Intro to ML. Part 3

Evgeny Burnaev, Alexey Zaytsev

Skoltech, Moscow, Russia

Skoltech

Skolkovo Institute of Science and Technology

Examples of Learning Tasks

- Image: annotation, segmentation, face recognition, OCR, face verification
- Autonomous technical systems (robots, cars)
- Medical diagnosis, fraud detection, network intrusions
- Playing games (chess, poker)
- Speech: recognition, synthesis, verification
- Text: topic modeling, spam detection

Math. ML Tasks

- **Dimensionality Reduction**: lower-dimensional features, preserving some properties of data
- **Regression**: predict some real-valued output variable for some input parameters (ship fuel consumption depending on weather conditions, route, etc.)
- **Classification**: set a label for each object (e.g. image classification)
- **Clustering**: partition objects into some "homogeneous" groups (e.g. divide documents into groups with similar topics)
- **Ranking**: rank objects according to some metric

What do we want?

- Algorithmic problems:
  - more efficient and more accurate algorithms
  - handle large-scale (dimensions, data volume) problems
  - handle diverse types of data sources, including non-structured data, data on graphs, etc.

- Theoretical problems:
  - what can be learned? under what conditions? restrictions?
  - learning guarantees?
  - learning algorithms performance?

This course: Our aims

- **Models and Algorithms**
  - **main algorithms and their efficiency**
  - **modern topics**
- Theory
  - learning guarantees
  - analysis of algorithms
- **Applications**

Definitions

- **Example**: item, instance of data, related to some object
- **Features** $\mathbf{x}$: input value (input parameters, an input vector, attributes, a point) characterizing an object
- **Labels** y: output value, categoric (classification) or real value (regression), associated to an object
- **Data**:
  - training data (usually contains labels)
  - test data (labels exist but not known)
  - validation data (labeled, used for tuning of hyperparameters)

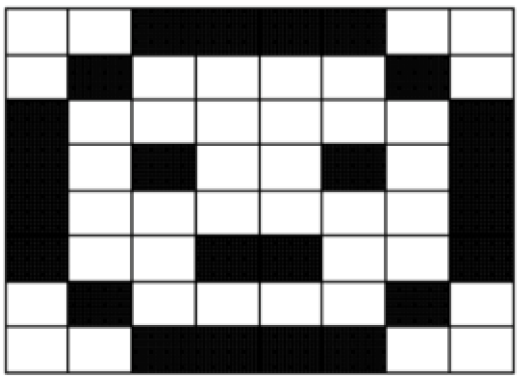
Machine Learning Problem

- o is an object
- $\mathbf{x}(o)$ is a set of features
- y is a label (class, category, etc.)
- For a new $\mathbf{x}$ we should define a corresponding class y

Machine Learning Problem: Example

O

x(O)



Y

Person

Bird

House

Definitions

- space of objects (input space) X
- space of labels (output space) Y
- unknown target function $f : X \to Y$
- **Given**:
  - Learning sample $S_m = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$
  - Objects $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \in X$
  - Labels $\{y_1, \ldots, y_m\} \in Y$, $y_i = f(\mathbf{x}_i)$
- **Find**:
  - $\widehat{f} : X \to Y$, approximating f on X
- Mainly ML is about how to
  - define description of objects $\mathbf{x}_i$
  - define "$\widehat{f}$ approximates f"
  - construct $\widehat{f}$ using S_m

Example: Shop revenue prediction

- **Object** o: place to open a new restaurant
- **Label** y: revenue after one year of operation
- **Features** $\mathbf{x} = \mathbf{x}(o)$: demographic properties of a considered city district, prices for real estate in a local neighborhood, availability of offices nearby, etc.
- **Challenges**:
  - small sample size
  - a lot of features ($d \gg 1$)
  - outliers/incorrect measurements
  - non-homogeneous data (big cities vs. local towns)

Features

- Usually as object $\mathbf{x}$ description we consider a set of features, i.e. $\mathbf{x} = (x_1, \ldots, x_d)$
- There are several types of features
  - binary, e.g. $x_j \in \{0, 1\}$
  - nominal, e.g. $x_j \in \{\textit{red}, \textit{green}, \textit{blue}\}$
  - ordinal, e.g. $x_j \in \{\textit{low}, \textit{middle}, \textit{high}\}$
  - real number, i.e. $x_j \in \mathbb{R}$
- Thus objects $\{\mathbf{x}_1, \ldots, \mathbf{x}_m\} \in X$ can be represented as an $m \times d$ matrix

$$\begin{pmatrix} x_{11} & \ldots & x_{1d} \\ \ldots & \ldots & \ldots \\ x_{m1} & \ldots & x_{md} \end{pmatrix}$$

Types of problems

- Classification
  - two-class classification: $Y \in \{0, 1\}$
  - multi-class classification (mono-label case): $Y = \{1, \ldots, K\}$
  - multi-class classification (multi-label case): $Y = \{0, 1\}^K$
- Regression: $Y = \mathbb{R}$ or $Y = \mathbb{R}^K$
- Ranking (learning to rank): Y is a finite ordered set of categories

Learning Scenarios

- Settings

batch: a learner get full sample, learn a model and performs predictions for unseen points

on-line: a learner receives one sample at a time and makes prediction for that sample

- Queries

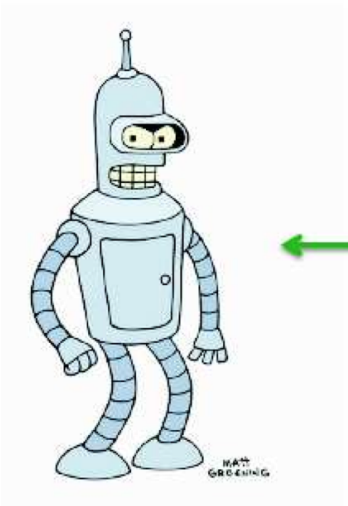
active: a learner can request the label of a point

passive: a learner always receives labeled points

(Passive) Supervised Learning

raw unlabeled data
$x_1, x_2, x_3, \ldots$

random sample



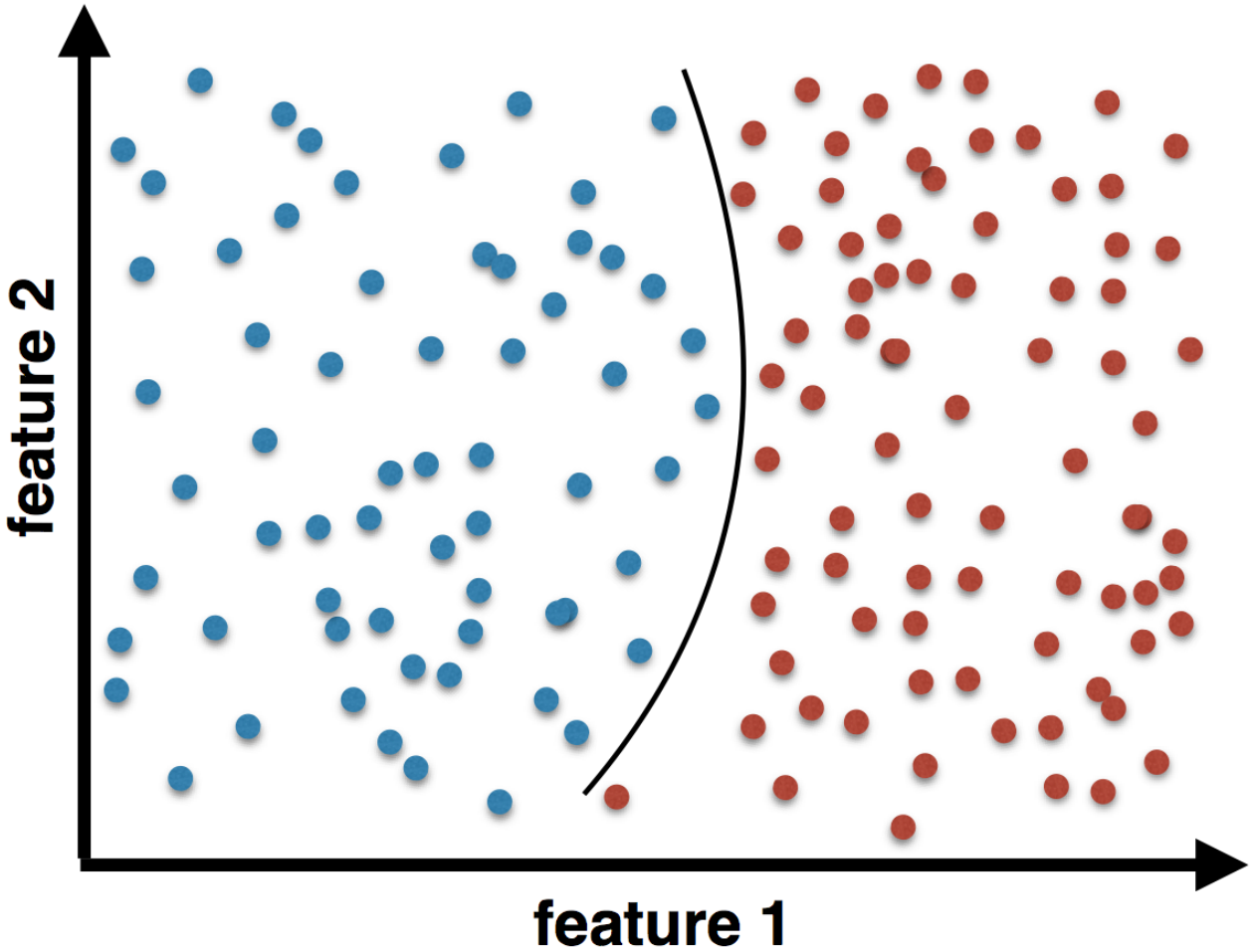
labeled training instances

$\langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle, \langle x_3, y_3 \rangle, \ldots$

supervised learner
induces a classifier

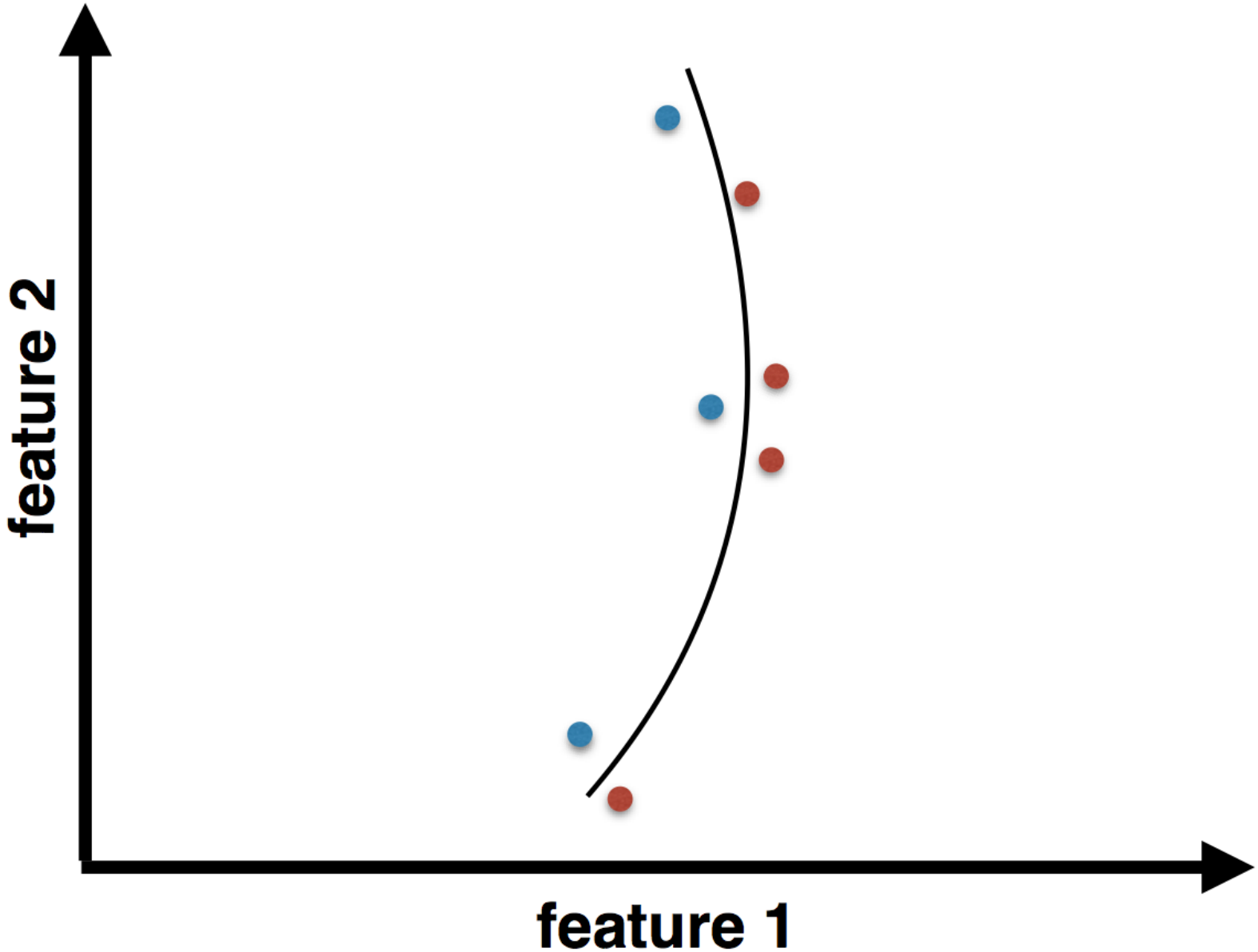
expert / oracle
analyzes experiments
to determine labels

So what's wrong with Supervised Learning

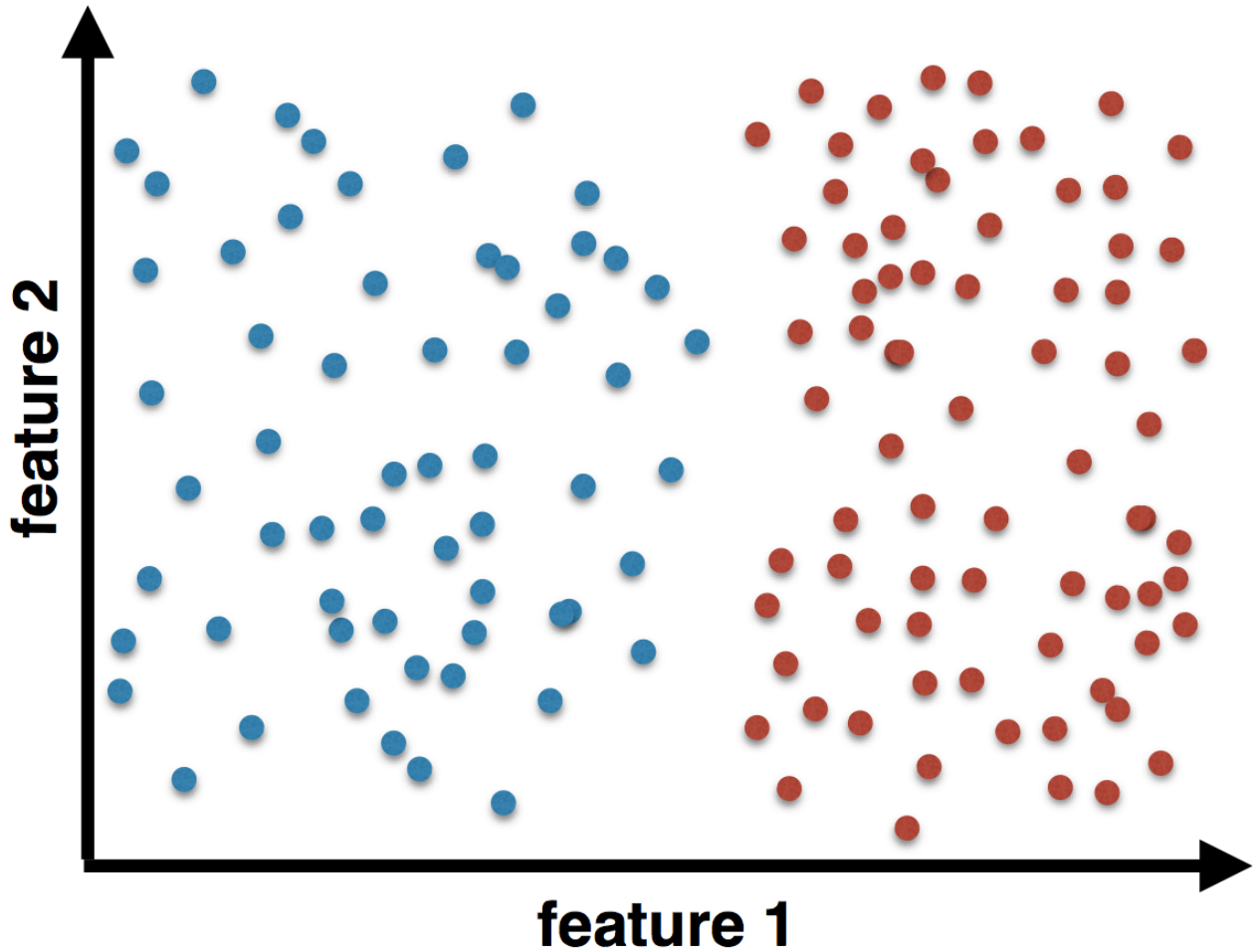


- Traditional approach almost universally adopted

Well, we actually only needed this!

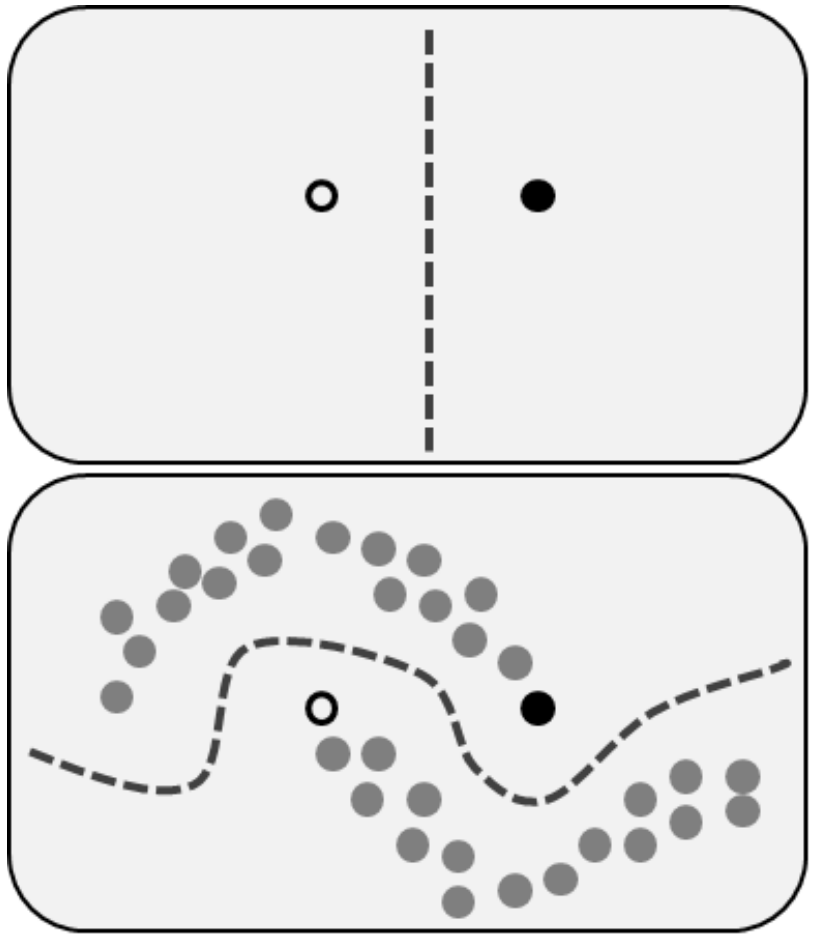


So this was a complete waste of time!

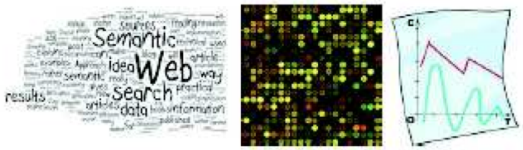


- Random sampling inevitably leads to redundancy

Semi-Supervised Learning



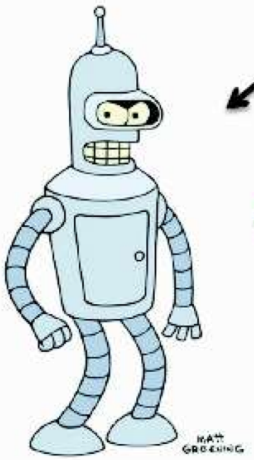
Semi-Supervised Learning



exploit the structure
in unlabeled data

raw unlabeled data
$x_1, x_2, x_3, \ldots$

random sample



labeled training instances

$\langle x_1, y_1 \rangle, \langle x_2, y_2 \rangle, \langle x_3, y_3 \rangle, \ldots$

semi-supervised learner
induces a classifier

expert / oracle
analyzes experiments
to determine labels

Active Learning

raw unlabeled data
$x_1, x_2, x_3, \ldots$

inspect the unlabeled data

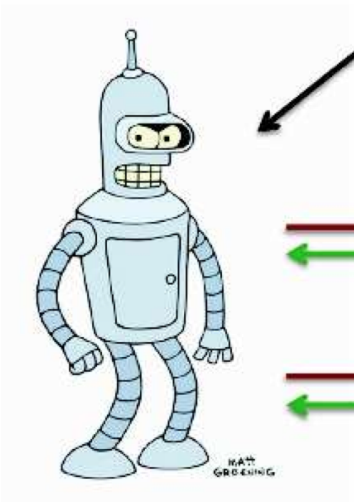
request labels for selected data

$\langle x_1, ? \rangle$

$\langle x_1, y_1 \rangle$

$\langle x_2, ? \rangle$

$\langle x_2, y_2 \rangle$

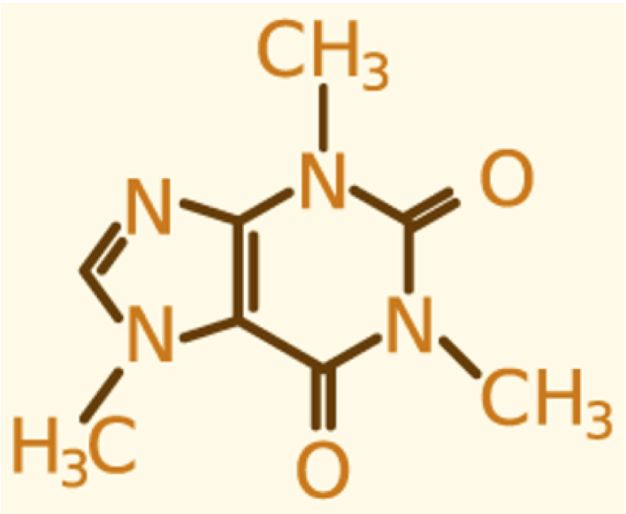


active learner
induces a classifier

expert / oracle
analyzes experiments to determine labels

Active Learning example: drug design

- Goal: find compounds which bind to a particular target



Large collections of compounds from:

- vendor catalogs
- corporate collections
- combinatorial chemistry

unlabeled point $\equiv$ description of chemical compound

label $\equiv$ active (binds to target) vs. inactive

getting a label $\equiv$ chemistry experiment

- **Hypothesis set** $F \subset Y^X$ is a subset of functions out of which the learner selects his hypothesis
  - represents a prior knowledge about the task at hand
  - depends on available features
- Predictive model belongs to a parametric family of functions

$$F = \{f(\mathbf{x}; \boldsymbol{\theta}) | \boldsymbol{\theta} \in \Theta\},$$

  where
  - $f : X \times \Theta \to Y$ is a fixed family of functions,
  - Θ is a feasible set of parameters
- Example: linear model with $\boldsymbol{\theta} = (\theta_1, \ldots, \theta_p)$, $\Theta = \mathbb{R}^p$, and features $\{\phi_j(\mathbf{x})\}_{j=1}^p$
  - regression $f(\mathbf{x}; \boldsymbol{\theta}) = \sum_{j=1}^p \theta_j \phi_j(\mathbf{x})$, $Y = \mathbb{R}^1$
  - classification $f(\mathbf{x}; \boldsymbol{\theta}) = \text{sign}\left(\sum_{j=1}^p \theta_j \phi_j(\mathbf{x})\right)$, $Y = \{-1, +1\}$

Example: Linear regression

- $X = Y = \mathbb{R}^1$, $m = 200$, $d = 3$ features: $\{x, x^2, 1\}$ or $\{x, \sin x, 1\}$

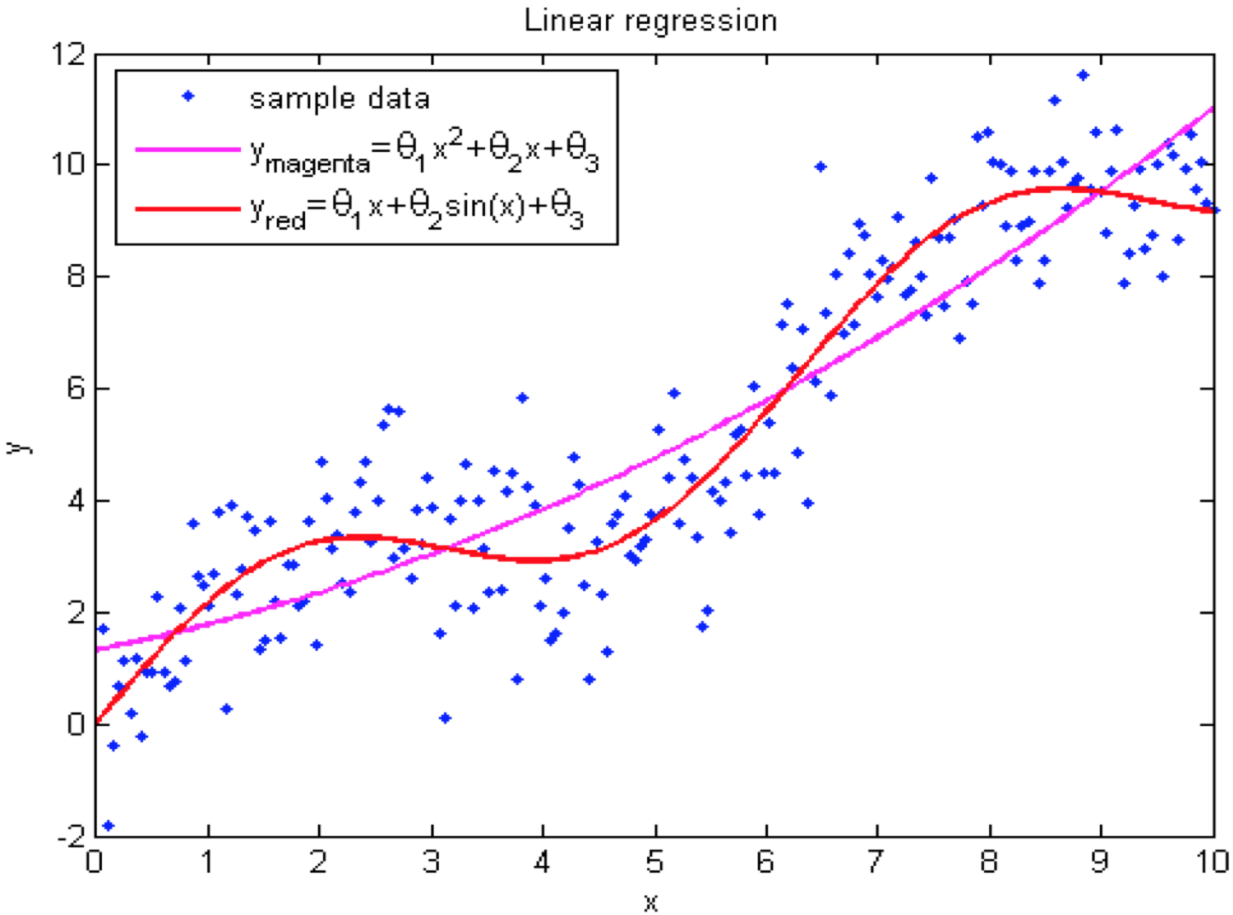


Figure – Linear regression [Vorontsov]

- **Training data**: sample S_m of size m drawn $i.i.d.$ according to distribution D on $X \times Y$

$$S = \{(\mathbf{x}_1, y_1), \ldots, (\mathbf{x}_m, y_m)\}$$

- **Problem** find hypothesis $\widehat{f} \in F$ with small generalization error
  - deterministic case: $y = f(\mathbf{x})$ is a deterministic function, only $\mathbf{x} \sim D$
  - stochastic case: output is a probabilistic function of input, e.g. $y = f(\mathbf{x}) + \varepsilon$

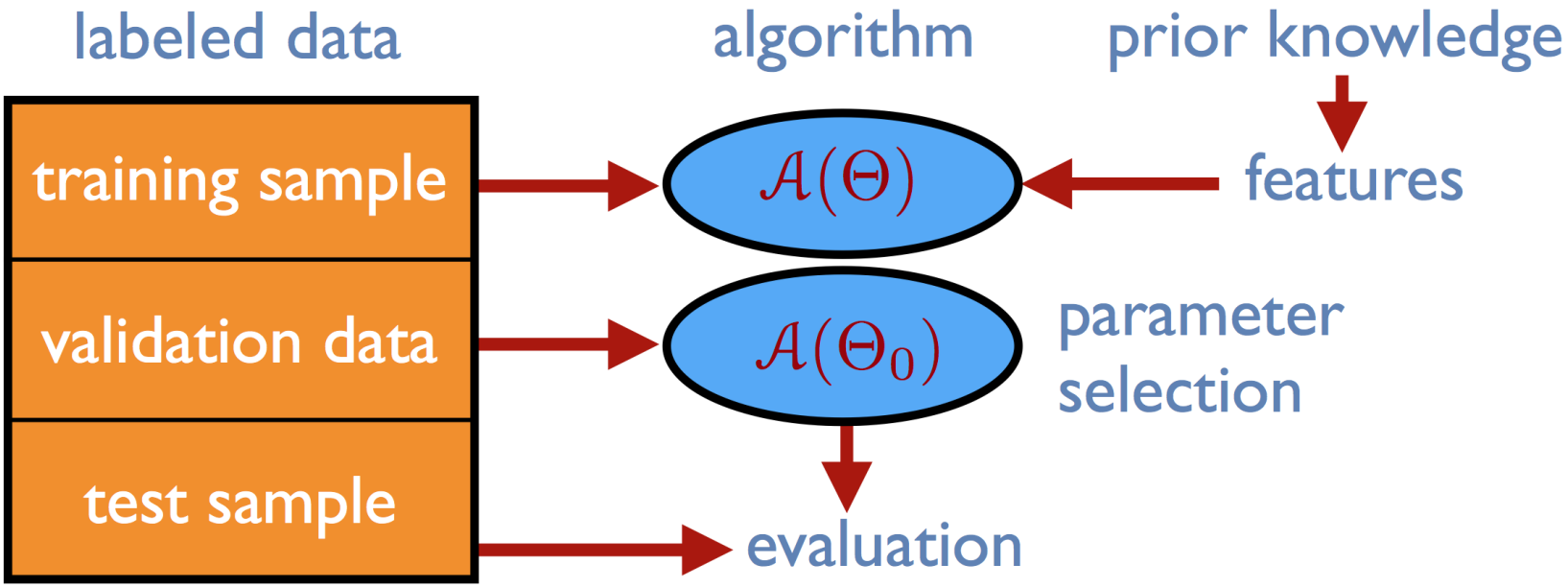


Figure – Learning scheme of predictive model [Mohri, 2016]

- ML algorithm $\mathcal{A} : (X \times Y)^m \to F$
- Train phase: using algorithm $\mathcal{A}$ we get $\widehat{f} = \mathcal{A}(S_m)$
- Test phase: calculate predictions $\widehat{f}(\mathbf{x}'_i)$ for new $\mathbf{x}'_i$, $i = 1, \ldots, m'$

Loss function $L : Y \times Y \to \mathbb{R}$

- $L(y, \widehat{y})$ is the error of predicting $\widehat{y}$ instead of y
- $0 - 1$ loss $L(y, \widehat{y}) = 1_{y \neq \widehat{y}}$ in case of binary classification
- $L(y, \widehat{y}) = (y - \widehat{y})^2$ in case of regression with $Y \subseteq \mathbb{R}$

- **Empirical error** for $f \in F$ and sample S_m

$$\widehat{R}(f) = \frac{1}{m} \sum_{i=1}^{m} L(f(\mathbf{x}_i), y_i)$$

- **Generalization error**: for $f \in F$

$$R(f) = \mathbb{E}_{(\mathbf{x},y)\sim D}[L(f(\mathbf{x}), y)]$$

- **Bayes error**

$$R^* = \inf_f R(f)$$

- **Noise**:
  - data generation process: $y = f(\mathbf{x}) + \varepsilon$, ε is a white noise
  - in regression for any $\mathbf{x} \in X$, L_2-loss and white noise model

$$f^* = \mathbb{E}(y|\mathbf{x})$$

  - observe that

$$R^* = \mathrm{Var}(\varepsilon)$$

Learning $\neq$ Fitting

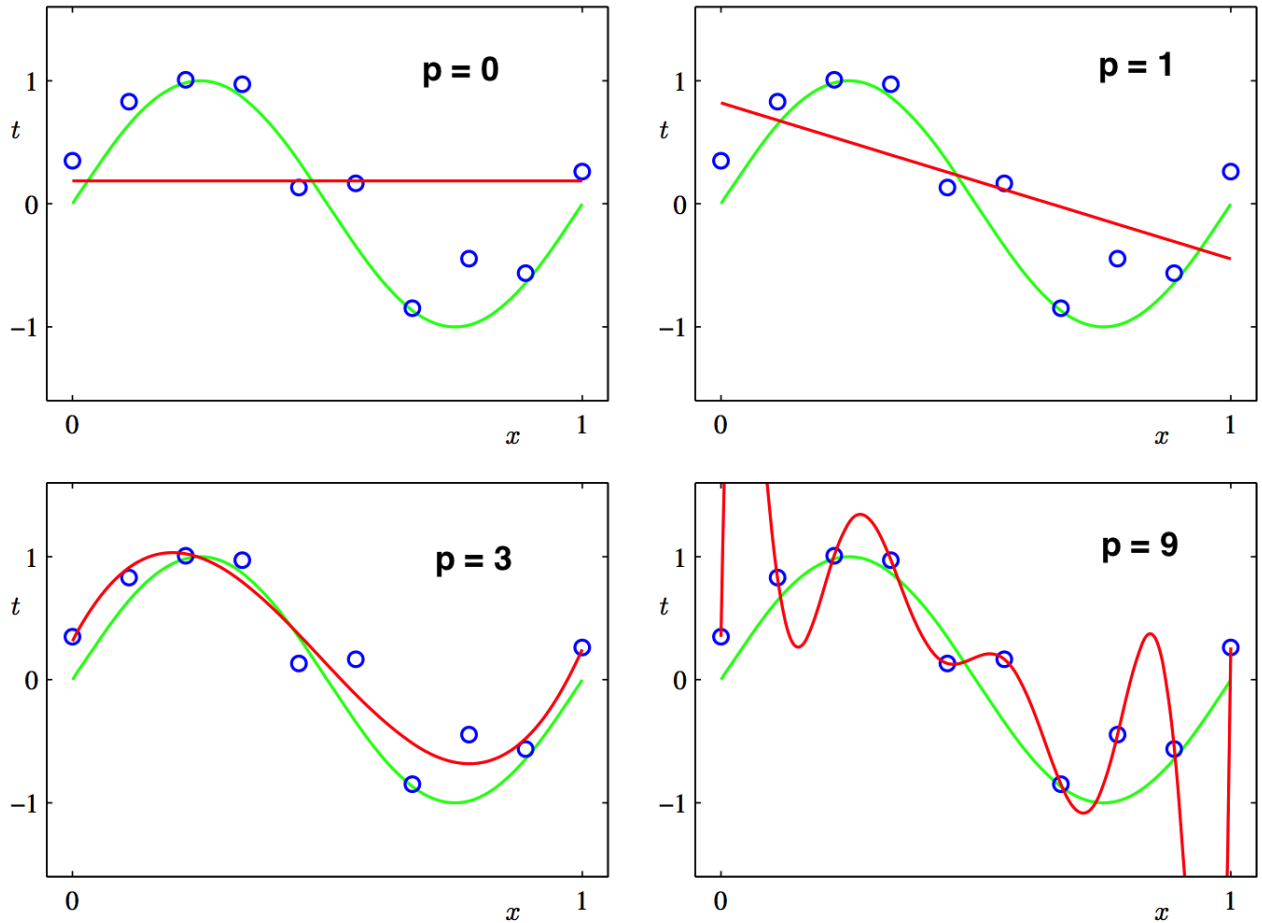


Figure – Notion of simplicity/complexity. How do we define complexity? [Bishop]

- A set of polynomials $f(x; \boldsymbol{\theta}) = \sum_{j=0}^{p} \theta_j x^j$
- Squared loss function $L(\widehat{y}, y) = (\widehat{y} - y)^2$

Learning $\neq$ Fitting

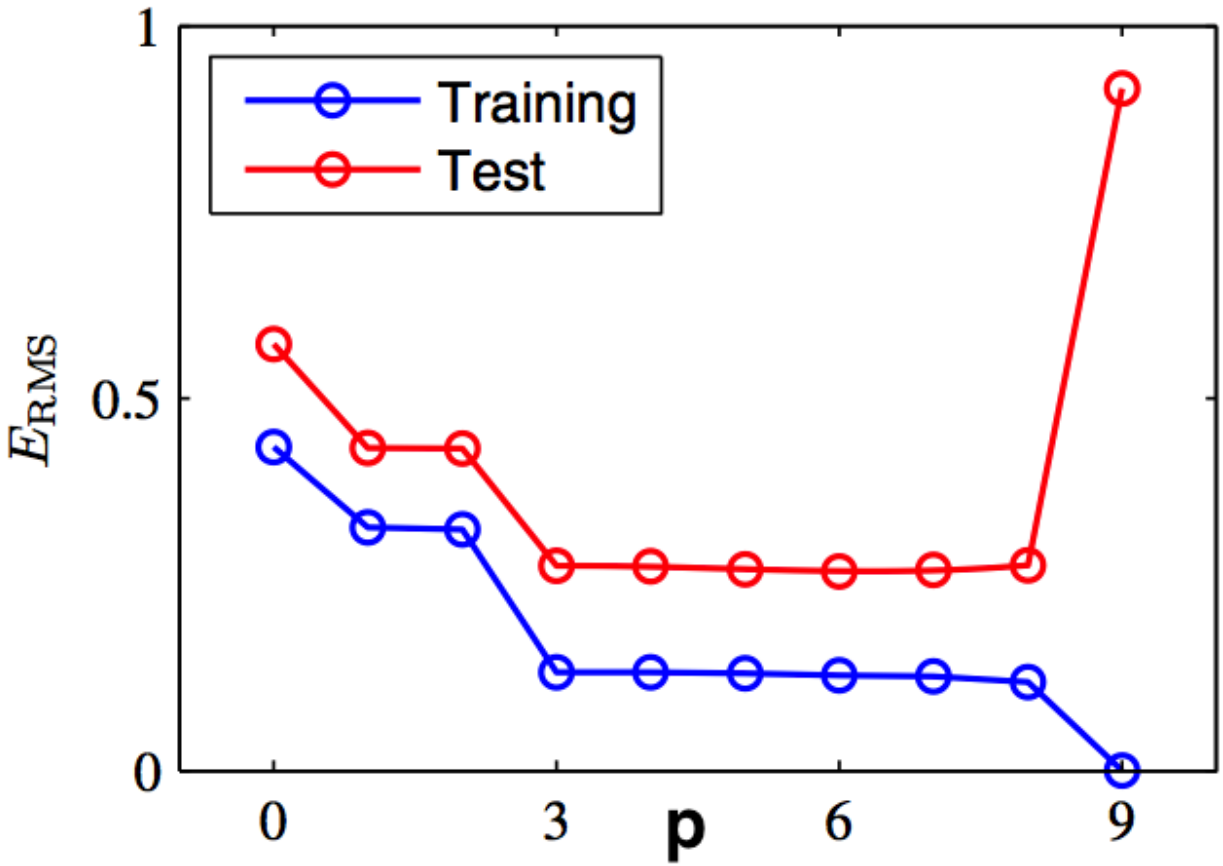


Figure – Notion of simplicity/complexity. How do we define complexity? [Bishop]

Overfitting: error on the test set $\gg$ error on the train set

Empirical Risk Minimization

- Select Hypothesis set F
- Find hypothesis $f \in F$ minimizing empirical error

$$\widehat{f} = \arg\min_{f \in F} \widehat{R}(f)$$

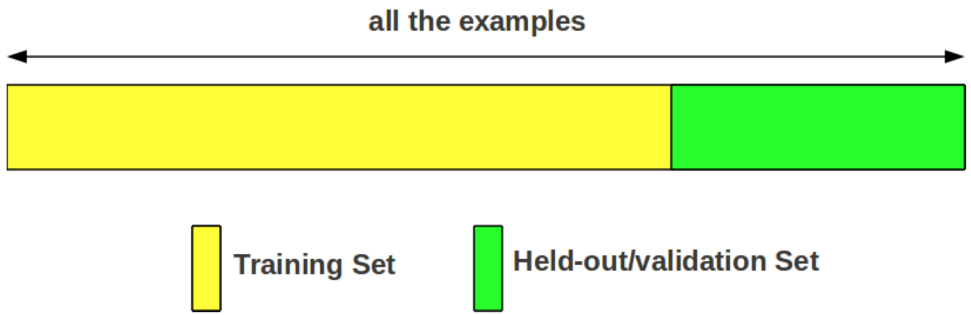
- F may be too complex
- Sample size may not be large enough

Empirical observations

- the best hypothesis on the sample may not be the best overall
- generalization is not memorization
- complex rules can provide poor predictions
- trade-off: complexity vs. sample size (underfitting/overfitting)
- detection: use cross-validation for random splitting in train/test subsets

Hold-out data

- Set aside a fraction (say $10\% - 20\%$) of the training data
- This part becomes our hold-out data (validation or development data)



- Remember: hold-out data is NOT the test data
- Train each model using the remaining training data
- Evaluate error on the hold-out data
- Choose the model with the smallest hold-out error
- Problems:
  - Wastes training data, so typically used when we have plenty of training data
  - Hold-out data may not be good if there was an unfortunate split (use random splitting!)

Afterwords

- Main steps to solve applied problem
  - understand problem and data
  - feature engineering
  - model selection and reduction of the problem to optimization one
  - accuracy evaluation
  - business deployment and use
- When developing ML algorithms
  - use synthetic data to explore limits of the algorithm
  - use applied data (from available data storages) to test under various real conditions

M-fold Cross-Validation

- Create M equal sized partitions of the training data
- Each partition has m/M examples
- Train using $M-1$ partitions, validate on the remaining partitions
- Repeat the same M times, each with a different validation partition

- Finally, choose the model with smallest average validation error
- Usually M is chosen as $4-10$

Cross-Validation II

$N \times M$-fold Cross-Validation

- We divide the training sample N times into M equal sized partitions
- Results of all N M-fold cross-validations are aggregated (e.g. averaged)
- By increasing N we can improve accuracy
- Each object is used in a test set N times
- We can construct confidence intervals using results of N repetitions

Structural Risk Minimization Principle

- Consider an infinite sequence of hypothesis sets ordered for inclusion

$$F_1 \subset F_2 \subset \ldots \subset F_n \subset \ldots$$

$$f = \arg \min_{f \in F_n,\, n \in \mathbb{N}} \widehat{R}(f) + \text{penalty}(F_n, m)$$

- Strong theoretical guarantees

- Typically computationally intensive

- Empirical risk minimization (ERM)

$$f = \arg\min_{f \in F} \widehat{R}(f)$$

- Structural Risk Minimization (SRM) for $F_n \subseteq F_{n+1}$

$$f = \arg\min_{f \in F_n,\, n \in \mathbb{N}} \widehat{R}(f) + \text{penalty}(F_n, m)$$

- Regularization-based algorithms

$$f = \arg\min_{f \in F} \widehat{R}(h) + \lambda \|f\|^2,\ \lambda > 0$$