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Deep Learning Summer School 2015

Introduction to Machine Learning

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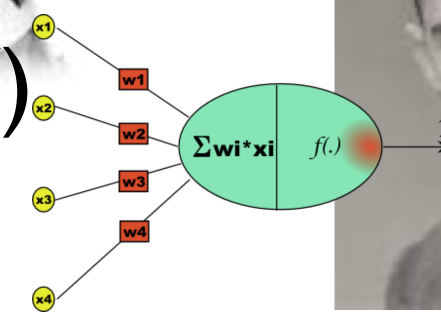
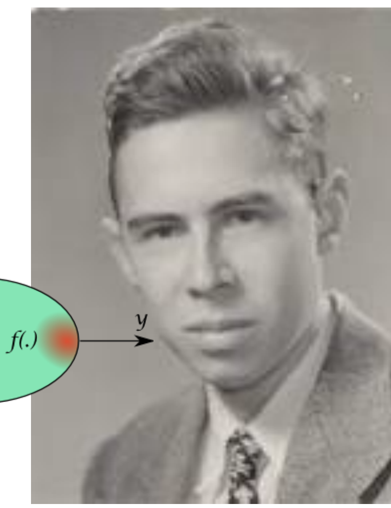
What is machine learning ?

Historical perspective

- Born from the ambitious goal of **Artificial Intelligence**
- Founding project:
  The **Perceptron** (Frank Rosenblatt 1957)
  First artificial neuron **learning** form examples





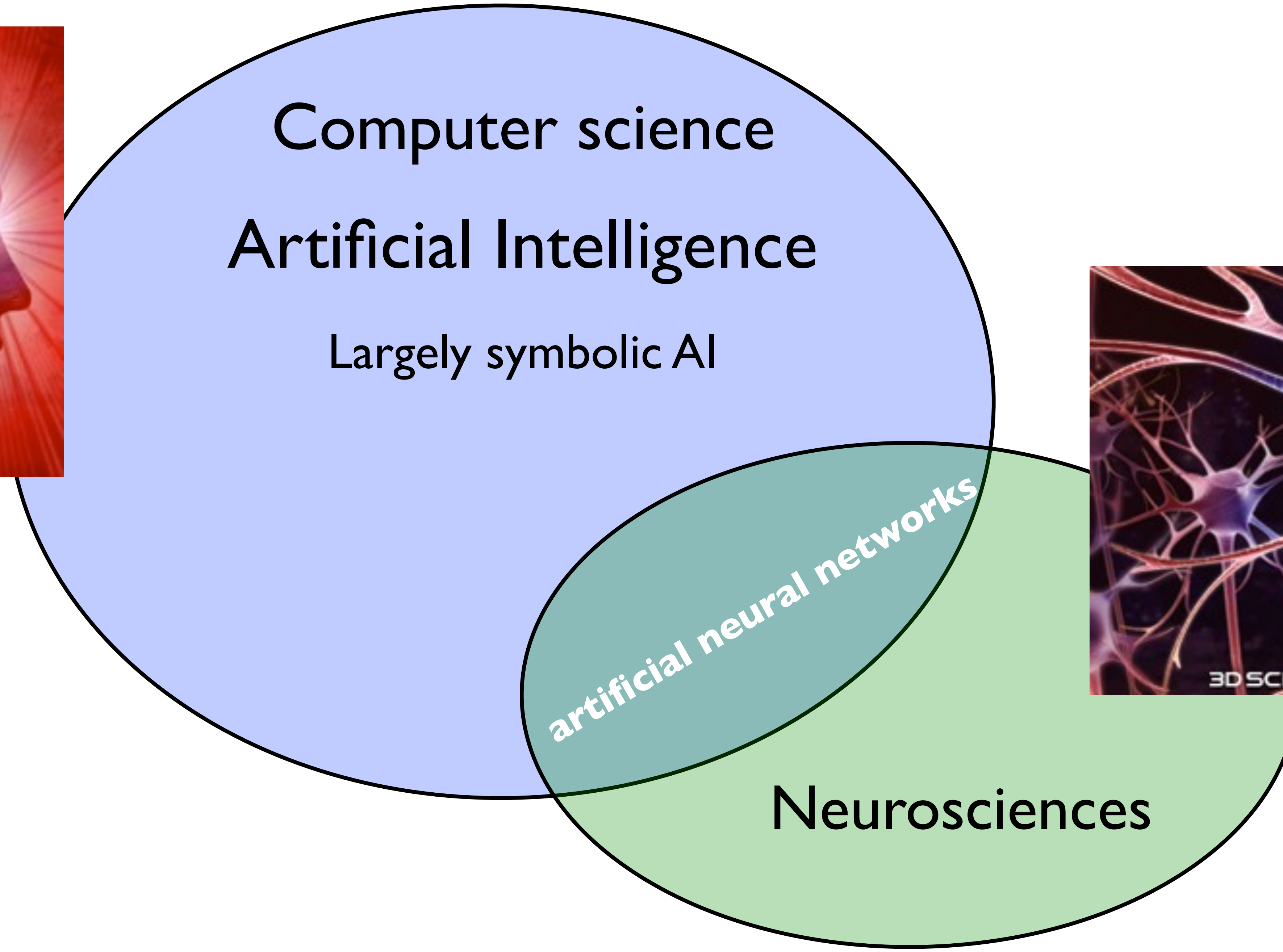
- Two historically opposed approaches to AI:

Neuroscience inspired:
➪ neural nets learning from examples for artificial perception

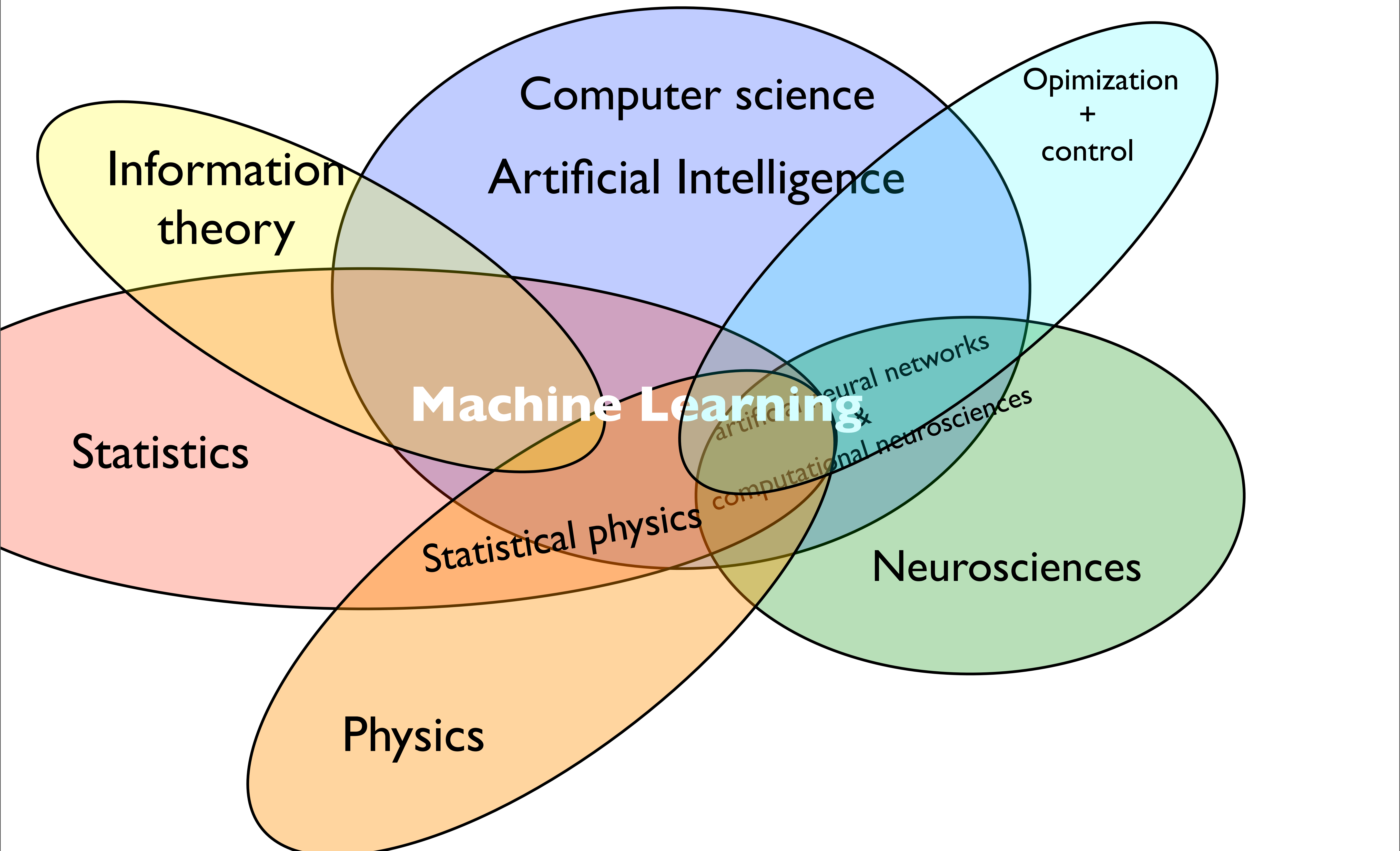
Classical symbolic AI:
Primacy of logical reasoning capabilities
➪ No learning (humans coding rules)
➪ poor handling of uncertainty
Got eventually fixed (Bayes Nets...)

Learning and probabilistic models largely won ➪ machine learning

Artificial Intelligence in the 60s



Current view of ML founding disciplines



What is machine-learning?

A (hypnotized) user's perspective

A scientific (witchcraft) field that

- researches fundamental principles (potions)
- and **develops** magical **algorithms** (spells to invoke)
- capable of leveraging collected data to (automagically) ***produce accurate*** ***predictive*** ***functions*** applicable to similar data (in the future!)

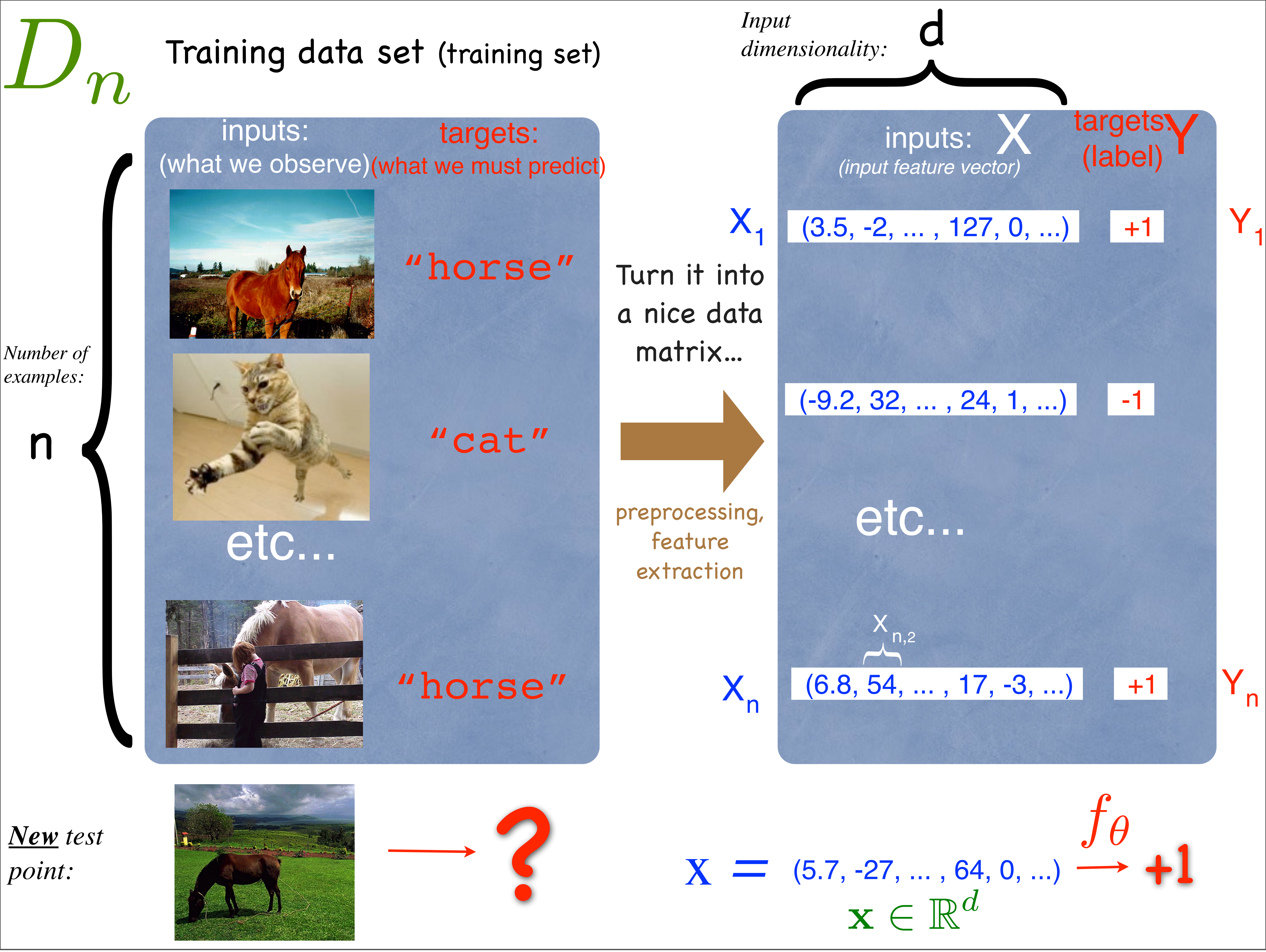
(may also yield informative *descriptive* functions of data)

The key ingredient of machine learning is...

- Collected from nature... or industrial processes.
- Comes stored in many forms (and formats...), strucutred, unstructured, occasionally clean, usually messy, ...
- In ML we like to view data as a **list of examples** (or we'll turn it into one)

➡ ideally ***many** examples* of the *same nature*.

➡ preferably with each example a *vector of numbers* (or we'll first turn it into one!)


D_n
Training data set (training set)
Input dimensionality: d
inputs: (what we observe)
targets: (what we must predict)
"horse"
"cat"
etc...
"horse"
Number of examples:
n
Turn it into a nice data matrix...
preprocessing, feature extraction
inputs: X
(input feature vector)
targets: Y (label)
X_1
(3.5, -2, ... , 127, 0, ...)
+1
Y_1
(-9.2, 32, ... , 24, 1, ...)
-1
etc...
$X_{n,2}$
X_n
(6.8, 54, ... , 17, -3, ...)
+1
Y_n
New test point:
?
$x = (5.7, -27, ... , 64, 0, ...) \xrightarrow{f_\theta} +1$
$x \in \mathbb{R}^d$

Importance of the

Problem dimensions

⇨ Détermines which learning algorithms will be practically applicable (based on their algorithmic complexity and memory requirements).

- Number of examples: **n**
  (sometimes several millions)
- Input dimensionality: **d**
  number of input features characterizing each example
  (often 100 to 1000, sometimes 10000 or much more)
- Target dimensionality ex. number of classes **m**
  (often small, sometimes huge)

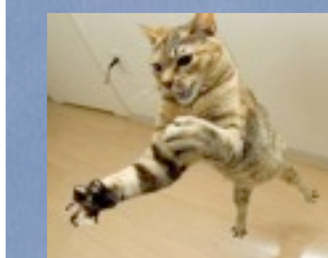
→ Data suitable for ML will often be organized as a matrix: n x (d+1) ou n x (d+m)

Turning messy data into a nice list of examples

data-plumbing

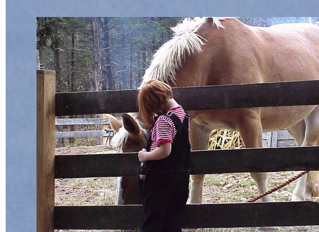
inputs: targets:

"horse



"cat

etc..

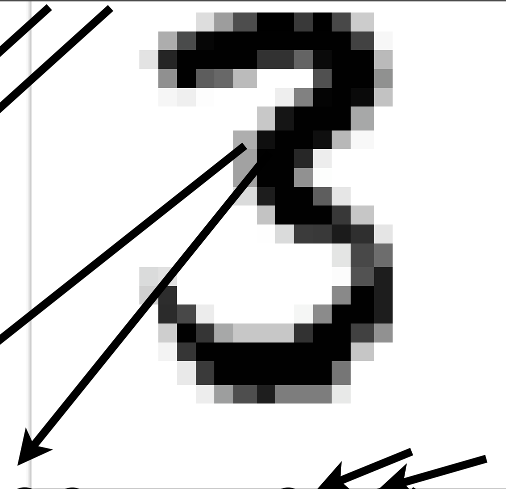


"horse

Key questions to decide what «examples» should be:

- **input:** What is **all** the (potentially relevant) **information** I will have **at my disposal** about a case **<u>when</u>** I will have to make a prediciton about it?(at test time)
- **target:** what I want to predict: Can I get my hands on <u>many</u> such examples that are actually labeled with prediciton targets?

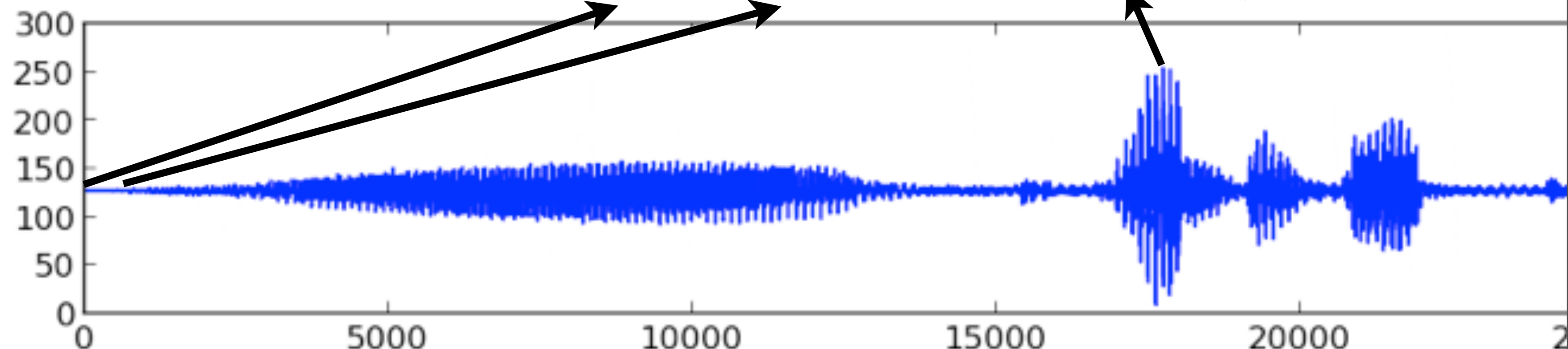
Turning an example into an input vector $\mathbf{x} \in \mathbb{R}^d$



Raw input representation:

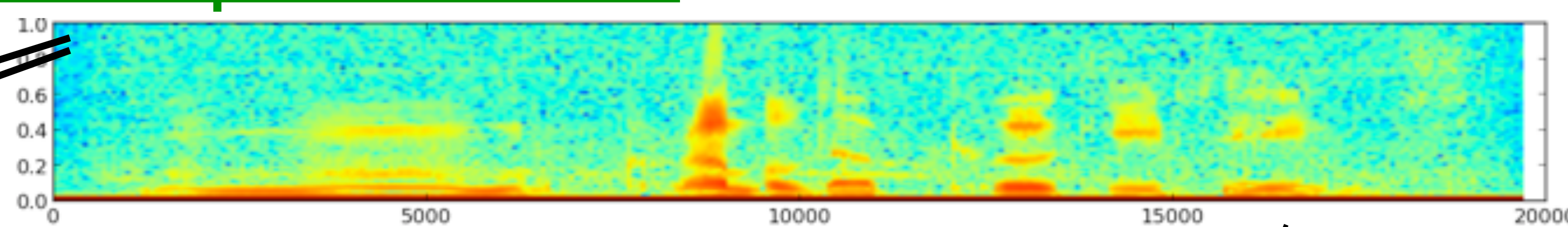
$x = (0, 0, \ldots, 54, 120, \ldots, 0, 0)$

$x = (125, 125, \ldots, 250, \ldots)$



OR some preprocessed representation:

$x = (\ ,\ \ ,\ \ ,\ \ ,\ \ldots)$



we the jumped jumping run elephant dog cat horse

Bag of words for «The cat jumped»: $x = (\ldots 0 \ldots, 0, 1, \ldots 0 \ldots, 1, 0, 0, \ldots, 0, 0, 1, 0, \ldots 0 \ldots$

OR vector of hand-engineered features:

$x = (\text{feature } 1, \ldots, \text{feature } d)$

ex: Histograms of Oriented Gradients

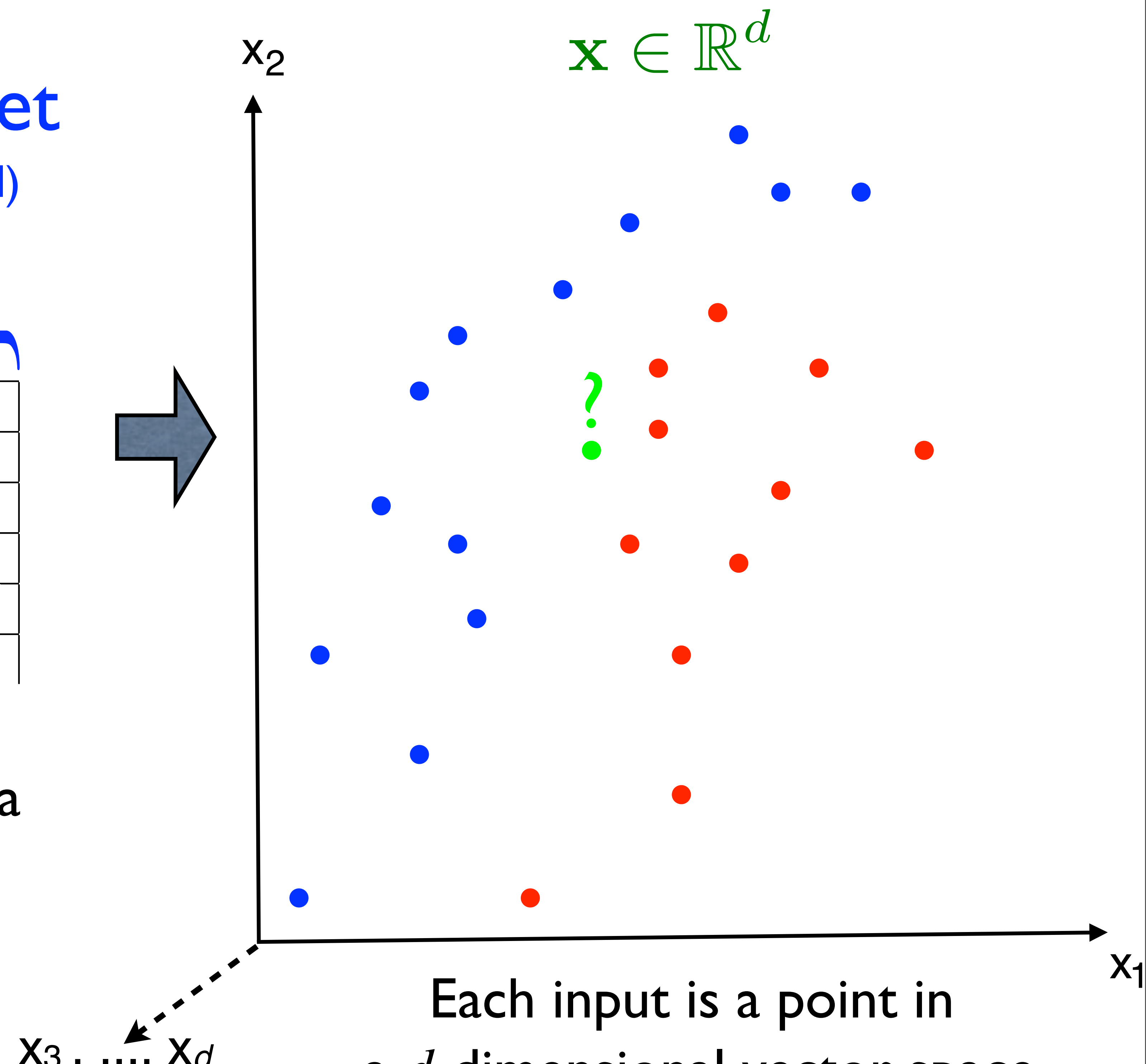
Dataset imagined as a point cloud in a *high-dimensional* vector space

input $\mathbf{x} \in \mathbb{R}^d$ | target (label) y

n examples

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$	$\mathbf{x}_5$	
0.32	-0.27	+1	0	0.82	1
-0.12	0.42	-1	1	0.22	0
0.06	0.35	-1	1	-0.37	1
0.91	-0.72	+1	0	-0.63	1
...	...	...	...	...	...

Each example (row) is now a d+1-dimensional vector



Each input is a point in a d-dimensional vector space

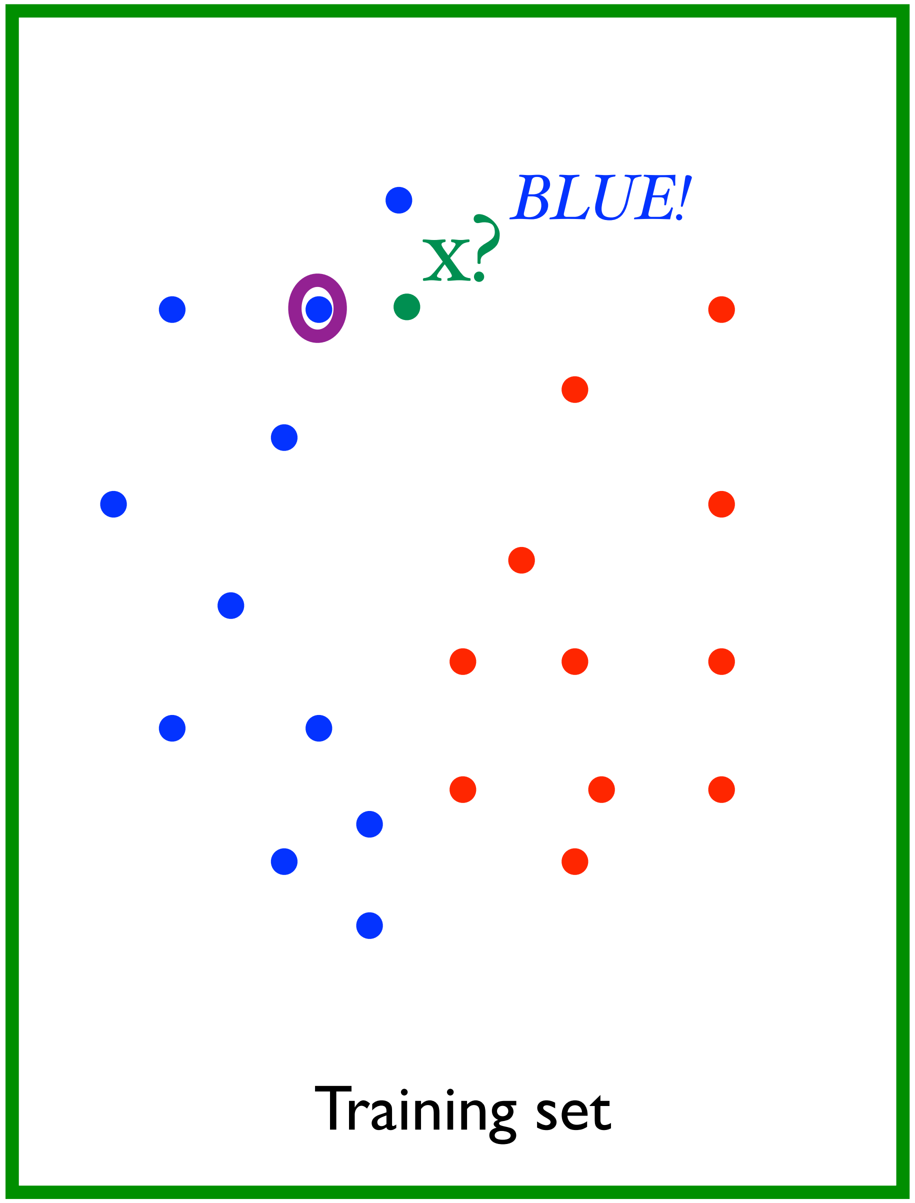
Ex: nearest-neighbor classifier

Algorithm:

For test point x:

- Find **nearest neighbor** of x among the training set according to some distance measure (eg: Euclidean distance).

- Predict that x has the same class as this nearest neighbor.



Machine learning tasks (problem types)

Supervised learning = predict a target y from input x

(and *semi*-supervised learning)

- y represents a category or "class"
  - ➠ classification — binary : $\mathbf{y} \in \{-1, +1\}$ or $\mathbf{y} \in \{0, 1\}$; multiclass : $\mathbf{y} \in \{1, m\}$ or $\mathbf{y} \in \{0, m-1\}$
- y is a real-value number
  - ➠ regression — $\mathbf{y} \in \mathbb{R}$ or $\mathbf{y} \in \mathbb{R}^m$

} Predictive models

Unsupervised learning: no explicit prediciton target y

- model the probability distribution of x
  - ➠ density estimation
- discover underlying structure in data
  - ➠ clustering
  - ➠ dimensionality reduction
  - ➠ (unsupervised) representation learning

} Descriptive modeling

Reinforcement learning: taking good sequential decisions to maximize a reward in an environment influenced by your decisions.

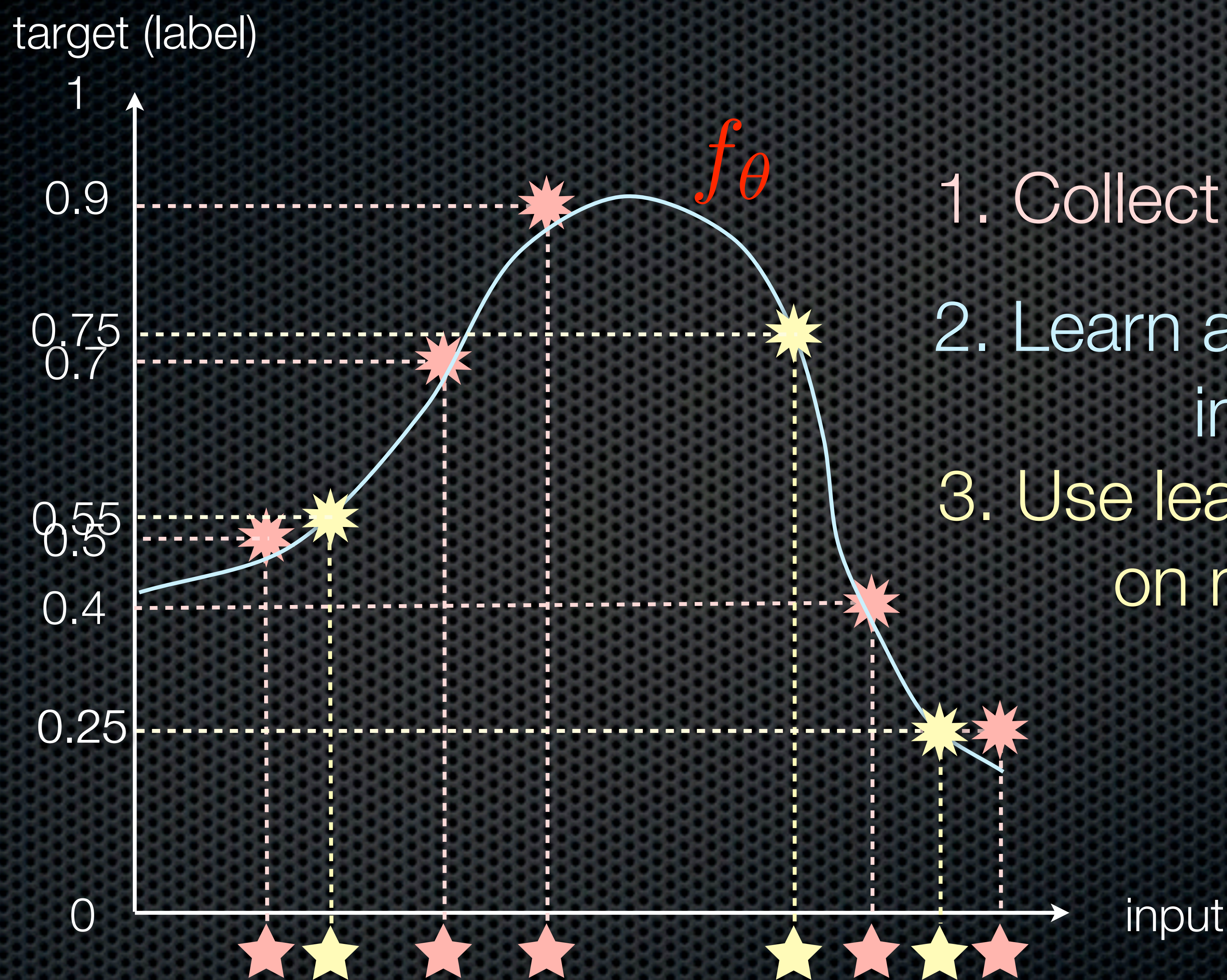
Learning phases

- **Training**: we learn a predictive function f_θ by optimizing it so that it predicts well on the training set.
- **Use** for prediction: we can then use f_θ on new (test) inputs that were not part of the training set.

⇨ The GOAL of learning is *NOT* to learn perfectly *(memorize)* the training set.

⇨ What's important is the ability for the predictor to ***generalize*** well on new (future) cases.

Ex: 1D regression



1. Collect training data
2. Learn a function (predictor)
   input → target
3. Use learned function
   on new inputs

Original slide by Olivier Delalleau

Supervised task:

predict y from x

input $\mathbf{x} \in \mathbb{R}^d$

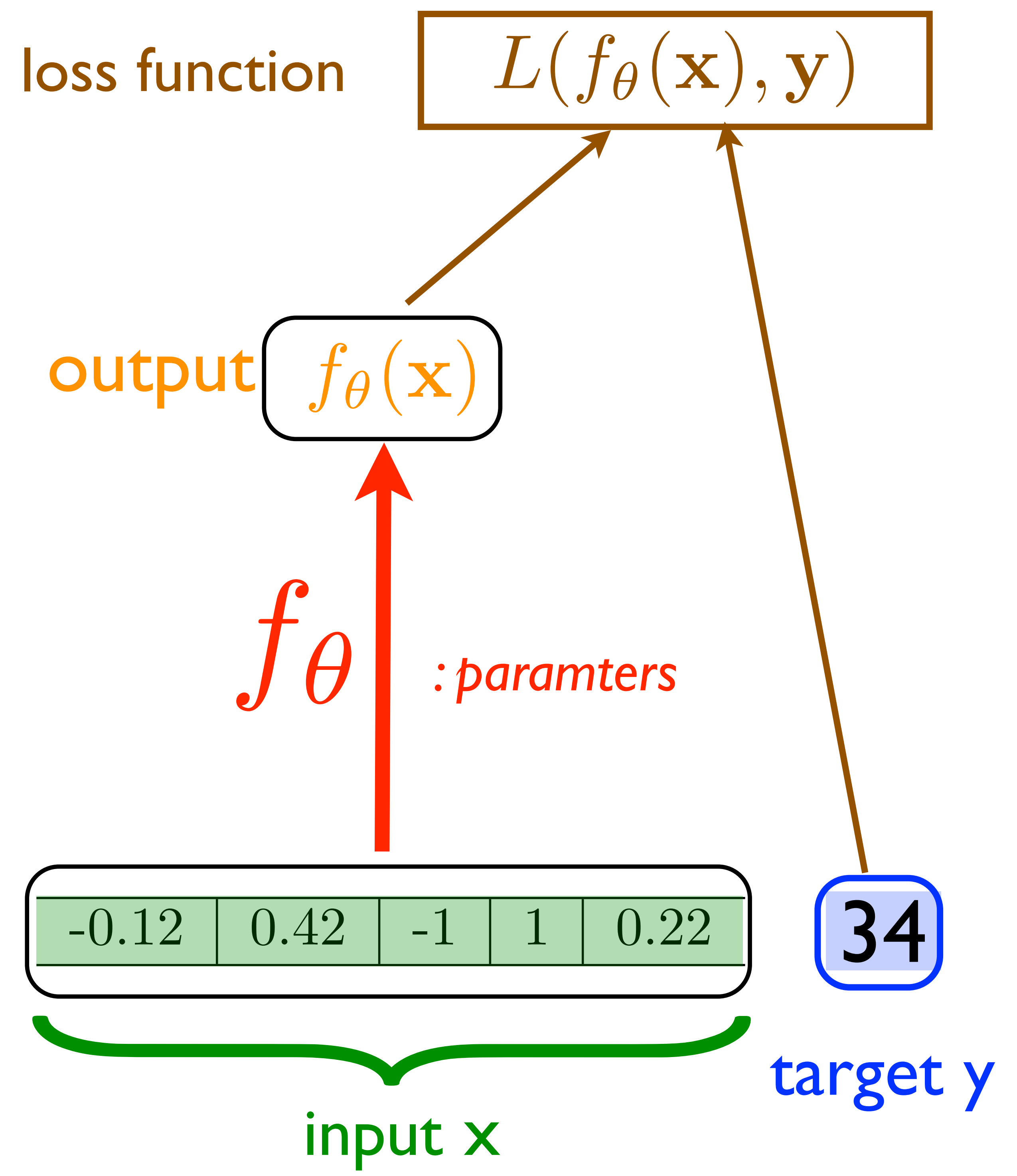
target (label) y

n examples

$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$	$\mathbf{x}_5$	t
0.32	-0.27	+1	0	0.82	113
-0.12	0.42	-1	1	0.22	34
0.06	0.35	-1	1	-0.37	56
0.91	-0.72	+1	0	-0.63	77
...	...	...	...	...	...

Training set D_n

Learn a function f_θ that will minimize prediciton errors as measured by cost (loss) L.



A machine learning algorithm usually corresponds to a combination of the following 3 elements:

(either explicitly specified or implicit)

- ✓ the choice of a specific function family: F
  (often a parameterized family)
- ✓ a way to evaluate the quality of a function $f \in F$
  (typically using a cost (or loss) function L
  mesuring how wrongly f prédicts)
- ✓ a way to search for the «best» function $f \in F$
  (typically an optimization of function parameters to minimize the overall loss over the training set).

Evaluating the quality of a function $f \in F$

and

Searching for the «best» function $f \in F$

Evaluating a predictor $f(x)$

The performance of a predictor is often evaluated using **several** different evaluation metrics:

- Evaluations of true quantities of interest ($ saved, #lifes saved, ...) when using predictor inside a more complicated system.
- «Standard» evaluation metrics in a specific field (e.g. BLEU (Bilingual Evaluation Understudy) scores in translation)
- Misclassification error rate for a classifier (or precision and recall, or F-score, ...).
- The loss actually being optimized by the ML algorithm (often different from all the above...)

Standard loss-functions

- For a density estimation task: $f : \mathbb{R}^d \to \mathbb{R}^+$ a proper probability mass or density function

  negative log likelihood loss: $L(f(x)) = -\log f(x)$

- For a regression task: $f : \mathbb{R}^d \to \mathbb{R}$

  squared error loss: $L(f(x), y) = (f(x) - y)^2$

- For a classification task: $f : \mathbb{R}^d \to \{0, \ldots, m-1\}$

  misclassification error loss: $L(f(x), y) = I_{\{f(x) \neq y\}}$

Surrogate loss-functions

- For a classification task: $f : \mathbb{R}^d \rightarrow \{0, \ldots, m-1\}$

  misclassification error loss: $L(f(x), y) = I_{\{f(x) \neq y\}}$

Problem: it is hard to *optimize* the misclassification loss directly

(gradient is 0 everywhere. NP-hard with a linear classifier) Must use a surrogate loss:

	Binary classifier	Multiclass classifier
Probabilistic classifier	Outputs probability of class 1 $g(x) \approx P(y=1 \mid x)$ Probability for class 0 is $1-g(x)$ Binary cross-entropy loss: $L(g(x),y) = -(y \log(g(x)) + (1-y) \log(1-g(x))$ Decision function: $f(x) = I_{g(x)>0.5}$	Outputs a vector of probabilities: $g(x) \approx (P(y=0 \mid x), \ldots, P(y=m-1 \mid x))$ Negated conditional log likelihood loss $L(g(x),y) = -\log g(x)_y$ Decision function: $f(x) = \operatorname{argmax}(g(x))$
Non-probabilistic classifier	Outputs a «score» $g(x)$ for class 1. score for the other class is $-g(x)$ Hinge loss: $L(g(x),t) = \max(0, 1-tg(x))$ where $t=2y-1$ Decision function: $f(x) = I_{g(x)>0}$	Outputs a vector $g(x)$ of real-valued scores for the m classes. Multiclass margin loss $L(g(x),y) = \max(0,1+\max_{k \neq y}(g(x)_k)-g(x)_y)$ Decision function: $f(x) = \operatorname{argmax}(g(x))$

Expected risk v.s. Empirical risk

Examples (x,y) are supposed drawn i.i.d. from an unknown true distribution $p(x,y)$ (from nature or industrial process)

- Generalization error = Expected risk (or just «Risk»)
  «how poorly we will do on average on the infinity of future examples from that unknown distribution»

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

- Empirical risk = average loss on a finite dataset
  «how poorly we're doing on average on this finite dataset»

$$\hat{R}(f,D) = \frac{1}{|D|} \sum_{(\mathbf{x},\mathbf{y})\in D} L(f(\mathbf{x}),\mathbf{y})$$

where $|D|$ is the number of examples in D

Empirical risk minimization

Examples (x,y) are supposed drawn i.i.d. from an unknown true distribution p(x,y) (nature or industrial process)

- We'd love to find a predictor that minimizes the generalization error (the expected risk)
- But can't even compute it! (expectation over unknown distribution)
- Instead: **Empirical risk minimization principle**
  «Find predictor that minimizes average loss over a trainset»

$$\hat{f}(D_{\text{train}}) = \underset{f \in F}{\operatorname{argmin}}\, \hat{R}(f, D_{\text{train}})$$

This is the training phase in ML

Evaluating the generalization error

- We can't compute expected risk $R(f)$
- But $\hat{R}(f, D)$ is a good estimate of $R(f)$ provided:
  - D was not used to find/choose f
    otherwise estimate is biased ⇨ can't be the training set!
  - D is large enough (otherwise estimate is too noisy); drawn from p

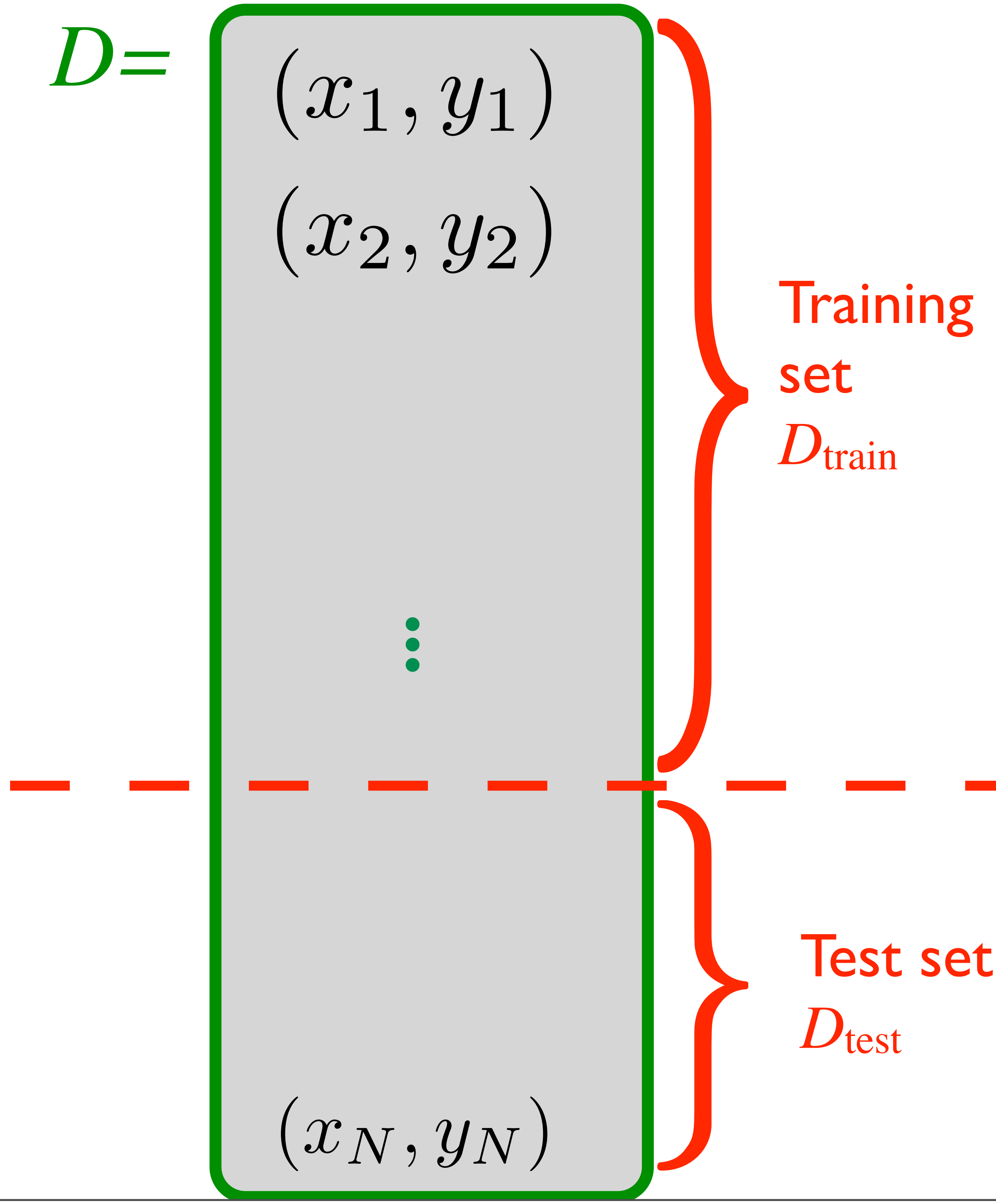
➡ Must keep a separate test-set $D_{\text{test}} \neq D_{\text{train}}$ to properly estimate generalization error of $\hat{f}(D_{\text{train}})$:

$$R(\hat{f}(D_{\text{train}})) \approx \hat{R}(\hat{f}(D_{\text{train}}), D_{\text{test}})$$

generalization error | average error on **test**-set (never used for training)

This is the <u>test</u> phase in ML

Simple train/test procedure



- Provided large enough dataset D drawn from $p(\mathrm{x,y})$
- Make sure examples are in random order.
- Split dataset in **two:** D_{train} and D_{test}
- Use D_{train} to choose/ optimize/find best predictor $f = \hat{f}(D_{\text{train}})$
- Use D_{test} to evaluate generalization performance of predictor f.

Model selection

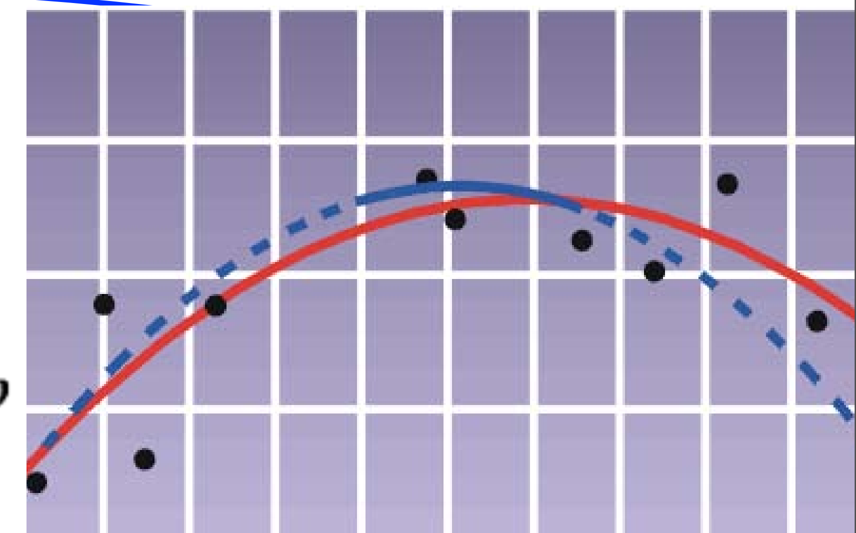
Choosing a specific function family F

Ex. of parameterized function families

$F_{polynomial\ p}$

Polynomial predictor (of degree p):

$$f(x) = b + a_1 x + a_2 x^2 + a_3 x^3 + \ldots + a_p x^p$$



F_{linear}

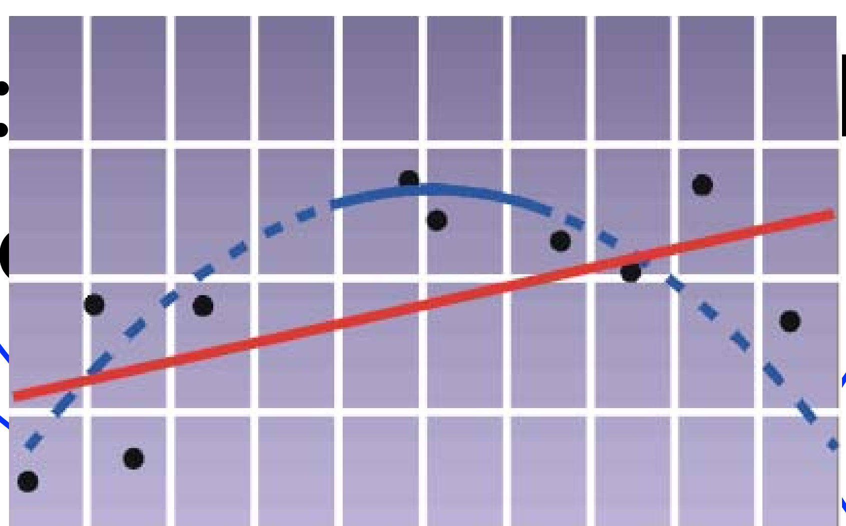
Linear (affine) predictor: $f_\theta(x) = wx + b$ (in 1 dimension)

(«linear regression») $f_\theta(x) = w^T x + b$ (in d dimensions)

$$\theta = \{w \in \mathbb{R}^d, b \in \mathbb{R}\}$$

Q: ... lest

pr...



F_{const}

Constant predictor: $f_\theta(x)=b$

where $\theta=\{b\}$

(always predict the same value or class!)

Capacity of a learning algorithm

- Choosing a specific Machine Learning algorithm means choosing a specific function family F.
- How «big, rich, flexible, expressive, complex» that family is, defines what is informally called the «capacity» of the ML algorithm.

  Ex: capacity($F_{polynomial\ 3}$) > capacity(F_{linear})
- One can come up with <u>several</u> formal measures of «capacity» for a function family / learning algorithm (e.g. VC-dimension Vapnik–Chervonenkis)
- One rule-of-thumb estimate, is the number of adaptable parameters: i.e. how many *scalar* values are contained in θ.

  Notable exception: chaining many linear mappings is still a linear mapping!

Effective capacity, and capacity-control hyper-parameters

The «effective» capacity of a ML algo is controlled by:

- Choice of ML algo, which determines big family F
- Hyper-parameters that further specify F
  e.g.: degree p of a polynomial predictor; Kernel choice in SVMs;
  #of layers and neurons in a neural network
- Hyper-parameters of «regularization» schemes
  e.g. constraint on the norm of the weights w
  (⇨ ridge-regression; L_2 weight decay in neural nets);
  Bayesian prior on parameters; noise injection (dropout); ...
- Hyper-parameters that control early-stopping of the iterative search/optimization procedure.
  (⇨ won't explore as far from the initial starting point)

Popular classifiers

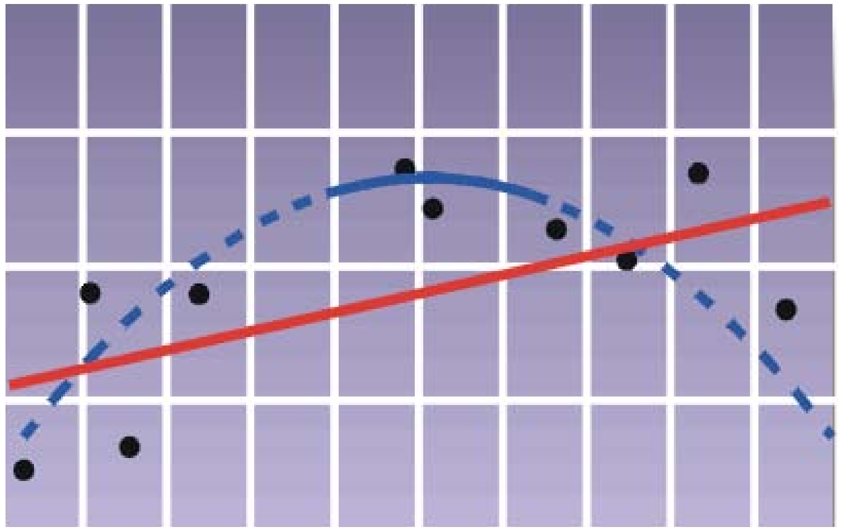
their parameters and hyper-parameters

Algo	**Capacity-control hyperparameters**	**Learned parameters**
logistic regression (L2 regularized)	strength of L2 regularizer	w,b
linear SVM	C	w,b
kernel SVM	C; kernel choice & params (σ for RBF; degree for polynomal)	support vector weights: α
neural network	layer sizes; early stop; ...	layer weight matrices
decision tree	depth	the tree (with index and threshold of variables)
k-nearest neighbors	k; choice of metric	memorizes trainset

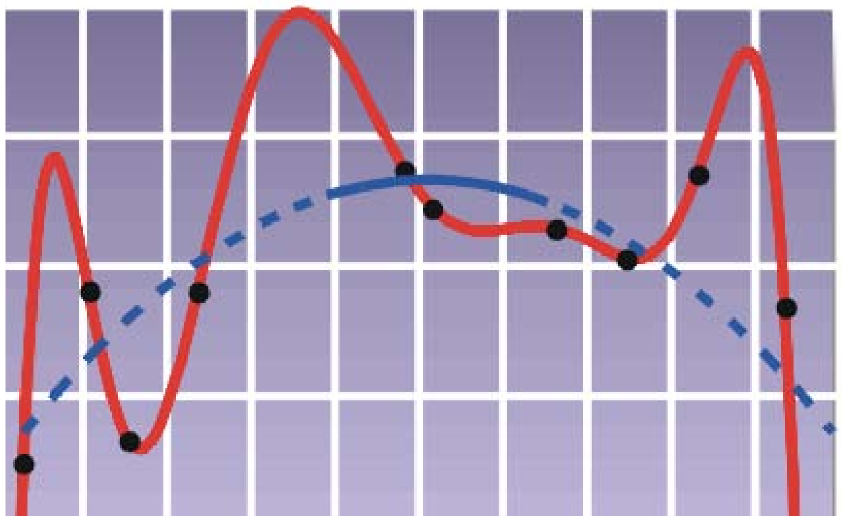
Tuning the capacity

- Capacity must be optimally tuned to ensure good generalization
- by choosing Algorithm and hyperparameters
- to avoid under-fitting and over-fitting.

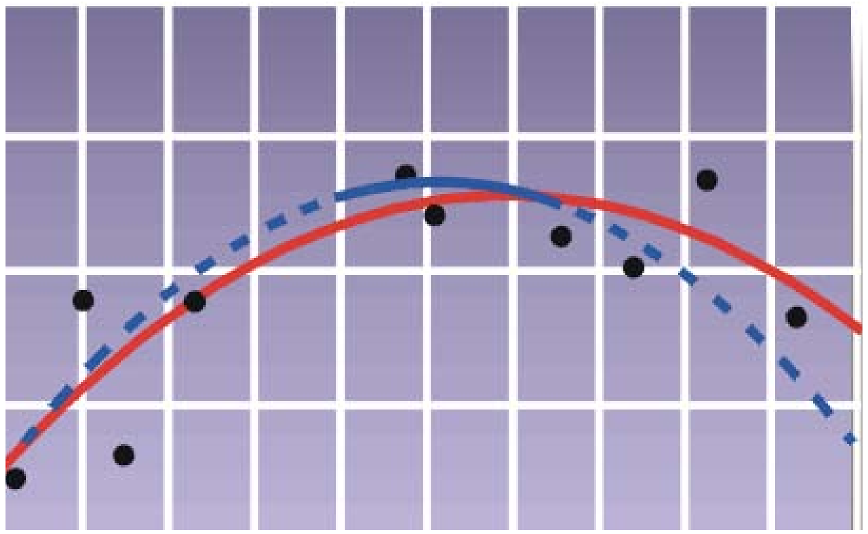
Ex: 1D regression with polynomial predictor



capacity too low
⇨under-fitting



capacity too high
⇨over-fitting



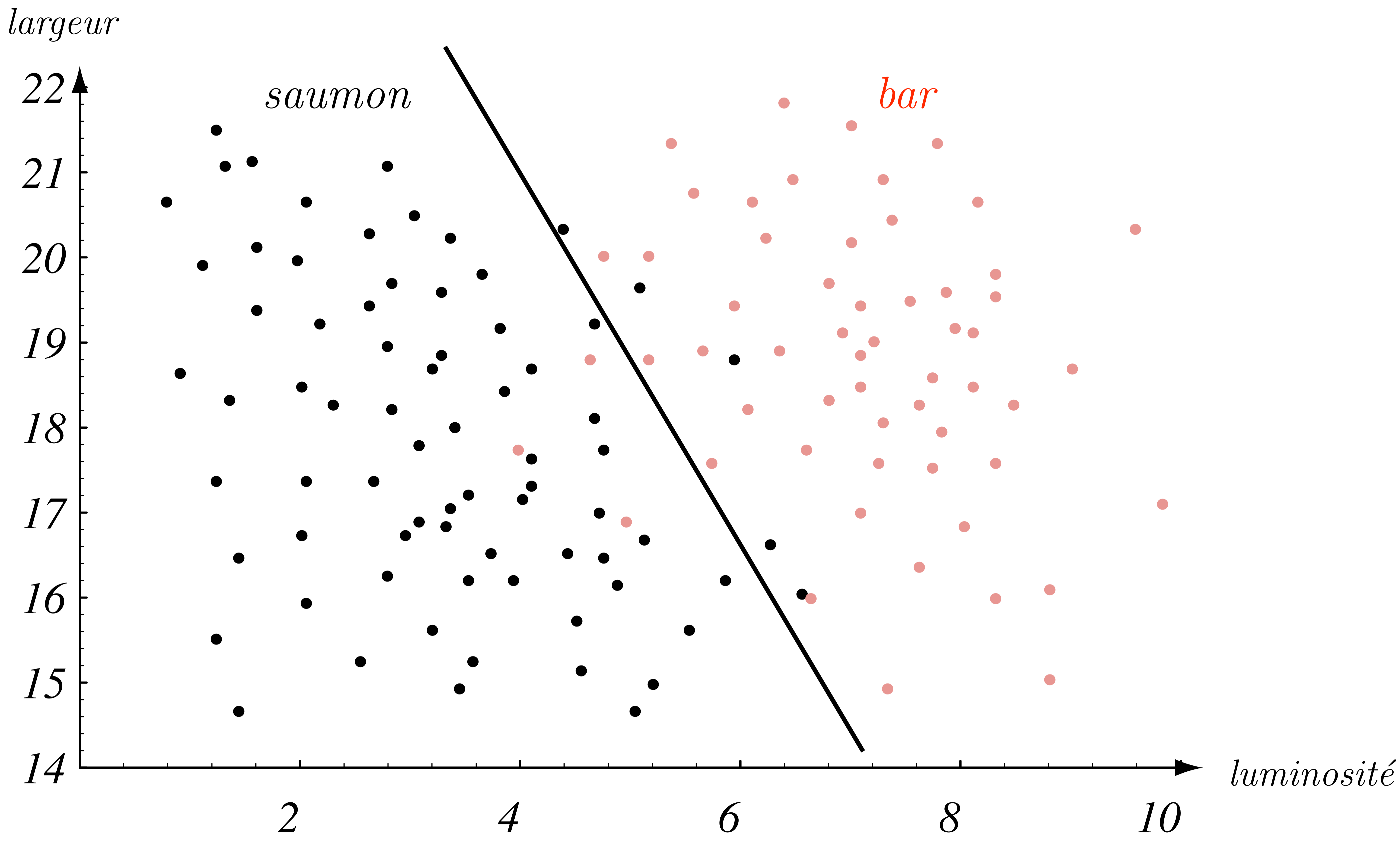
optimal capacity
⇨good generalisation

performance on training set is not a good estimate of generalization

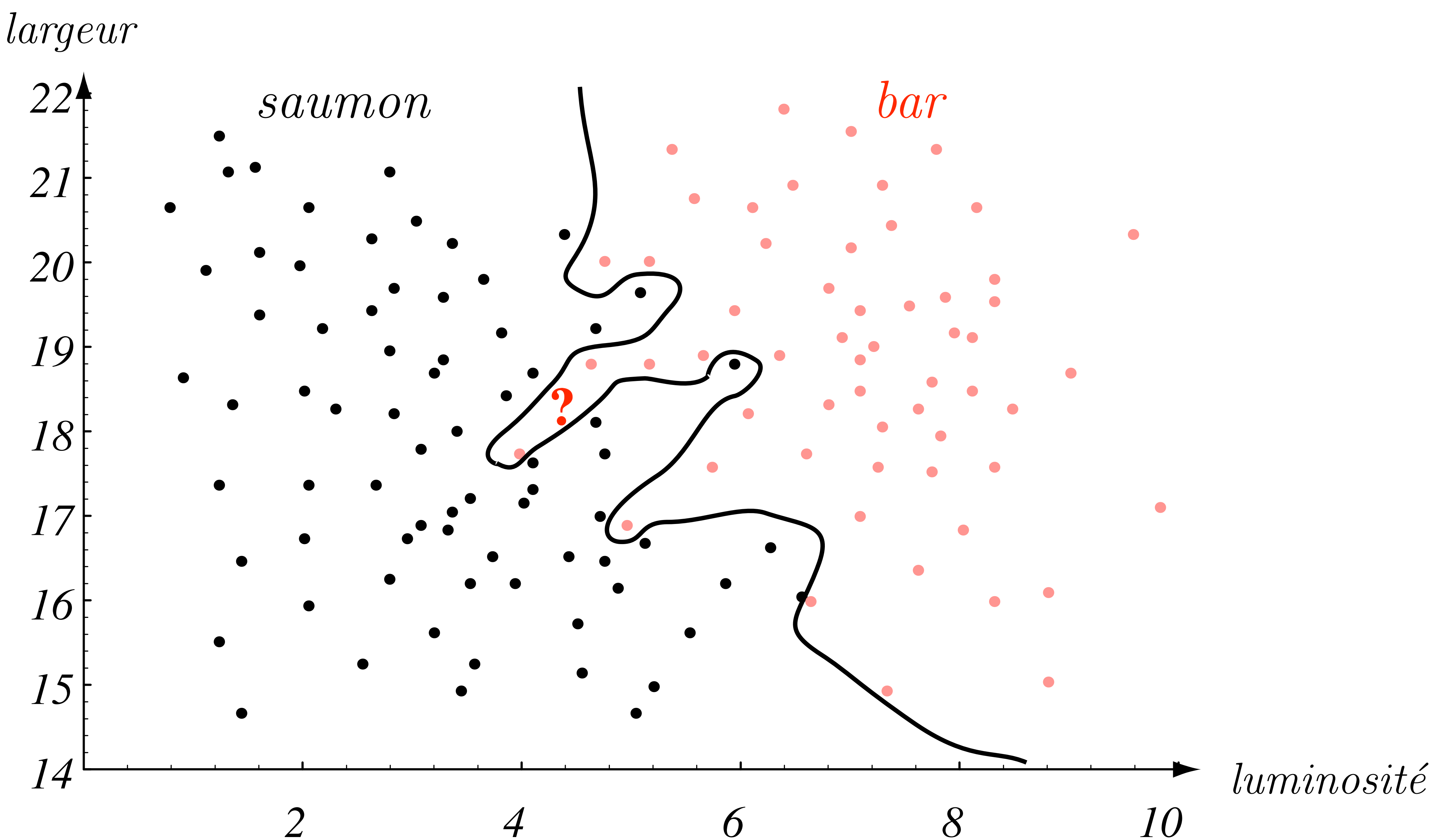
Ex: 2D classification

Linear classifier

- Function family too poor
  (too inflexible)
- = **Capacity too low** for this problem
  (relative to number of examples)
- => Under-fitting

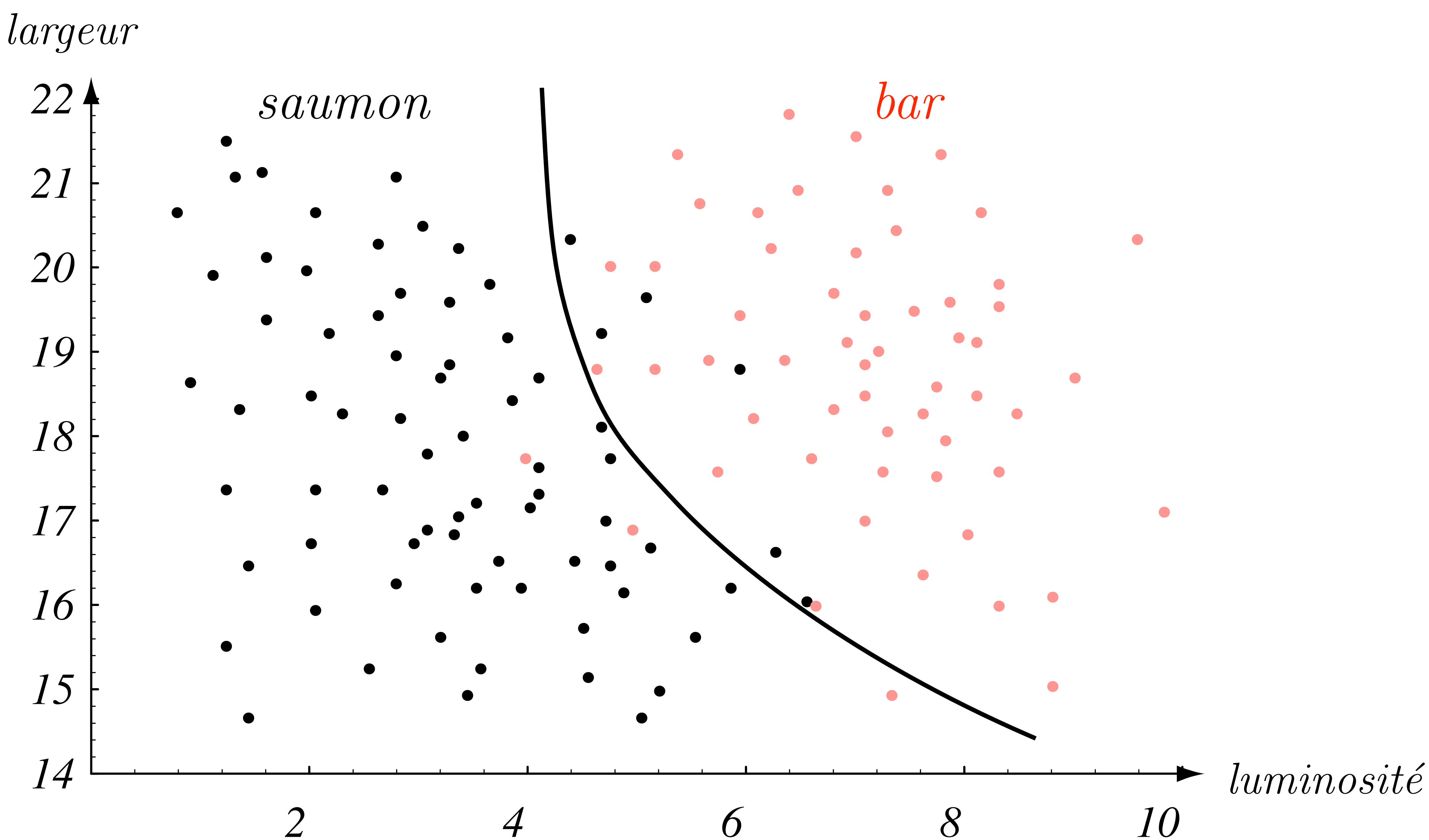


- Function family too rich
  (too flexible)
- = **Capacity too high** for this problem
  (relative to the number of examples)
- => Over-fitting

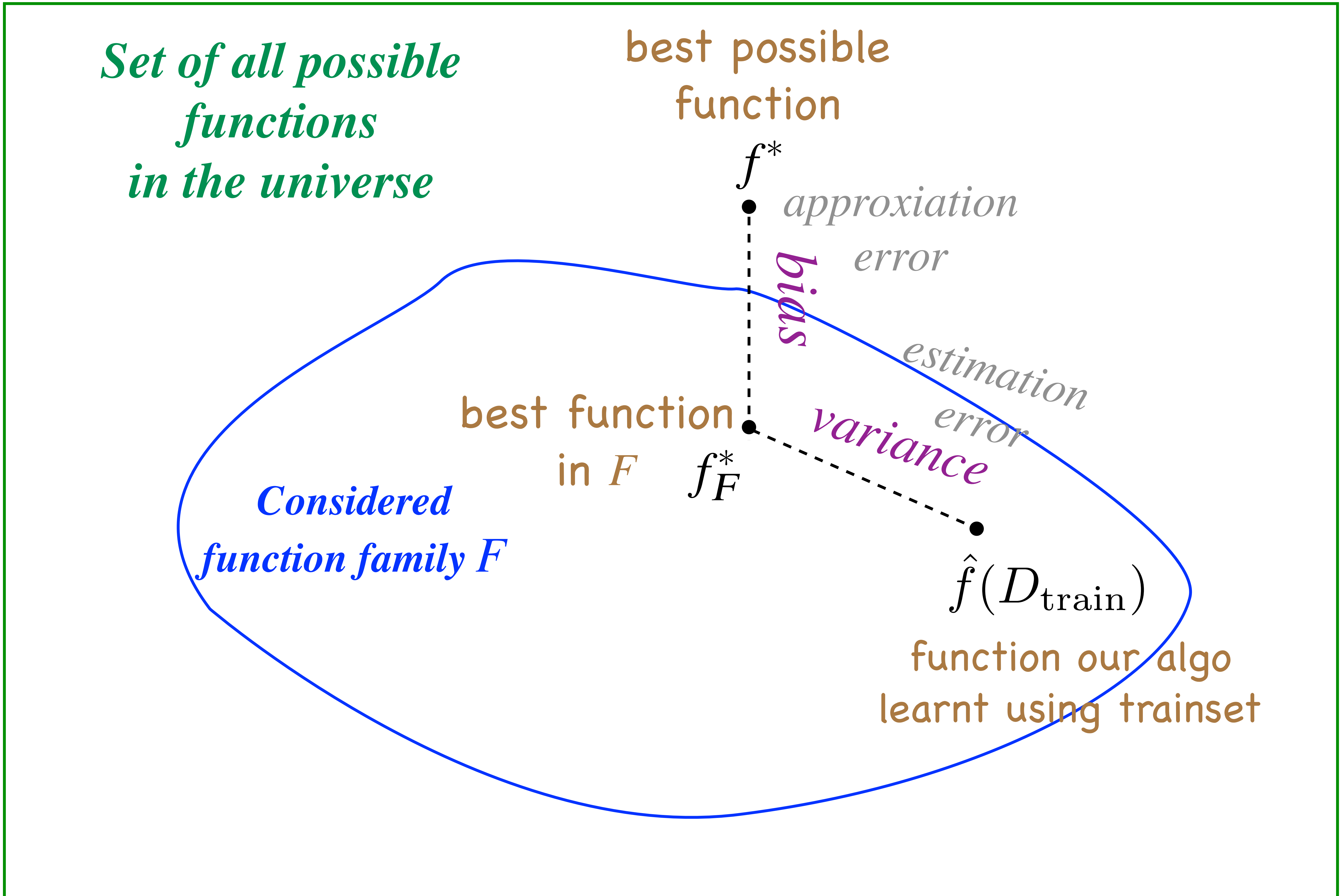


Nombre d'erreurs d'entrainement: 0

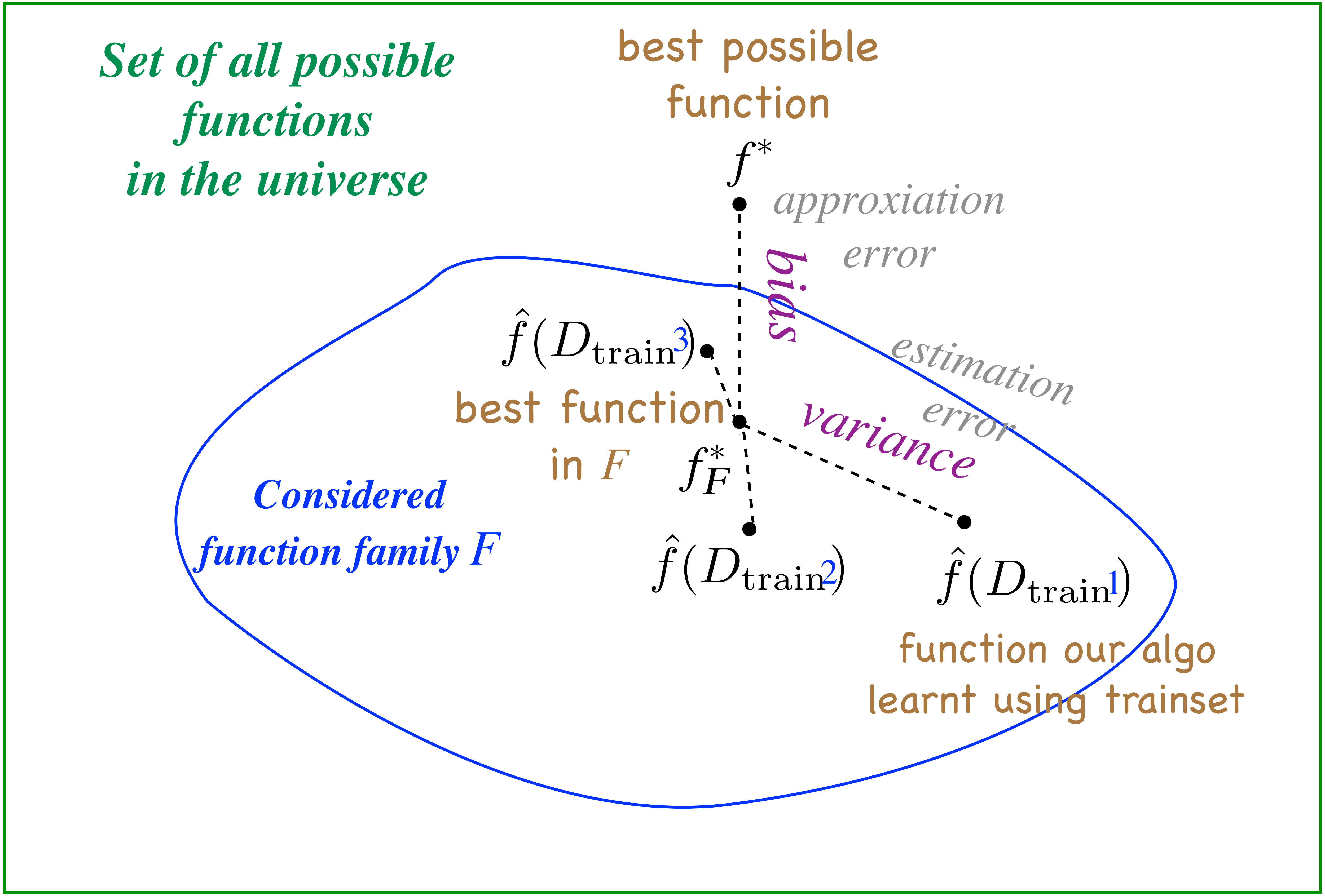
- **Optimal capacity** for this problem
  (par rapport à la quantité de données)
- => Best generalization
  (on future test points)



Decomposing the generalization error



What is responsibe for the variance?



Optimal capacity
& the biais-variance dilemma

- Choosing richer F: capacity ↑
  ➪ bias ↓ *but* variance ↑.
- Choosing smaller F : capacity ↓
  ➪ variance ↓ *but* bias ↑.
- Optimal compromise... will depend on number of examples ***n***
- Bigger ***n*** ➪ variance ↓
  So we can afford to increase capacity (to lower the bias)
  ➪ can use more expressive models
- The best regularizer is more data!

Model selection how to

Make sure examples are in random order

Split data D in 3: D_{train} D_{valid} D_{test}

$D=$

(x_1, y_1)

(x_2, y_2)

⋮

(x_N, y_N)

Training set D_{train}

Validation set D_{valid}

Test set D_{test}

Model selection meta-algorithm:

For each considered model (ML algo) $\mathbf{A}$:

For each considered hyper-parameter config λ:

- train model $\mathbf{A}$ with hyperparams λ on D_{train}

$$\hat{f}_{\mathbf{A}_\lambda} = \mathbf{A}_\lambda(D_{\text{train}})$$

- evaluate resulting predictor on D_{valid} (with preferred evaluation metric)

$$e_{\mathbf{A}_\lambda} = \hat{R}(\hat{f}_{\mathbf{A}_\lambda}, D_{\text{valid}})$$

Locate $\mathbf{A}^*, \lambda^*$ that yielded best $e_{\mathbf{A}_\lambda}$

Either return $f^* = f_{\mathbf{A}^*_{\lambda^*}}$

Or retrain and return

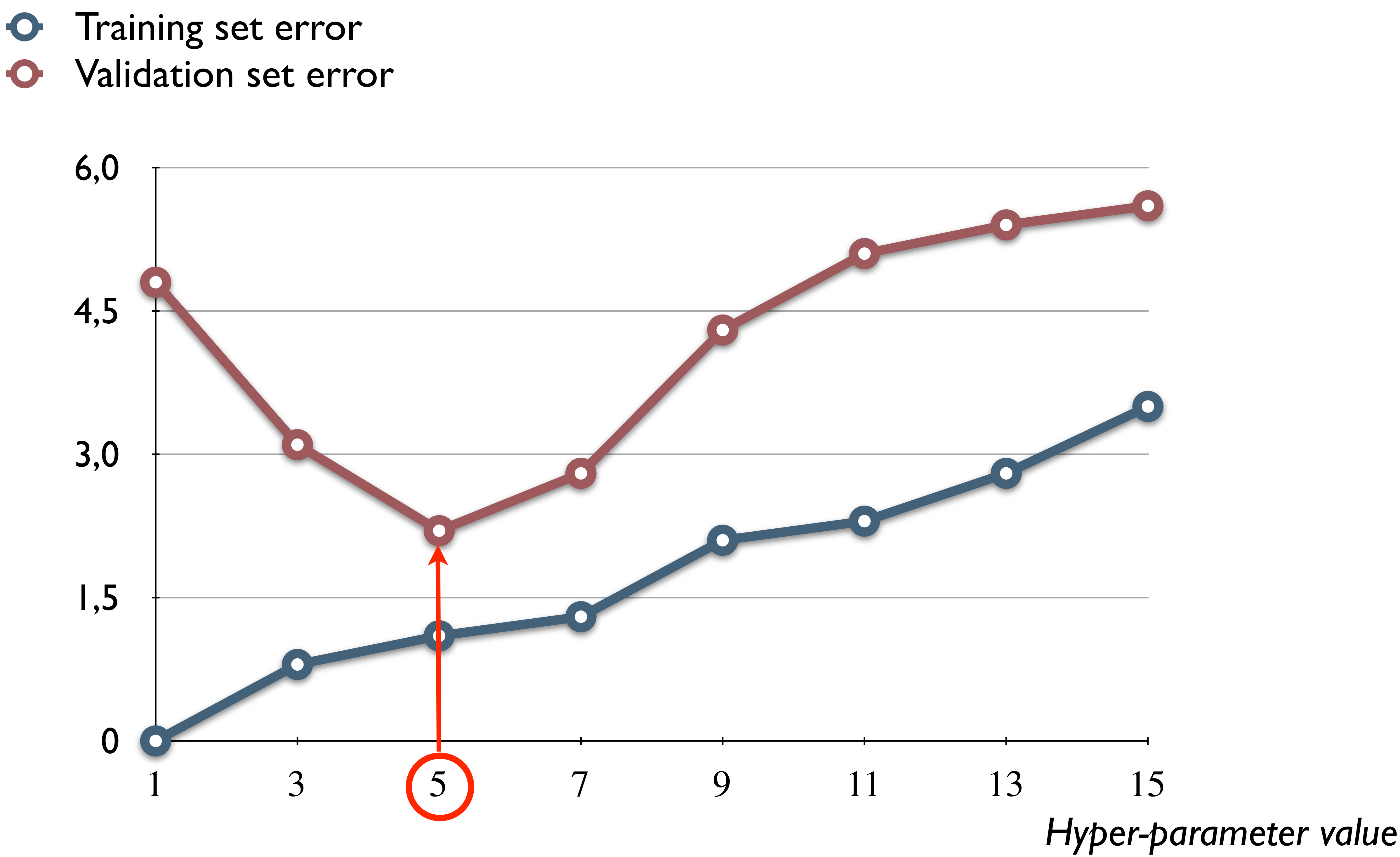
$$f^* = \mathbf{A}^*_{\lambda^*}(D_{\mathbf{train}} \cup D_{\mathbf{valid}})$$

Finally: compute unbiased estimate of generalization performance of f^* using D_{test}

$$\hat{R}(f^*, D_{\mathbf{test}})$$

D_{test} must never have been used during training or model selection to select, learn, or tune anything.

Ex of model *hyper-parameter* selection



Hyper-parameter value which yields smallest error on validaiton set is 5
(it was 1 for the training set)

Question

What if we selected capacity-control hyper-parameters that yield best performance on the training set?

What would we tend to select?

Is it a good idea? Why?

Model selection procedure summary:

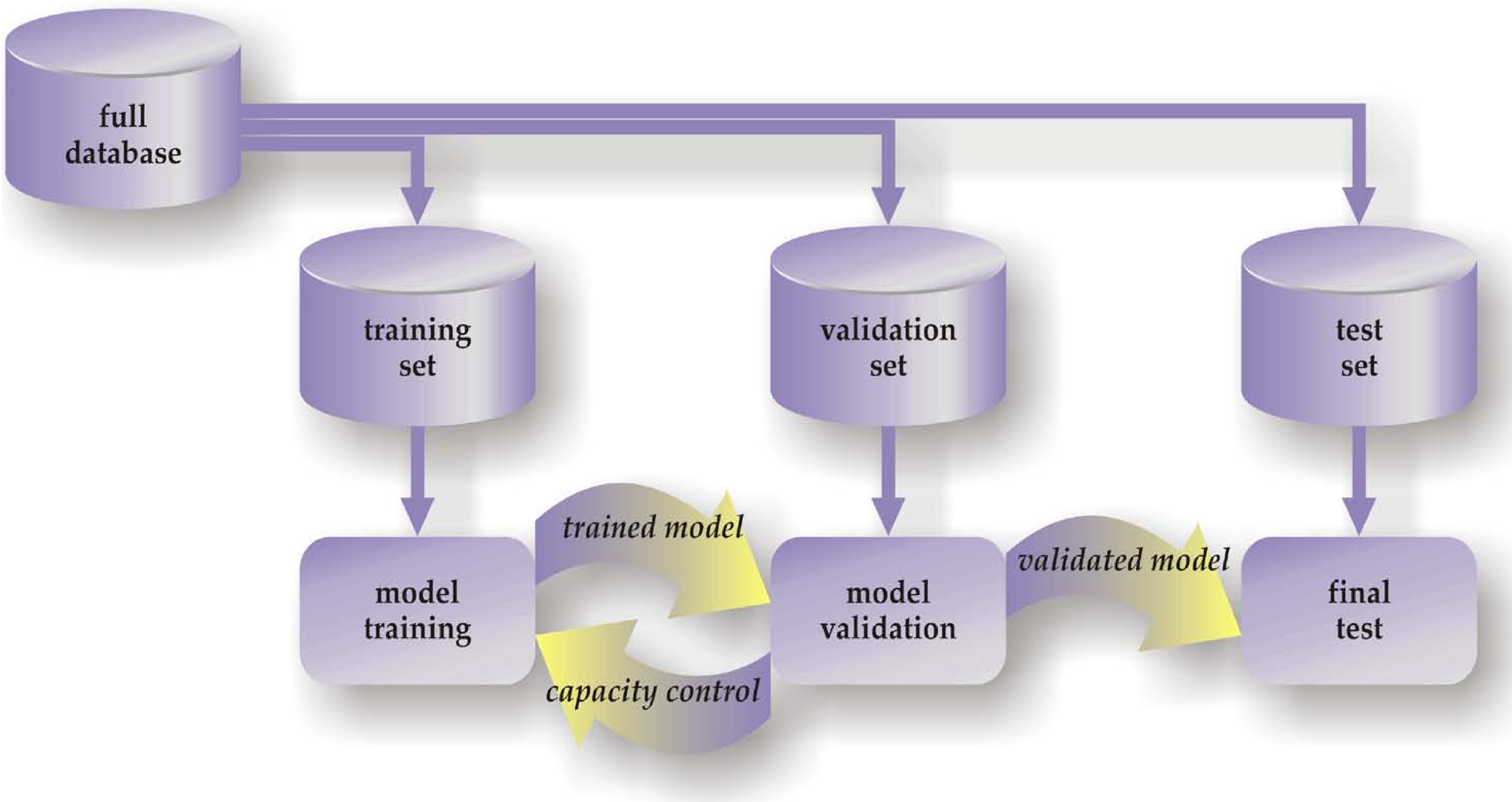
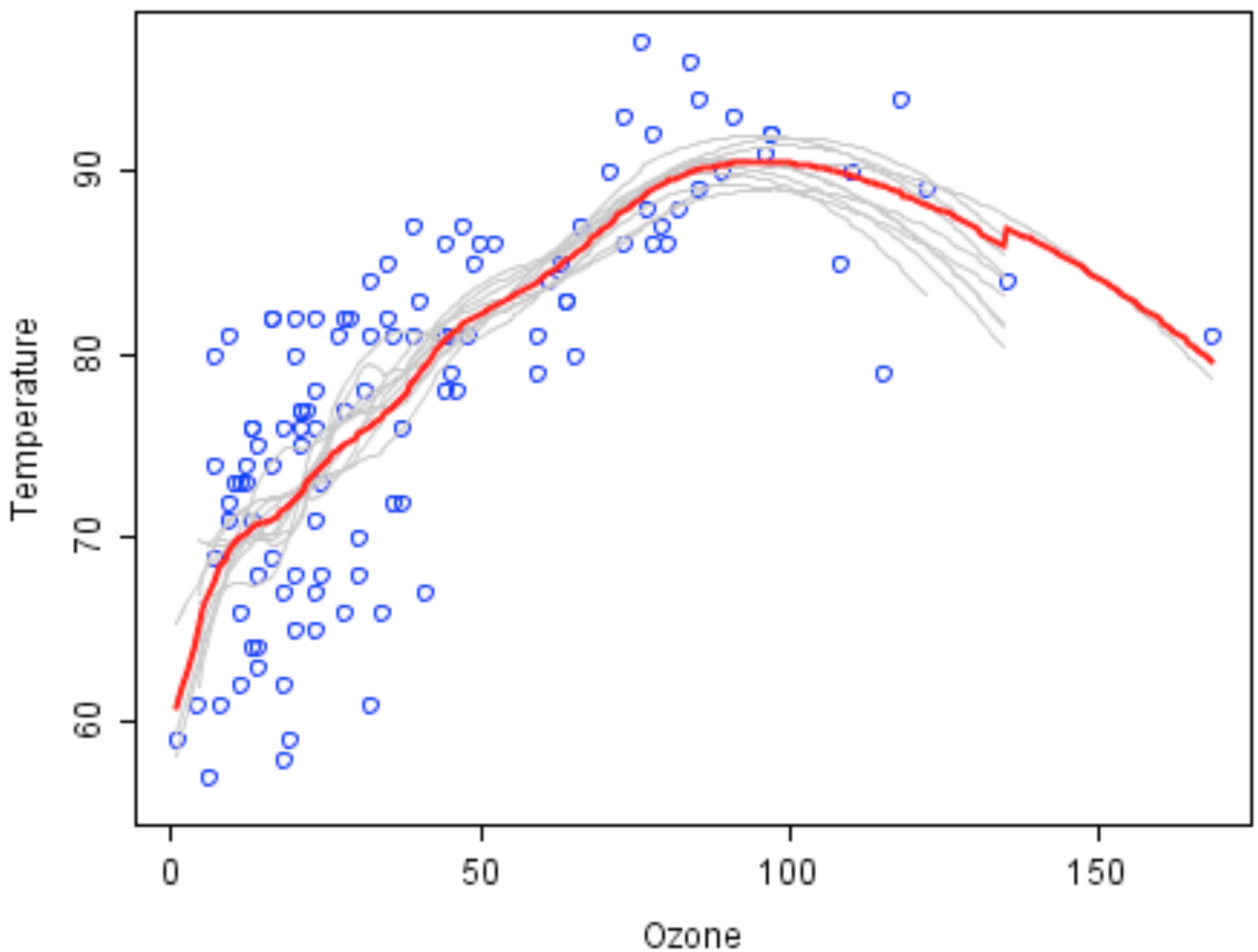


Figure by Nicolas Chapados

Ensemble methods

- Principle: train and combine multiple predictors to good effect
- Bagging: average many high-variance predictors
  ➪ variance ↓
  (e.g.: average deep trees ➪ Random decision forests)
- Boosting: build weighted combination of low-capacity classifiers
  ➪ bias ↓ and capacity ↑
  (e.g. boosting shallow trees; or linear classifiers)

Bagging
for reducing variance on a regression problem



How to obtain non-linear predictor with a linear predictor

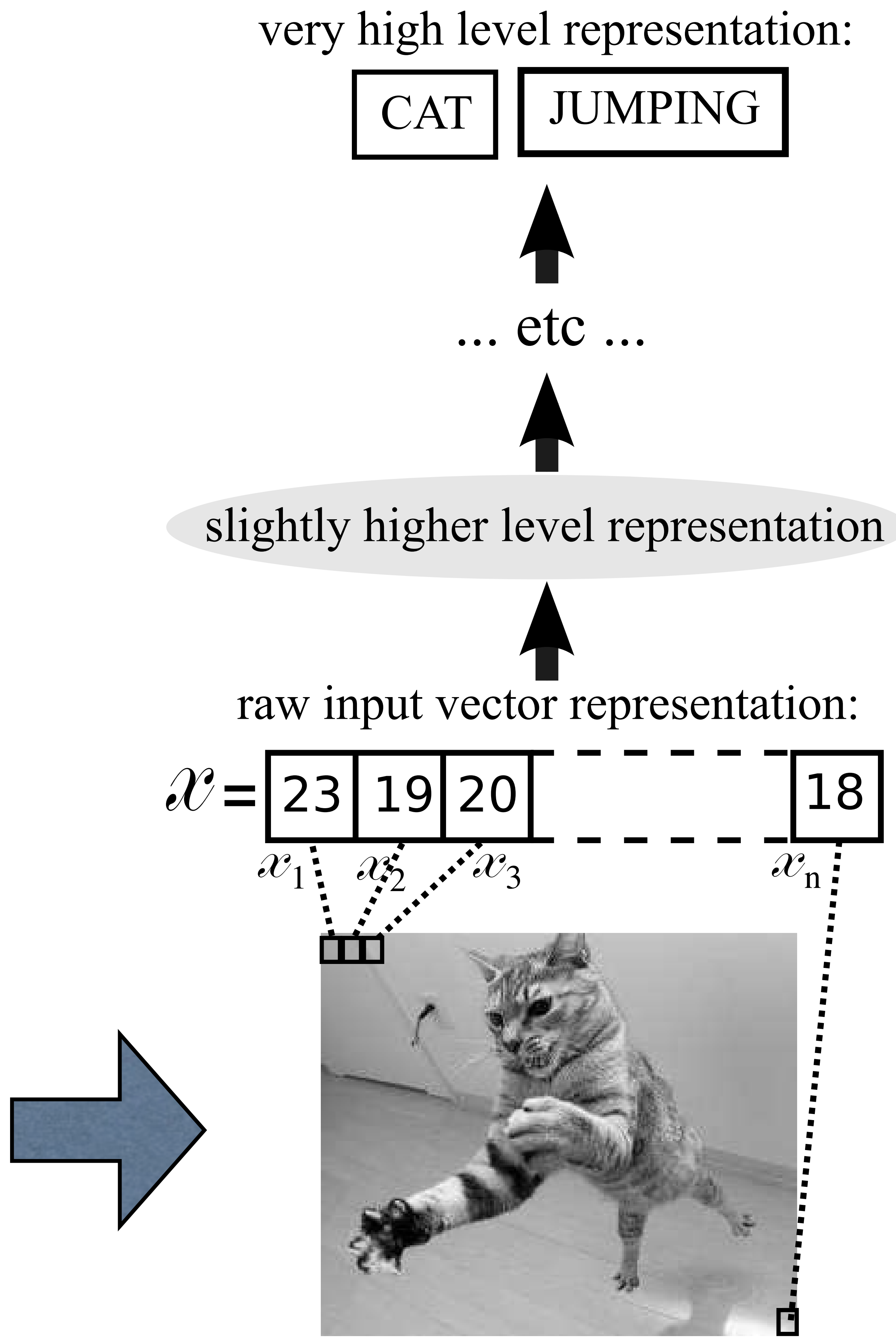
Three ways to map x to a feature representation $\tilde{\mathbf{x}} = \phi(\mathbf{x})$

- Use an explicit fixed mapping (ex: hand-crafted features)

- Use an implicit fixed mapping
  ➠Kernel Methods (SVMs, Kernel Logistic Regression ...)

- Learn a parameterized mapping
  (i.e. let the ML algo learn the new representation)
  ➠ Multilayer feed-forward Neural Networks
  such as Multilayer Perceptrons (MLP)

Levels of representation



Questions ?