Introduction to Machine Learning

based on slides of

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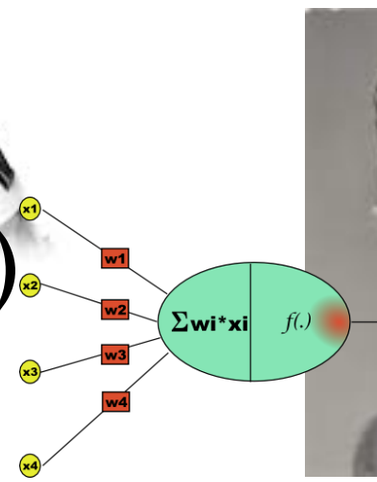
What is machine learning ?

Historical perspective

- Born from the ambitious goal of **Artificial Intelligence**

- <u>Founding project:</u>
  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

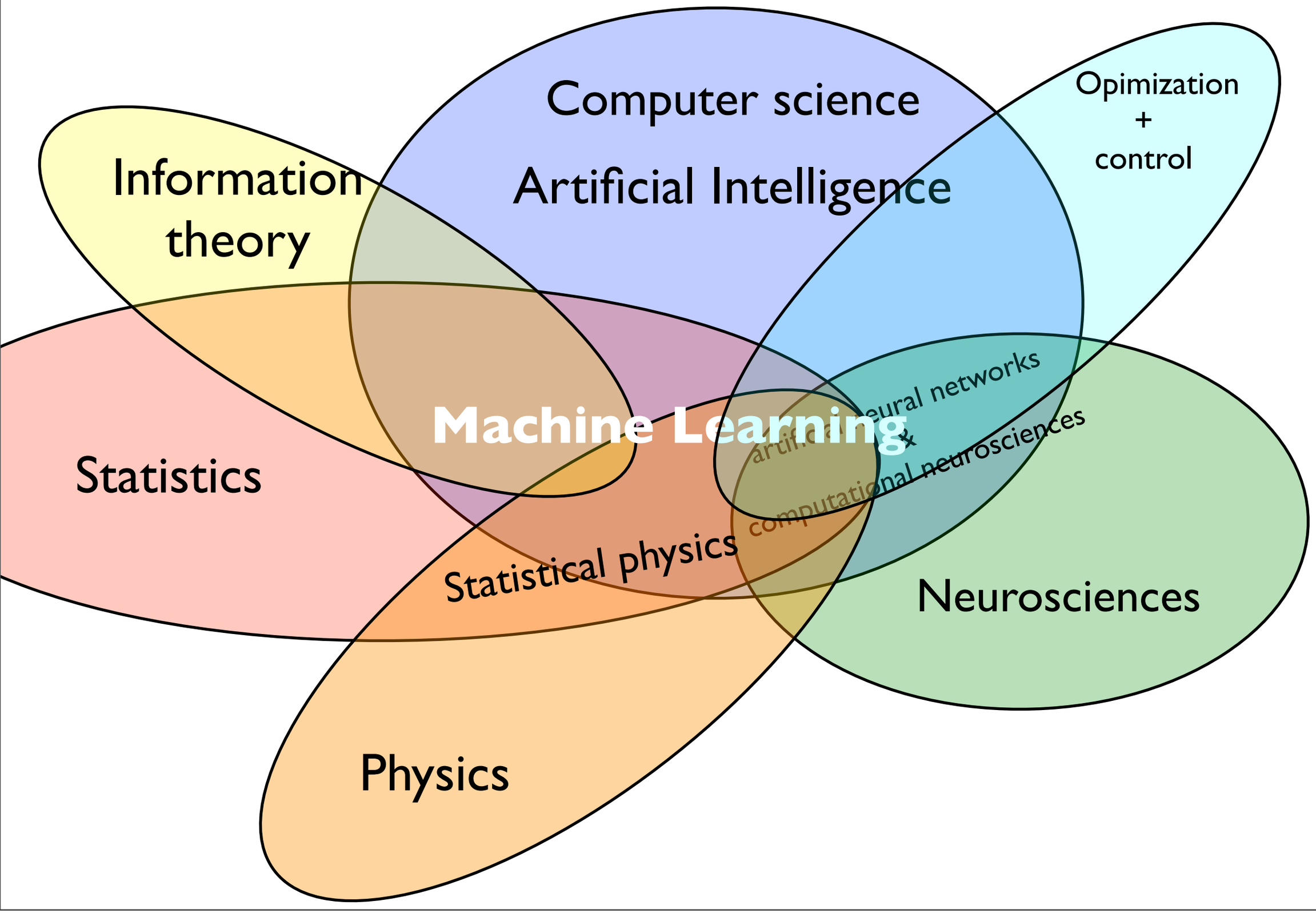
⇨ <u>No learning</u> (humans coding rules)

⇨ <u>poor handling of uncertainty</u>

Got eventually fixed (Bayes Nets...)

Learning and probabilistic models largely won ⇨ machine learning

Current view of ML founding disciplines



What is machine-learning?

A scientific field that

- researches fundamental principles
- and **develops algorithms**
- capable of leveraging collected data to (automatically) **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)

Number of examples: n

"horse"

"cat"

etc...

"horse"

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
	(-9.2, 32, ... , 24, 1, ...)	-1
	etc...	
X_n	(6.8, 54, ... , 17, -3, ...)	+1

$X_{n,2}$

Y_1

Y_n

New test point:

?

$\mathbf{x} = (5.7, -27, \ldots, 64, 0, \ldots) \xrightarrow{f_\theta} +1$

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

Importance of the
Problem dimensions

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

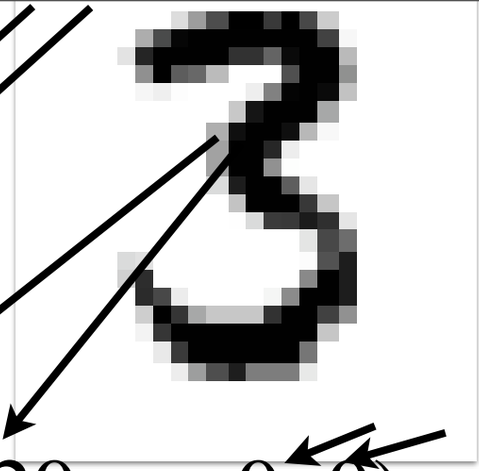
- Number of examples: **n**
  (sometimes several millions)

- 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)

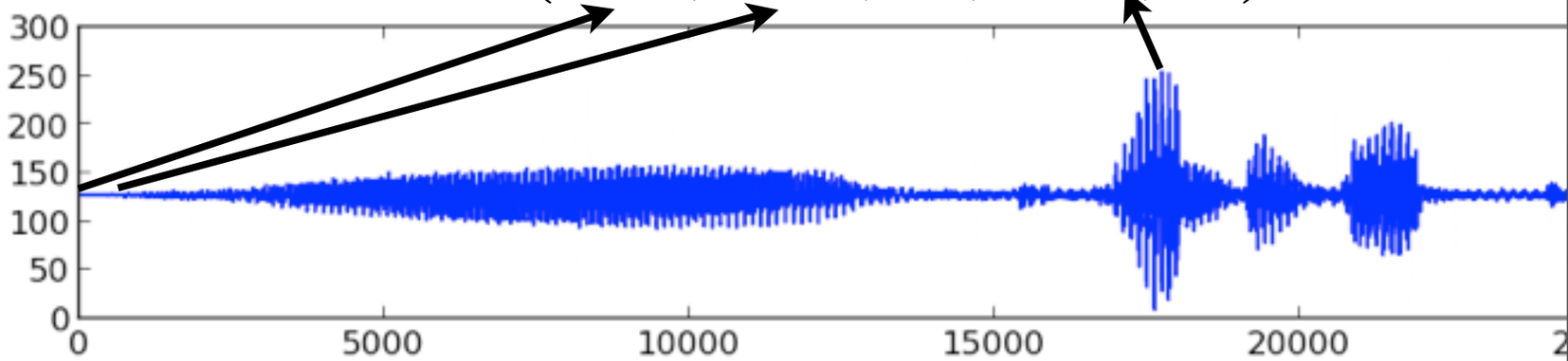
Turning an example into an input vector $\mathbf{x} \in \mathbb{R}^d$



Raw input representation:

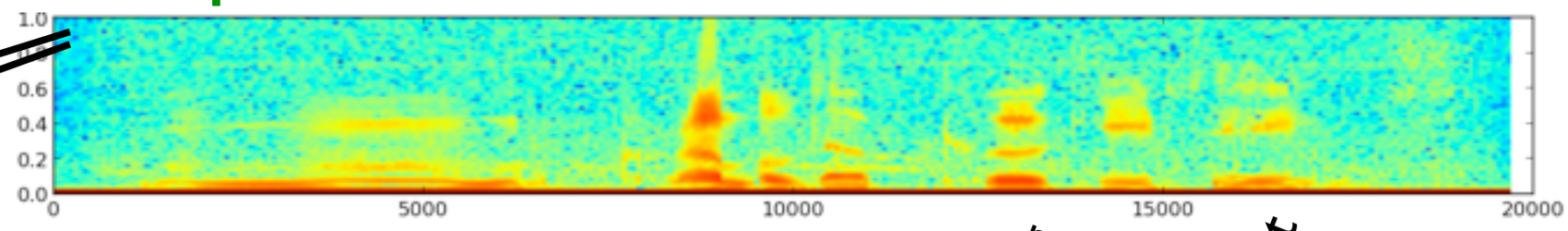
$x = (0, 0, ..., 54, 120, ..., 0, 0)$

$x = (125, 125, ..., 250, ...)$



OR some preprocessed representation:

$x = (, \quad , \quad , \quad , \quad , \quad ....)$



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

we the jumped jumping run elephant dog cat horse

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

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

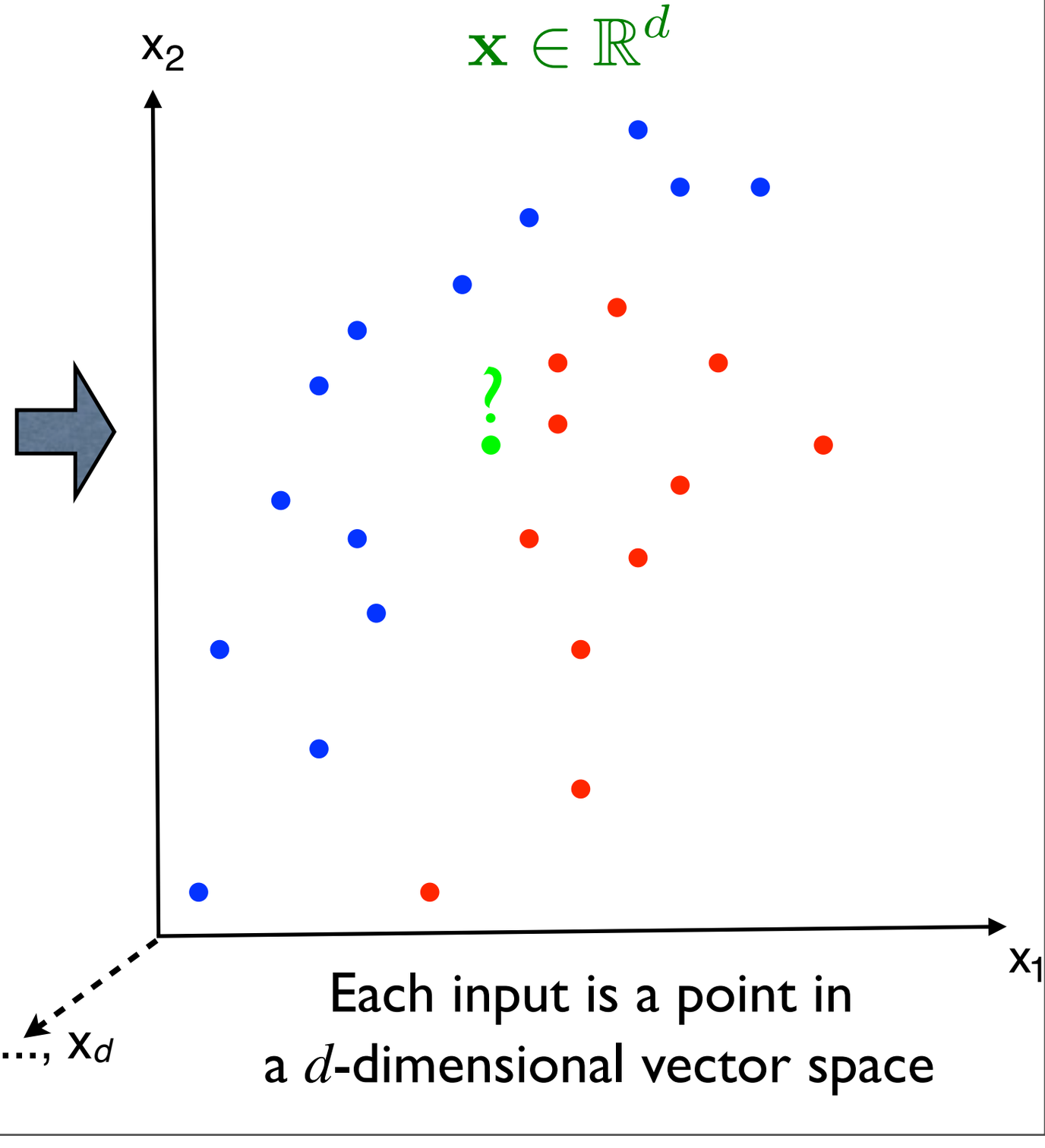
target

(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
...	...	...	...	...	...



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

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

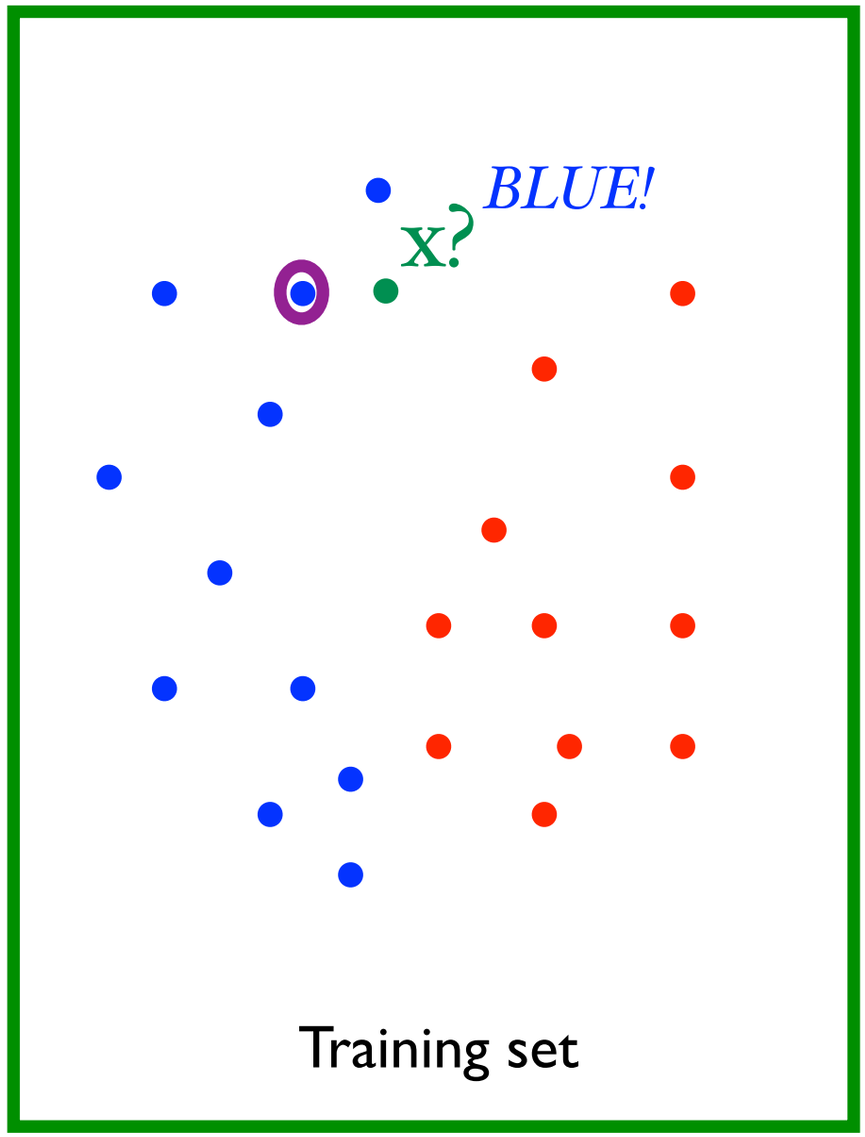
Ex: nearest-neighbor classifier

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 categories

Supervised learning = predict a target y from input x

- y represents a category or "class"
  - ➠ classification $\text{binary} : \mathbf{y} \in \{-1, +1\}$ or $\mathbf{y} \in \{0, 1\}$
    $\text{multiclass} : \mathbf{y} \in \{1, m\}$ 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 prediction 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 the reward from the environment

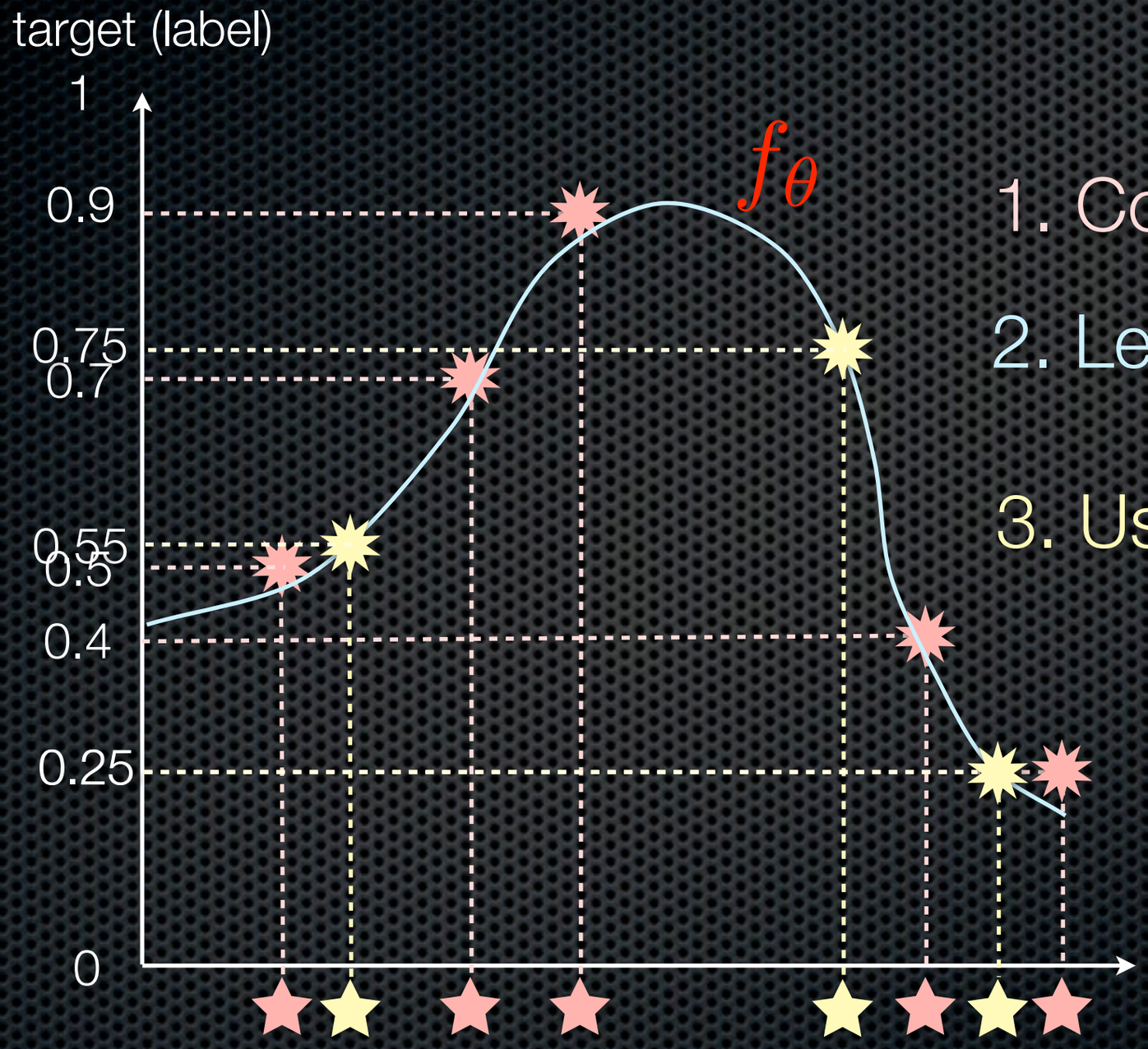
Model-Based Learning

- **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 $\mathbf{x} \in \mathbb{R}^d$

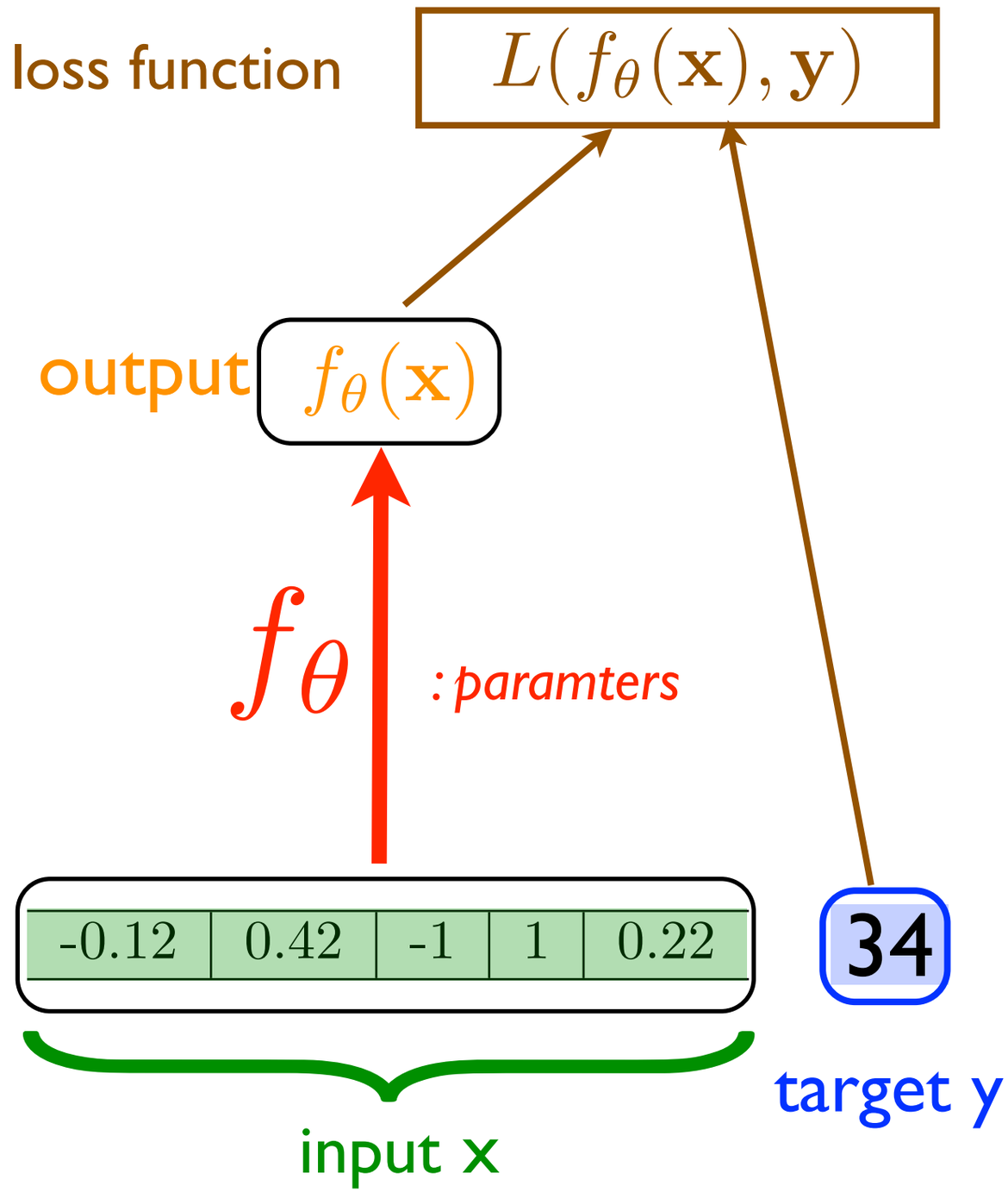
target (label) y

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 prediction 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 implicitly)

✓ 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 predicts)

✓ 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: $f : \mathbb{R}^d \to \{0, \ldots, m-1\}$
  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: $g(x) \approx (P(y=0\|x), \ldots, P(y=m-1\|x))$ Negated conditional log likelihood loss $L(g(x),y) = -\log g(x)_y$ Decision function: $f(x) = \text{argmax}(g(x))$
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: $f(x) = \text{argmax}(g(x))$

Expected risk v.s. Empirical risk

Examples (x,y) are supposed drawn i.i.d. from an unknown true distribution $p(\mathrm{x},\mathrm{y})$ (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 $p(\mathrm{x},\mathrm{y})$ (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 $\hat{f}(D_{\text{train}})$:

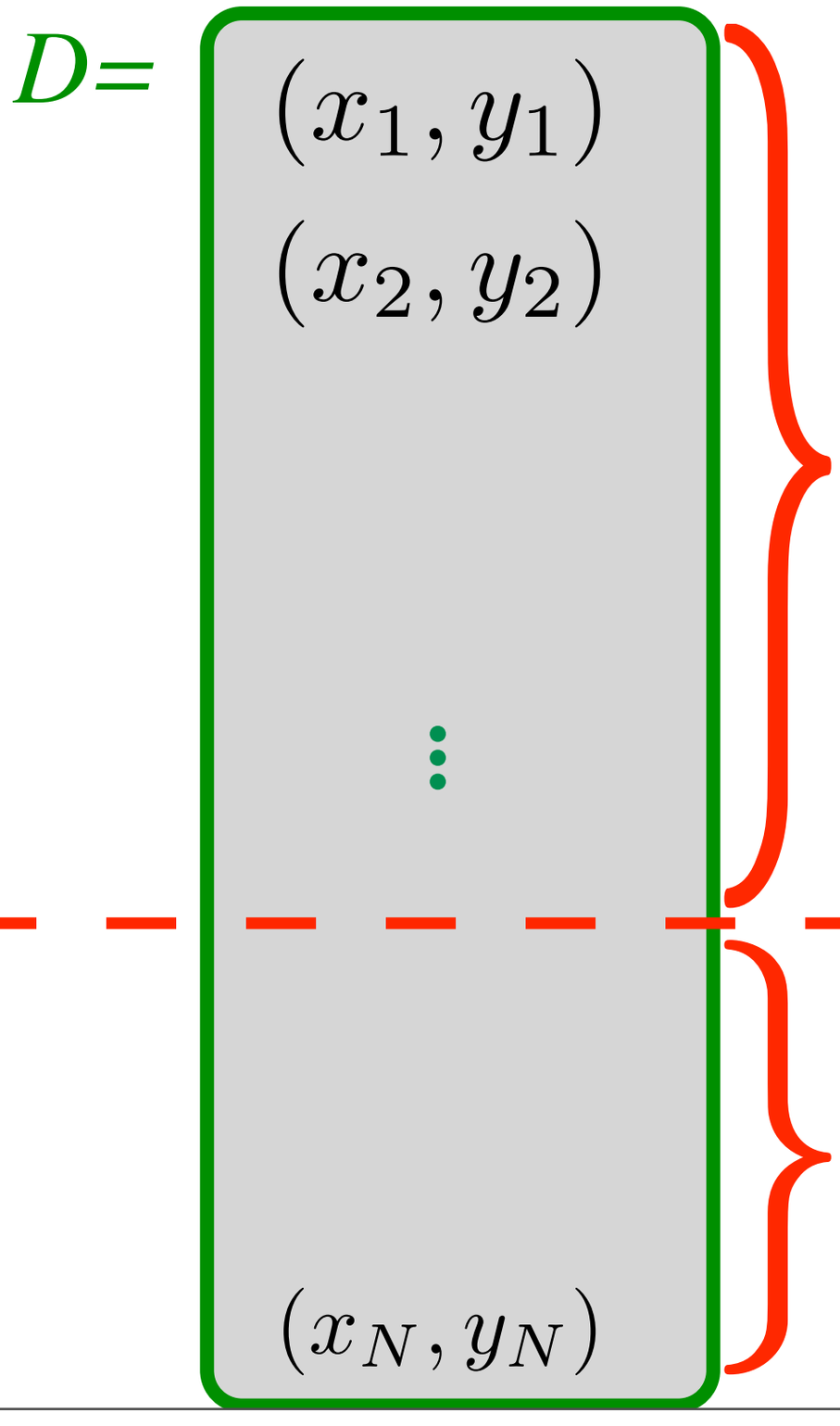
$$R(\hat{f}(D_{\text{train}})) \approx \hat{R}(\hat{f}(D_{\text{train}}), D_{\text{test}})$$

generalization error

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

This is the test phase in ML

Simple train/test procedure



- Provided large enough dataset D drawn from $p(\text{x,y})$
- 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

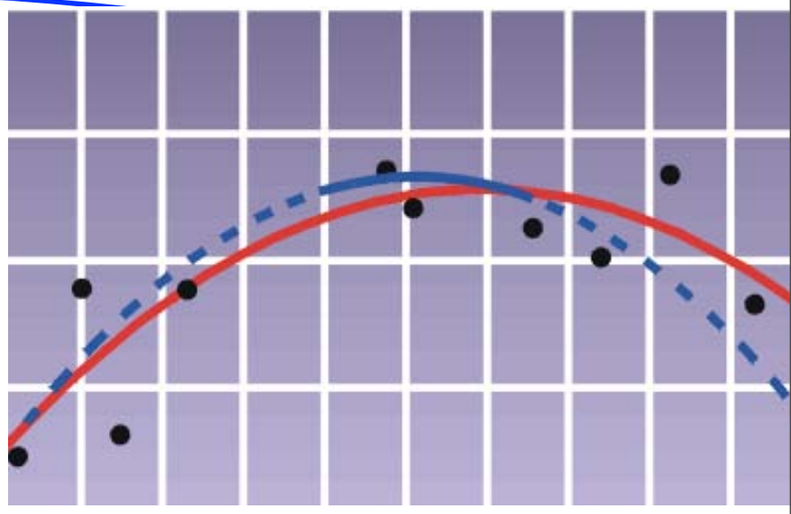
Choosing a specific function family F

Ex. of parameterized function families

$F_{polynomial\ p}$

Polynomial predictor (of degree p):

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



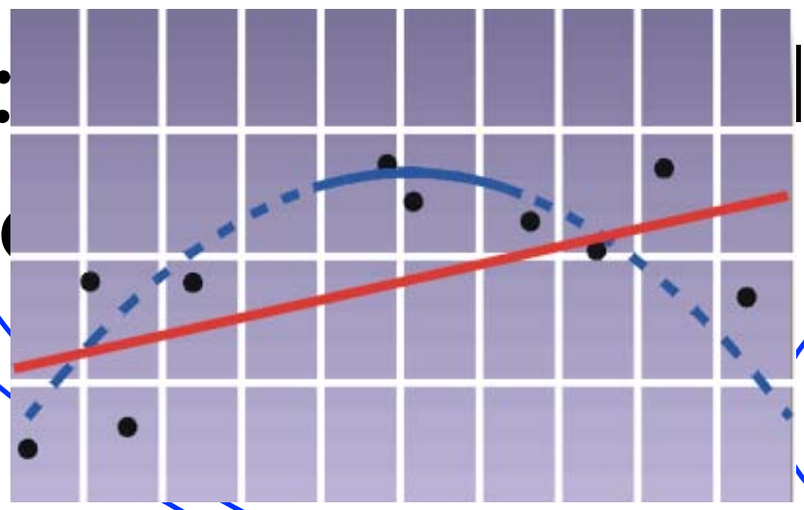
F_{linear}

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

(«linear regression»)

Q: [illegible]lest

pr[illegible]



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 several 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

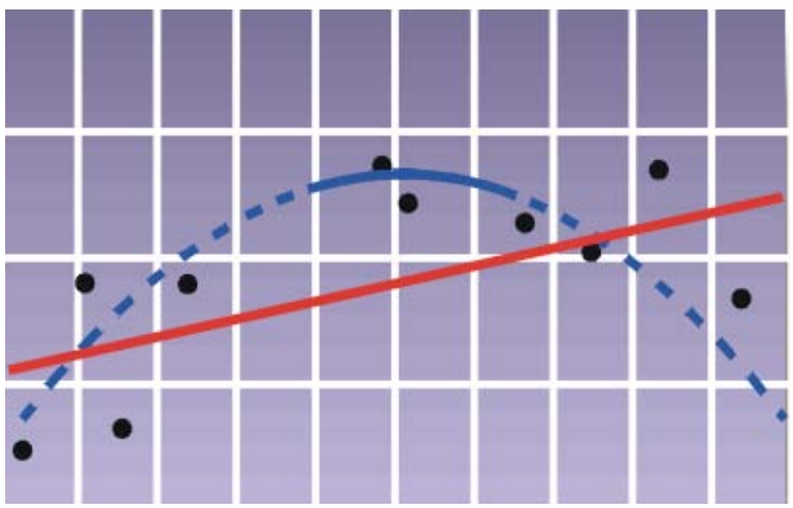
their parameters and hyper-parameters

Algo	**Capacity-control hyperparameters**	**Learned parameters**
logistic regression (L_2 regularized)	strength of L_2 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

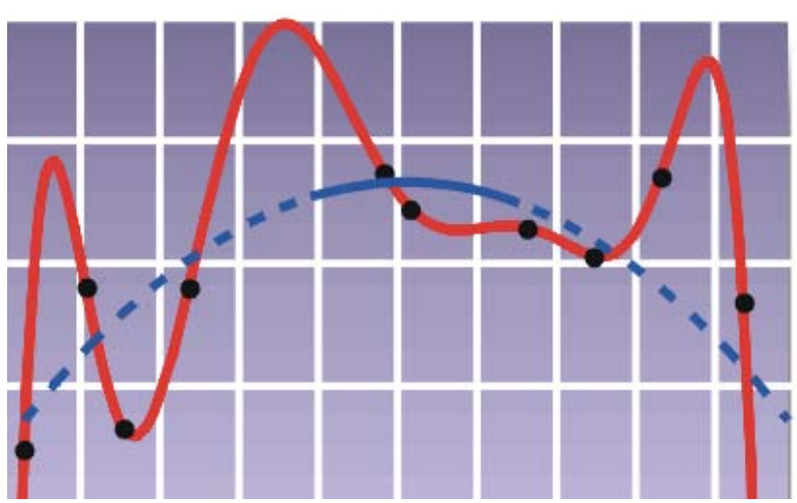
Tuning the capacity (model order)

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

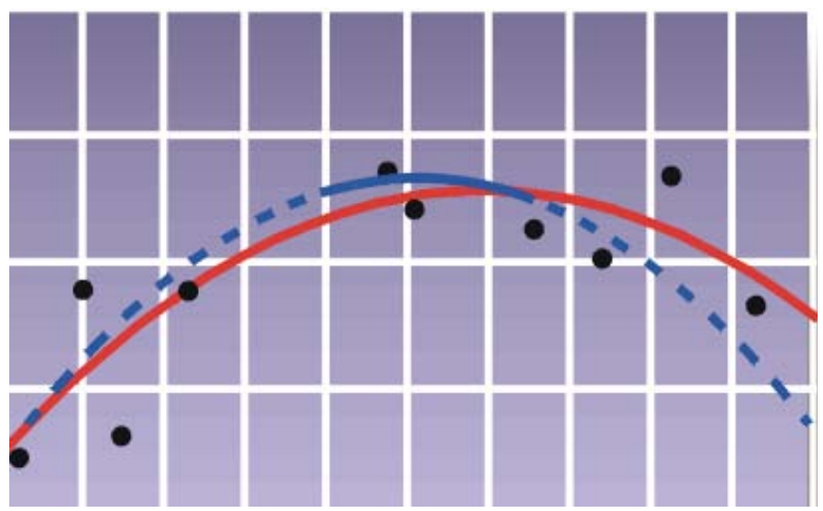
Ex: 1D regression with polynomial predictor



capacity too low
⇨under-fitting



capacity too high
⇨over-fitting



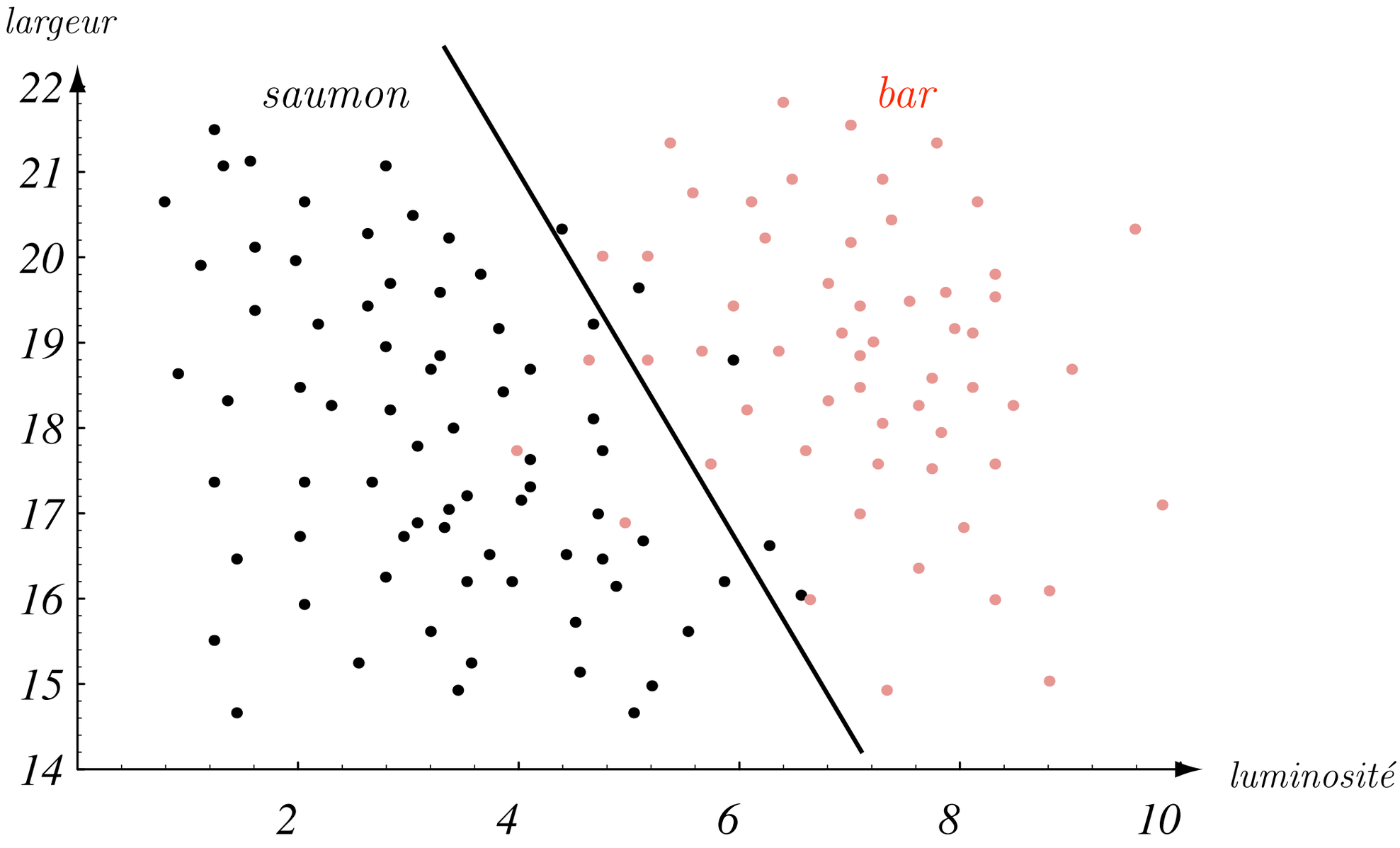
optimal capacity
⇨good generalisation

performance on training set is not a good estimate of generalization,
because as capacity increases, the loss (error) in the training set decreases.

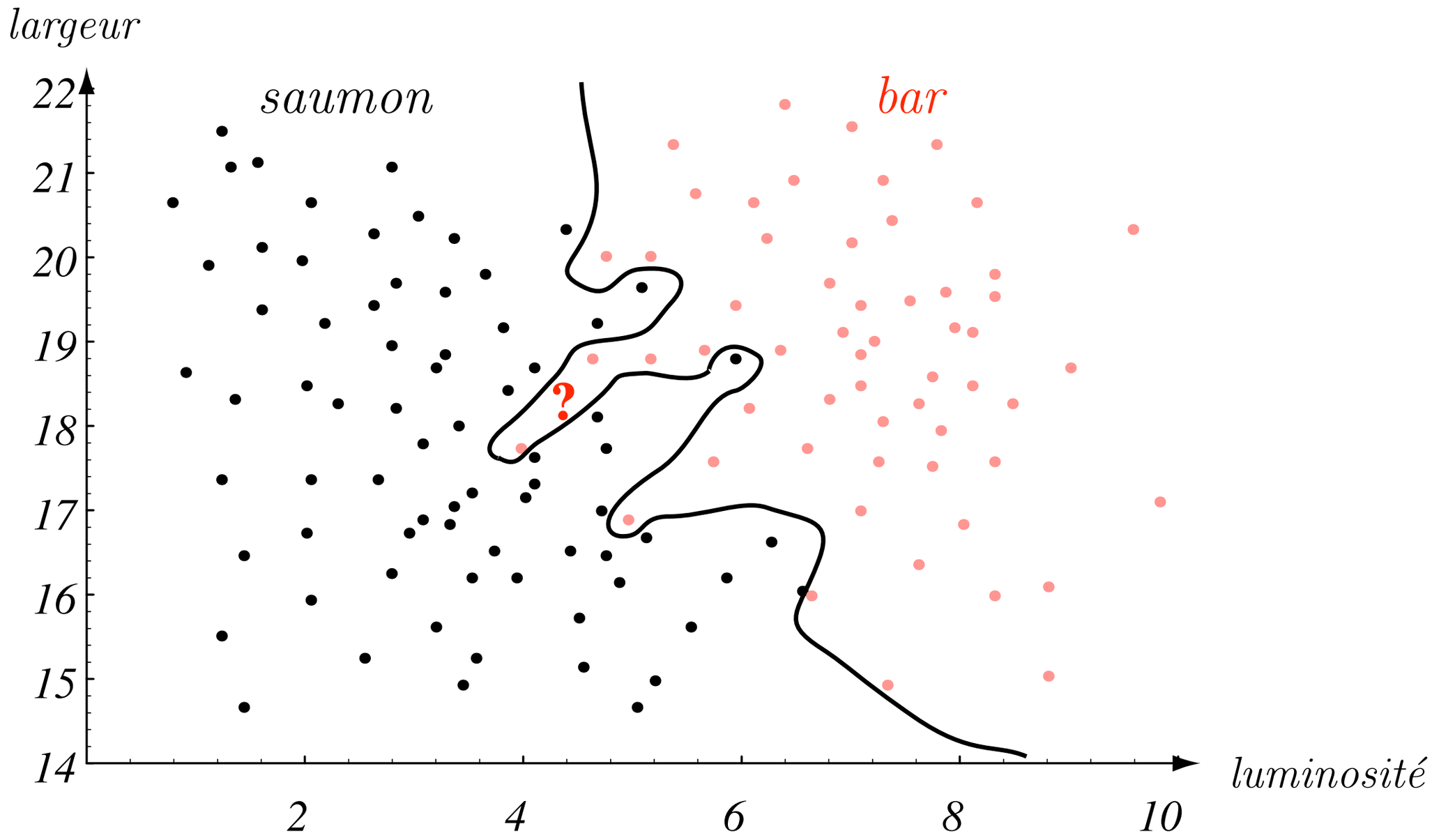
Ex: 2D classification

Linear classifier

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

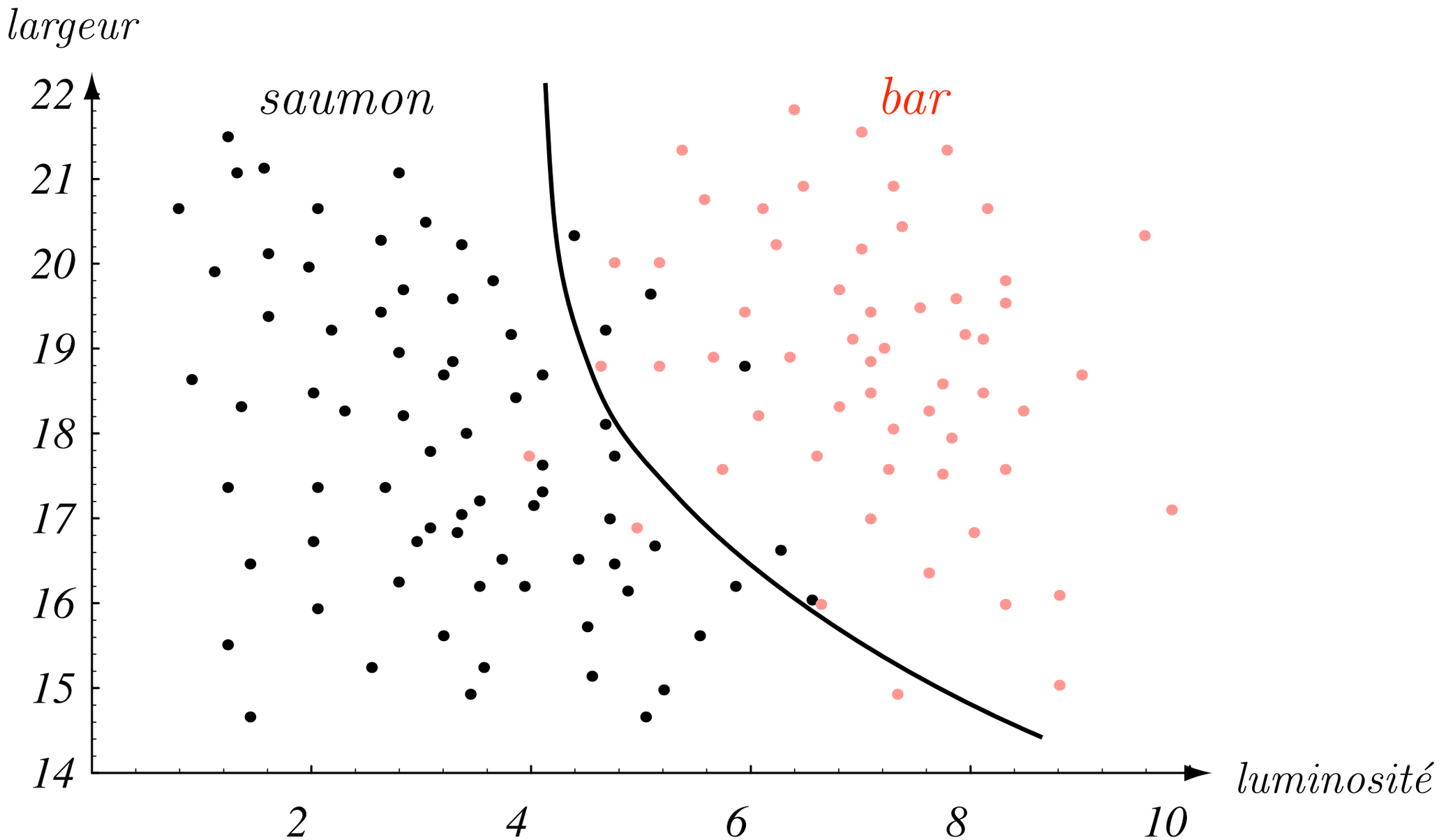


- Function family too rich
  (too flexible)
- = **Capacity too high** for this problem
  (relative to the number of examples)
- => Over-fitting

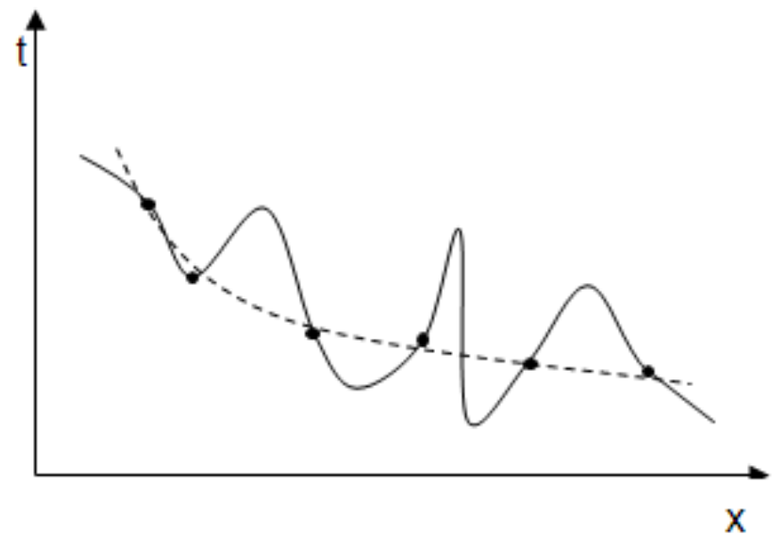


number of errors: 0

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



- **Generalization: successful predictions on unseen examples**
- **Occam's razor:**
  - Prefer the simplest model that fits well to the data.
- **Alternatively: Bias variance dilemma**
  - **generalization error = bias + variance**
  - **Bias:** how well the model fits the training data (small for large models)
  - **Variance:** how small perturbations in the training set affect the training results (large for large models)



Optimal capacity & the bias-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)

$\vdots$

(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

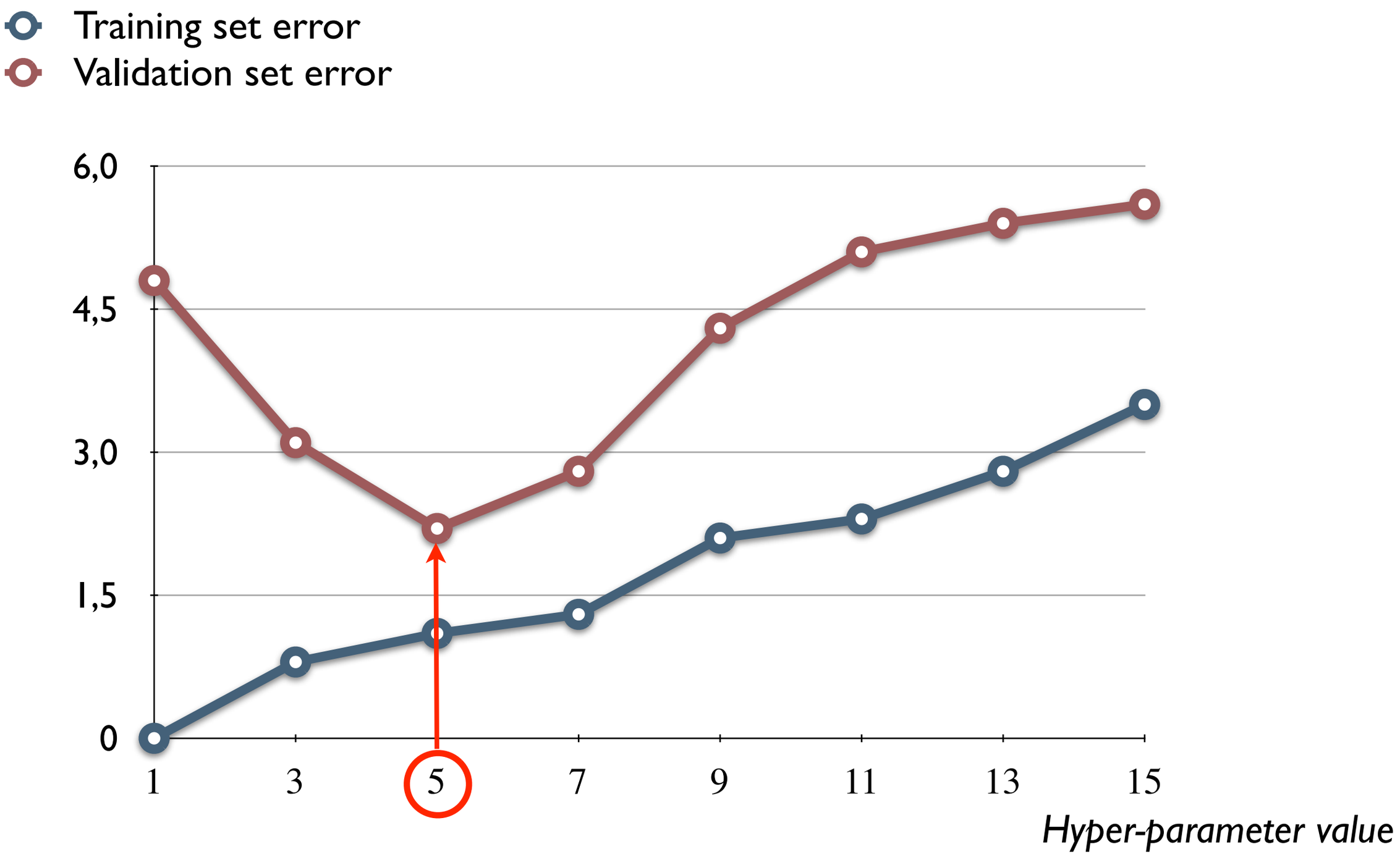
$$f^* = \mathbf{A}^*_{\lambda^*}(D_{\mathbf{train}} \cup D_{\mathbf{valid}})$$

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)

Model/hyperparameter selection using validation set

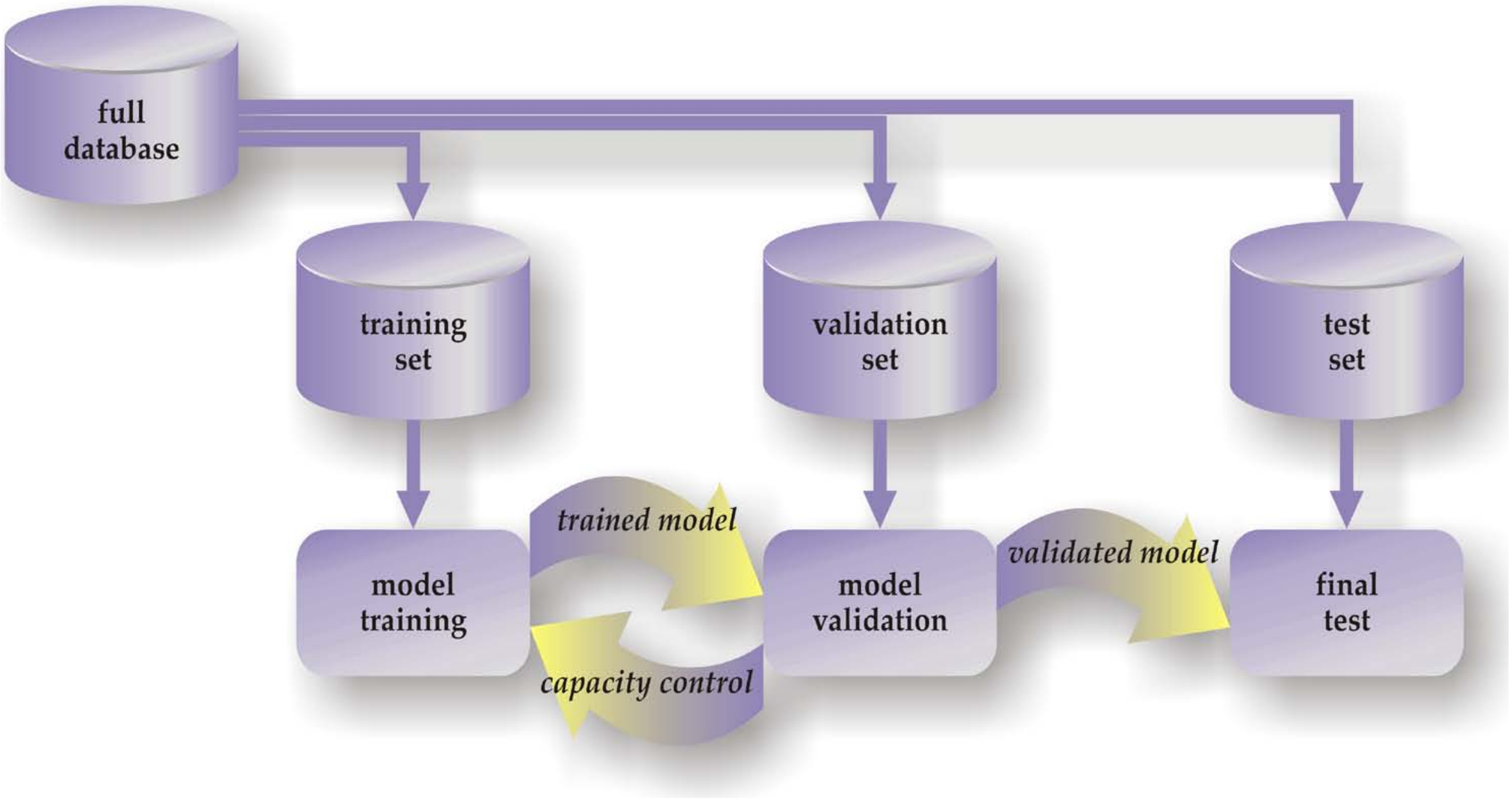


Figure by Nicolas Chapados

- **K-fold cross-validation (**K-CV):
  - Split dataset D into K *disjoint* subsets (folds) D_1 ,…, D_K (usually K=10).
  - For each subset D_i (i=1 ,…, K), train a model using D-D_i as training set and compute generalization error (ge_i) using D_i as test set.
  - Compute ge = average(ge_i)
  - Depends (somehow) on initial splitting
- **Leave-one-out (**K=N): deterministic, more reliable, but computationally expensive
- We use cross-validation to select the best model (e.g. network architecture) .
- The final solution is obtained by training the selected model on the whole dataset.