IFT6390
Fondements de l'apprentissage machine

General framework of learning
Evaluation of the generalization performance.
Model selection
Learning curves.

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Probabilistic approach to learning

- It is assumed that the data is generated by an unknown process.
- X,Y is seen as a pair of random variables, distributed according to an unknown probability law P (X,Y).
- X (a vector variable) is itself seen as a set of scalar random variables.

$$P(X,Y) = P(X_{[1]}, \ldots, X_{[d]}, Y)$$

General framework of learning: the dataset

- Data
  - $D_n = (Z_1, Z_2, \ldots, Z_n)$ generated by "nature"
- IID: "independent and identically distributed"
  - drawn from the same UKNOWN distribution $p(Z)$
  - independently

General framework of learning: three classic problems

- The three problems we consider
  - classification: $Z = (X,Y) \in \mathbb{R}^d \times \{1,\ldots,N\}$ $(\mathbb{R}^d \times \{-1,1\})$
  - regression: $Z = (X,Y) \in \mathbb{R}^d \times \mathbb{R}$
  - density estimation: $Z \in \mathbb{R}^d$

- Collection of functions $\mathbf{F}$ (possible solutions), $f \in \mathbf{F}$:
  - classification: $f : \mathbb{R}^d \to \{-1,1\}$
  - regression: $f : \mathbb{R}^d \to \mathbb{R}$
  - density estimation: $\mathbf{F}$ contains density functions

Phases of learning

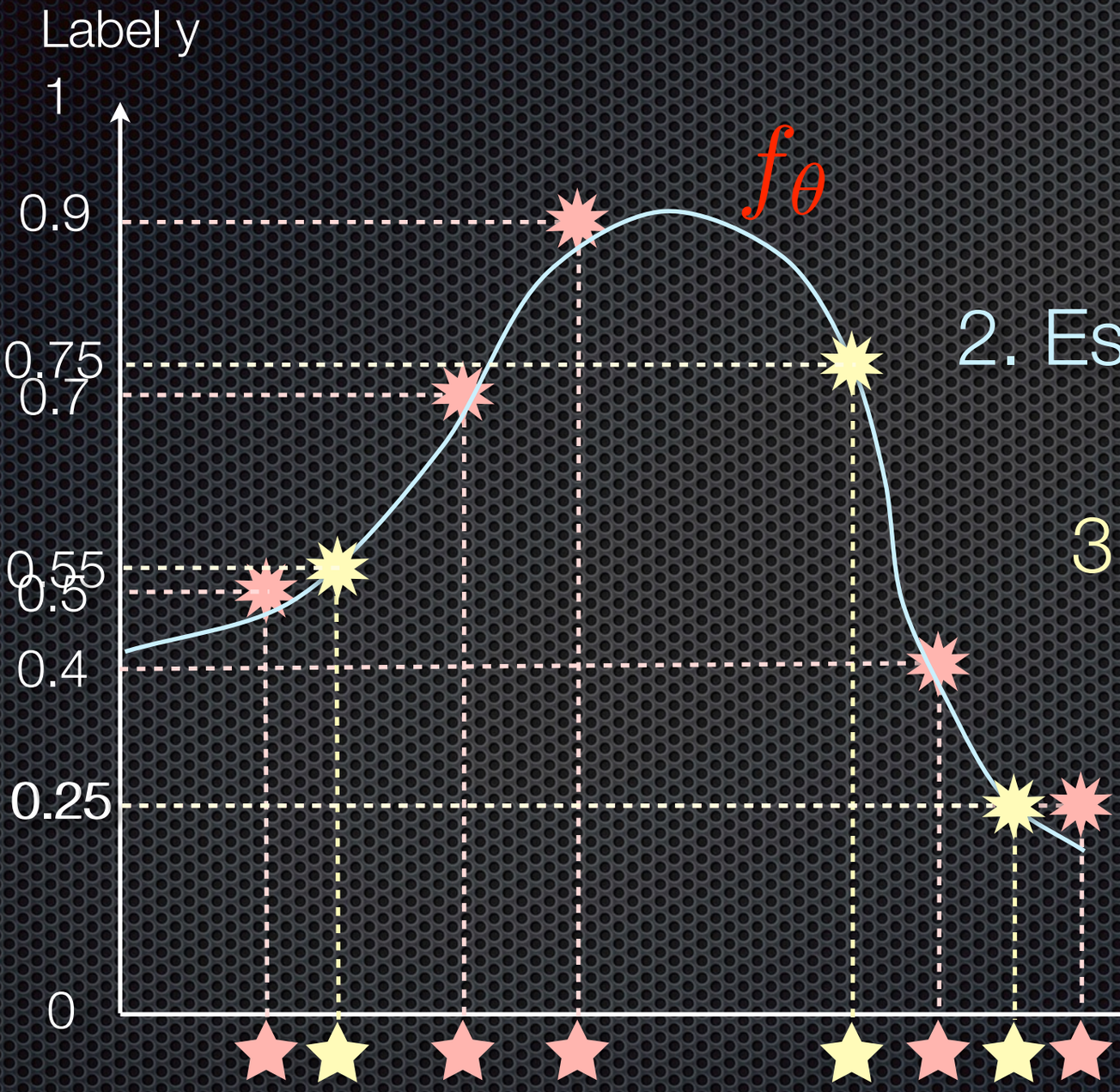
- Training: we learn a function f_θ optimizing its parameters θ so that it works well on the training set.

- Prediction / testing : then we can use the function on new points (test examples) that are not part of the training set.

⇨ It is *not important* to learn perfectly *(memorise)* the training set.

⇨ It is important to be able to *generalise* on new cases (points/examples).

Eg: regression 1D



1. Collect data
2. Estimate the function
   Input $\longmapsto$ Label
3. Use that function on new data

Supervised task

predict y from x

target

input

(label)

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

$\mathbf{y}$

n examples

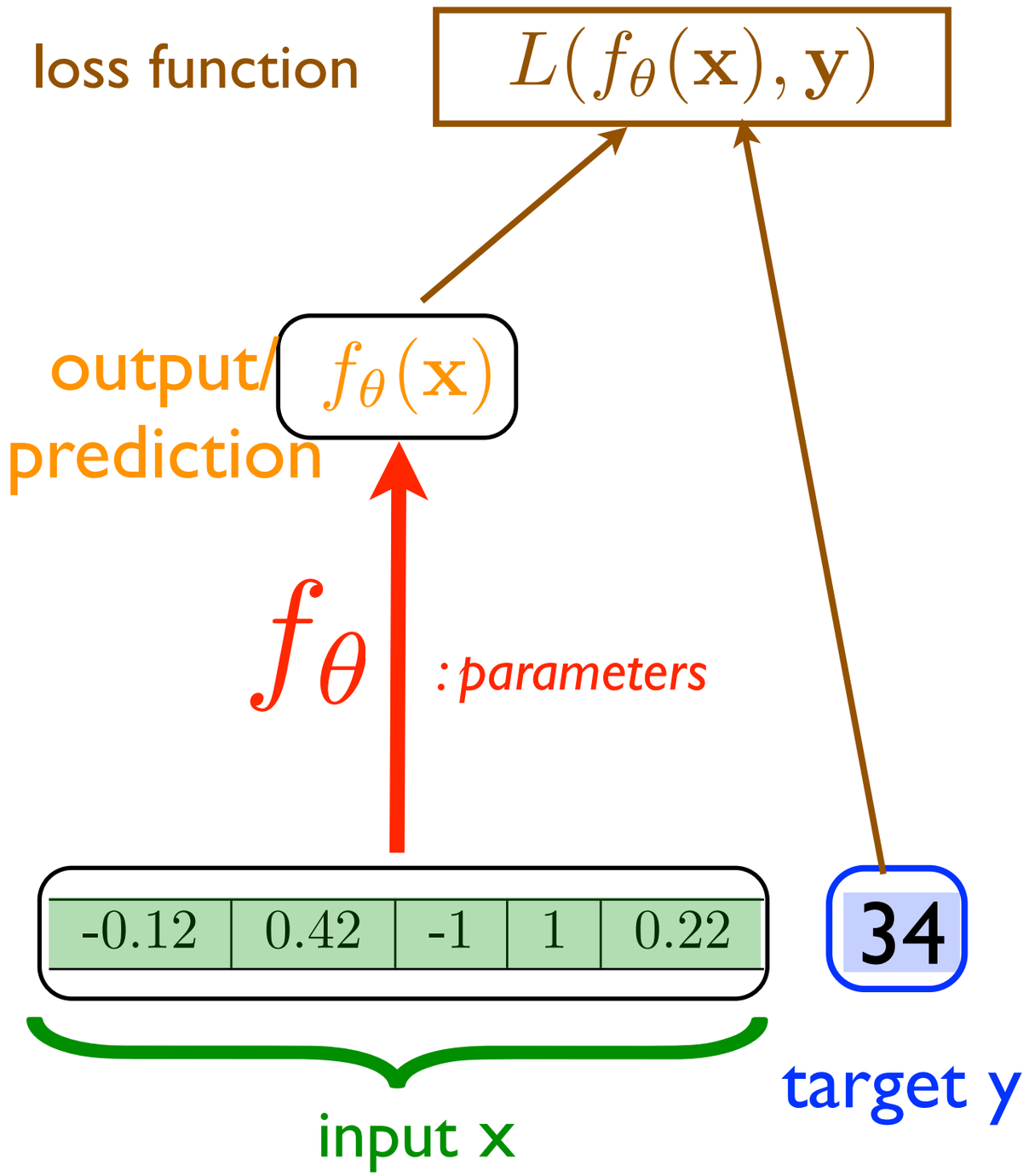
$\mathbf{x}_1$	$\mathbf{x}_2$	$\mathbf{x}_3$	$\mathbf{x}_4$	$\mathbf{x}_5$	t
0.32	-0.27	+1	0	0.82	113
-0.12	0.42	-1	1	0.22	34
0.06	0.35	-1	1	-0.37	56
0.91	-0.72	+1	0	-0.63	77
...	...	...	...	...	...

Training set D_n

Learn a function

$f = f_\theta$ which

minimizes a cost (loss).



A learning algorithm is often the combination of the following:

(given explicitly or implicitly)

✓ the specification of a family of functions F
(often a *parametric* family)

✓ a method to evaluate the quality of a function $f \in F$ (typically using a cost function (loss) L eg: count how many points are misclassified by f)

✓ a way to search the «best» function $f \in F$ (ie, optimization of parameters to minimize the loss).

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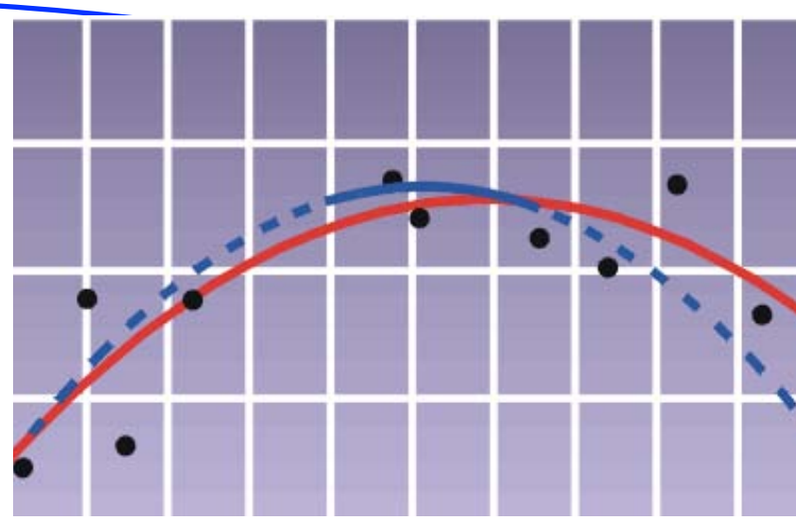
Examples of parametric function family

$F_{polynomial\ p}$

polynomial predictor (of degree p):

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

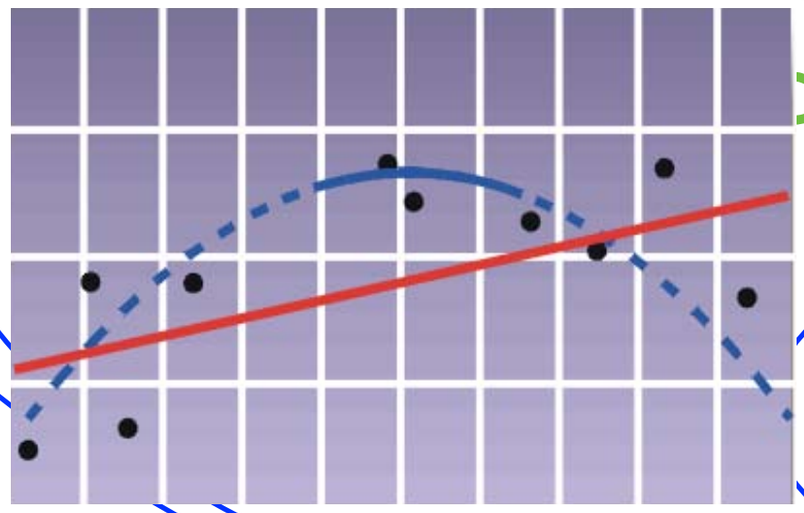


F_{linear}

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

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

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



class

F_{const}

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

or $\theta=\{b\}$

(Always predict the same value or class!)

There exist many different function families

- Constant
- Linear / affine
- polynomial
- Histograms “staircase functions”
- Weighted sum of kernels (eg Parzen or SVM with kernel)
- Decision trees
- Neural networks (composition of non-linear functions)
  Each neural network "architecture" corresponds to a different family of functions..

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Evaluate the quality of a predictor $f(x)$

The performance of one of a prediction function f (x) is often evaluated with **many** different evaluation metrics:

- Evaluation of the true quantity of interest ($ saved/gained, #lives saved, ...) when using the predictor within a complex complete system.
- "Standard" performance measures specific to a particular field (eg BLEU score Bilingual Evaluation Understudy for translation)
- Classification error rate for a classifier (or precision and recall, or F-score, ...).
- The cost that is actually optimized by the machine learning algorithm.

Simples cost (loss) functions for performance evaluation

(« cost function » or « loss function »)

- Classification task

  classification error

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

$$L(f(x), y) = I_{\{f(x) \neq y\}}$$

- Regression task:

  quadratic error:

$$f : \mathbb{R}^d \to \mathbb{R}$$

$$L(f(x), y) = (f(x) - y)^2$$

- Density estimation task

  negative log likelihood:

$$f : \mathbb{R}^d \to \mathbb{R}^+$$

a probability density (or mass) function

$$L(f(x)) = -\log f(x)$$

Performance evaluation is often the average of a cost (loss) function on a set of test data

Surrogate losses

- For a classification task: $f : \mathbb{R}^d \to \{0, \ldots, m-1\}$
  classification error: $L(f(x), y) = I_{\{f(x) \neq y\}}$

Problem: difficult to directly optimize the classification error rate
(gradient 0 everywhere. NP-hard with a linear classifier) Use a surrogate loss!

	Binary classifier	Multiclass classifier
Probabilistic classifier	Give the probability that the class is 1 $g(x) \approx P(y=1 \mid x)$ Probability of class 0 is $1-g(x)$ Binary cross entropy: $L(g(x),y) = -(y \log(g(x)) + (1-y) \log(1-g(x))$ Decision function: $f(x) = I_{g(x)>0.5}$	Outputs a vector of probabilities: $g(x) \approx (P(y=0\|x), \ldots, P(y=m-1\|x))$ Negative conditional log-likelihood $L(g(x),y) = -\log g(x)_y$ Decision function: $f(x) = \text{argmax}(g(x))$
Non-probabilistic classifier	Give a «score» $g(x)$ for class 1. the score for the other class is $-g(x)$ Hinge loss: $L(g(x),t) = \max(0, 1-tg(x))$ où $t=2y-1$ 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

"Risk" = "average" loss

Example (x,y) drawn i.i.d. from unknown distribution $p(\mathrm{x},\mathrm{y})$
(from nature or an industrial process)

- Generalization error = Expected risk
  (or just «Risk» = expected loss)
  «the loss/error we will get on average over infinitely many future examples from this unknown distribution»

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

- Empirical risk = the average loss over a finite dataset D (drawn from p)
  «the average error on the examples in this dataset»

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

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

Estimating the expected risk

- We cannot calculate it exactly… because $p(\mathrm{x},\mathrm{y})$ is unknown!
- We can estimate it approximately:
  If we did not use D at all to choose f the empirical risk is an unbiased estimate (though noisy) of the expected risk:

$$R(f) \approx \hat{R}(f, D)$$

because $\mathbb{E}_{p(\mathbf{x},\mathbf{y})}[L(f(\mathbf{x}), \mathbf{y})] \approx \frac{1}{|D|} \sum_{(\mathbf{x},\mathbf{y}) \in D} L(f(\mathbf{x}), \mathbf{y})$

More precisely unbiased estimator means that:

$$\mathbb{E}_{D \sim p}[\hat{R}(f, D)] = R(f)$$

which is also reflected in $\lim_{|D| \to \infty} \hat{R}(f, D) = R(f)$

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✓ a method to evaluate the quality of a function $f \in F$ (typically using a cost function (loss) L eg: count how many points are misclassified by f)

✓ a way to search the «best» function $f \in F$ (ie, optimization of parameters to minimize the loss).

Learning is choosing a function from a set of functions

Set of all possible functions "in the universe"

F set of functions considered

$\hat{f}(D_{\text{train}})$

function found by the algorithm using the training set

what principle do we use to find it?

Empirical Risk Minimization (ERM)

- We would like to find a predictor that minimizes the error of generalization (expected risk)
- But we can not even calculate it!
- Instead: **Principle of ERM minimization**
  «Find the predictor that minimizes the average loss on a training set»

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

This is the training phase

Estimate the generalization error of the predictor $\hat{f}(D_{\text{train}})$

The problem:

- ERM minimization principle: we train a model (we adapt its parameters) so that it makes a minimum of errors on the training set.

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

- BUT what really interests us is to generalize on new examples.
- Since the parameters of the model are chosen, specialized, to minimize training error, this way underestimates the generalization error.
- So training error is not a good estimate for generalization error (there is an estimation *bias*).

Estimate the generalization error of the predictor $\hat{f}(D_{\text{train}})$

- $\hat{R}(f, D)$ is a good estimator for $R(f)$ under the condition:
  - D was not used to find / choose f
    otherwise biased ⇨ we can not use the training set!
  - D is sufficiently big (otherwise estimate is noisy); drawn from p

➡ We must keep a separate test set $D_{\text{test}} \neq D_{\text{train}}$ to correctly estimate the 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 the test set (never used for training)

This is the test phase

Generalization error estimation:
Simple validation

All of the labeled data we have:

$D=$

(x_1, y_1)

(x_2, y_2)

$\vdots$

(x_N, y_N)

We split our data in two

(it may be necessary to first mix the rows of data)

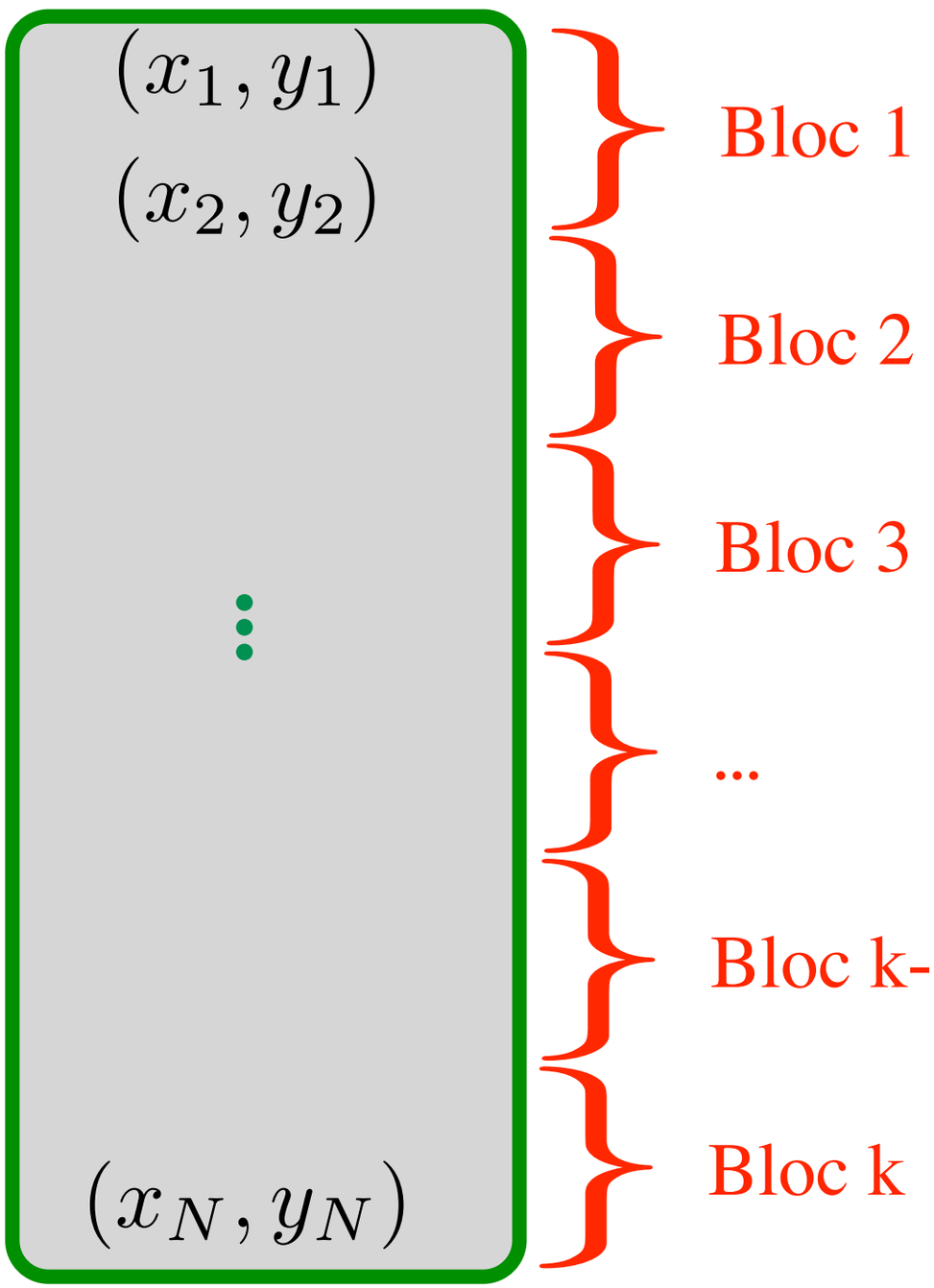
Training set (size n)

*We **train the model** to minimize the error on the training set*

Test set (size m)

*The **generalization performance** is evaluated by measuring errors on the test set that was never viewed during training.*
(performance measure "out of sample").

If we do not have enough data: cross-validation (in k blocks)



Simple idea: the training / test procedure is repeated several times by dividing the data set differently.

Training on	*Test error calculation on*
$D \setminus$ Bloc 1	Bloc 1
$D \setminus$ Bloc 2	Bloc 2
...	...
$D \setminus$ Bloc k	Bloc k

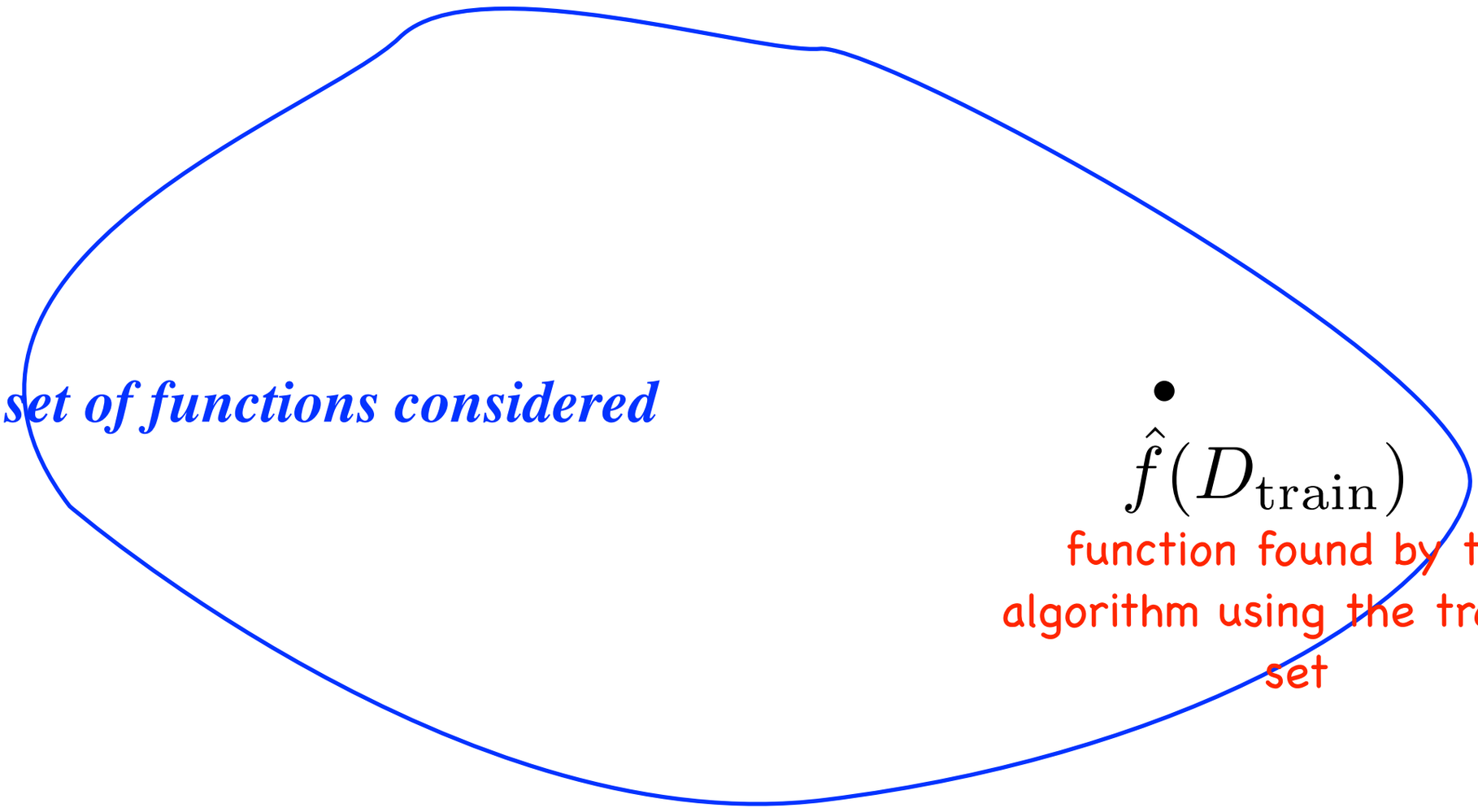
Our estimate of the generalization error of the algorithm on this problem is deduced from the sum of the errors obtained on all the blocks.

We will this method *k-fold cross validation.*
The case k=N is called *leave-one-out* or *jackknife*.

Notions of capacity of overfitting or underfitting

Learning is choosing a function from a set of functions

Set of all possible functions "in the universe"



Concept of capacity or complexity of model

- Corresponds to the "size" or "richness" of the function set considered (± flexible functions)
- Often related to the **number of free parameters** (to learn from the training set) Usually the more, the greater the capacity.
- But not always ... it is rather the number of effective degrees of freedom of the function (effective capacity).
- There are formal measures for some restricted frameworks. Ex: VC-dimension (Vapnik-Chervonenkis).

Examples of parametric function family

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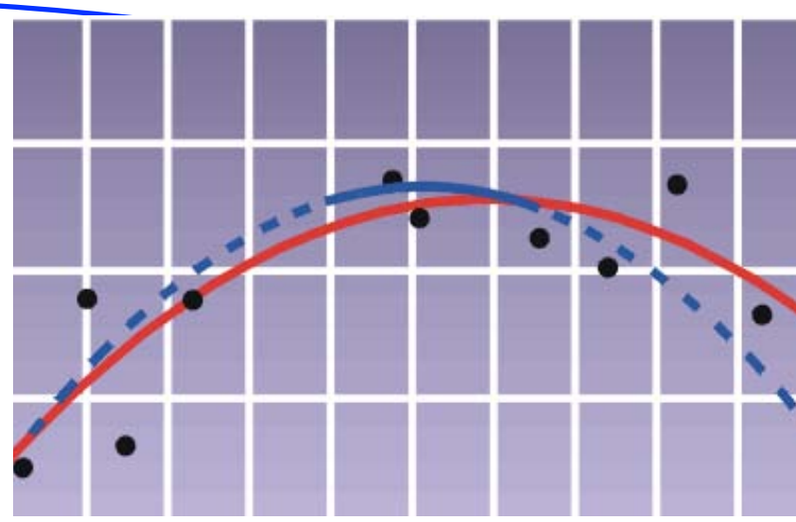

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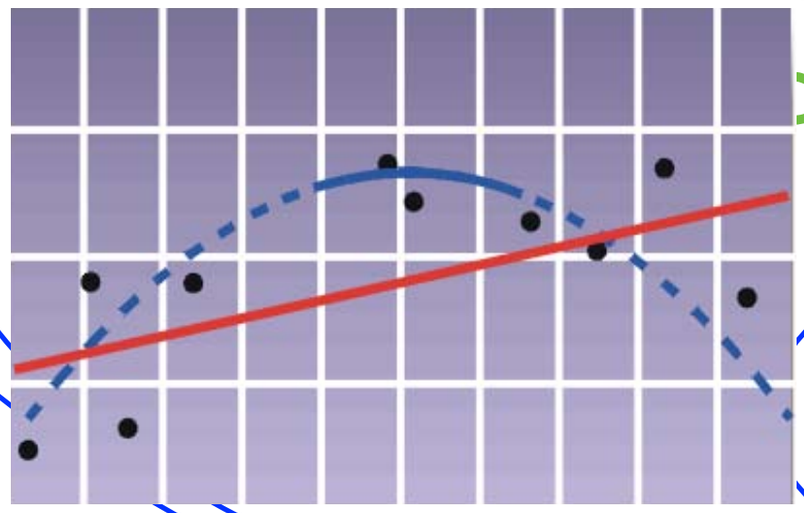

class

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

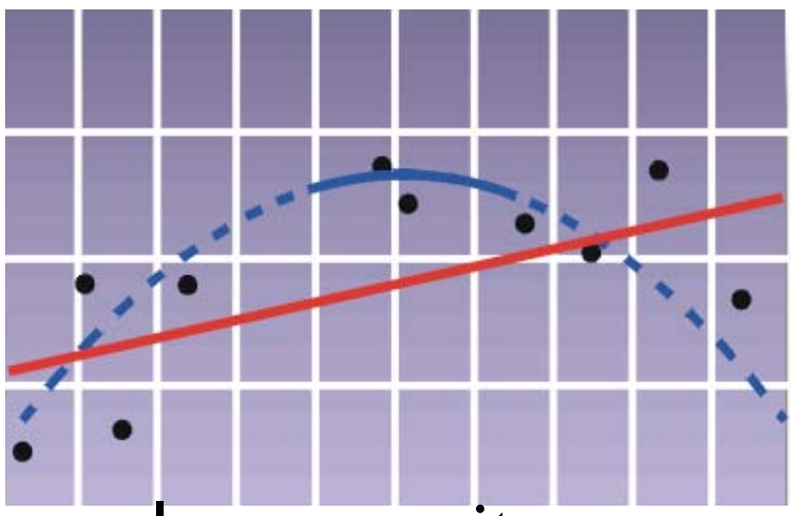
or $\theta=\{b\}$

(Always predict the same value or class!)

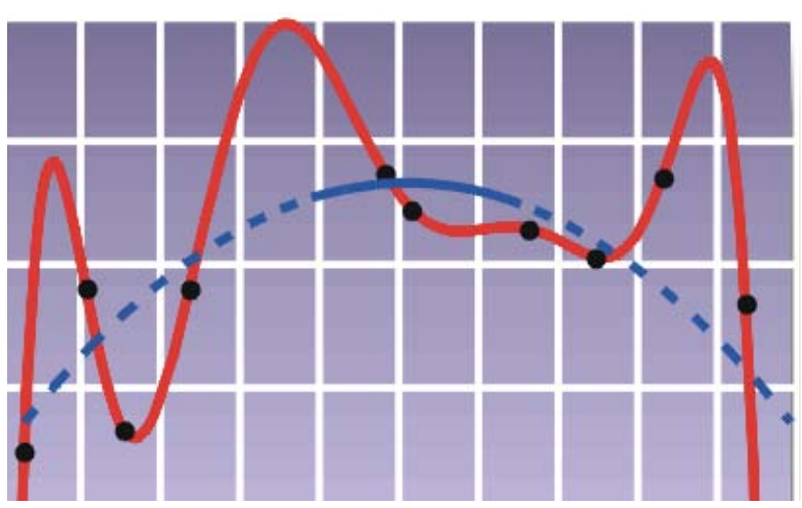
Capacity control

- The choice of the function set and the hyper-parameters of the algorithms make it possible to control the capacity of the model.
- It is essential to have a good generalization.

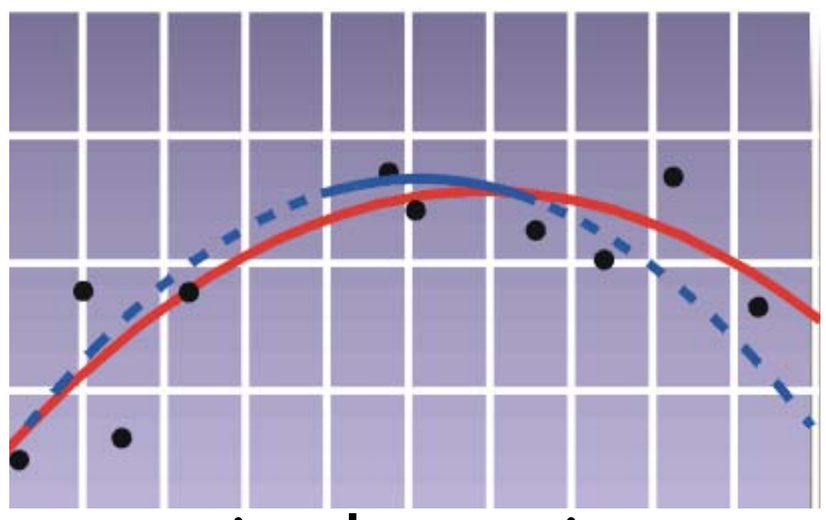
Ex: Regression 1D



low capacity
⇨underfitting



too high capacity
⇨overfitting



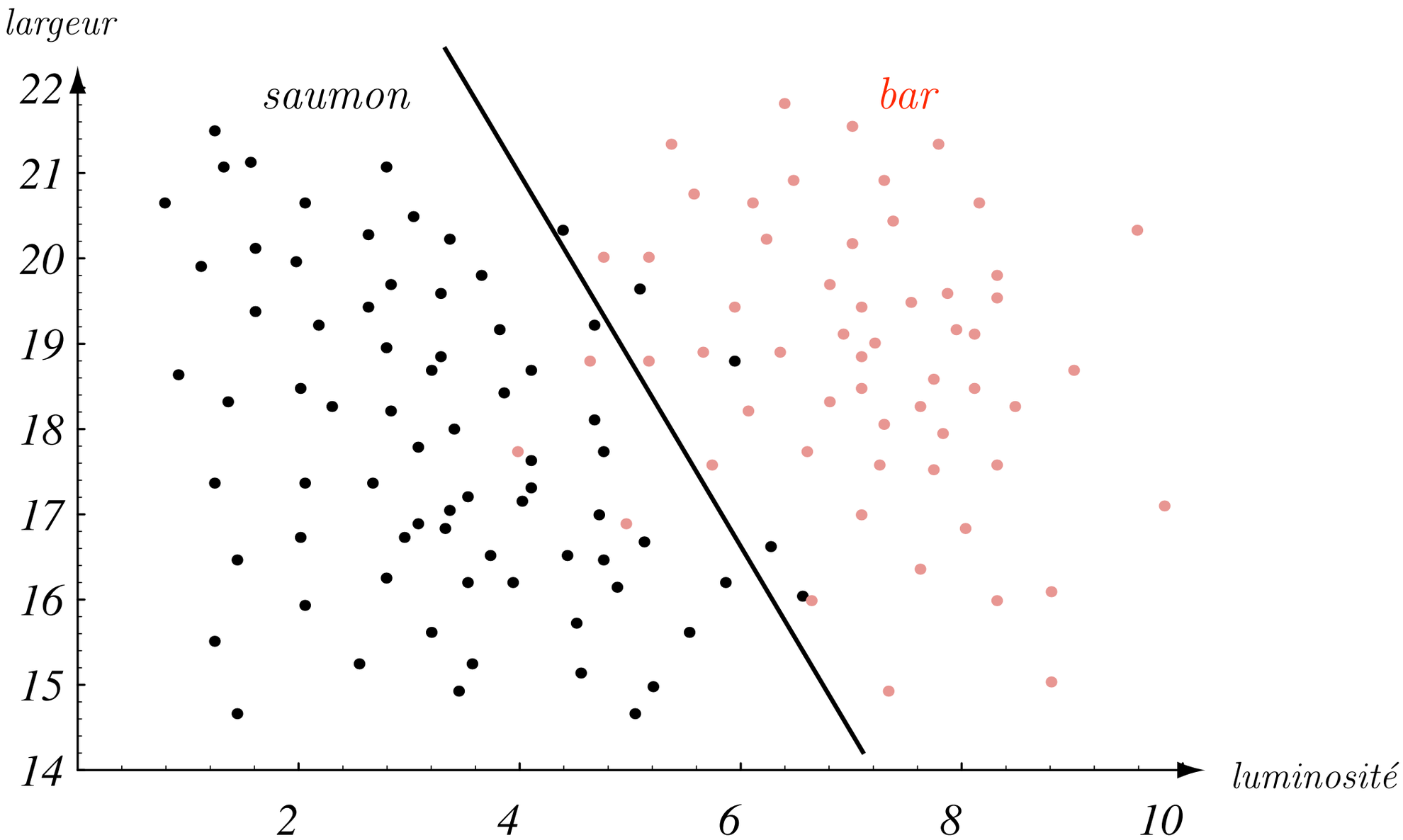
optimal capacity
⇨good generalization

the performance on the training set is not a good estimate of the generalization

Ex: classification 2D

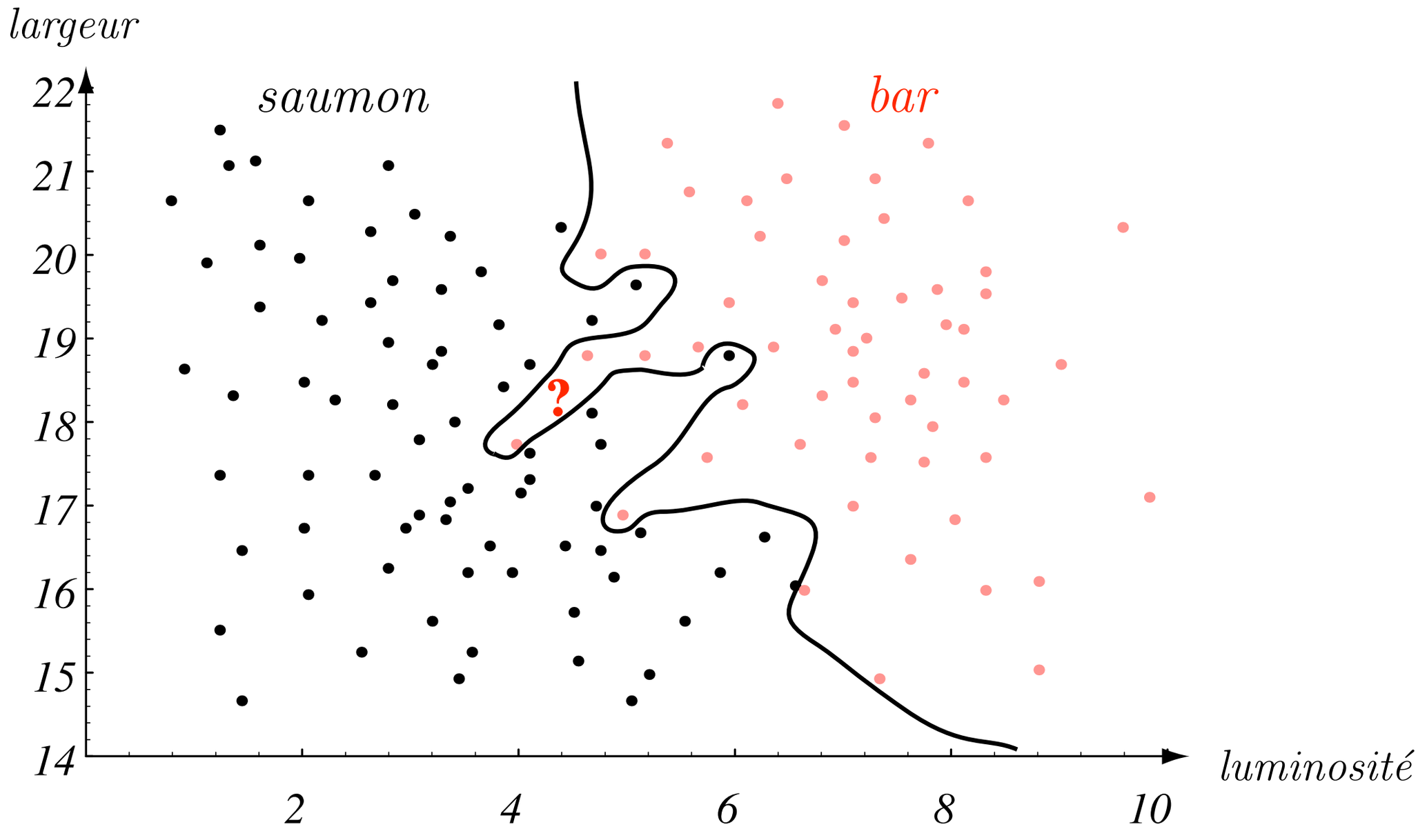
Linear classifier

- Function family poor (too little expressivity)
- = Capacity too small for this problem (relative to the amount of data)
- => Underfitting



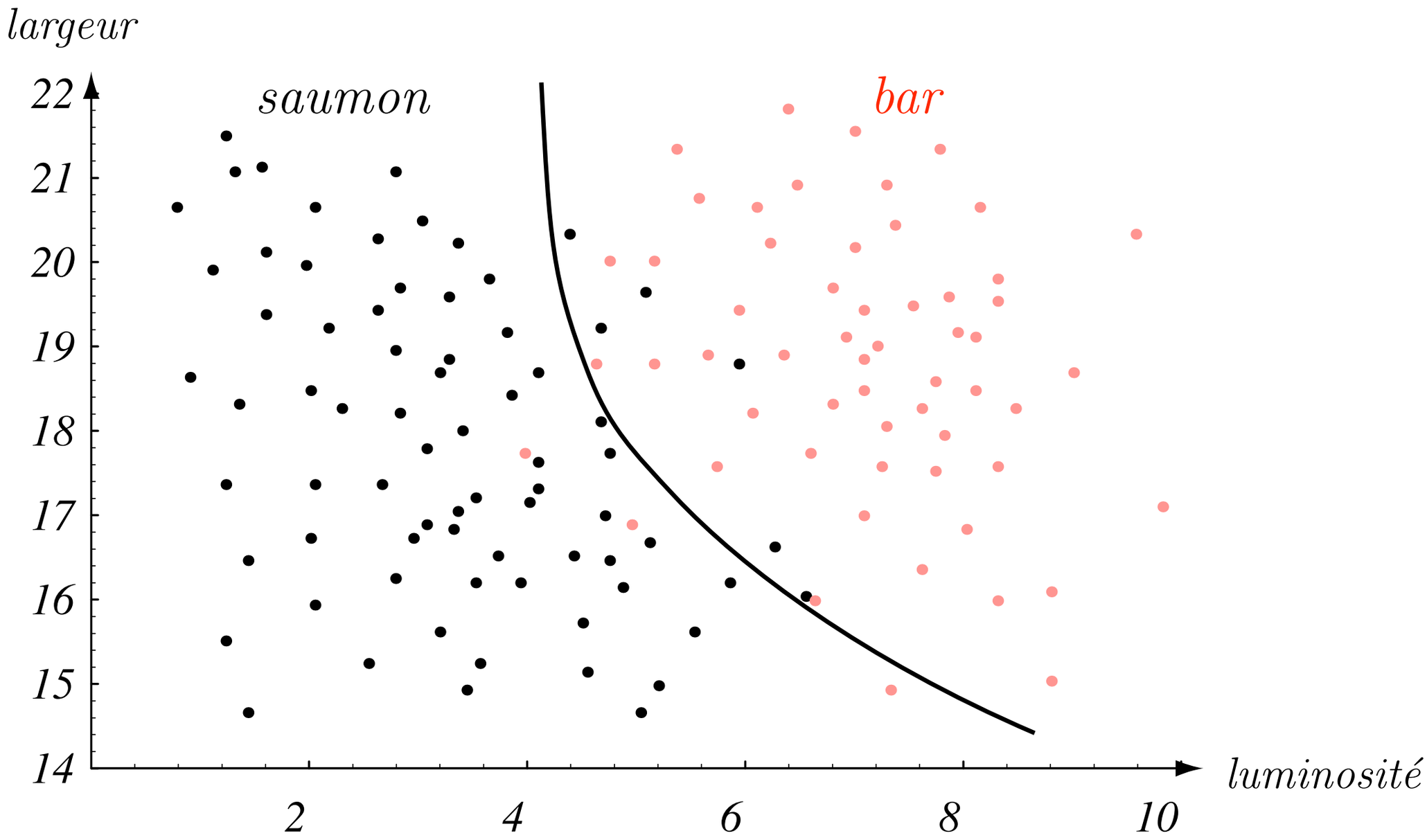
Number of training errors: 3+5 = 8

- Function set too rich (too expressive)
- = Capacity too high for this problem (relative to the amount of data)
- => Overfitting



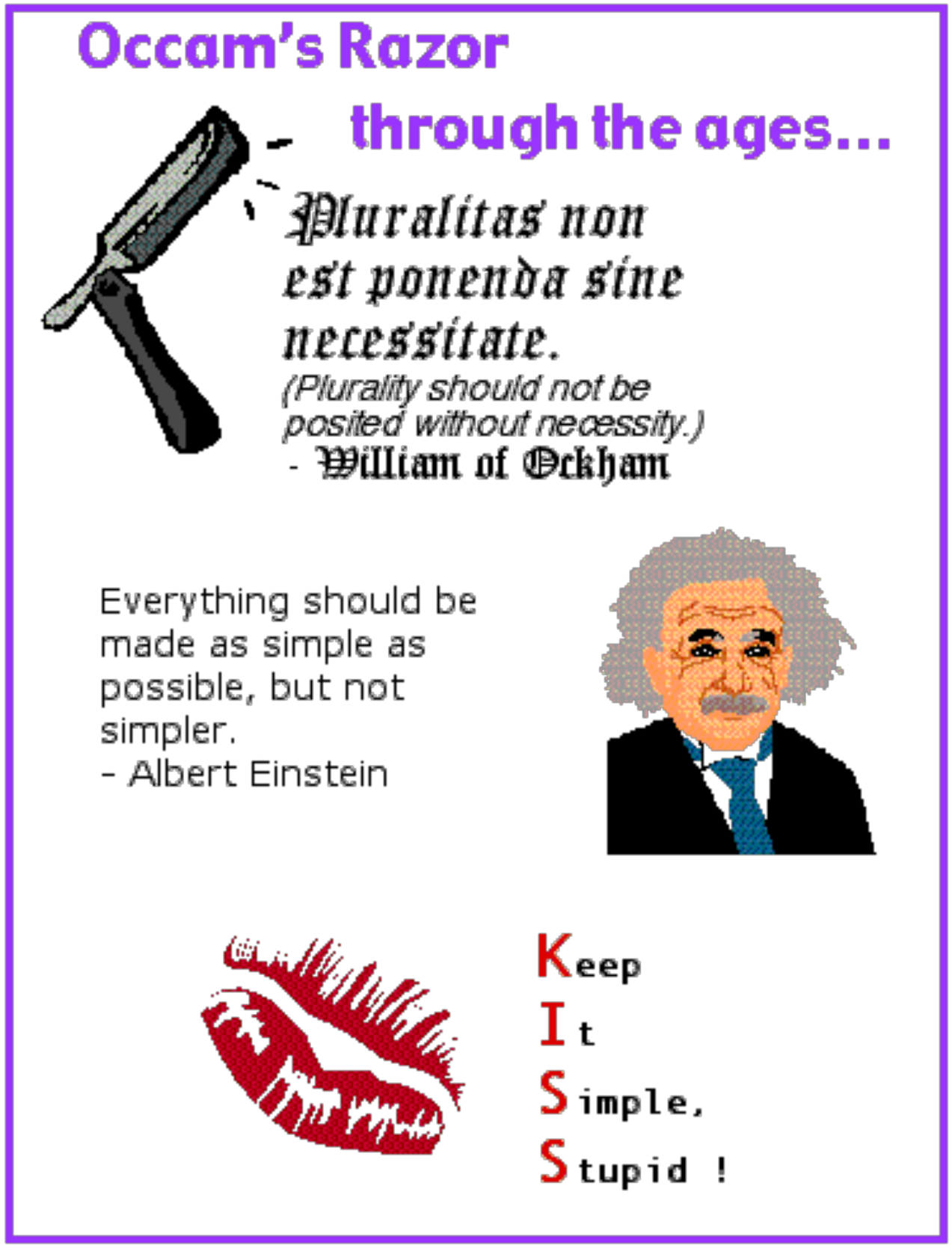
Number of training errors: 0

- Optimum capacity for this problem (relative to the amount of data)
- => Better generalization (on future test points)



Number of training errors: 3+6 = 9

Occam's razor



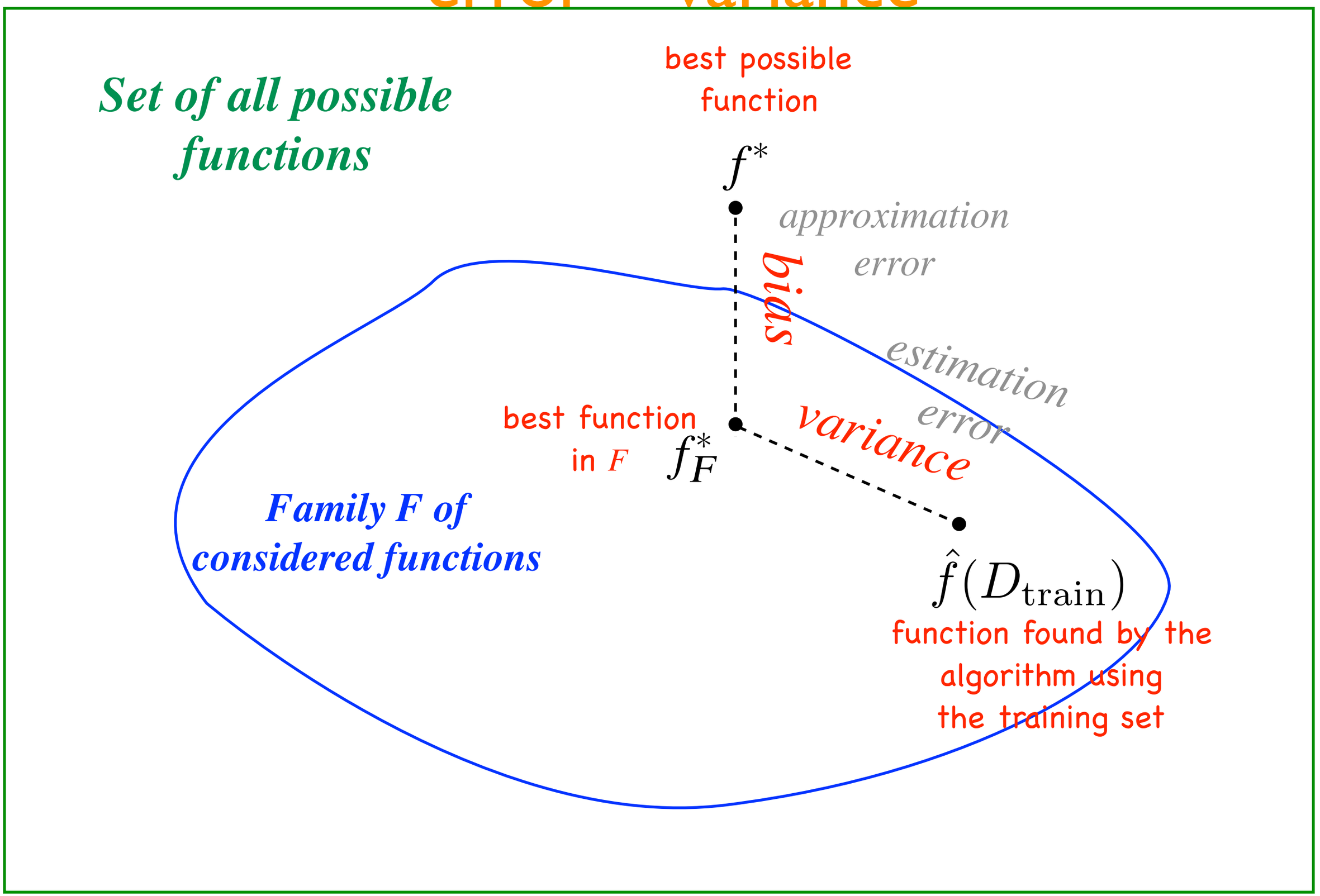
William of Ockham

In learning:

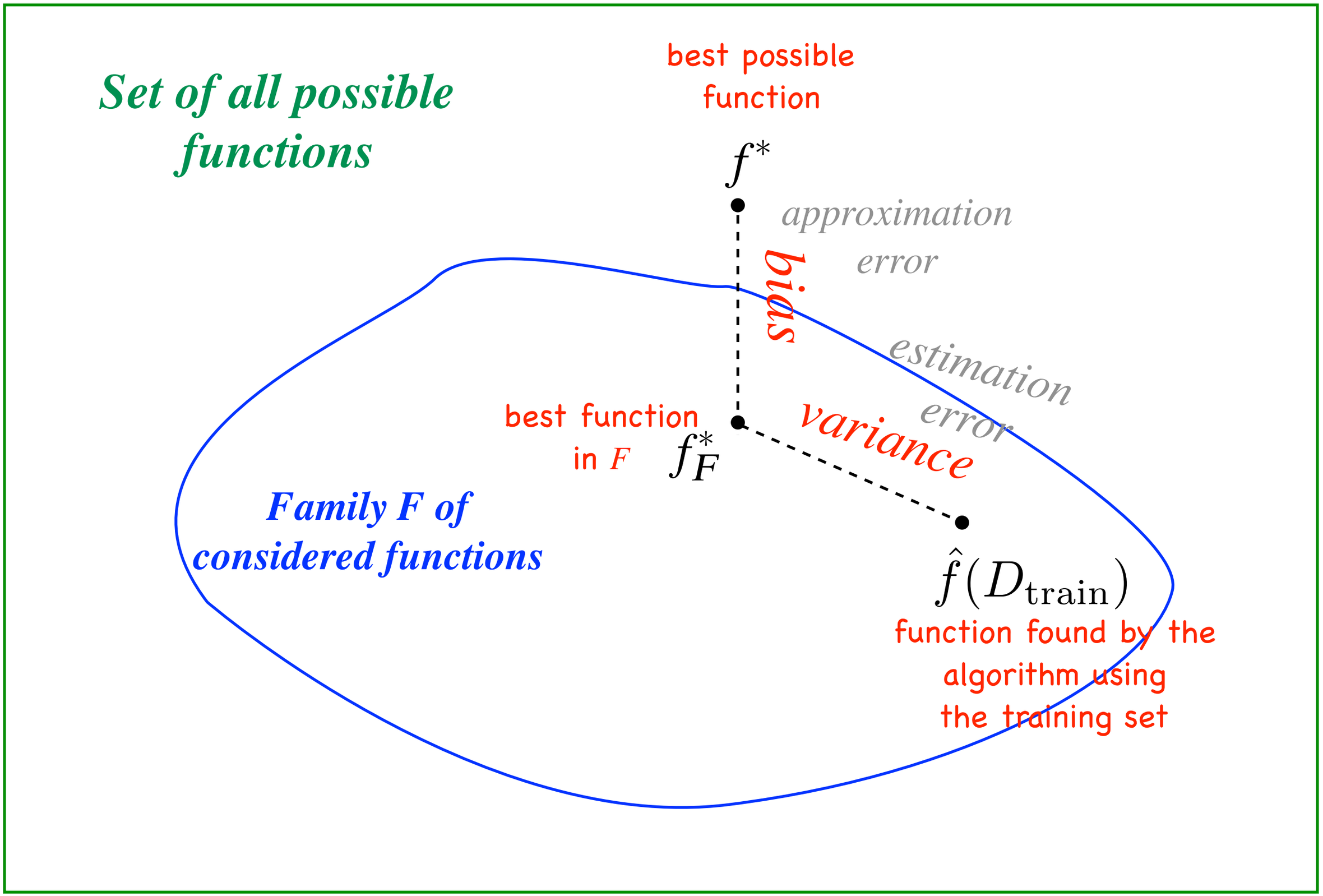
Choose the simplest possible model that learns the data well.

Issue: the more the function family is rich (complex) the more the training data are well "learned" ...

Decomposition of the generalization error + variance



What is the source of variance?



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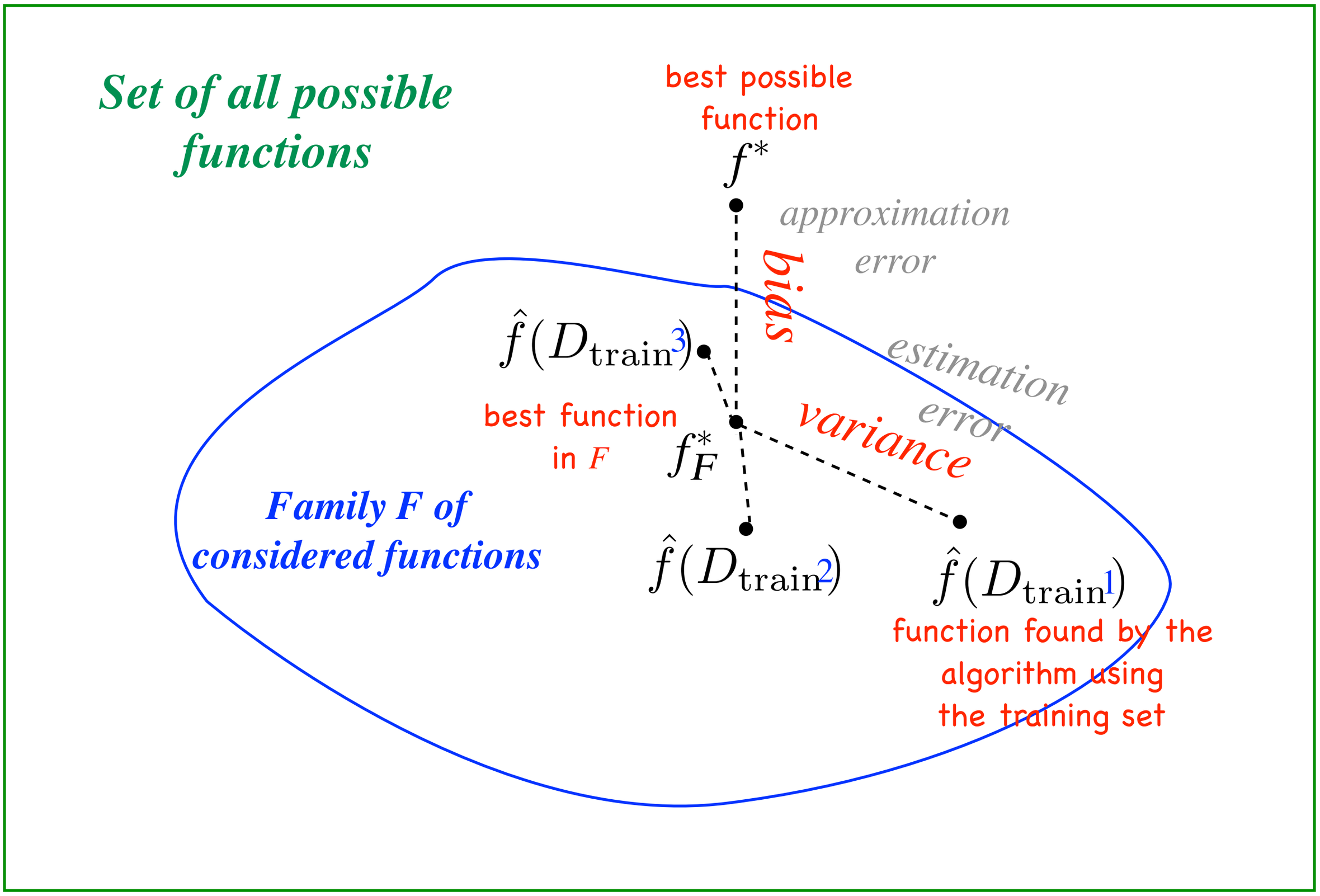


What is the right capacity?
The **bias-variance tradeoff**

- If we choose a rich set F: capacity ↑
  ⇨ bias ↓ *but* variance ↑.

- If we choose a more limited set F: capacity ↓
  ⇨ variance ↓ *but* bias ↑.

- The optimal compromise… will depend on the problem and the number of training examples ***n***

- Bigger ***n*** ⇨ variance ↓
  We can then afford to increase the capacity (to decrease the bias)
  ⇨ we can afford more complex models.

- The best regularizer is more data :)

Model selection
Selection of hyper-parameters
in practice

Model selection

We will consider:

- **Several** learning algos.
- For each algo, **several** choices of values of its hyper-parameters (eg nb of neighbors k in k-NN, nb of neurons in a neural network, ...)

For each case, we will train a model (optimize its parameters on a training set)
then evaluate its out-of-sample generalization performance (on a validation set)

Model selection (and hyperparameters)

Make sure the examples in D are in random order. Divide 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 model considered model (algo) $\mathbf{A}$:

For each configuration of hyper-parameters λ:

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

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

- evaluate the predictor of D_{valid} (with an appropriate evaluation metric)

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

Identify $\mathbf{A}^*, \lambda^*$ that give the best $e_{\mathbf{A}_\lambda}$

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

Or re-train and return

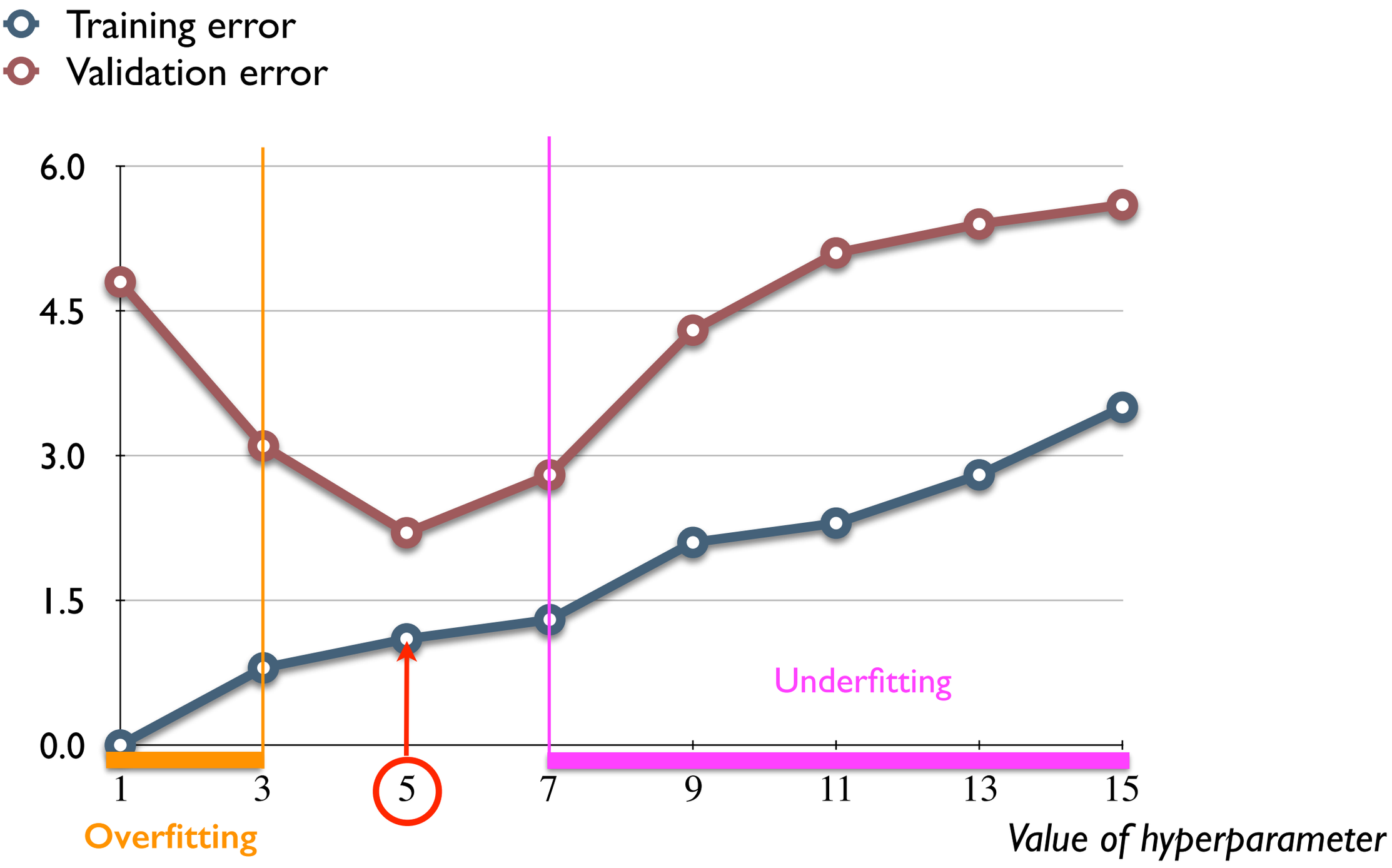
$$f^* = \mathbf{A}^*_{\lambda^*}(D_{\mathbf{train}} \cup D_{\mathbf{valid}})$$

Finally, calculate an unbiased estimate of the generalization performance of f^* using D_{test}

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

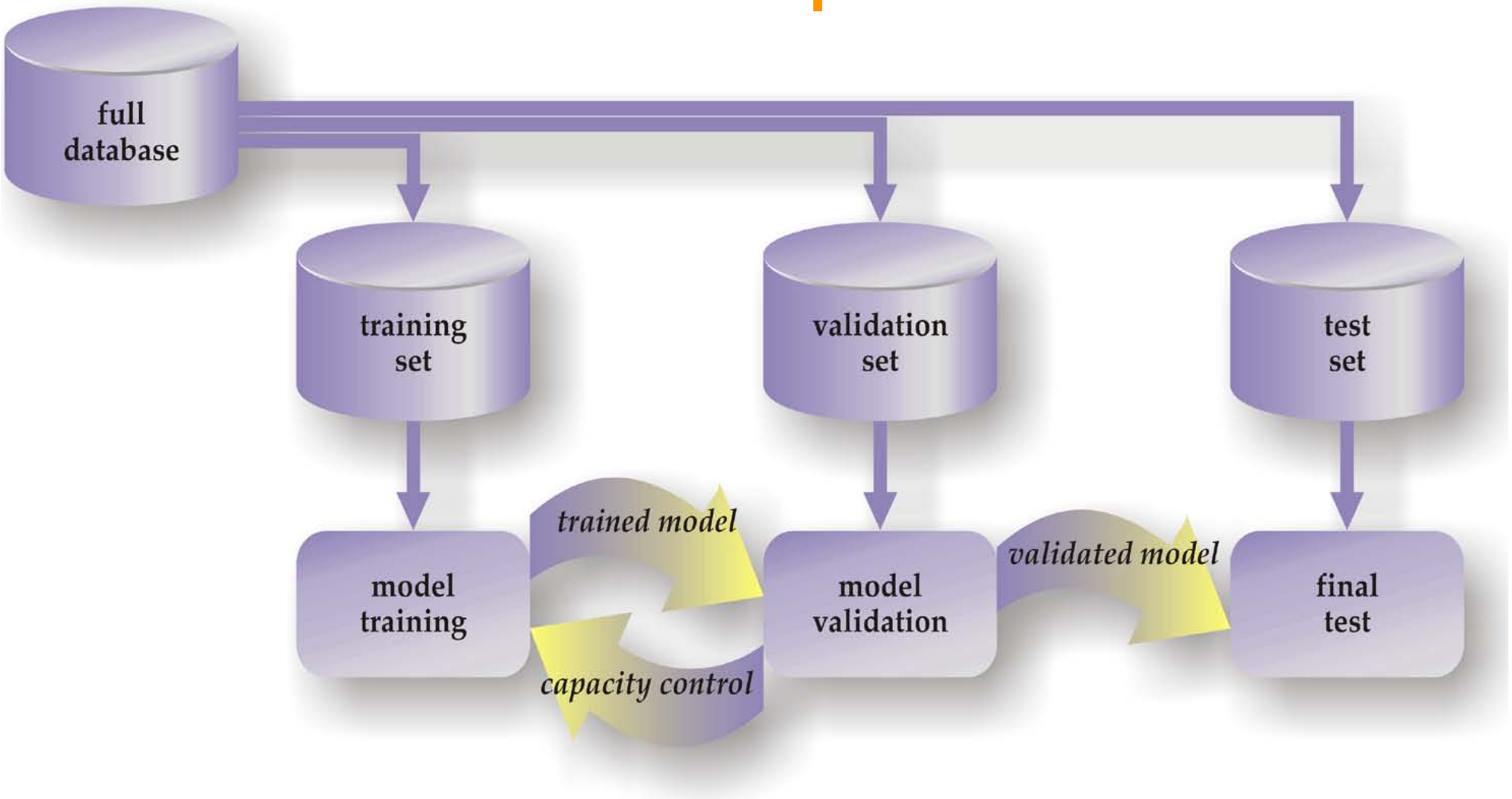
D_{test} must never have been used during training or model selection to select, learn, or adjust anything

Learning curves



The value of the hyper-parameter giving the minimum error on the validation set is **5** (while it's 1 for the training set)

Model Selection: How to proceed



The final performance evaluation must be based on data that has not been used for training or selection of models or capacity.

Parameters v.s. hyperparameters?

- Parameters are optimized on the training set (learned by the algorithm).
- Hyper-parameters are fixed by the user generally before training.
  We optimize them on a validation set (external loop) Generally they control capacity
- What would happen if we chose both hyper-parameters and optimal parameters on the training set?

➡ Would tend to choose the highest possible capacity (to make the least mistake on the training set)

➡ Overfitting

➡ Bad generalization

Parameters?
Hyper-parameters?

Eg: for histogram methods

- Which are the hyper-parameters?
- Which are the parameters?

Parameters?
Hyper-parameters?

Eg: for histogram methods

- Which are the hyper-parameters?
  - Number of bins (subdivisions/cases)
- Which are the parameters?
  - The count (how many examples) in each bin

Parameters?
Hyper-parameters?

Eg: For k-NN

- Which are the hyper-parameters?
- Which are the parameters?

Parameters?
Hyper-parameters?

Eg: For k-NN

- Which are the hyper-parameters?
  - Neighborhood size: k
- Which are the parameters?
  - We memorize the training data set

Parameters?
Hyper-parameters?

Eg: for Parzen windows

- Which are the hyper-parameters?
- Which are the parameters?

Parameters?
Hyper-parameters?

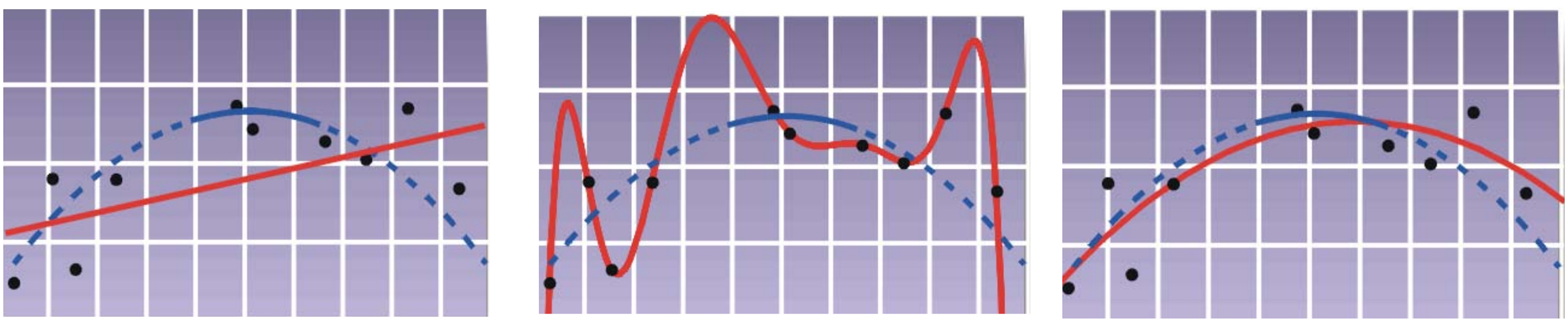
Eg: for Parzen windows

- Which are the hyper-parameters?
  - Neighborhood Size: Kernel width
- Which are the parameters?
  - We memorize the training data set

Parameters?
Hyper-parameters?

Eg: For polynomial regression

- Which are the hyper-parameters?
  - degree of the polynomial
- Which are the parameters?
  - learned polynomial coefficients



Hyper-parameters?

There may be several hyper-parameters

- Controlling the "size" of the function family
- Inducing a more-or-less restrictive preference among the functions of a family
- Choosing one of several families
- Controlling certain aspects of parameter optimization (which will be performed on the training set).

Regularization

- To more finely control overfitting, we can induce a soft preference among the functions in *F*

$$\Omega : F \rightarrow \mathbb{R}$$

a small $\Omega(f)$, indicates preference for function f.

- Rather than minimize the empirical risk:

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

- We will minimize regularized empirical risk

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

λ is a scalar that control the power of regularization:

the tradeoff between empirical risk and the "a priori" preference between functions in F.

  - *Eg: for F=polynomials we can have* $\Omega(polynomial_p)=p$

For the prediction of time series: sequential validation