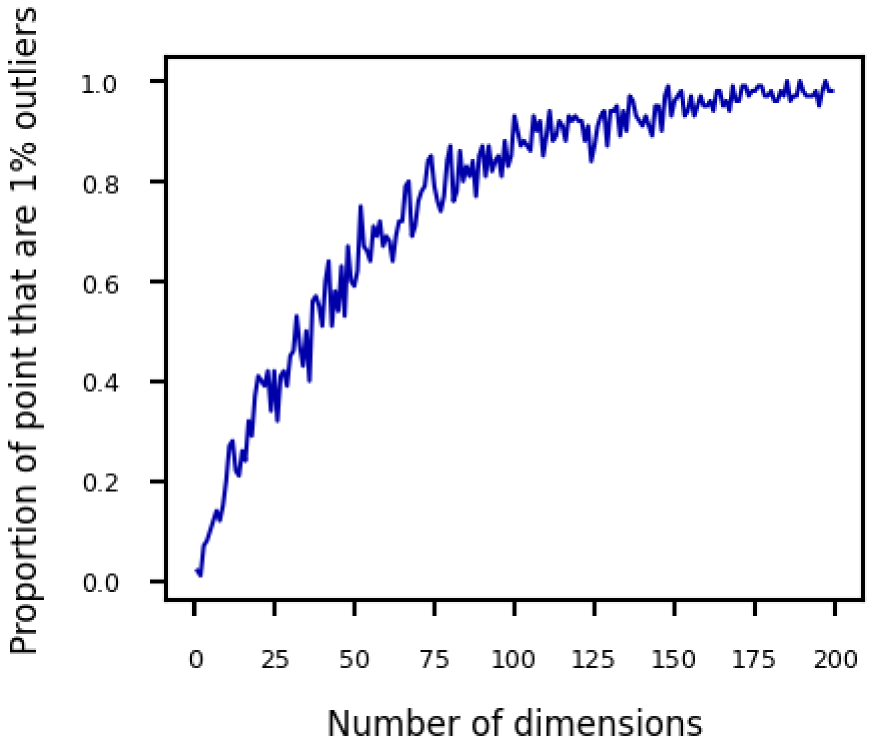
Example: digit classification

- Input pixels go in, each layer transforms them to an increasingly informative representation for the given task
- Often less intuitive for humans



Curse of dimensionality

- Just adding lots of features and letting the model figure it out doesn't work
- Our assumptions (inductive biases) often fail in high dimensions:
    - Randomly sample points in an n-dimensional space (e.g. a unit hypercube)
    - Almost all points become outliers at the edge of the space
    - Distances between any two points will become almost identical



Practical consequences

- For every dimension (feature) you add, you need exponentially more data to avoid sparseness
- Affects any algorithm that is based on distances (e.g. kNN, SVM, kernel-based methods, tree-based methods,...)
- Blessing of non-uniformity: on many applications, the data lives in a very small subspace
    - You can drastically improve performance by selecting features or using lower-dimensional data representations

”More data can beat a cleverer algorithm”

(but you need both)

- More data reduces the chance of overfitting
- Less sparse data reduces the curse of dimensionality
- *Non-parametric* models: number of model parameters grows with amount of data
    - Tree-based techniques, k-Nearest neighbors, SVM,...
    - They can learn any model given sufficient data (but can get stuck in local minima)
- *Parametric* (fixed size) models: fixed number of model parameters
    - Linear models, Neural networks,...
    - Can be given a huge number of parameters to benefit from more data
    - Deep learning models can have millions of weights, learn almost any function.
- The bottleneck is moving from data to compute/scalability

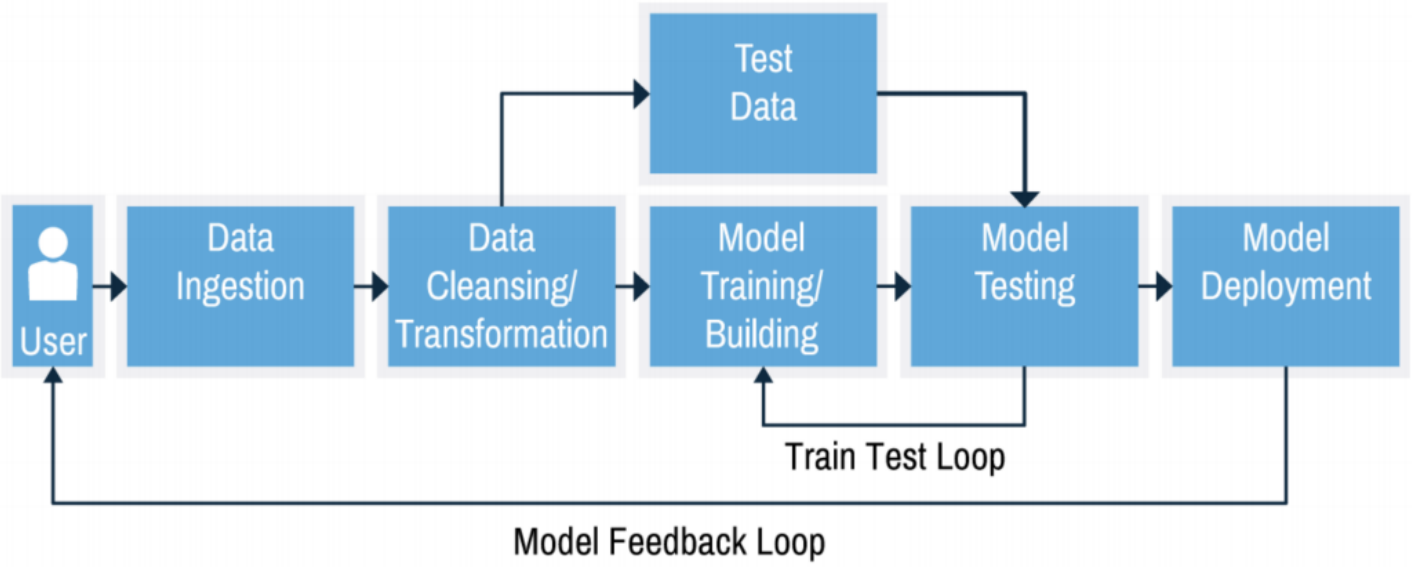
Building machine learning systems

A typical machine learning system has multiple components, which we will cover in upcoming lectures:

- Preprocessing: Raw data is rarely ideal for learning
    - Feature scaling: bring values in same range
    - Encoding: make categorical features numeric
    - Discretization: make numeric features categorical
    - Label imbalance correction (e.g. downsampling)
    - Feature selection: remove uninteresting/correlated features
    - Dimensionality reduction can also make data easier to learn
    - Using pre-learned embeddings (e.g. word-to-vector, image-to-vector)

- Learning and evaluation
    - Every algorithm has its own biases
    - No single algorithm is always best
    - *Model selection* compares and selects the best models
        - Different algorithms, different hyperparameter settings
    - Split data in training, validation, and test sets
- Prediction
    - Final optimized model can be used for prediction
    - Expected performance is performance measured on *independent* test set

- Together they form a *workflow* of *pipeline*
- There exist machine learning methods to automatically build and tune these pipelines
- You need to optimize pipelines continuously
    - *Concept drift*: the phenomenon you are modelling can change over time
    - *Feedback*: your model's predictions may change future data



Summary

- Learning algorithms contain 3 components:
    - Representation: a model f that maps input data X to desired output y
        - Contains model parameters θ that can be made to fit the data X
    - Loss function $\mathcal{L}(f_\theta(X))$: measures how well the model fits the data
    - Optimization technique to find the optimal θ: $\underset{\theta}{\operatorname{argmin}} \mathcal{L}(f_\theta(X))$
- Select the right model, then fit it to the data to minimize a task-specific error $\mathcal{E}$
    - Inductive bias b: assumptions about model and hyperparameters
      $\underset{\theta,b}{\operatorname{argmin}} \mathcal{E}(f_{\theta,b}(X))$
- Overfitting: model fits the training data well but not new (test) data
    - Split the data into (multiple) train-validation-test splits
    - Regularization: tune hyperparameters (on validation set) to simplify model
    - Gather more data, or build ensembles of models
- Machine learning *pipelines*: preprocessing + learning + deployment