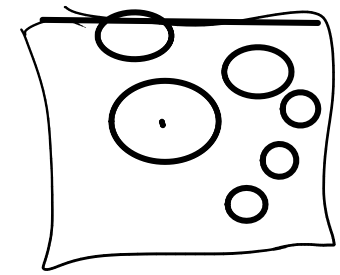
Overfitting Intuitions

Lecture 2:
Over-fitting – the "enemy"



Why such *cheap* minimization algorithms ? (e.g. GD)

→ Do we *really* want to minimize $J(\theta, X_{train})$
The **true objective:** obtain **good performance** on new (unseen) data, which are *different*, but *similar*

$X_{train} \sim \mathcal{P}(x,y)$

$X_{test} \sim \mathcal{P}(x,y)$

We want ***"generalization"***

It's a very ***ill-posed*** problem !

$\mathcal{P}(x,y)$

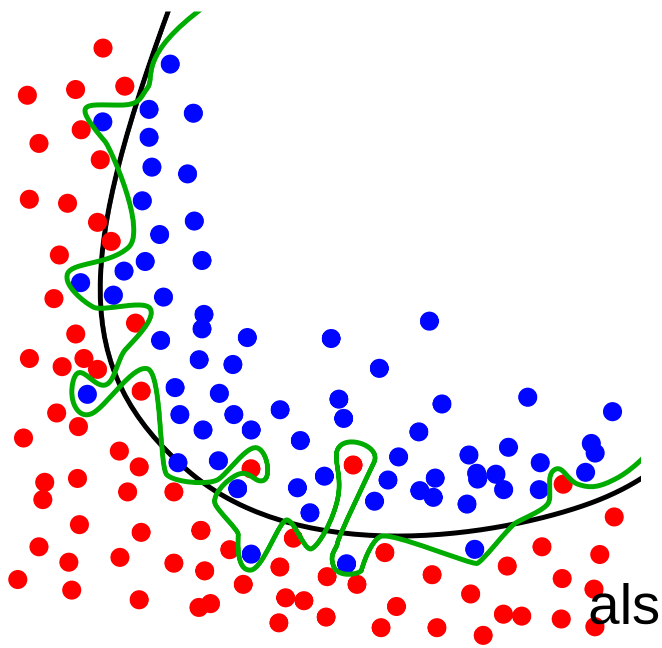
- Example:
  Can we define the probability distribution of the *subspace of dog pictures*, within the space of *100x100 pixels RGB pictures*?
  → We can picture the space of *100x100 pixels RGB pictures*. It's a 3.10^4-dimensional hypercube, easy. R^{30 000}
  → *Subspace of dog pictures* : **no** (unthinkable-of manifold, and it makes no human sense to define this mathematically)
  → We may just assume simple things, like, probably that manifold has a smaller *intrinsic dimension*. But it'll be difficult to measure, etc.
  → so instead, we use **data**

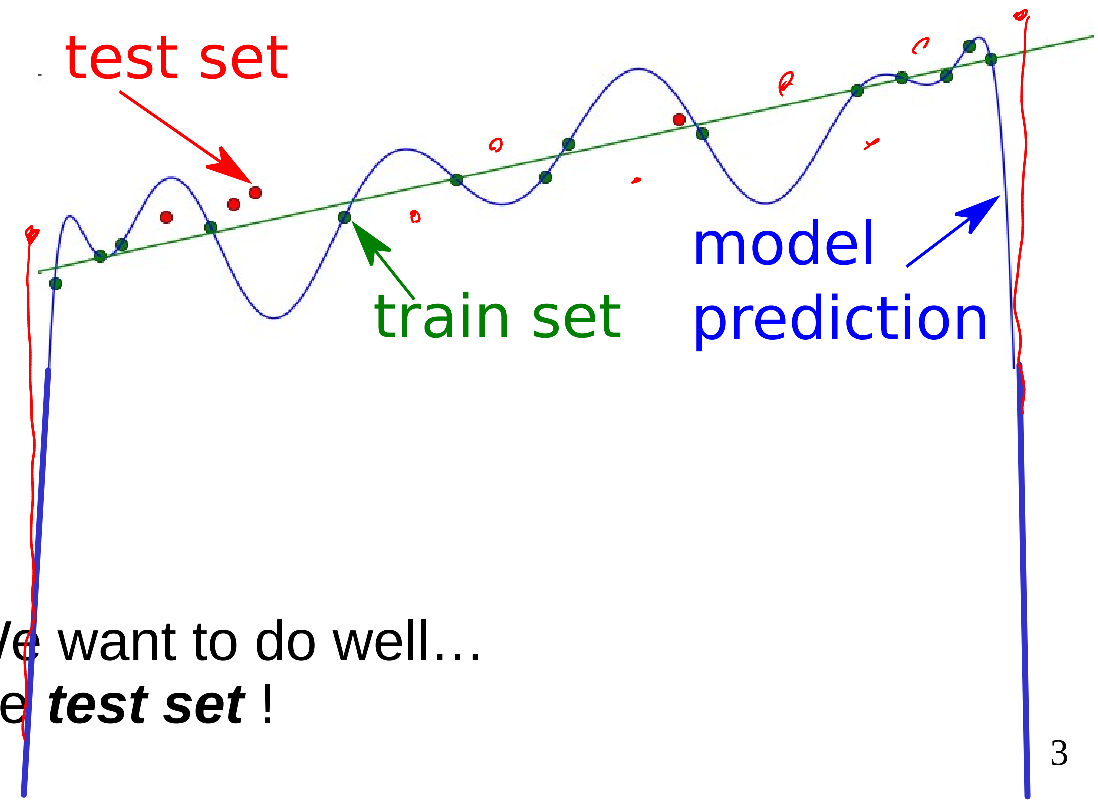
$x_n \in \mathbb{R}^{30000}$, $f_\theta(x_n) = \begin{cases} \text{dog}, 1 \\ \text{no-dog}, 0 \end{cases}$

Over-fitting
intuitive definition

Reminder:
N points are always ***exactly*** interpolated by an **(N-1)$^{\text{th}}$-order** polynomial.
→ Yes, but with **horrible over-fitting:**

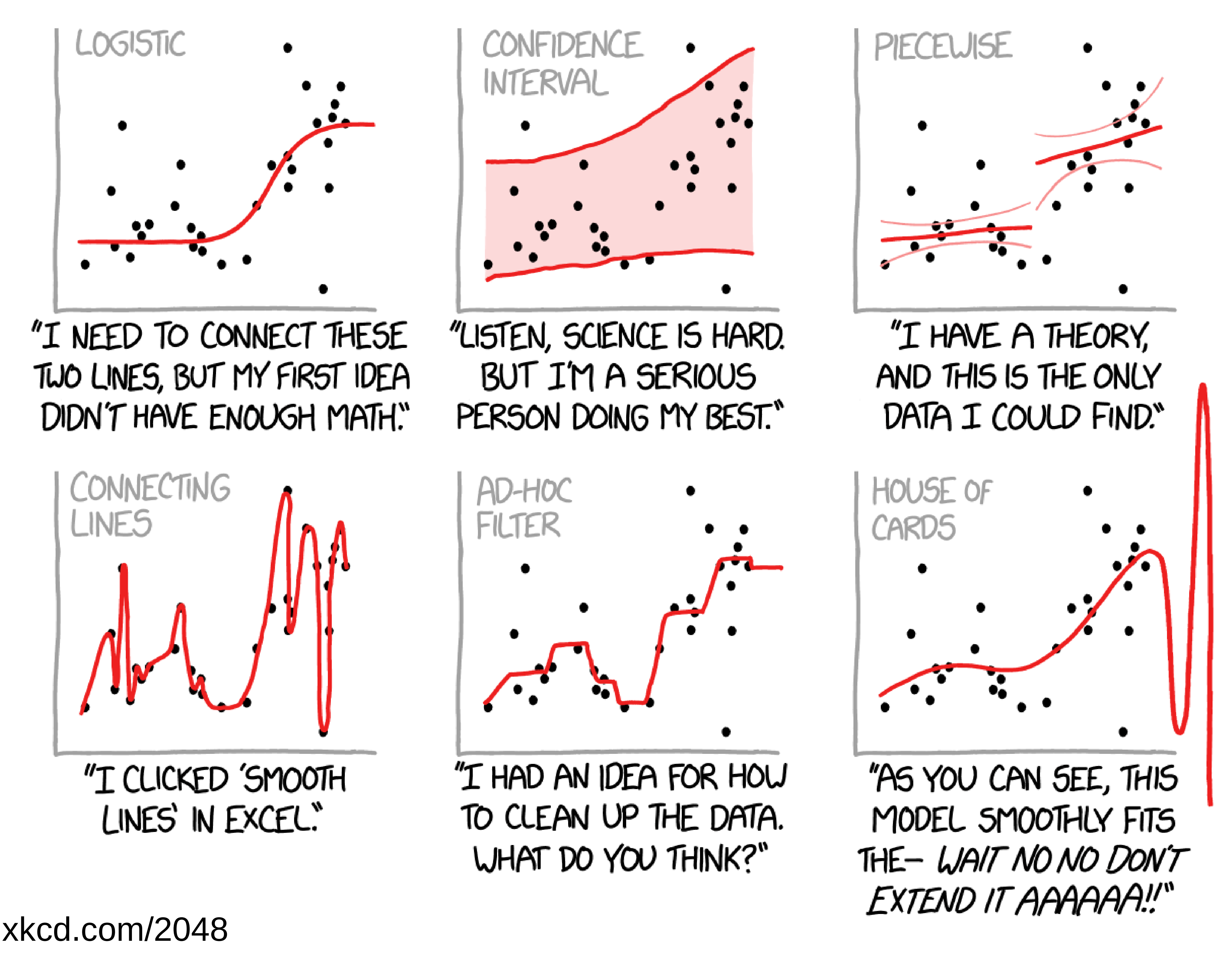
Classification: Cover theorem states that N points are always linearly separable in N dimensions
→ Same problem:





We want to do well…
also on the ***test set*** !

curve-fitting: https://xkcd.com/2048/



xkcd.com/2048

Measuring the over-fitting: concept of ***Test set***

Over-fitting: visually, in 2D, easy to see

→ but how to characterize it **quantitatively** ?

With only N data points:

- We simulate the arrival of **new data** by setting aside some examples. N_{test}
- We **train** the model with the $N_{train} = N - N_{test}$ examples (opimization of the parameters *Θ*)
- We **test** the model (measure performance) on the "new" data N_{test}
(test: *model prediction* vs. *Ground Truth*)

Measuring the over-fitting: concept of ***Test set***

- Few errors ≃ good performance
- The difference between

  - ***train*** set error

  \- ***test*** set error

  is <u>*a*</u> **measure of *over-fitting***

→ Low overfitting = good generalization

→ High overfitting = bad generalization

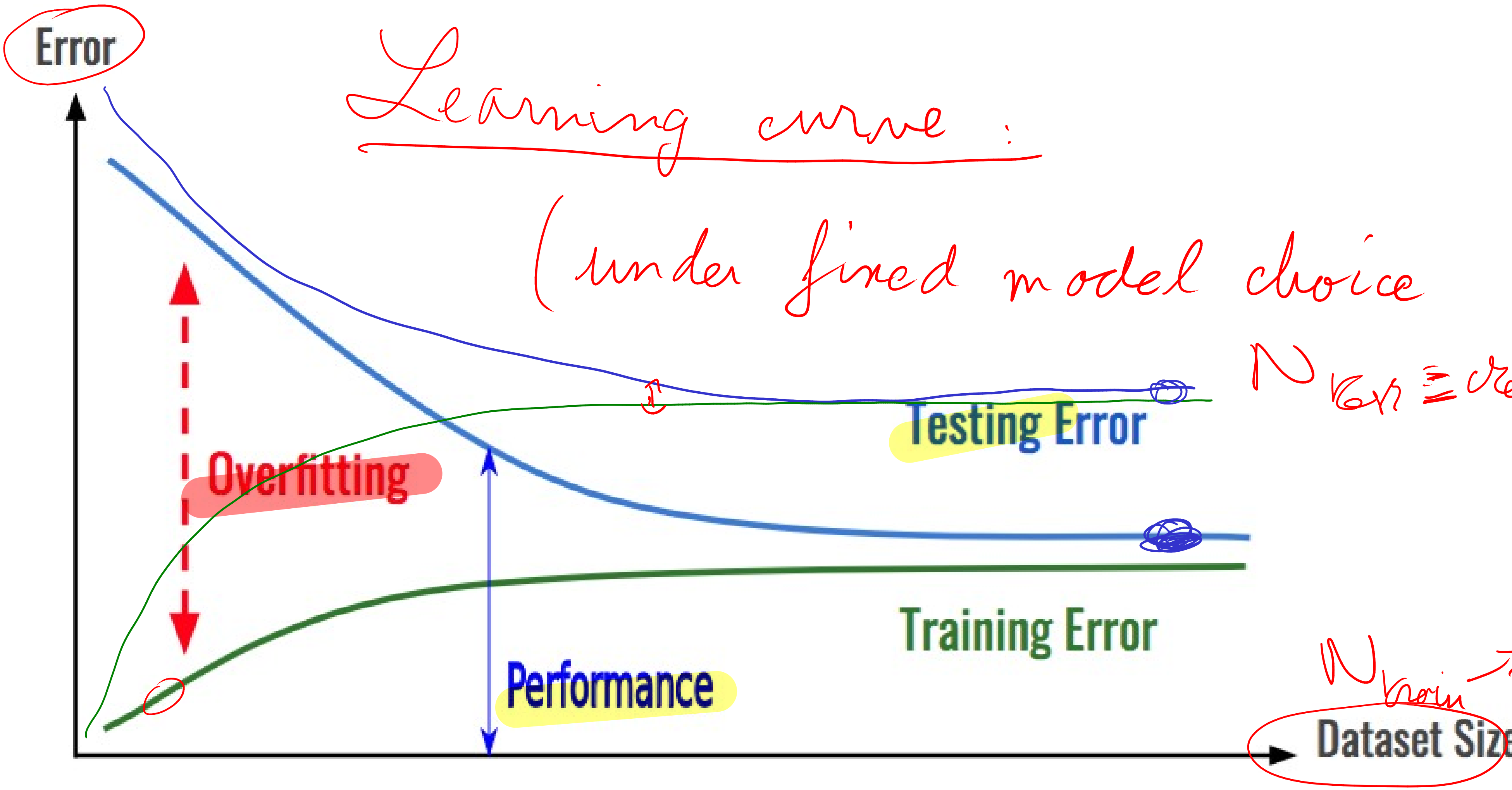
- **Amount of overfitting ≠ performance**

Overfit vs Train set size

- For instance, set: $N_{test} = 0.2N, N_{train} = 0.8N$

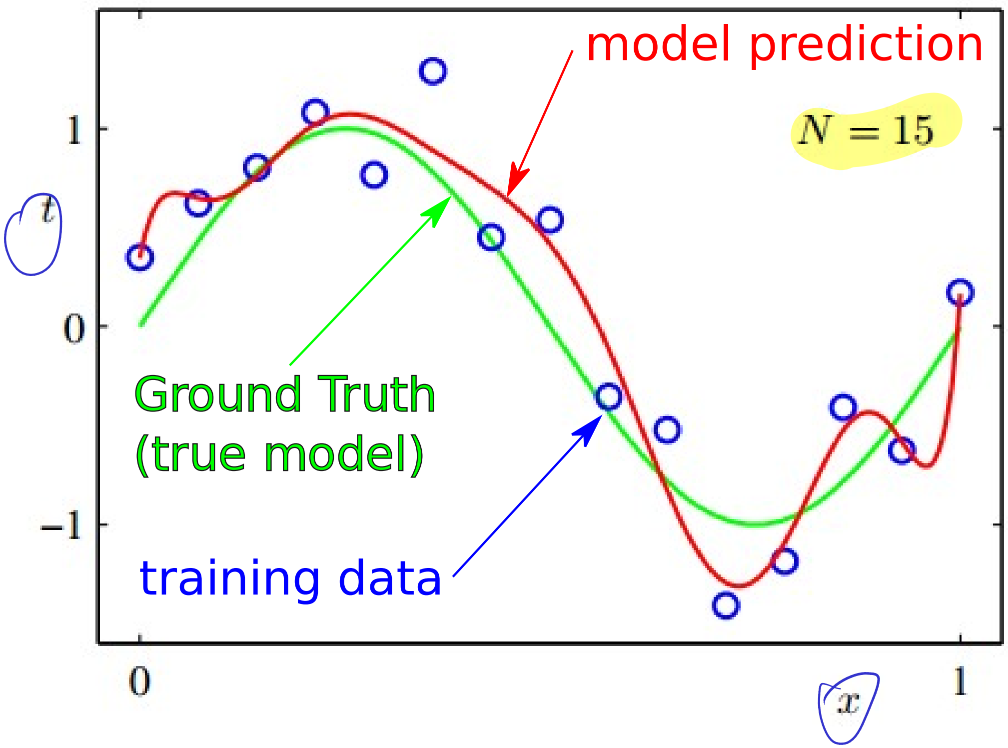
Learning curve :

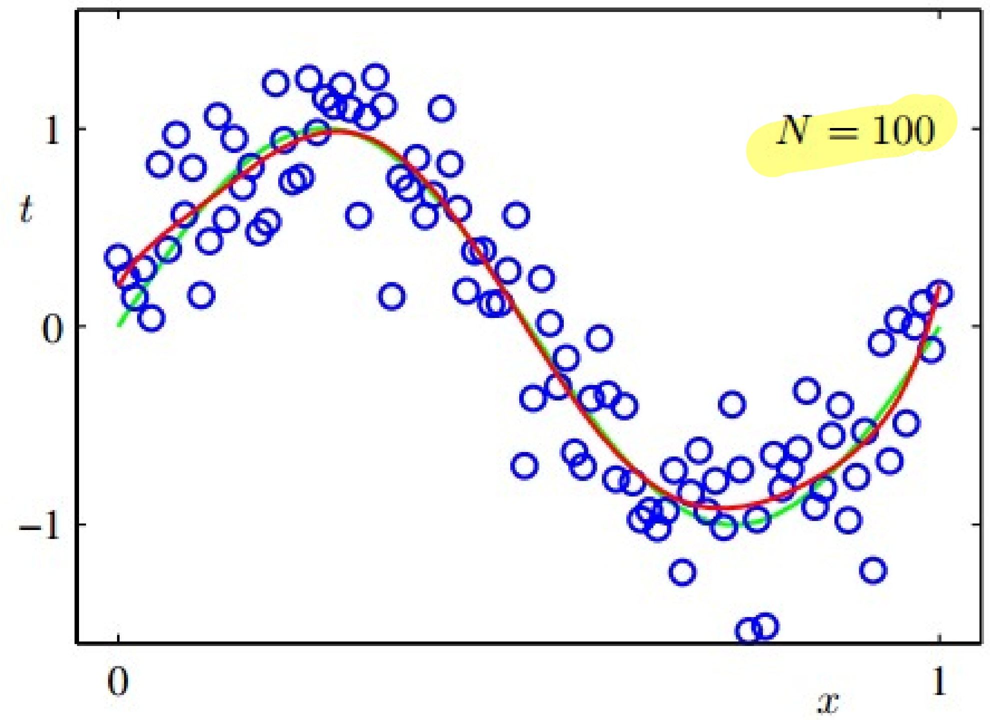
(under fixed model choice



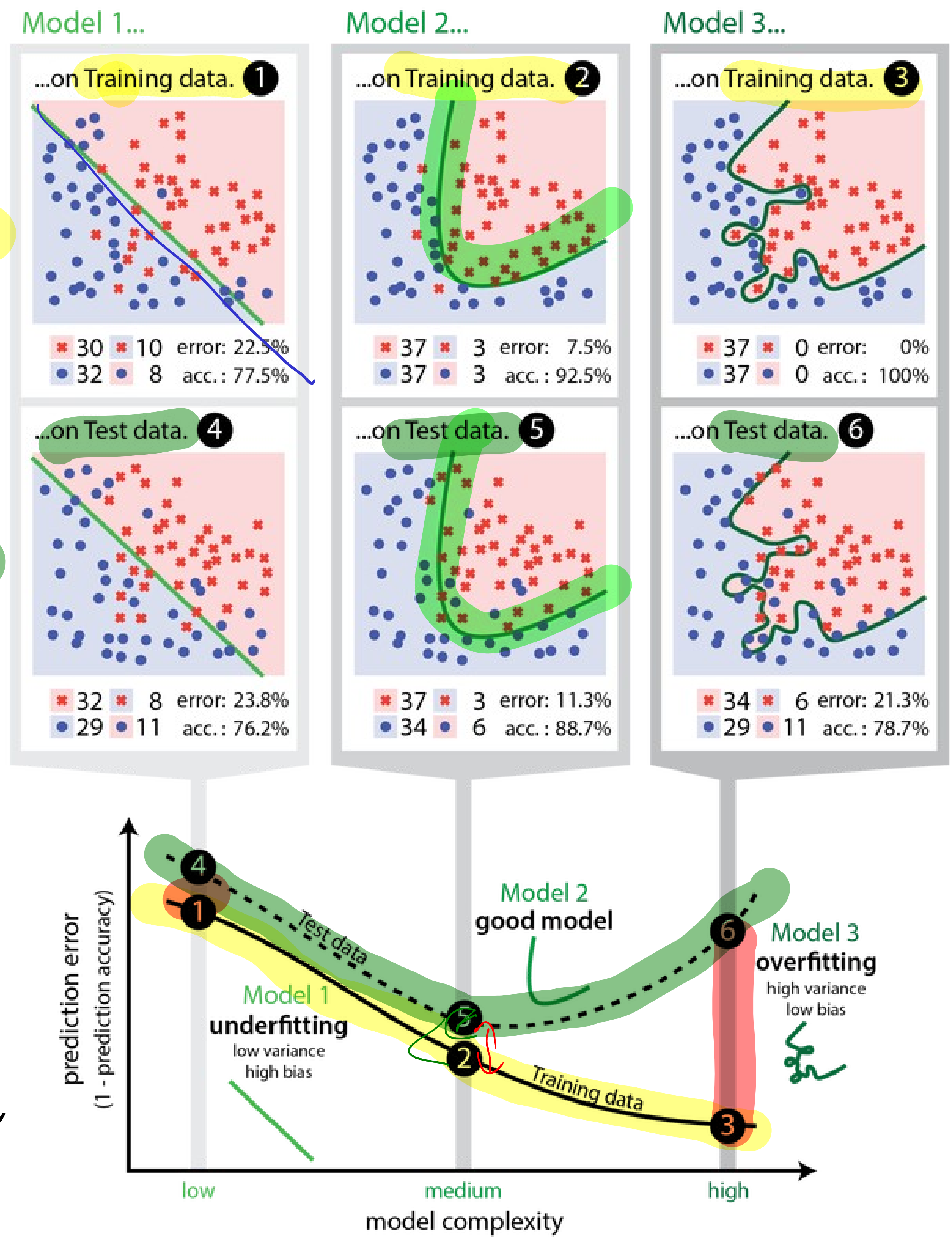
Overfit vs Train set size

- Restrain overfitting by adding more training data (here, using a 9th order polynomial)





Overfit vs model complexity



2-D dataset

available for all problems.

Model *complexity*
= model *capacity*

Hypothesis Space

- Useful concept:

$$H = \{\ f \mid f \text{ can be expressed by your model}\}$$

$$= \{\ f_\theta \mid \theta \in \Theta\ \}$$

Concept of **hyper-parameter**

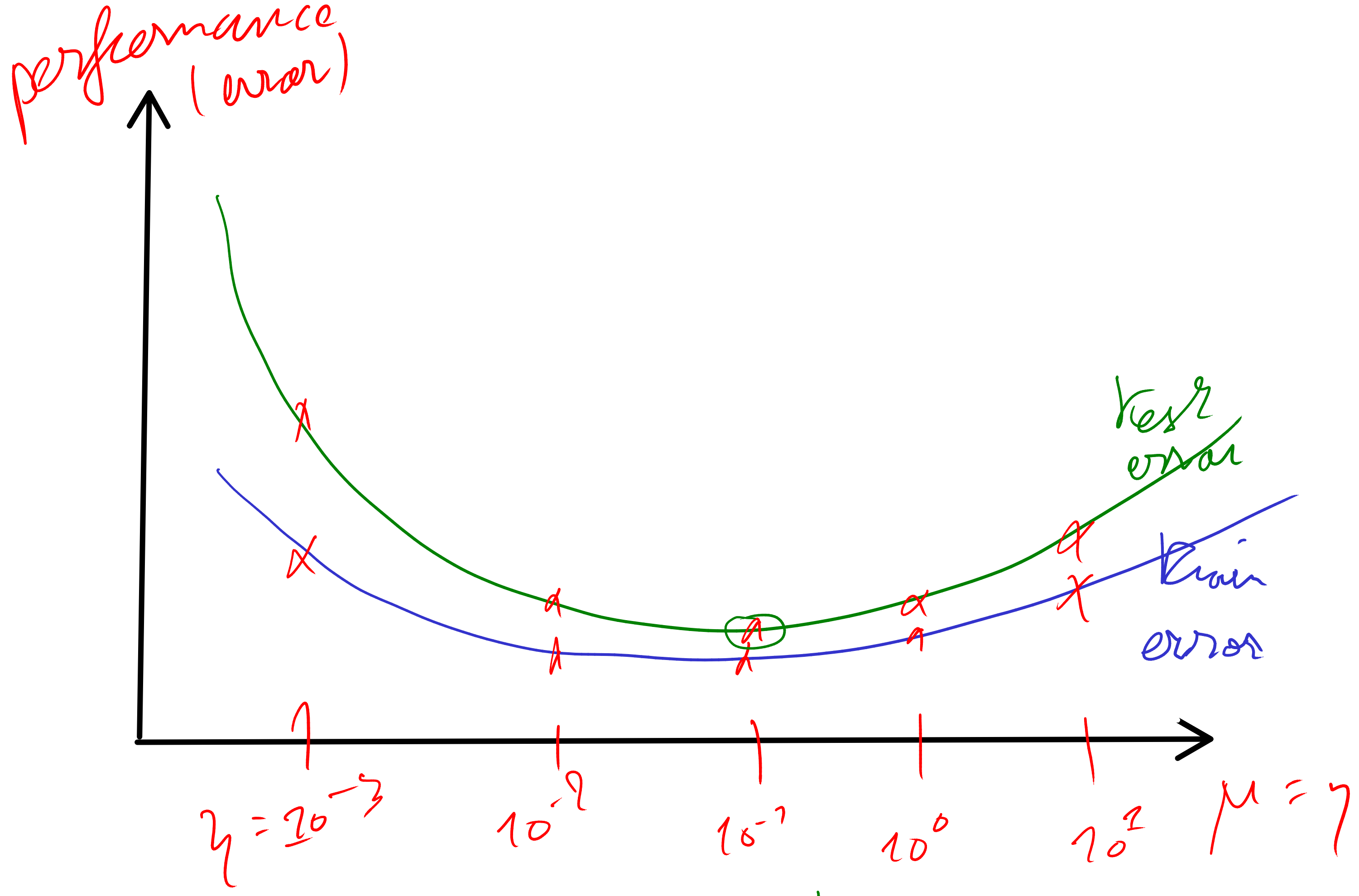
Not really a choice: Train set size $Ntrain$ (quite fundamental)
→ use as much as available, + study the *learning curve*

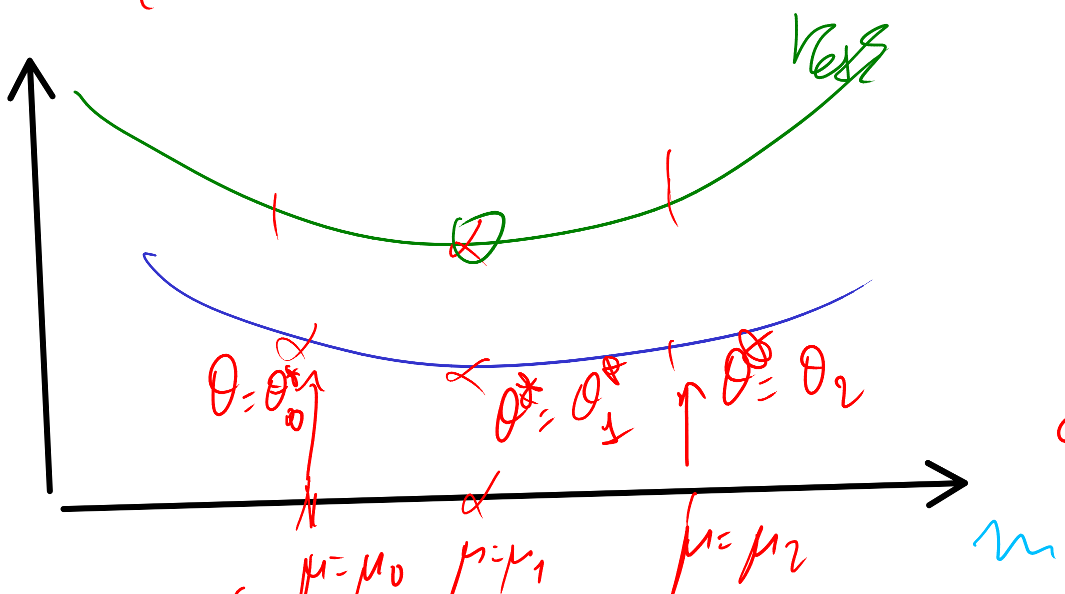
Overfitting depends on many choices: the **hyper-parameters** ***μ***

- ***Learning rate*** η $\mathbb{P}(\theta_0)$
- **Initialization** of parameters
- Learning strategy (size m of the mini-batch for instance)
- **Stopping criterion** (iterative methods: *MaxIter* or *tolerance*)
- **Pre-processing** choices (standardization or not, etc)
- Model ***capacity*** (or ***complexity***): not well defined. It's a bit of everything. Concretely: number of parameters (Cardinal of Θ), architecture, Kernel,…

→ Basically, everything that is not a parameter (a θ ∈ Θ) … is a hyper-parameter !

→ Let's optimize also these hyper-parameters *μ* !



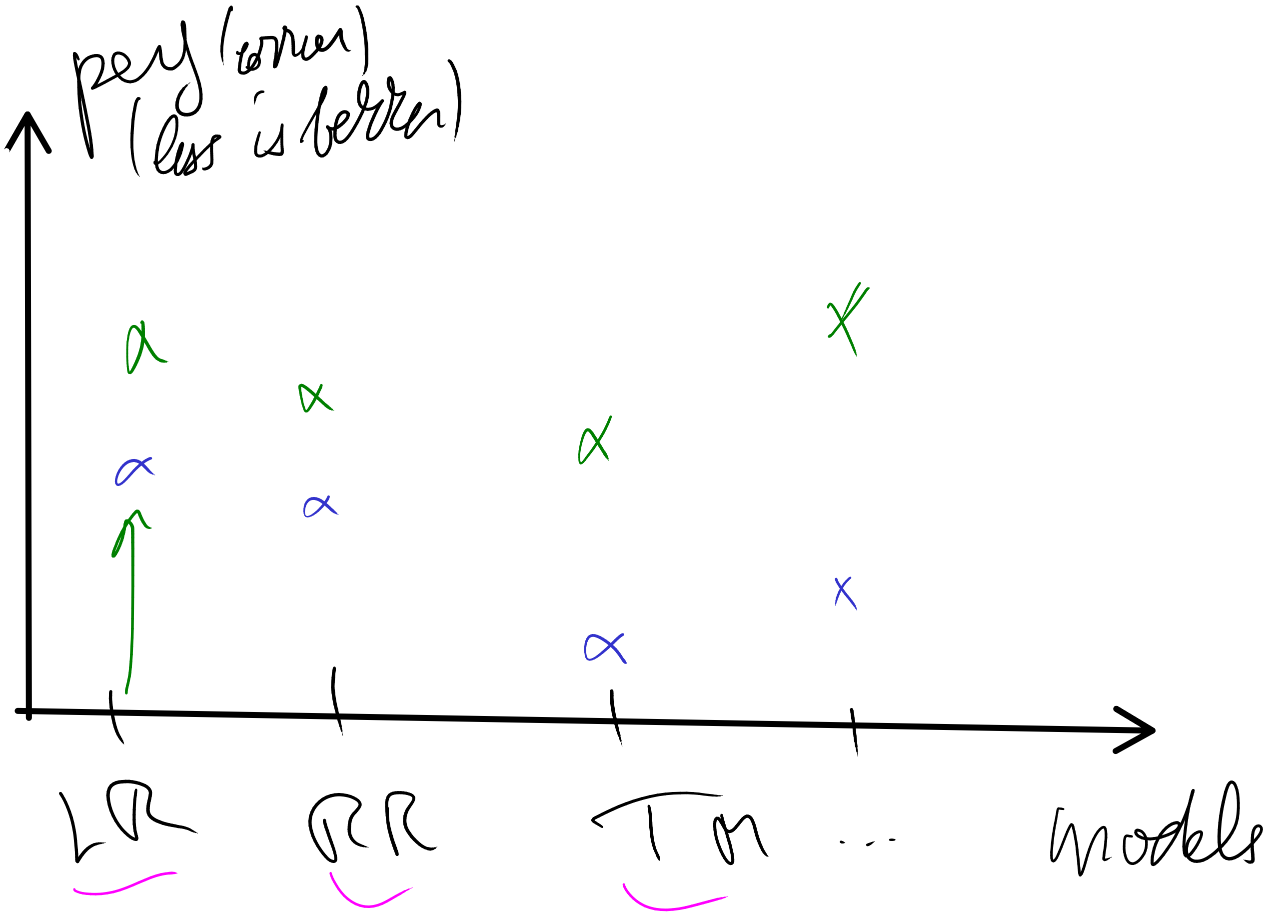


$\mathcal{L}$ = Loss

$$\mu = \left(\eta,\ n,\ P(\theta_0),\ \text{Archi},\ \dots \right)$$

$$\mu^* = \operatorname*{argmin}_{\mu_0} \left(\mathcal{L}\left(X_{test}, Y_{test}, \theta = \theta^*, \mu_0 \right) \right)$$

$$\theta^* = \operatorname*{argmin}_{\theta} \left(\mathcal{L}\left(X_{train}, Y_{train}, \theta, \mu_0 \right) \right)$$


perf (error)
(less is better)
LR
RR
Tr
...
models

Note: ML is a bi-level optimisat° pbm.

Validation Set

If we also optimize the hyper-params,
then we can also over-fit them !?!

Train set

Train parameters $\theta \rightarrow \theta^*$

(Hyper-param. fixed) $\mu = \mu_0$

$\operatorname{argmin}_{\theta} (\mathcal{L})$

Validation set

Optimize hyper-param. $\mu \rightarrow \mu^*$

(Parameters fixed) $\theta \Rightarrow \theta^*$

$\operatorname{argmin}_{\mu,\ \theta = \theta^*} (\mathcal{L})$

Test set (single use!)

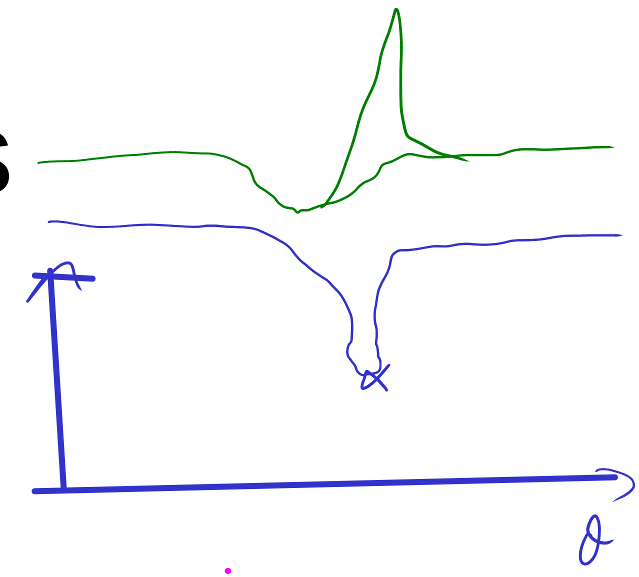
(Hyper-param. fixed) $\mu = \mu^*$

(Parameters fixed) $\theta = \theta^*$

→ measure performances

estimate future performance

Over-fitting
General things

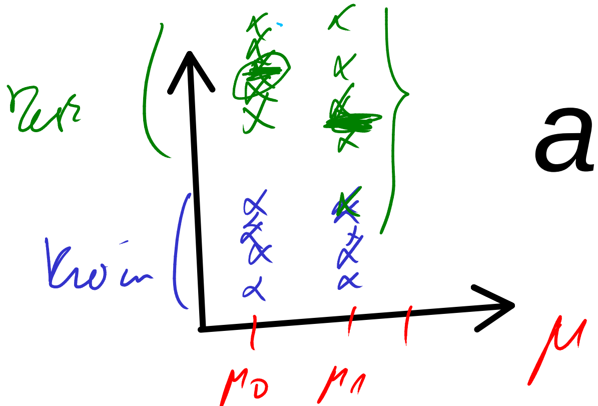


How to improve performance ?

- Seeing a lot of overfitting ?
  → **reduce the model complexity**
  (try **simpler** models)
- Little to no overfit ?
  → try more ***expressive***, more ***flexible*** models

Searching the ***global minimum*** $J(\theta, X_{train})$ .. or not ?
→ “best fit” possible but… on the *train set* !
→ in general, global min. = large over-fit.

- Ill-defined problem: what is *generalizability* ?
  → How to sample “the set of all 2D images showing a dog” ? → *Generative Models*. Quality ??
  → *Transfer Learning*



a Cross-Validation
K-fold CV

- Make K folds , e.g. $K{=}5$ train/validation splits

$\mu = \mu_0$ fixed

Iteration 1	Valid.	Train	Train	Train	Train	test
Iteration 2	Train	Valid.	Train	Train	Train	test
Iteration 3	Train	Train	Valid.	Train	Train	test
Iteration 4	Train	Train	Train	Valid.	Train	test
Iteration 5	Train	Train	Train	Train	Valid.	test

$\theta \to \theta_1^*$, $\mu = \mu_0$

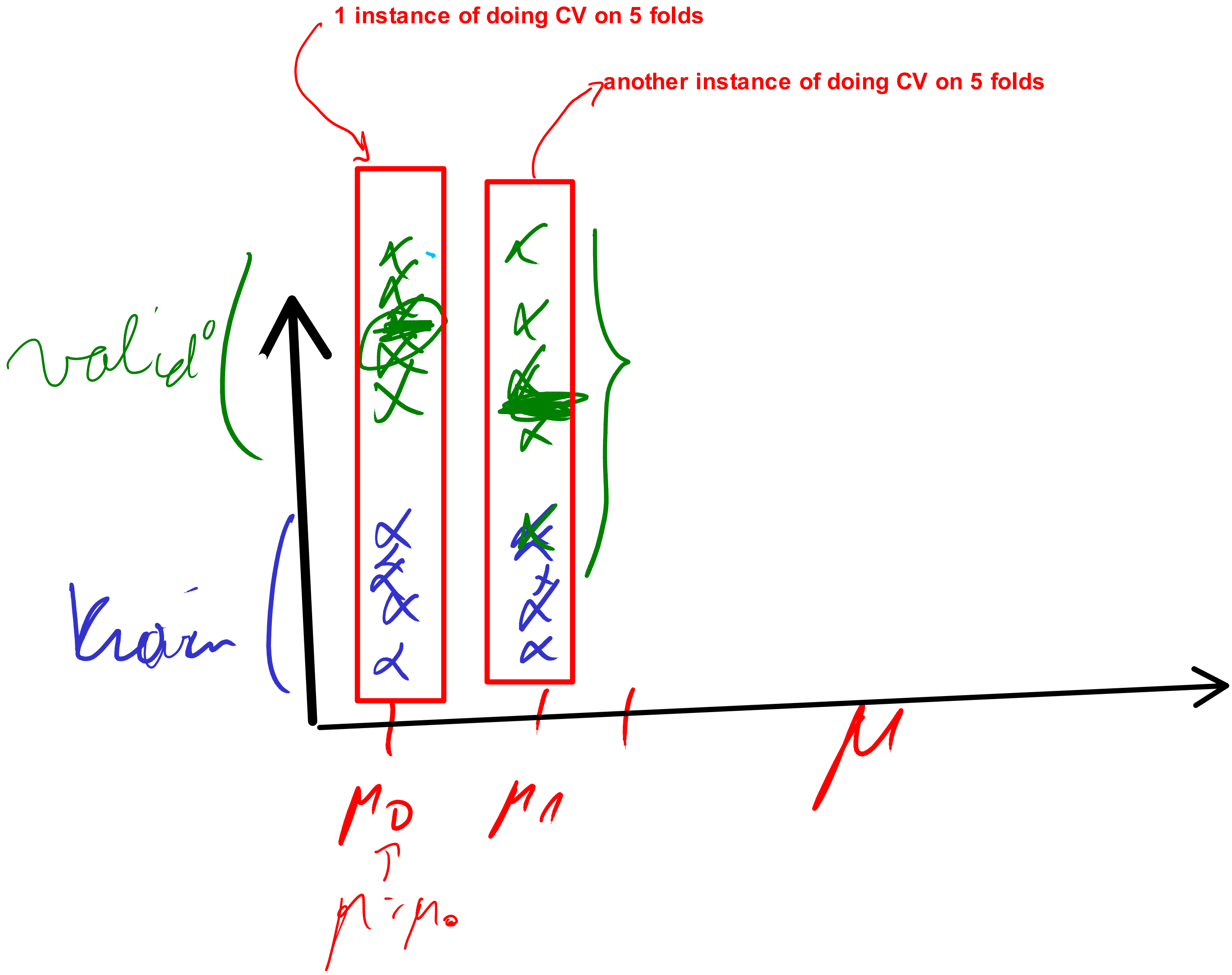
$\theta \to \theta_2^*$, $\mu = \mu_0$

$\theta \to \theta_3^*$, $\mu = \mu_0$

Bootstrapping

N — N out of N with replacement.

→ reduces the splitting-related noise



1 instance of doing CV on 5 folds
another instance of doing CV on 5 folds
valid
train
μ_0
μ_1
μ

Another Cross-Validation **Leave-one-out** CV (**LOO**)

Def: Like K-fold but with $\mathrm{K} = N_{\mathrm{train}}$.

- **Useful** esp. for small data sets (reduce N_{train} by only 1 example)

$N_{\text{train}} - 1$ train

1 val

- **Reasonable** only for small data sets (otherwise, too many computations)

Key concepts

- Generalization, ***over-fitting***, *under-fitting*, performance
- **The split : *Train, validation, test***
- **Amount of overfitting ≠ performance**
- Train set size
- **Hyper-parameters**
- Complexity ~ capacity ~ expressiveness
- Cross-Validation
- Curse of dimensionality

To go further: keywords

- I strongly encourage you to read :
  Bishop section 3.2 "Bias-Variance decomposition"
  It's very well explained and a quite basic argument – no time to cover it now

Simple

- **Basic stuff**: ***Hypothesis space***, finite vs infinite.

  1) **Double Descent**: *catastrophic overfitting* (without regul) happens esp. when N=P.
  \+ there is an *implicit regularization* obtained by over-parametrization (when P>N, provided some simple conditions).
  → see works of **Francis Bach**.

more advanced

  2) A rather classic, finite-dim, finite set approach:

- Vapnik–Chervonenkis dimension (**VC dimension**)
- Probably approximately correct learning (**PAC learning**)

  3) Another kind of approach:
  There are exact results for ***random data sets*** (some are physcists' or mathematicians works).
  More keywords: tensor PCA, planted solution, random constraint satisfaction problems (CSP), dynamic threshold (algorithmic threshold), Information Theoretic threshold (IT),

  → See works of **Gerard Ben-Arous, Lenka Zdeborova**, and others