Introduction to Validation and Theoretical Issues [IIA – Lect.______]

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In the course flow

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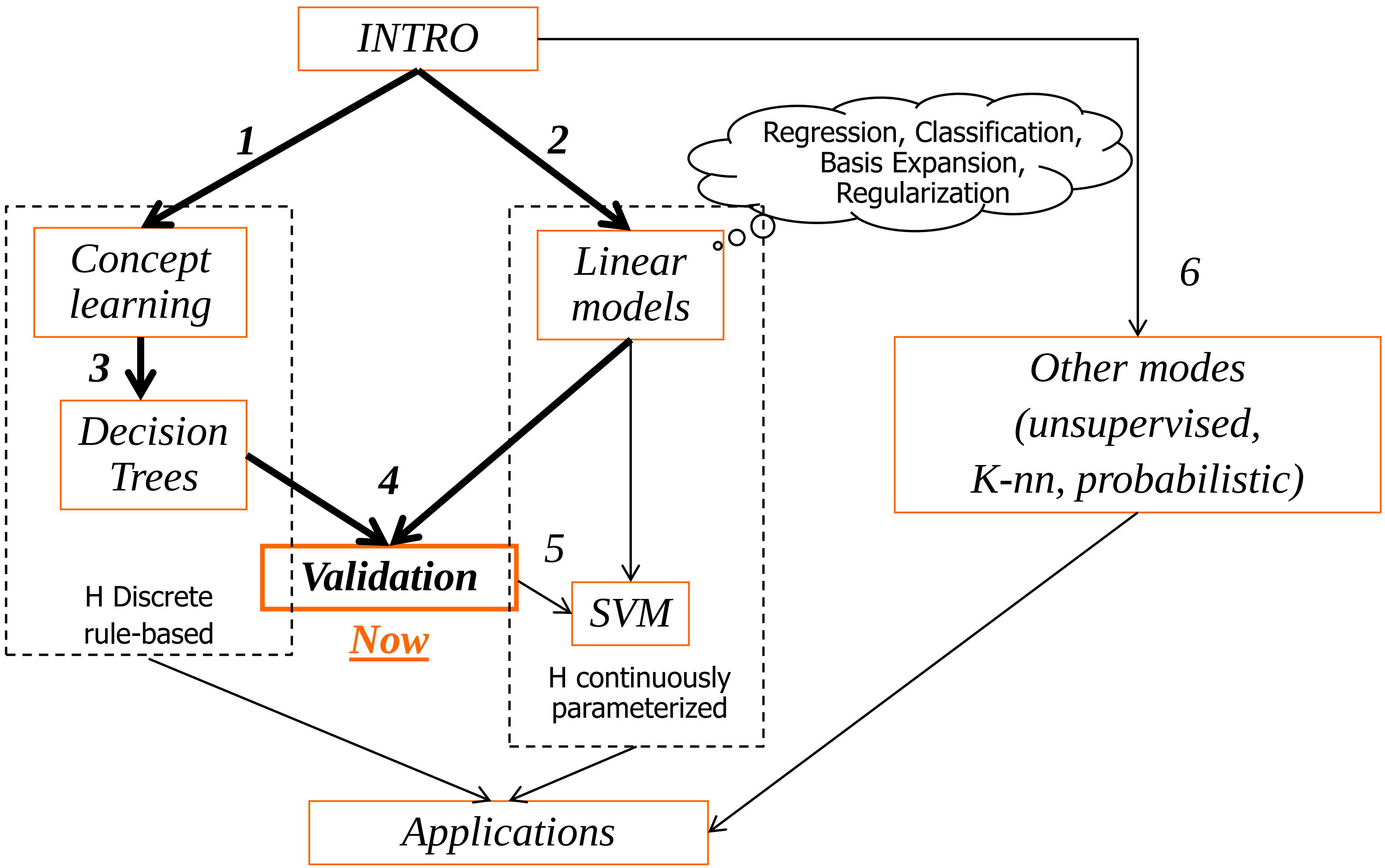

Obiettivi (overview)

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Questioni fondamentali del ML:

evaluate generalization capabilities (of your hp)

- ruolo <u>essenziale</u> della validazione
- cenni (dell'esistenza) di fondamenti teorici (supporto al significato del ML)

- Aspetto sia teorico che pratico per un uso *consapevole* del ML
- Raccogliamo gli spunti raccolti finora solo indirettamente dedicandoci una (questa) lezione

ML issues

Quando un modello di ML
è un buon modello?
Usare il ML versus usare bene il ML

NP

Machine Learning: generalization (I)

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- *Learning*: search for a *good function* in a function space from known data

Def

- Good w.r.t. generalization error: it measures how accurately the model predicts over novel samples of data (low error, high accuracy and vice versa)

[Repetita from lect. 1]

Generalization (II)

- Inductive learning hypothesis
  - Any *h* that approximates *f* well on training examples will also approximate *f* well on new (unseen) instances x (**?**)
  - I.e. is it really valid? And at which extent?

- Punto centrale, ma come obiettivo del ML:
  - Teoria che supporta in che condizioni ciò si verifca
  - Guida la scelta del "best model" (tra modelli diversi o configurazioni diverse: iperparametri, livello di training, …)
  - Va verificato nelle applicazioni

Generalization (III)

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[Repetita from lect. 1]

- Generalization: crucial point of ML!!!
- **Learning** phase **(training, fitting)**: build the model from know data – *training data* (and bias)
- **Predictive** phase **(test)**: apply to new examples
  (we take the inputs ***x'*** and we compute the response by the model; we compare with its target *d'* that the model has never seen):

  evaluation of the predictive hypothesis, i.e. of the generalization capability

Note: *performance* in ML = *predictive accuracy*

estimated by the error computed on the (Hold out) Test Set

Def

- [*repetita*] **Overfitting**: A learner overfits the data if

  it outputs a hypothesis h(·)∈H having true error ε and empirical (TR) error E, but there is another h'(·)∈H having E'>E and ε' < ε

Premise: which measure?

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Recap:

To evaluate typically we measure (see def. in previous lectures)

- For *classification*: MSE for the loss, accuracy or mean error rate for the outcome
  - but also precision, recall or specificity, sensitivity (accounting for False Positive, False Negative), …
- For *regression*: MSE, Root MSE (*S*), Mean Absolute Error, Max Absolute Error, ….
  - but also statistics measures such *R* (correlation coefficient/index), etc.
- Of course high error ←→ low accuracy (both for training, test, etc.)
  - E.g. poor fitting with high training error,
  - E.g. poor generalization with high test error, …

Validation: Two aims

Very important!

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Def

- ***Model selection:*** estimating the performance (*generalization error*) of different learning models in order to choose the best one (to generalize).
  - this includes search the best *hyper-parameters* of your model (e.g. polynomial order, lambda of ridge regression, …).

  It returns a model

Def

- ***Model assessment:*** having chosen a final model, estimating/evaluating its prediction error/ risk (*generalization error*) on new *test* data (measure of the quality/performance of the ultimately chosen model).

  It return an estimation

Gold rule: Keep separation between goals and use separate data sets

Defs

Hold out

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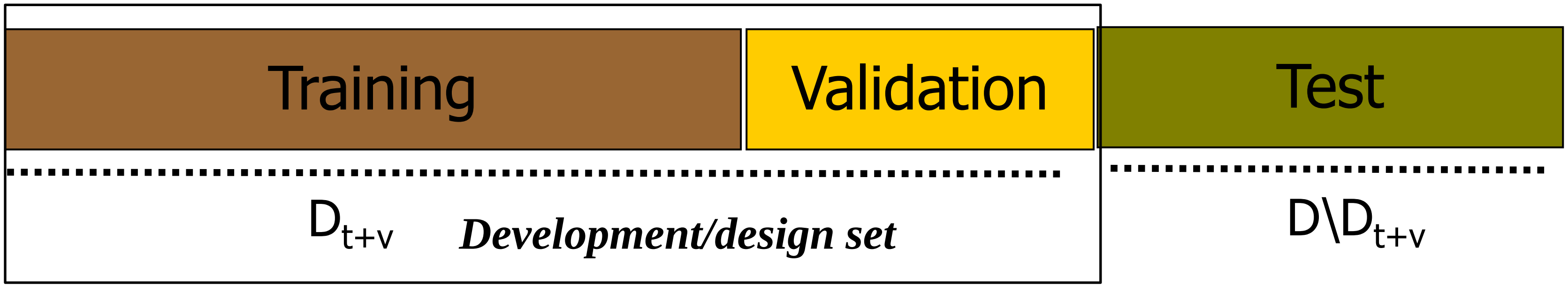
- If data set size is sufficient: e.g. 50% TR, 25% VL, 25% TS **disjoint sets**



- TR: *Training set* is used to fit [**training**]
- VL*: Validation set* (or *selection set*) is used to select the best models (among different models and/or hyper-parameters configurations) [**model selection**]
- TR+VL sometimes are joitnly called development/design set , i.e. used to build the final model
- TS*:Test set* is used for estimation of generalization error (of the final model) [**model assessment**]

Notes:

1) the estimation made for model selection (on vl set) [is for model selection purpose], it is not a good estimation for the assessment phase/risk test.

2) **Test set results** cannot be used for model selection (or call it validation set)

Test or model selection?

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- What if test set is used in a (repeated) design cycle?
  - We are making *model selection* and not reliable *assessment* (estimation of expected generalization error)
    - and *we wouldn't be able to do that on future examples*
    - Blind test set concept (e.g. for ML competitions)
    - Image an exam exercise: if you see the solutions it is not a test!
  - In that case, used test set error provides an overoptimistic evaluation of the true test error (→ we will see how easy is to obtain very high classification accuracy over a random task even using the test set only implicitly)

Gold rule:

Keep separation between goals and use separate sets

(**TR** for training, **VL** for model selection, **TS** for risk estimation)

TR=training set, VL= validation set, TS=test set

TR/VL/TS by a **simple** schema

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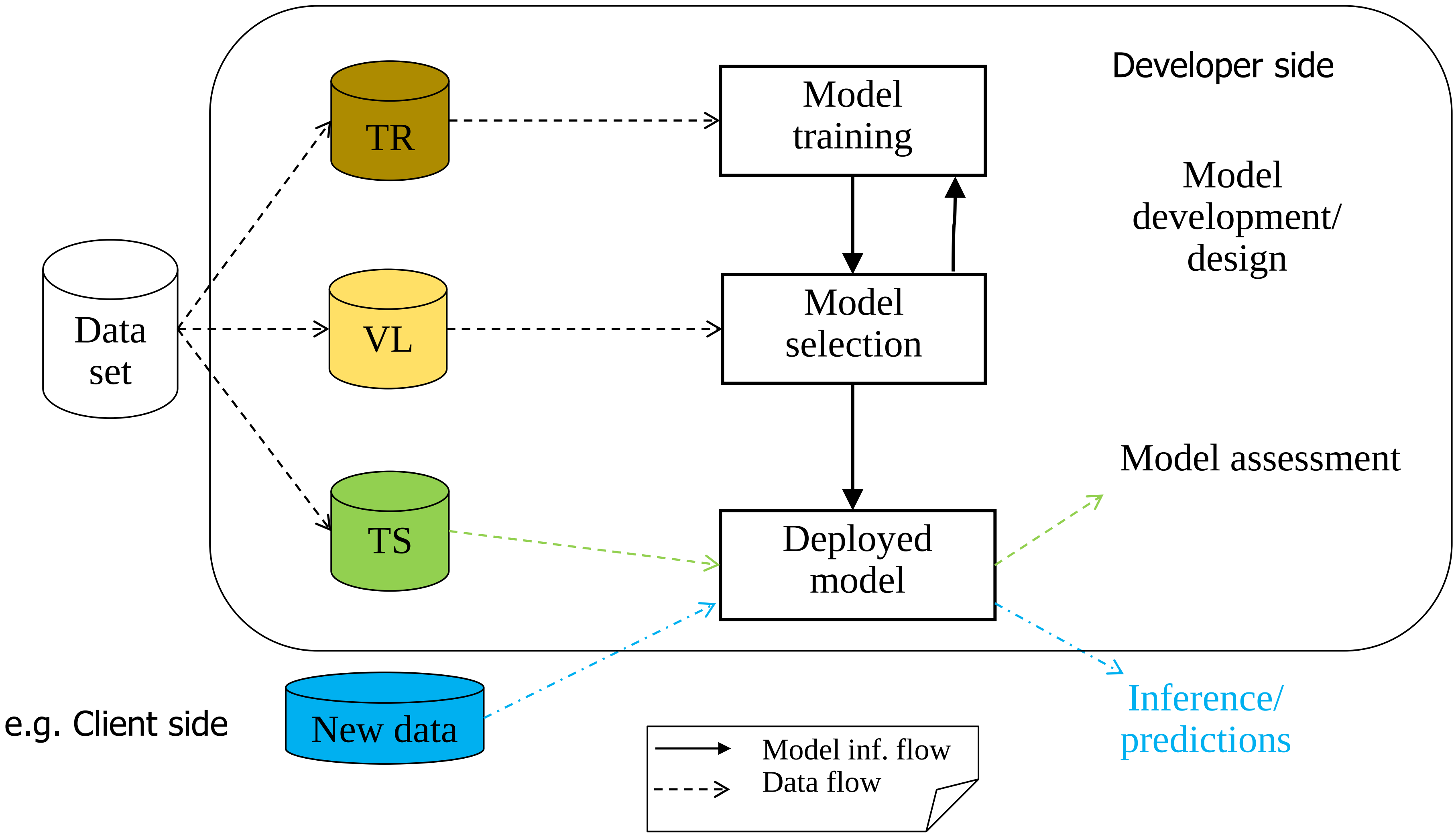

A simple meta-algorithm

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- Separate TR (training), VL (validation) and TS (test) sets
- Search best $h_{\mathbf{w},\lambda}()$ changing the model hyper-parameters λ [e.g. the polynomial order, the lambda for ridge regression]:
  - For each different values of λ (grid search)
    - Search best $h_{w,\lambda}()$ that minimize error/empirical loss (fitting the TR set) finding the best $\boldsymbol{w}$ parameters,

      where best = minimum error on TR set [e.g. $argmin_{\mathbf{w}}\ Loss(\mathbf{w})\ in\ L_2$]
- Select the best best $h_{w,\lambda}()$: where best = minimum error on the VL set
- (Optional: Now it is also possible to fit $h_{\mathbf{w},\lambda}(x)$ on TR+VL with best λ model)
- Evaluate the final $h_{w,\lambda}(x)$ on the TS

This is a double cycle: Search best can be a *for* on a grid of values in the external cycle: for each λ value you train a model $h_{\mathbf{w},\lambda}$ (in the internal cycle, e.g. the gradient descent cycle) and then compute the results (accuracy) on the VL set.
Then take the best value of λ i.e the model with min VL err or max VL accuracy etc..

Search on a grid (e.g. with 2 hyper-parameters)

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- Find *hyper-parameters* value (i.e. parameters that are not directly learnt, which are not modified by training)

Def

- Search best hyper-parameter can be a <<FOR>> over a grid of candidate values. For each trained model $h_{\mathbf{w},\lambda}$ compute the results (accuracy) on the VL set. Then take the one with the minimum error or the max accuracy.

Hyper-param.	Lambda 0.1	Lambda 0.01	Lambda 0.001
Degree 1	Res1	Res4	Res7
Degree 2	Res2	Res5	Res8
Degree 4	**Res3**	Res6	Res9

E.g. "Res1" is computed on the VL set, by the model with and Polynomial-Degree=1 and Lambda=0.1 trained on the TR set

- Example: The best one is *Res3* → (Degree 4, lambda=0.1) is the winner
- We can automatize it!!! Parallelization is easy (independence of the trials)
- Alternatives exist to reduce the cost or to automatize the search *

Exercise

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λ	TR	VL	TS
0.5	75	70	70
0.1	80	75	70
0.01	90	70	72

Accuracy (% di classificazione corretta)

- In che ordine si usano le porzioni di dati per calcolare i valori in tabella?
- Quale modello (ossia lambda) si sceglie?
- Che fenomeni si osservano?

Controesempio (separare TR, VL e TS)

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- 20-30 esempi, 1000 variabili di input random,
- *random target* 0/1
- Scelgo 1 modello con una sola variabile/feature che indovina *'per caso'* al 99% sul dataset e poi su qualsiasi split successivo in training, validation e test set.

Perfect result (a model with accuracy 99%)? What is wrong?

99% non è una buona stima dell' errore di test (quella corretta e' 50%)

1. Errore stimato su training o validation per model selection NON è utile per stima del rischio! Dati di TR o VL non vanno usati per scopi di test

2. Usare *tutto* il data set per feature/model selection lede la correttezza dell stima (risultati biased – «Feature Selection bias»).

- Test set è stato usato implicitamente all'inizio*.
- Test deve essere separato prima, prima di qualsiasi model selection o design del modello (incluso selezione di features)

Un test set esterno fornisce invece la stima corretta del 50% (*random coin result* !).

E' la <u>correttezza della stima</u> che è in giudizio, non la possibilità di risolvere il task!

Delicato confrontando metodi diversi e usando tecniche di K-fold cross-validation che in se non garantiscono corretteza della procedura di validazione

The table for the Counterexample

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Input variable value

Pattern

	1	2	…	26	27	28	…	1000	**Target**
1	…	…	…	1	1	1	…	…	1
2				0	0	0			0
3				1	1	1			1
4				0	0	0			0
…				0	0	0			0
…				1	1	1			1
…				0	0	0			0
20	…	…	…	1	1	1	…	…	1
TS1				1	0	0			1
TS2				0	1	0			0
TS2				1	1	1			1
Accuracy				100%	33%	66%			

Hold out and **K-fold** cross validation

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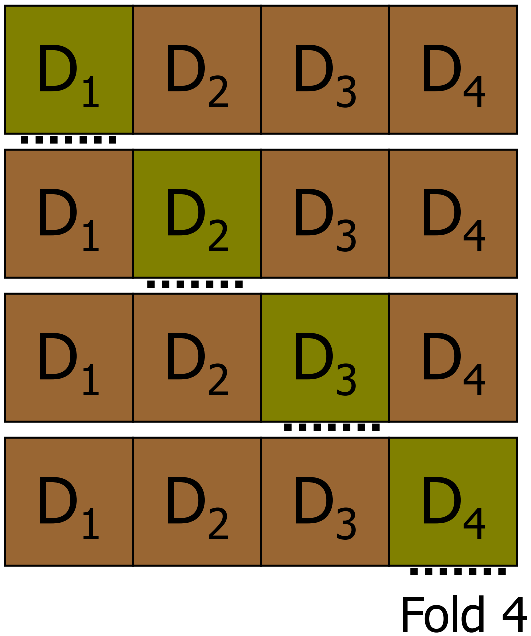
Hold out CV *can make insufficient use of data*



Def K-fold Cross-Validation

- Split the data set D into k mutually exclusive subsets $D_1, D_2, \ldots, D_K$
- Train the learning algorithm on $D \setminus D_i$ and test it on D_i
- Summarize averaging all the D_i results (*diagonal*)
- NOTE: This technique can be used both for the validation set or for the test set
- *It uses all the data for training and validation or testing*

Issues:

- How many folds? 3-fold, 5-fold , 10-fold, …., 1-leave-out
- Often computationally very expensive
- Combinable with validation set, double-K-fold CV, ….

An example of model selection and assessment (with K-fold CV)

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- Split data in TR and Test set (here simple hold-out or a K-fold CV)

- [Model selection] Use K-fold CV (internal) over TR set, obtaining new TR e VL set in each split, to find best hyper-parameters of your model (e.g. polynomial order, lambda of ridge regression, …): How?
  Apply a **grid-search** with many possible values of the hyper-par.
  - i.e. for example a k-fold-CV for λ =0.1, a k-fold-CV CV for λ =0.01 , ... and then take the best λ (comparing the mean errors computed over the validation sets obtained by the all the folds of each k-fold CV, … the results on the diagonal in the previous slide)

- Train on the whole TR set the final model

- [Model assessment] Evaluate it on the external Test set

Validation: summarizing

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- **Stima Empirica**: errore calcolato/stimato su (Hold out)
  - E.g. Hold out: training, validation set and test sets
  - K-fold cross validation (resampling)

- **Teoria**: E.g. Statistical Learning Theory [Vapnik] :
  - *sotto quali condizioni (matematiche) un modello è capace di generalizzare (buona generalizzazione)?* → cenni

Typical behavior of learning

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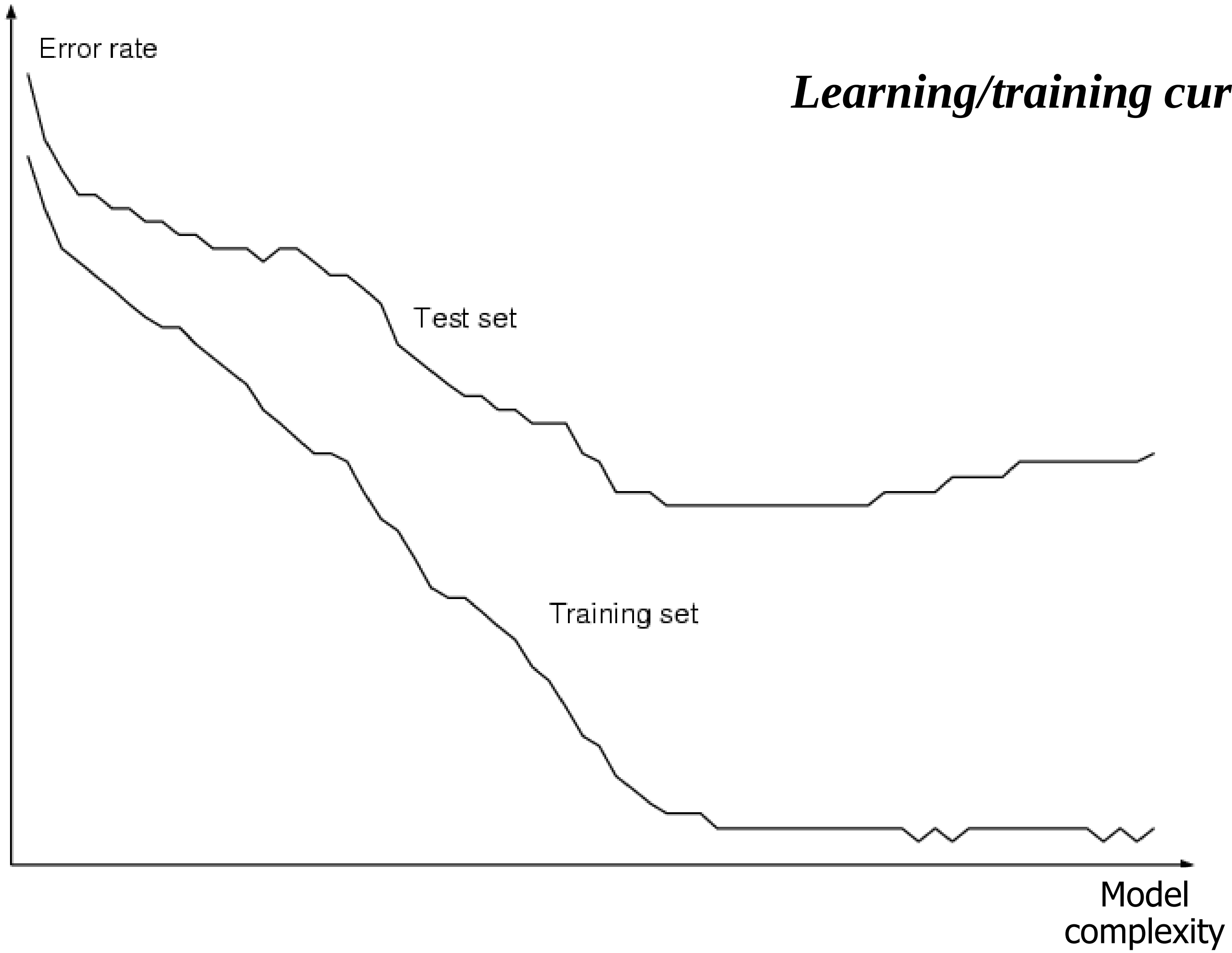
Learning/training curve



Typical behavior of learning

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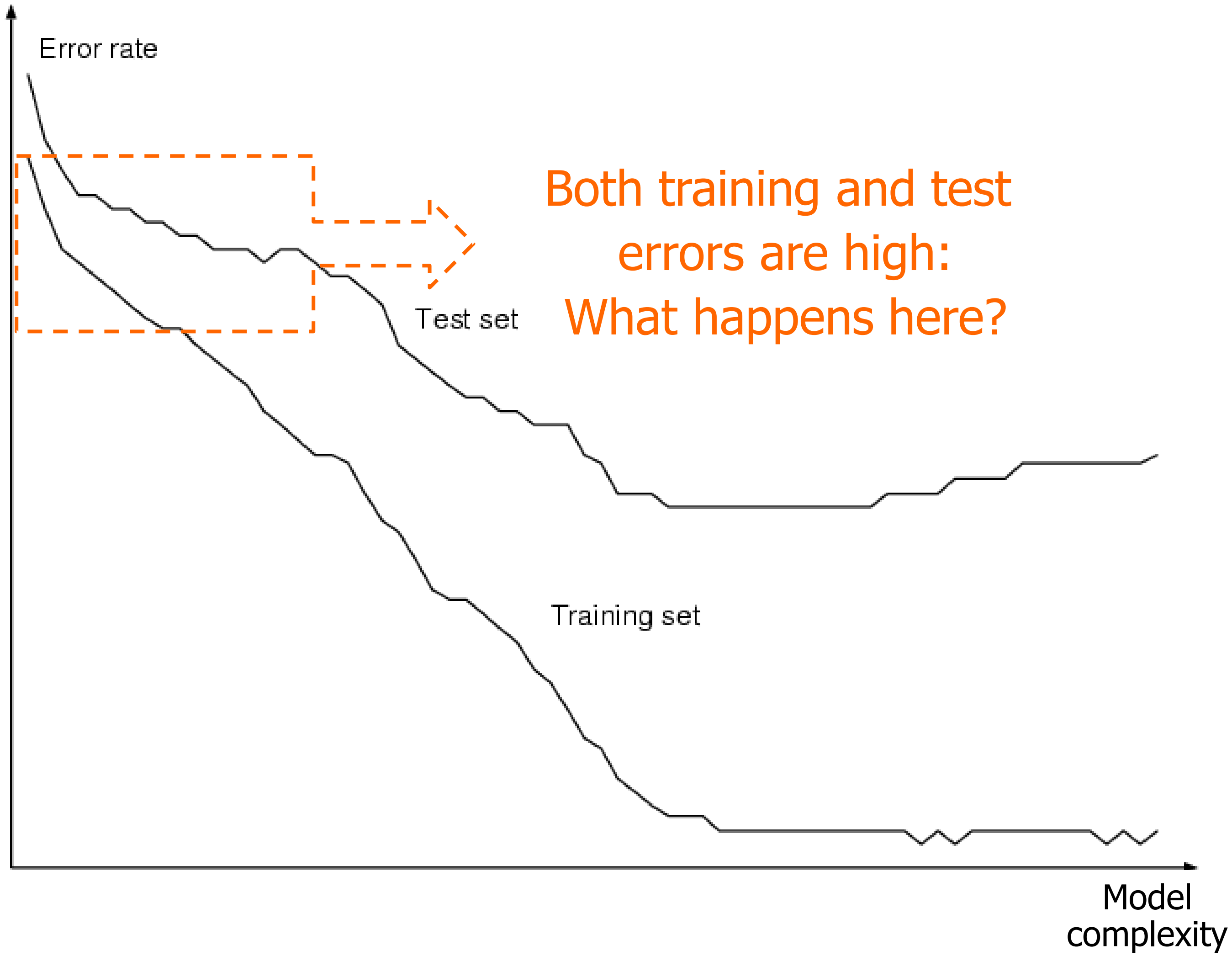

Both training and test errors are high:
What happens here?

Typical behavior of learning & Polynomial Curve Fitting (I)

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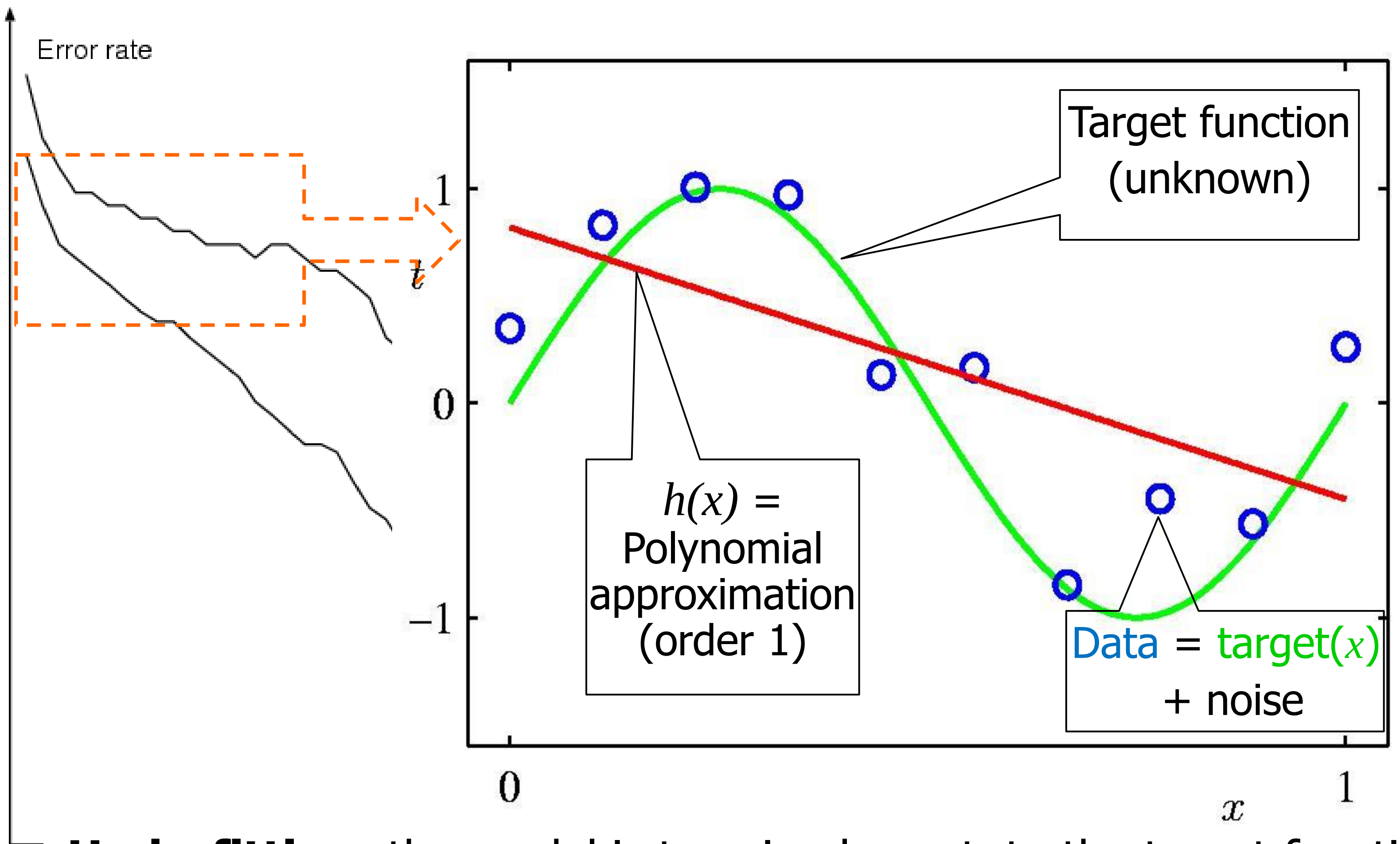

Underfitting: the model is too simple w.r.t. to the target function both for known data and new data

Typical behavior of learning

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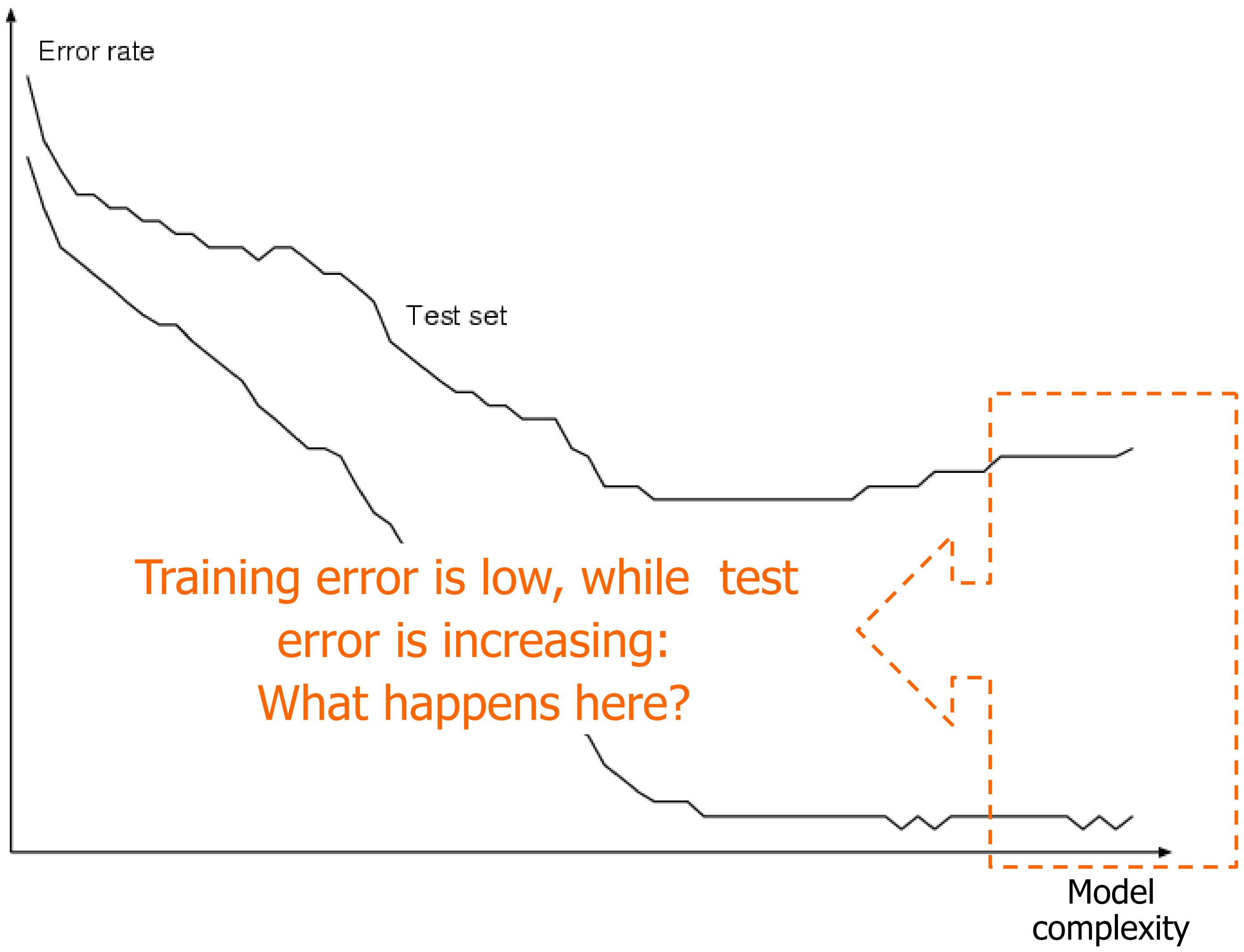

Training error is low, while test error is increasing:
What happens here?

Typical behavior of learning & Polynomial Curve Fitting (II)

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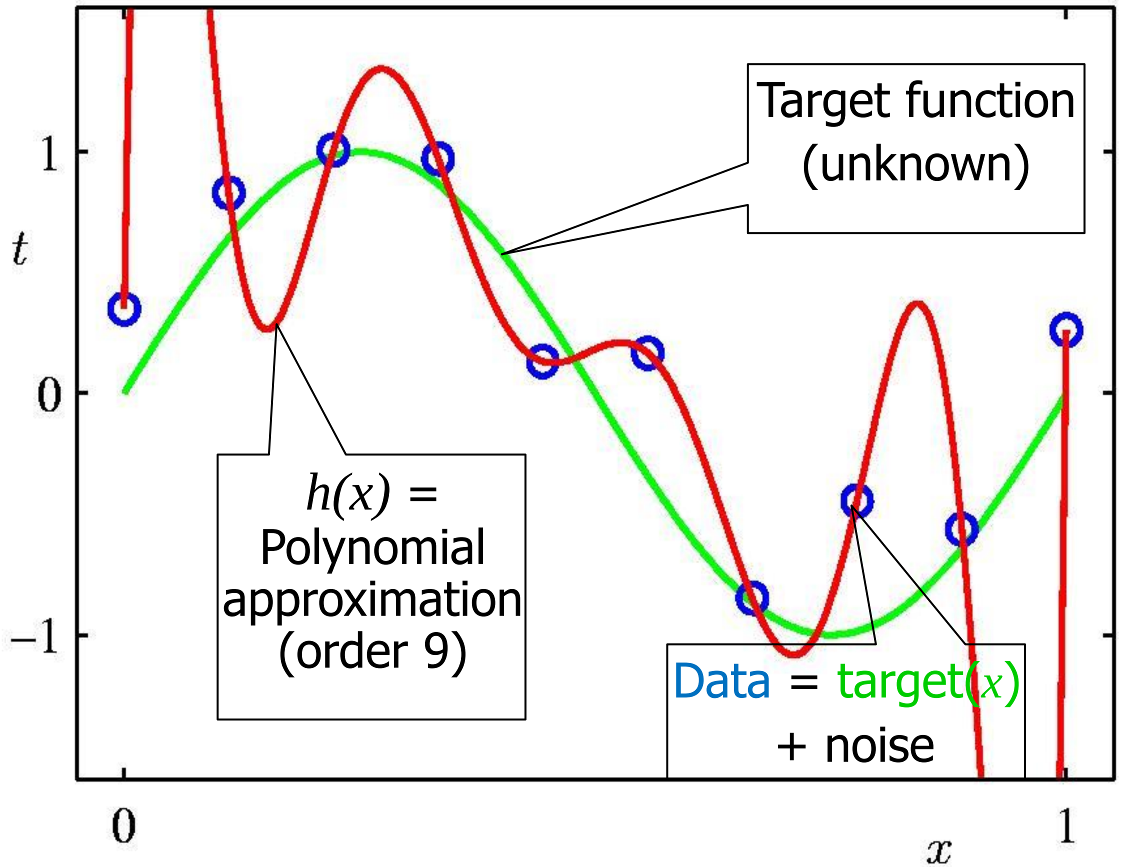

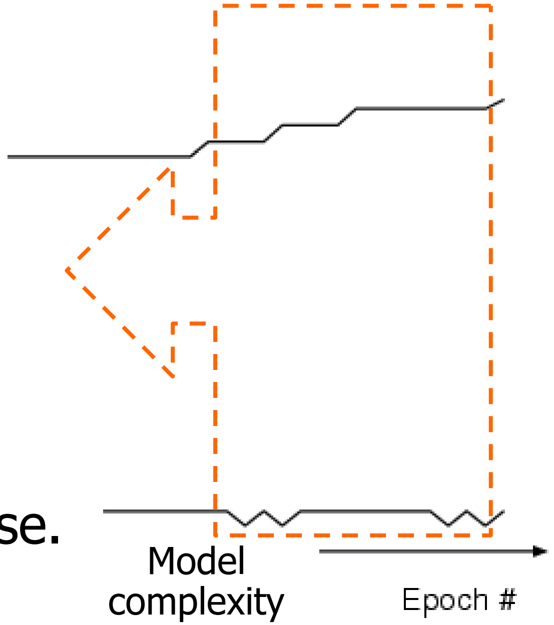

Overfitting: the model is too complex: Fit the noise.

Training error is very low, test error can be high

Data Set Size: l=15

previous was 10

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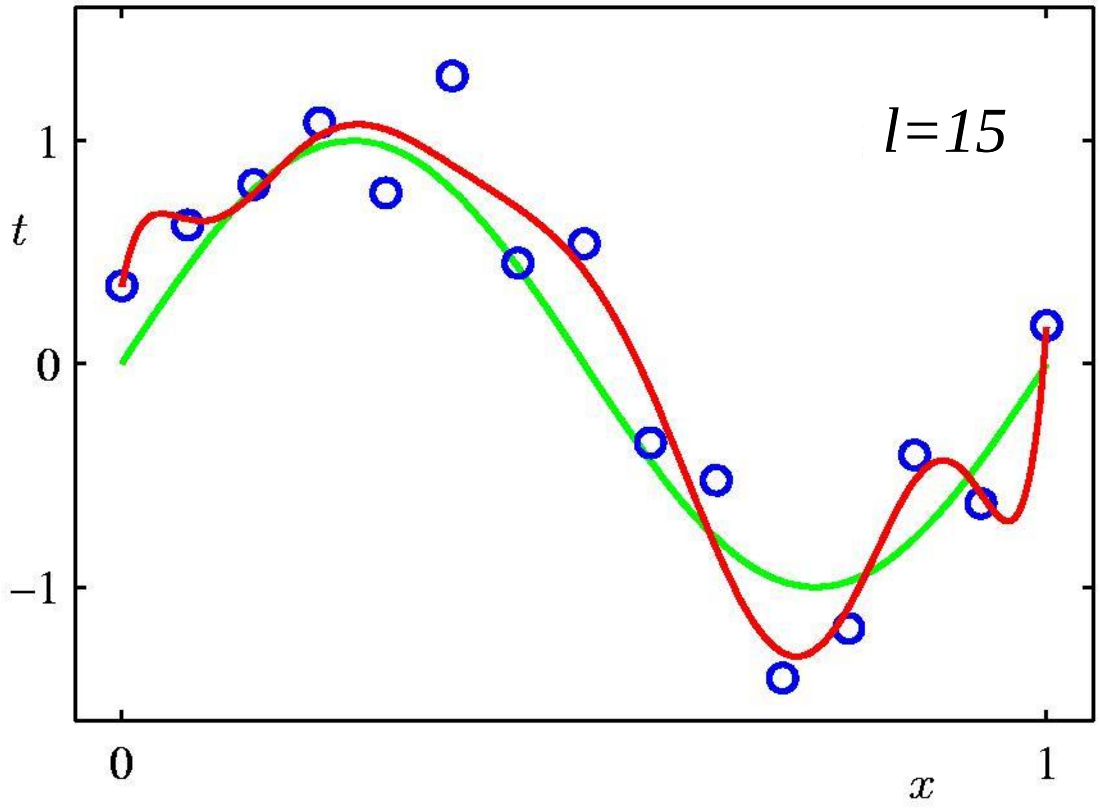
9th Order Polynomial (chancing the of number of data)



Data Set Size: $l=100$

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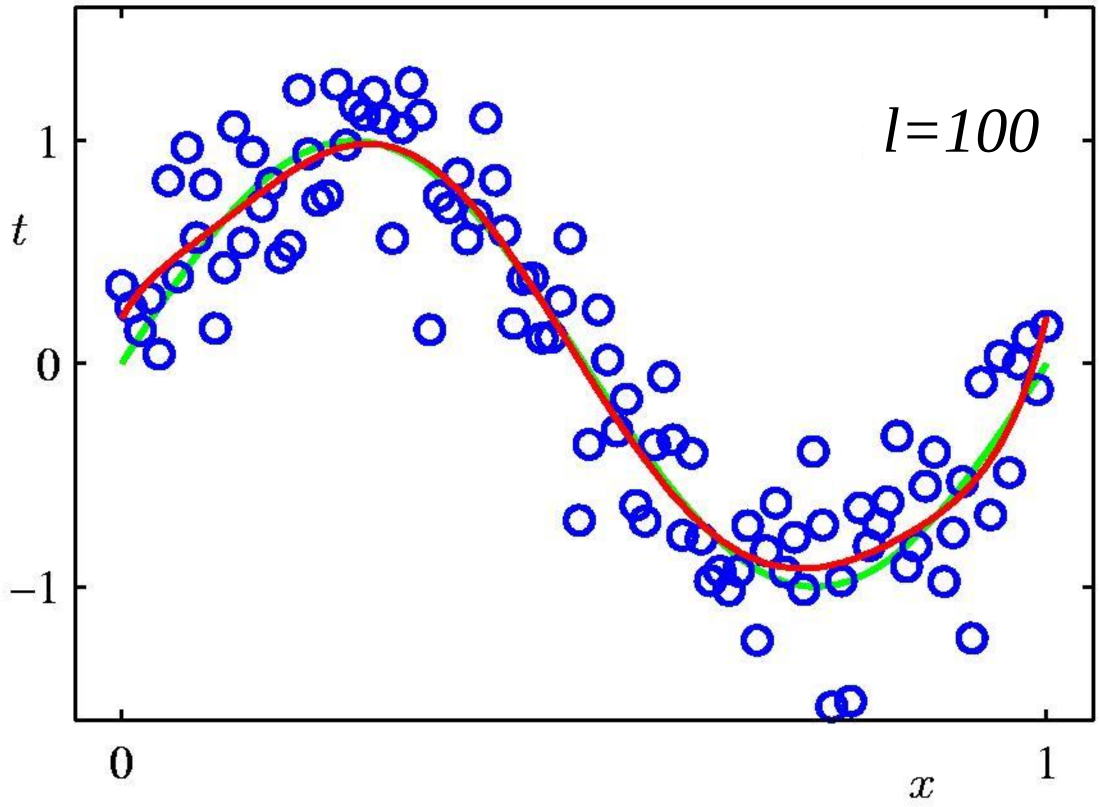
9^{th} Order Polynomial (even more data)



Toward SLT

Putting all together:

- The *generalization* capability (measured as a risk or test error) of a model
  - with respect to the training error
  - overfitting and underfitting zones

1. The role of model complexity
2. The role of the number of data

- Statistical Learning Theory (SLT): a general theory relating such topics

(Simplified) Formal Setting Statistical Learning Theory (SLT)

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Defs

- Approximate unknown $f(\boldsymbol{x})$, d *(or y or t) is the target (d=true f +noise)*
- Minimize *risk function* $R = \int L(d, h(\boldsymbol{x}))dP(\boldsymbol{x}, d)$ True Error Over *all* the data
- Given
  - value from teacher (d) and the probability distribution $P(\boldsymbol{x}, d)$
  - a loss (or cost) function, e.g. $L(h(\boldsymbol{x}), d) = (d - h(\boldsymbol{x}))^2$

- Search h in H : Min R
- But we have only the finite data set $TR = (\boldsymbol{x}_{p,} d_p), \quad p = 1 \dots l$
- To search h: minimize *empirical risk* (training error E), finding the best values for the model free parameters

$$R_{emp} = \frac{1}{l} \sum_{p=1}^{l} (d_p - h(\boldsymbol{x}_p))^2$$

- Emprical Risk Minimixzation (ERM) Inductive Principle
- *Can we use R_{emp} to approximate R?*

Vapnik-Chervonenkis-dim and SLT: a general theory (I)

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Def

- Given the *VC-dim* (VC), a measure *complexity* of *H (flexibility to fit data)* (e.g. Num. of parameters for linear models/polynomials)

Repetita: Can we use R_{emp} to approximate R?

Very important!

Def

- *VC-bounds in the form:* it holds with probability 1-δ that

guaranteed risk

$$R \boxed{\leq} \underline{R_{emp}} + \underbrace{\varepsilon(1/l, VC, 1/\delta)}_{VC\text{-confidence}}$$

- First (basic) explanation:
  - ε is a function that grows with VC *(VC-dim)*, that decreases with (higher) l and $delta$.
  - We know that R_{emp} decrease using complex models (with high *VC-dim*) (e.g. the polynomial degree in the example)
  - $delta$ is the confidence, it rules the probability that the bound holds (e.g. low delta 0.01, it holds with probability 0.99)
- Now we can see how it can "explain" the *underfitting* and *overfitting* and the aspects that control them.

Vapnik-Chervonenkis-dim and SLT: a general theory (II)

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Comments:

Very important!

Def

- *VC-bounds in the form:* it holds with probability 1-δ that

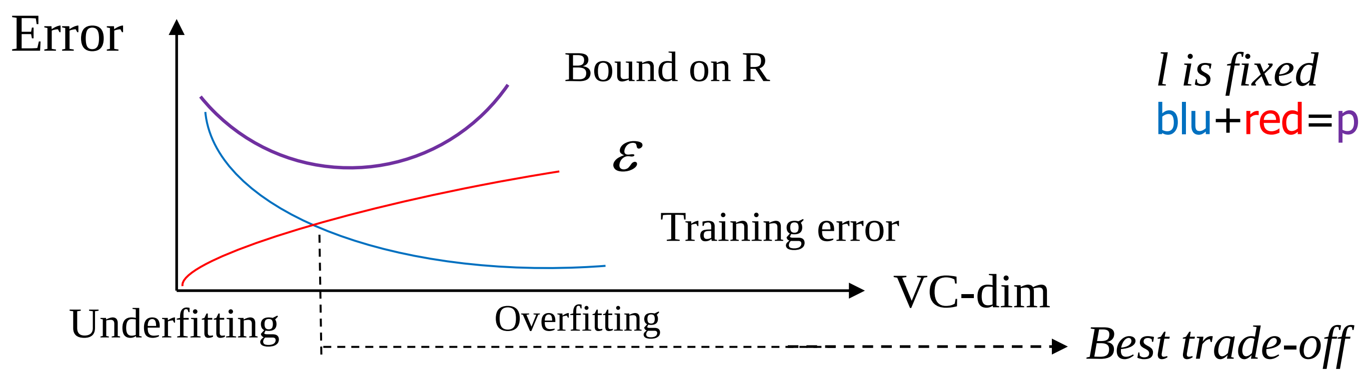
guaranteed risk $$R \boxed{\leq} \underline{R_{emp}} + \underline{\varepsilon}(1/l, VC, 1/\delta)$$ *VC-confidence*

Intuition:

- Higher l (data) → lower VC confidence and bound close to R
- Too simple model (low VC-dim) can be not suff. due to high R_{emp} (underfitting)
- Higher VC-dim (fix l) → lower R_{emp} but *VC-conf*. and hence R may increase (overfitting)

Def

- *Structural risk minimization*: minimize the bound !



l is fixed
blu+red=purple

- Concept of control of the model complexity (flexibility):
  trade-off between TR accuracy (fitting) and model complexity (VC-dim)

Discussion
Complexity control

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- **Statistical Learning Theory (SLT):**
  - Permette inquadramento formale del problema della generalizzazione e (underfitting/)overfitting, fornendono limitazioni superiori analitiche e quantitative al rischio R di predizione su tutti i dati, indipendemente dal tipo di learning algorithm o dettagli del modello.
  - Il ML è ben fondato:
    - Il rischio del learning (e l'errore di generalizzazione) può essere analiticamente limitato, e solo pochi concetti sono fondamentali !
    - Si può trovare un buona approssimazione dell f target da esempi, pur di avere un buon numero di dati e una adeguata complessità del modello (misurabile formalmente con la VC-dim)
  - Porta a nuovi modelli (SVM) (e altri metodi che direttamente considerino il controllo della complessità nella costruzione del modello)
  - Fonda uno dei principi induttivi sul *controllo della complessità*

Domande aperte:

- Quali (altri) principi vi sono per fondare il controllo della complessità e <u>come operare in pratica</u>?
  - Come misurare la complessità (flessibilità per il fitting)?
  - Come trovare il bilanciamento ottimo tra fitting e complessità ?

Some Examples for Complexity Control

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- Linear models (LM):
  - Complexity seems* related to number of free parameters *w*: input dimension / dim. of the basis expansion (e.g. polynomial degree)
  - Lambda parameter for the regularized version (using the model selection/validation techniques to find the proper value of lambda)
- Decision trees (DT): number of nodes (e.g. control by early stop, pruning)
- We will also see: direct approach to the complexity optimization through the SVM model
- **Exercise**: relate the complexity control to the approaches used in the different models, explaining the *underftting* and the *overfitting* from the point of view of the SLT upper bound on *R*: e.g. how to explain the role of the hyper-parameters lambda in Linear models or # of nodes in DT etc. in terms of SLT?

Conclusioni

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- ML models flexiblity →
  - Use the power of ML without control is a way to produce *illusory results*
  - Control the tradeoff between model fitting and complexity
  - Fundamental role of validation approaches (for model selection and estimations)

- Il ML è ben fondato teoricamente
  - Domande fondamentali tramite Statistical Learning Theory (#ML)
  - ed altre (e.g. PAC- probably approximately corerct learning con cenni in AIMA cap. 18.5)

Bibliography

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- AIMA , ed .3: **chap 18.4**
  (thought quite simplified !!!)

- Further readings (not mandatory!):
- Every good ML book:
  - see the bibliography of the SVM lecture

For fun

- Can I have just a look to the test set?

  See https://youtu.be/XvOsh15hLIs

By Sepe-Dukic past ML students

*

* It can hold also for the validation set used as test set ;-)

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