Model Validation and Selection

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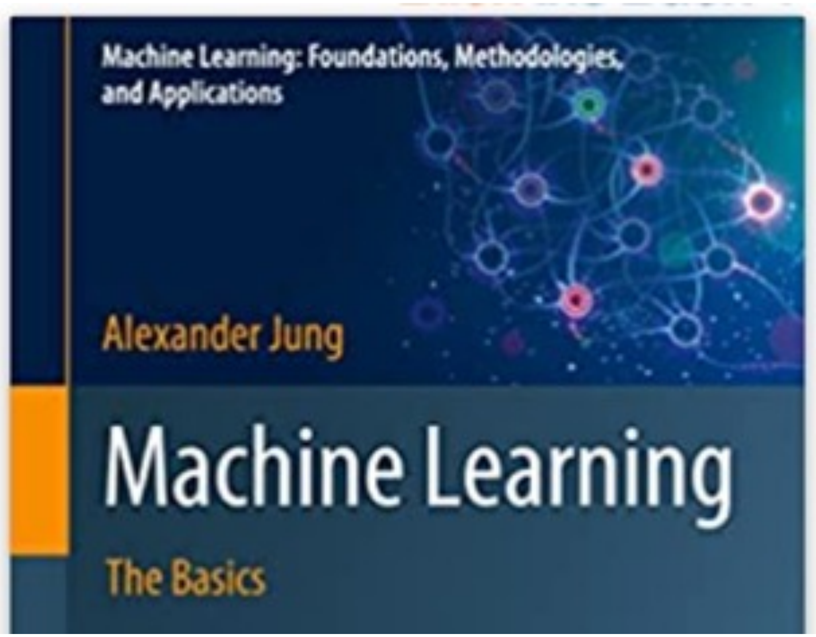
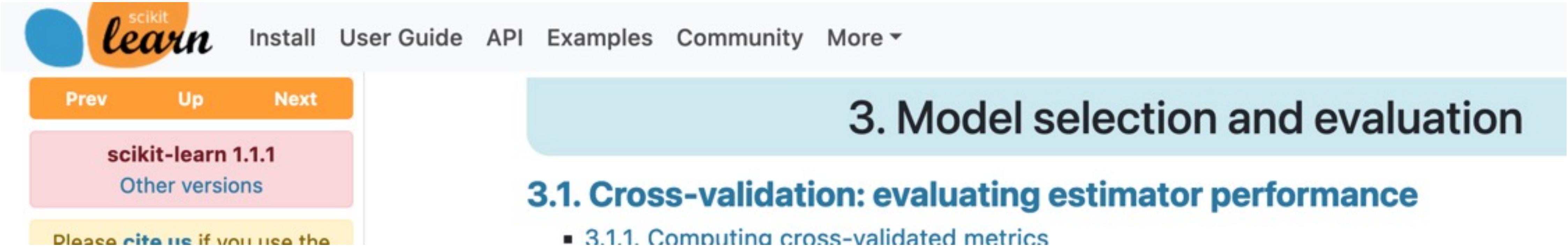
Reading.

Ch. 6 of https://mlbook.cs.aalto.fi





https://scikit-learn.org/stable/model_selection.html

”Model”

=

Hypothesis Space

Learning Goals

- know train err is bad quality measure for ML method

- val.err. is more useful as quality measure for a ML model

- basic idea of k-fold CV

- hyper-parameter tuning = model selection

- Python implementations of k-fold CV / gridsearch

ML – In a Nutshell

- learn hypothesis h(.) out of model such that for any data point $h(x) \approx y$
- approximation quality measured by loss $L((x,y),h)$
- approximate "any data point" by a training set

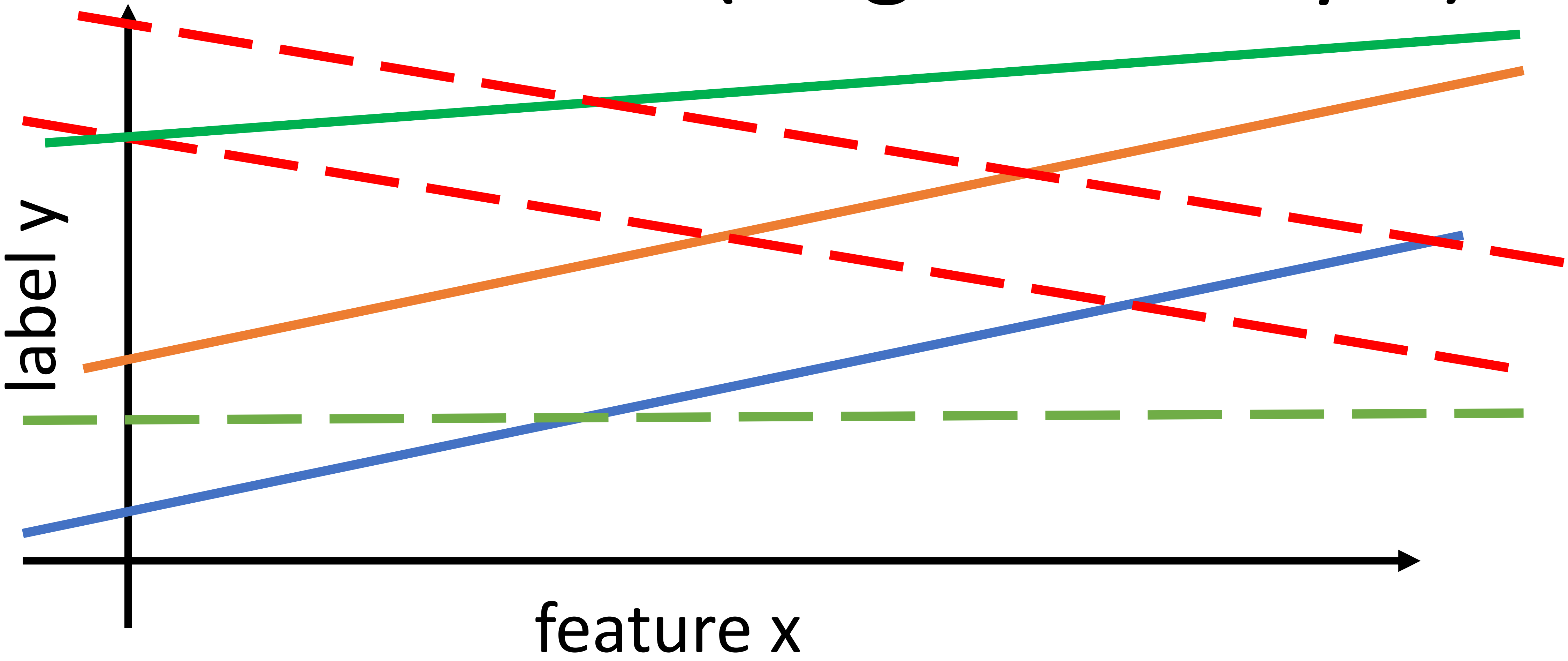
Model Validation

How do we know a model is any good ?

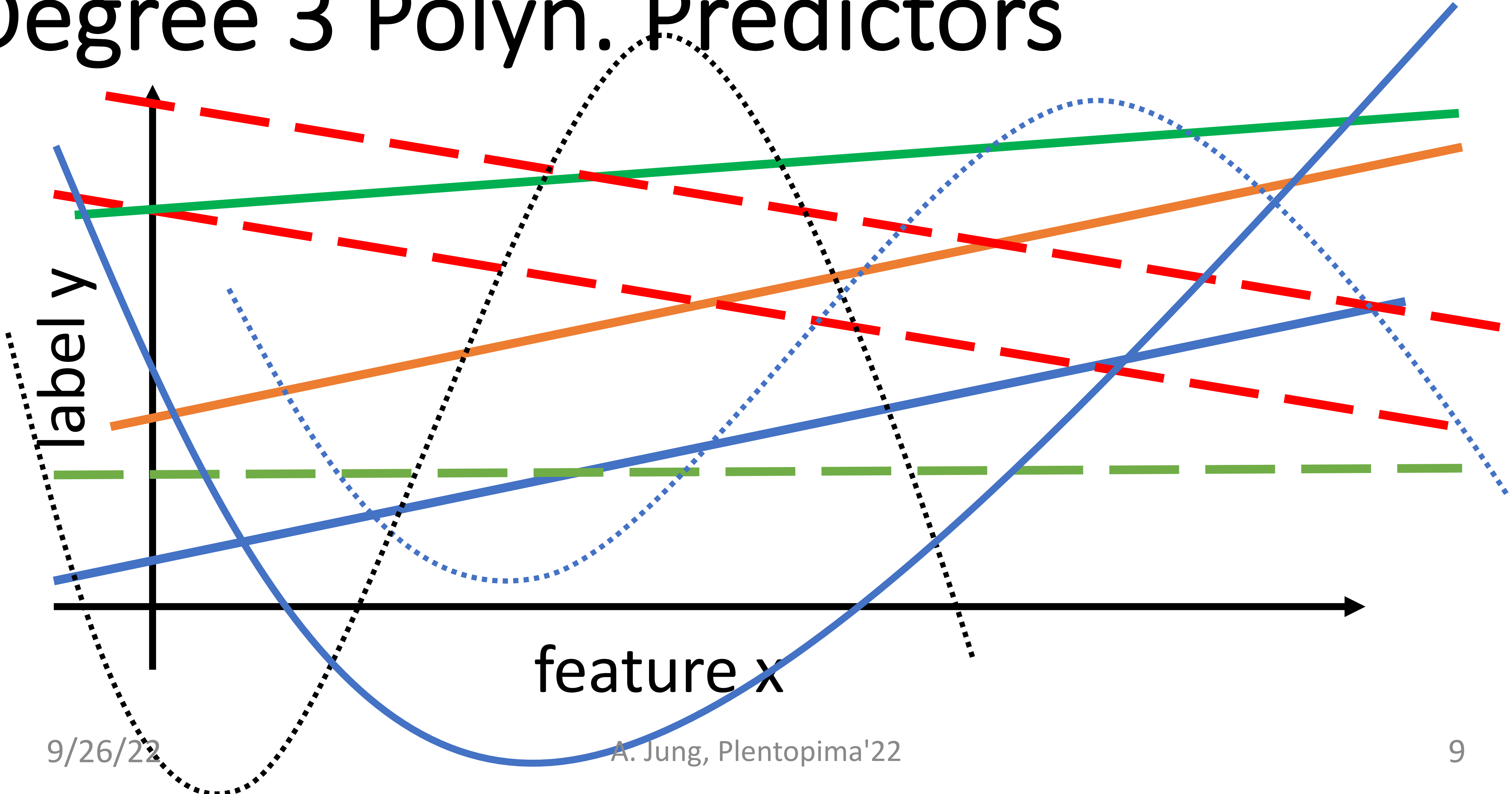
Model Selection

How to choose between different alternative models?

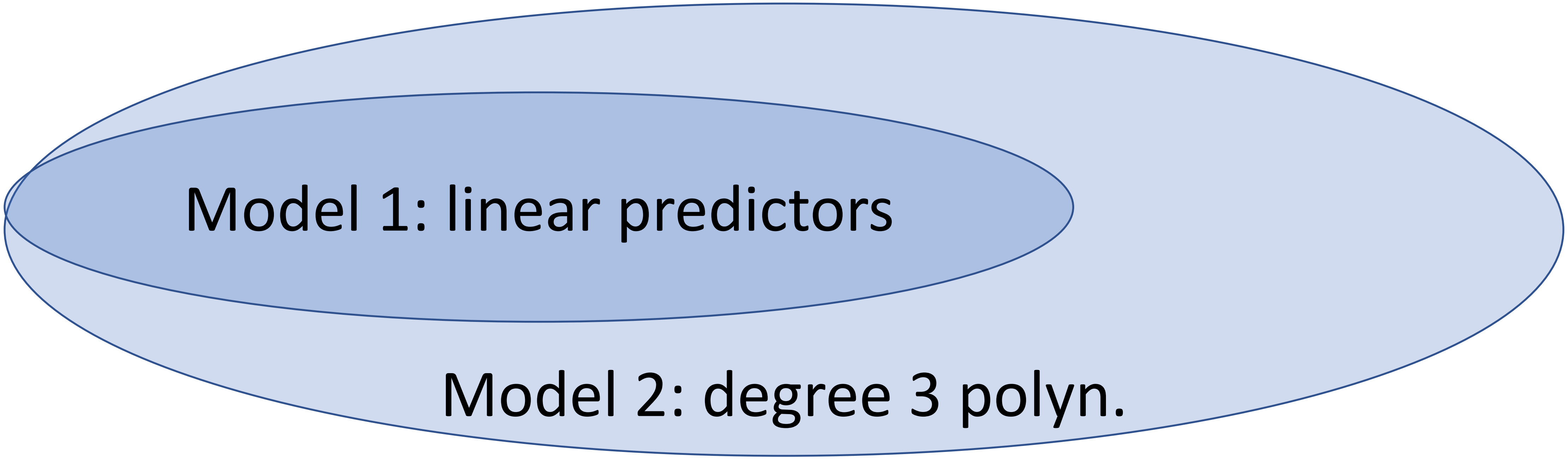
Model 1:
Linear Predictors (Degree 1 Polyn.)



Model 2:
Degree 3 Polyn. Predictors



Nested Models – I



Math Notation

$$\mathcal{H}^{(n)} = \left\{ h(x) = \sum_{l=0}^{n} w_l x^l \; with \; some \; w_l \right\}$$

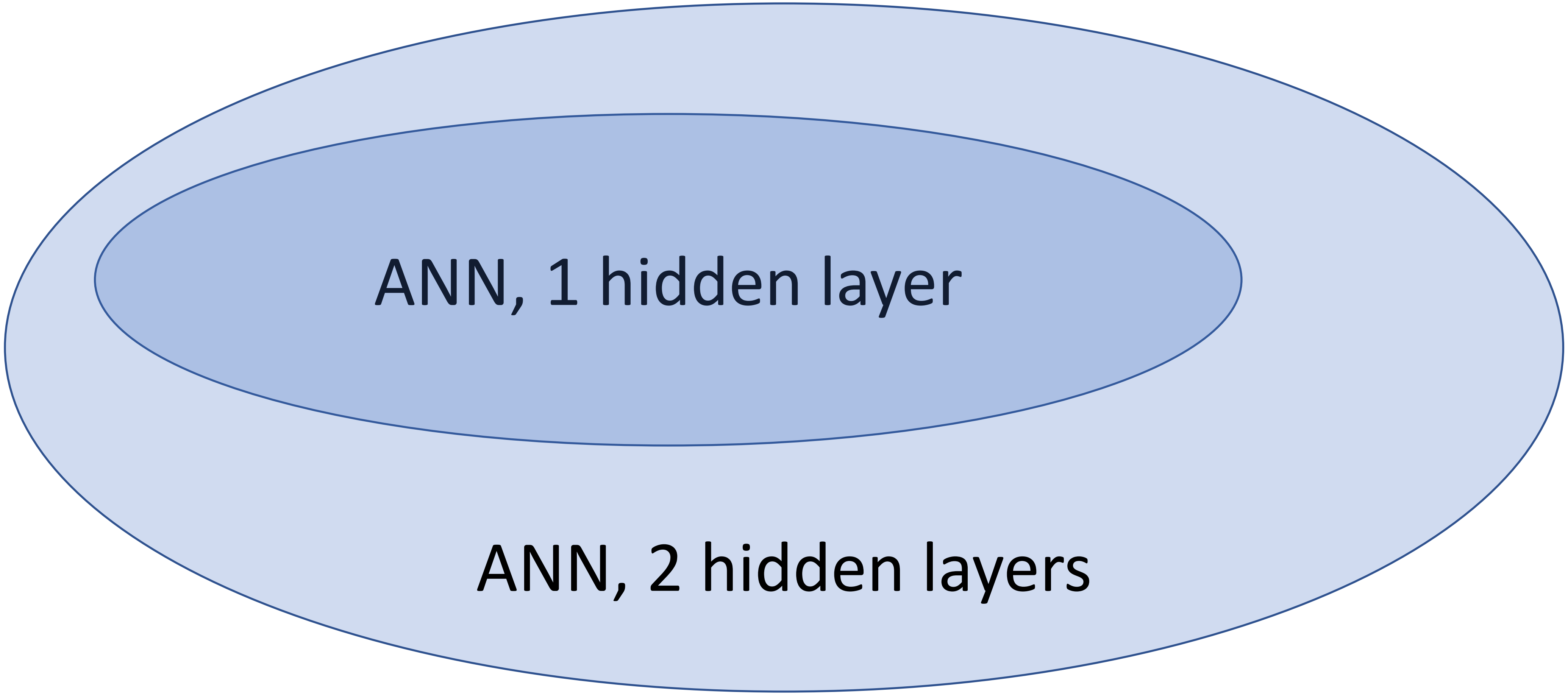
$\mathcal{H}^{(0)}$ … constant prediction (ignores feature)

$\mathcal{H}^{(1)}$ … linear hypotheses

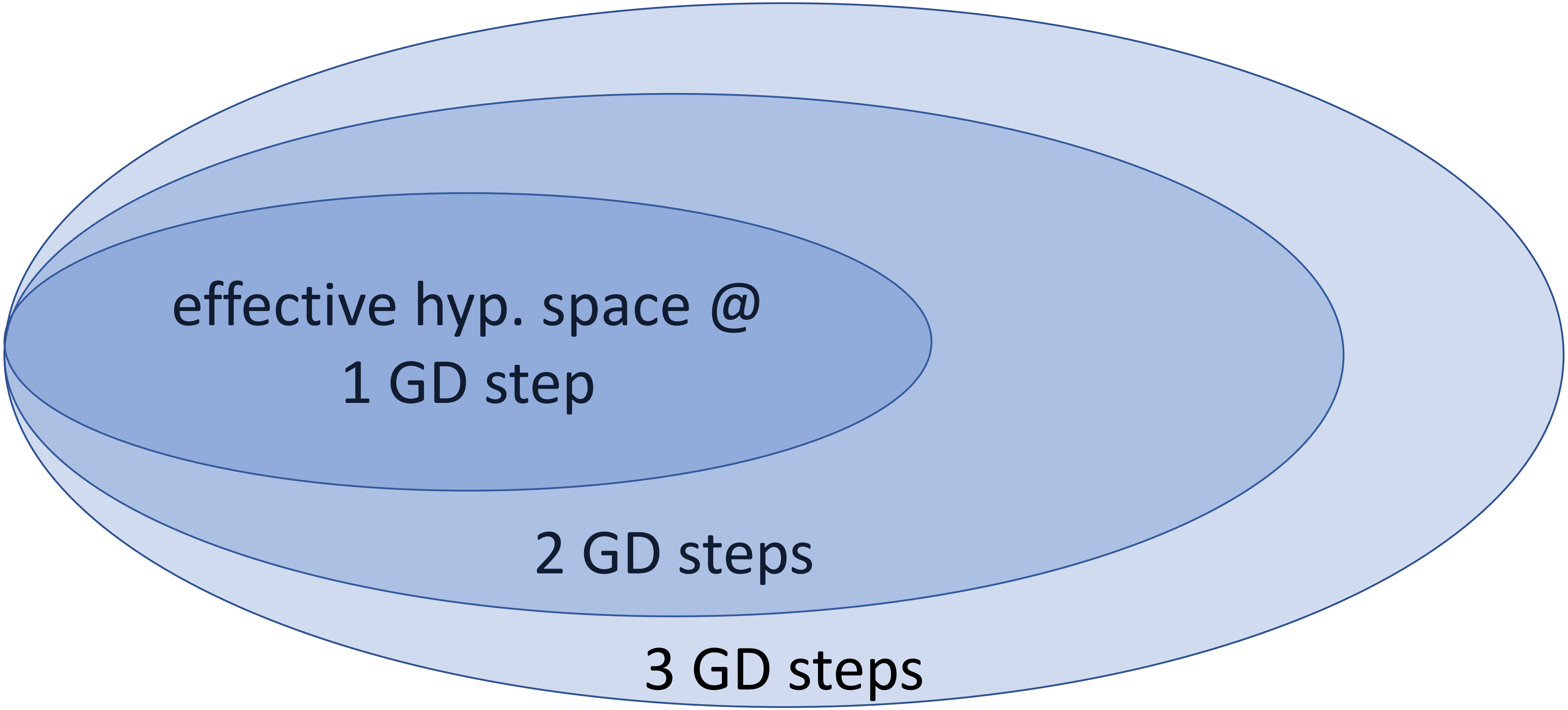
$\mathcal{H}^{(3)}$ … degree 3 polyn.

$$\mathcal{H}^{(0)} \subseteq \mathcal{H}^{(1)} \subseteq \mathcal{H}^{(2)} \subseteq \mathcal{H}^{(3)} \subseteq \ldots$$

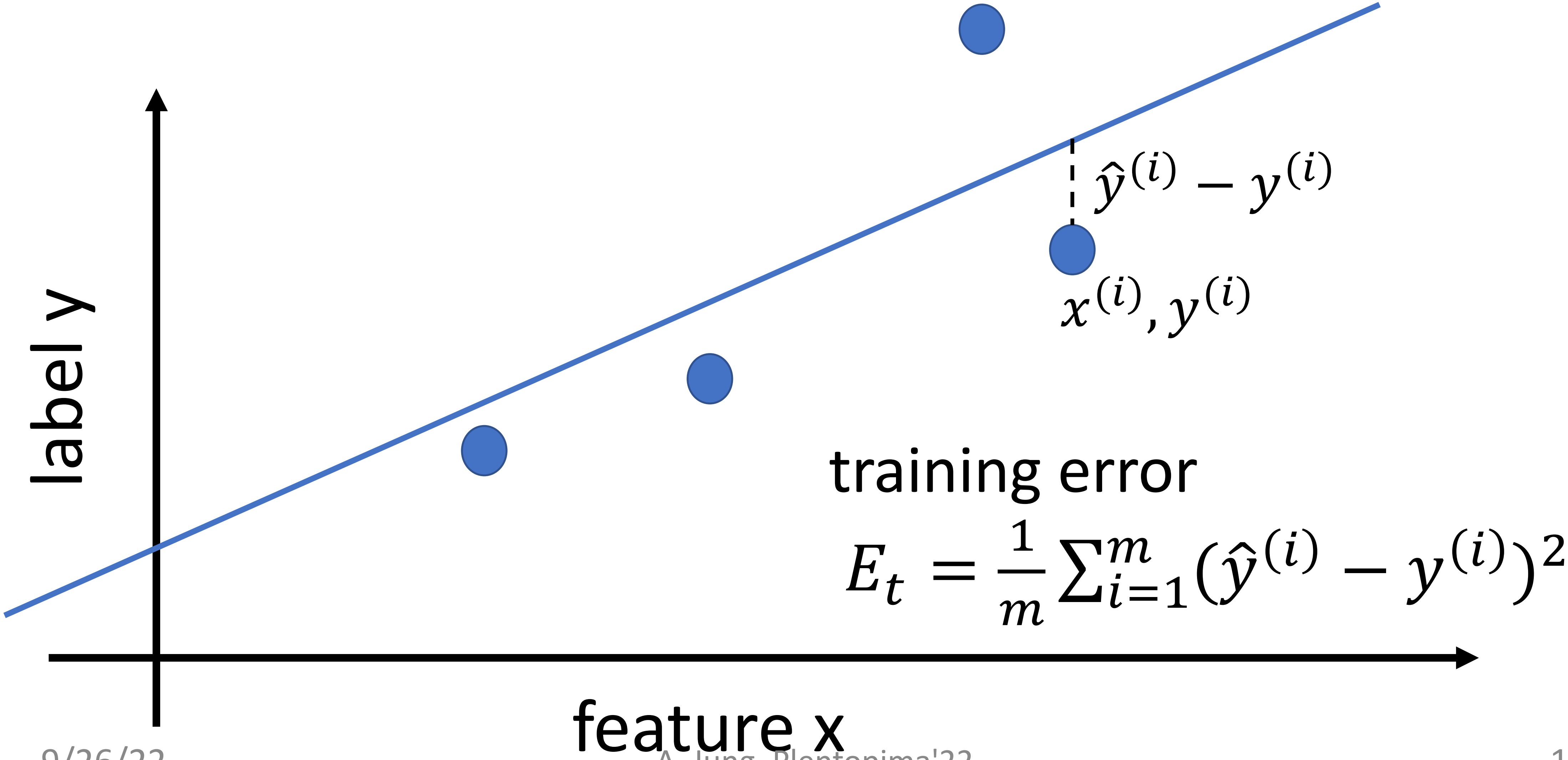
Nested Models - II



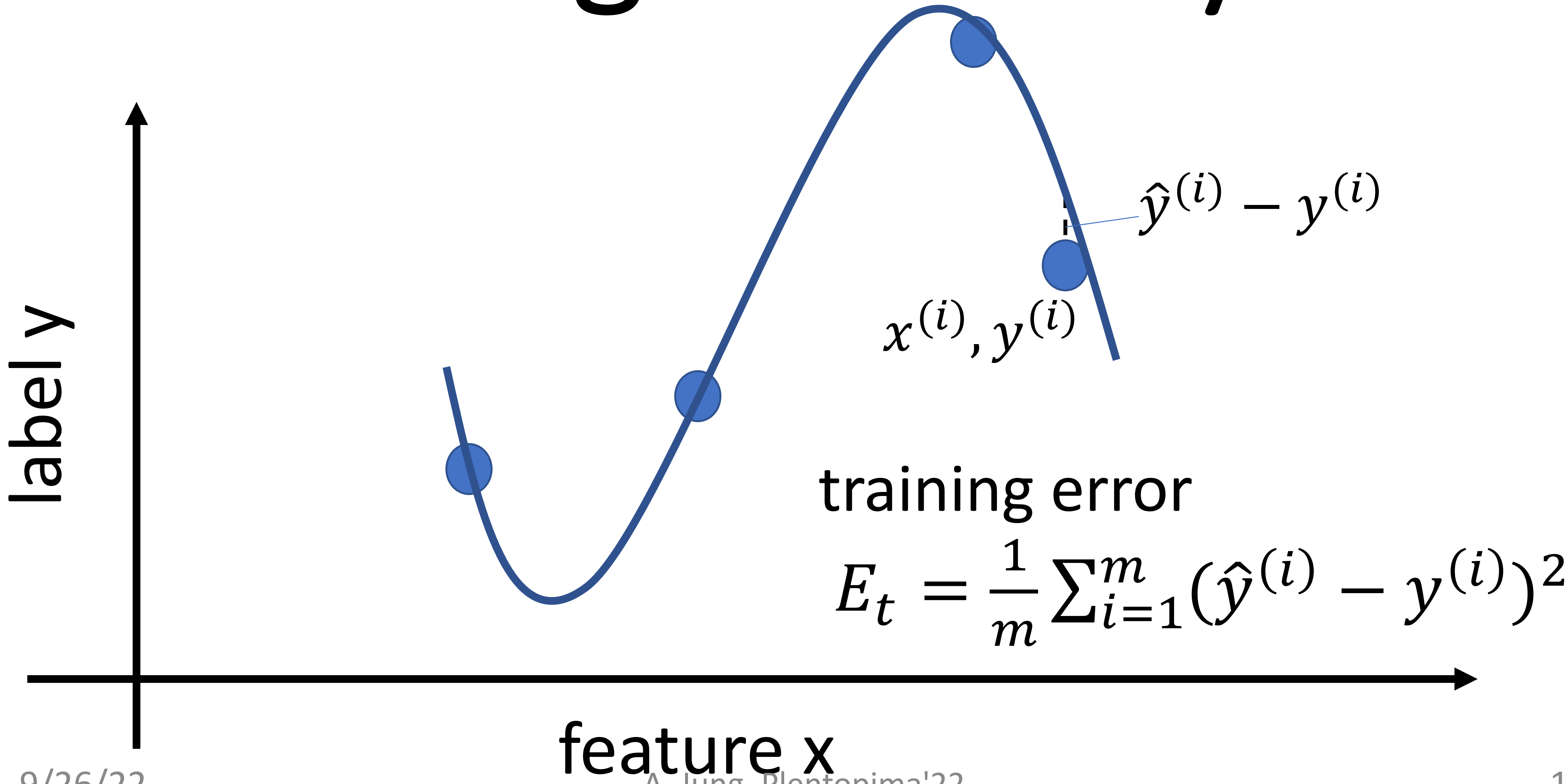
Nested Models - III



Learn Linear Predictor



Learn Degree 3 Polyn.

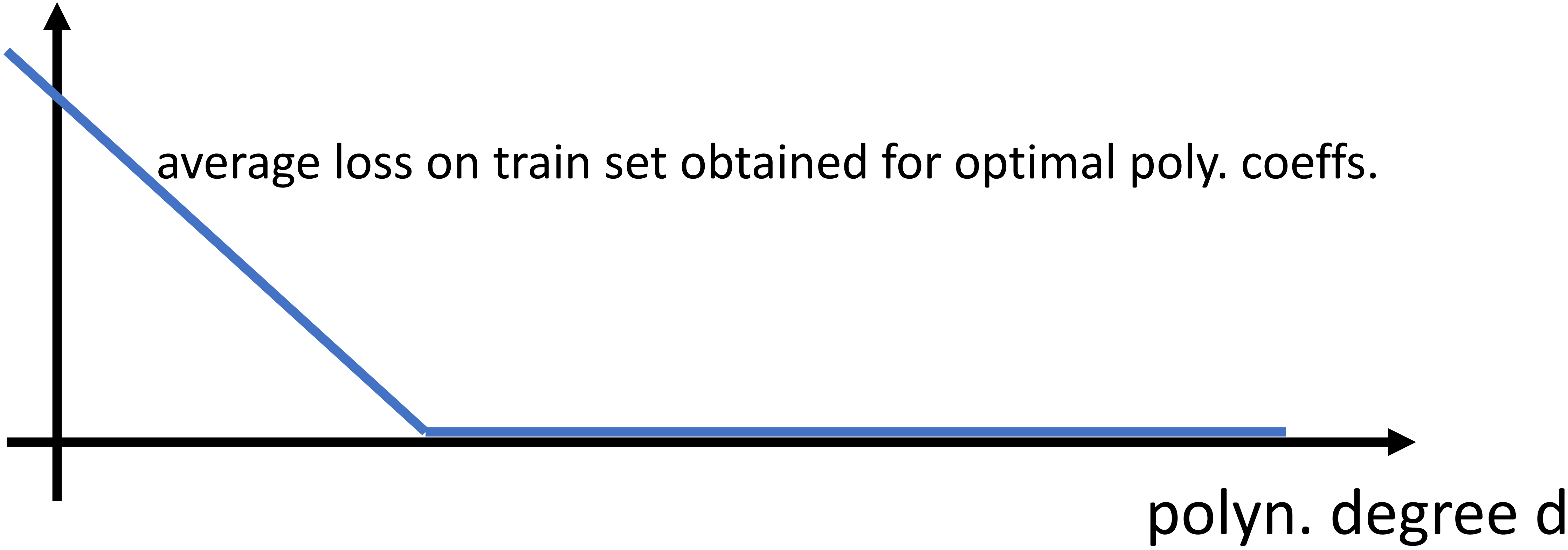


Training Errors

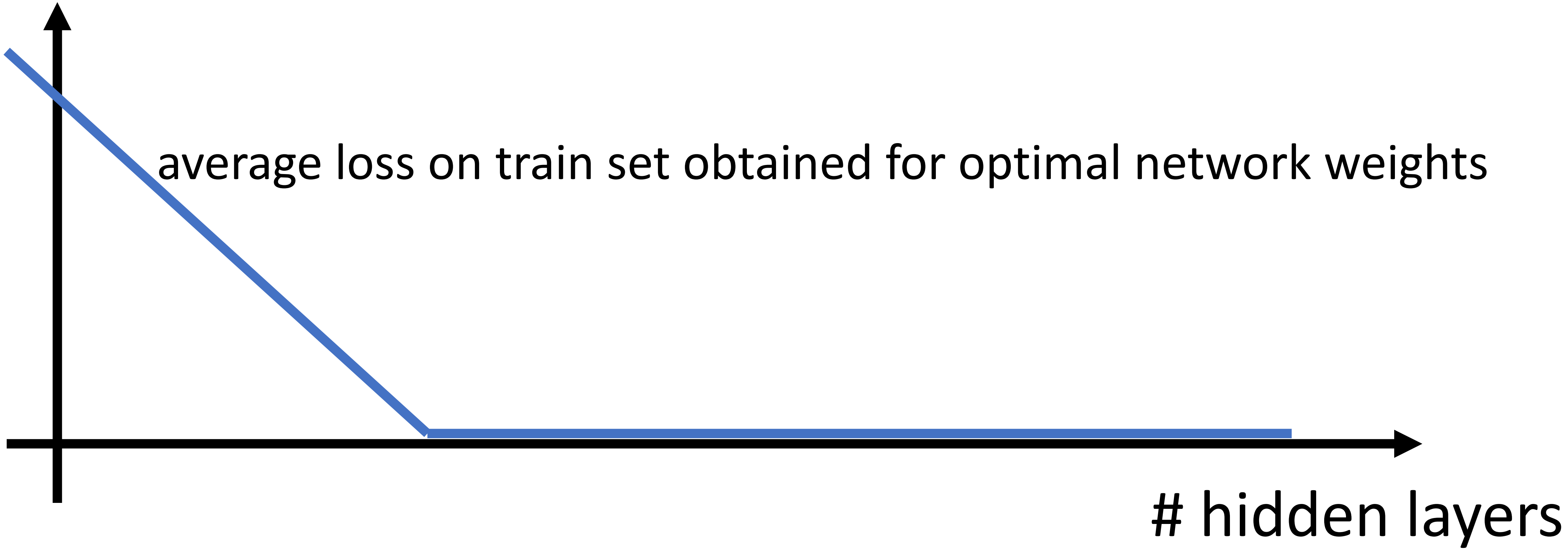
model 1
linear predictors

model 2:
degree 3 polyn.

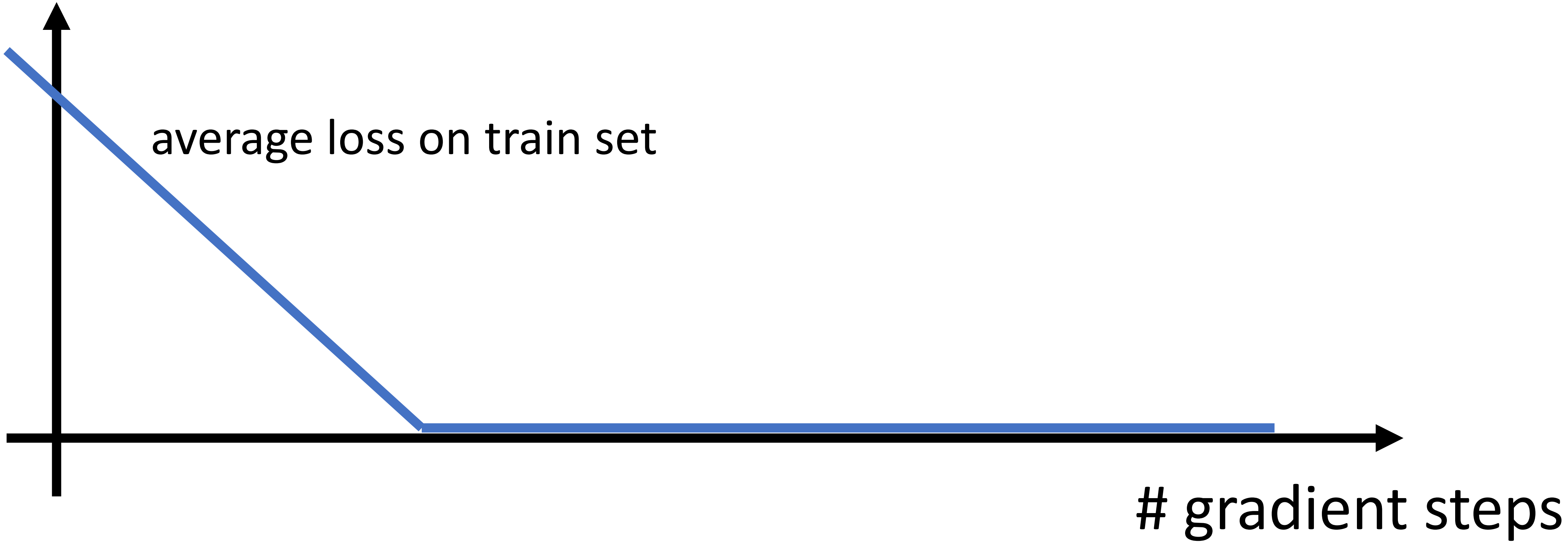
Train Error vs. Degree



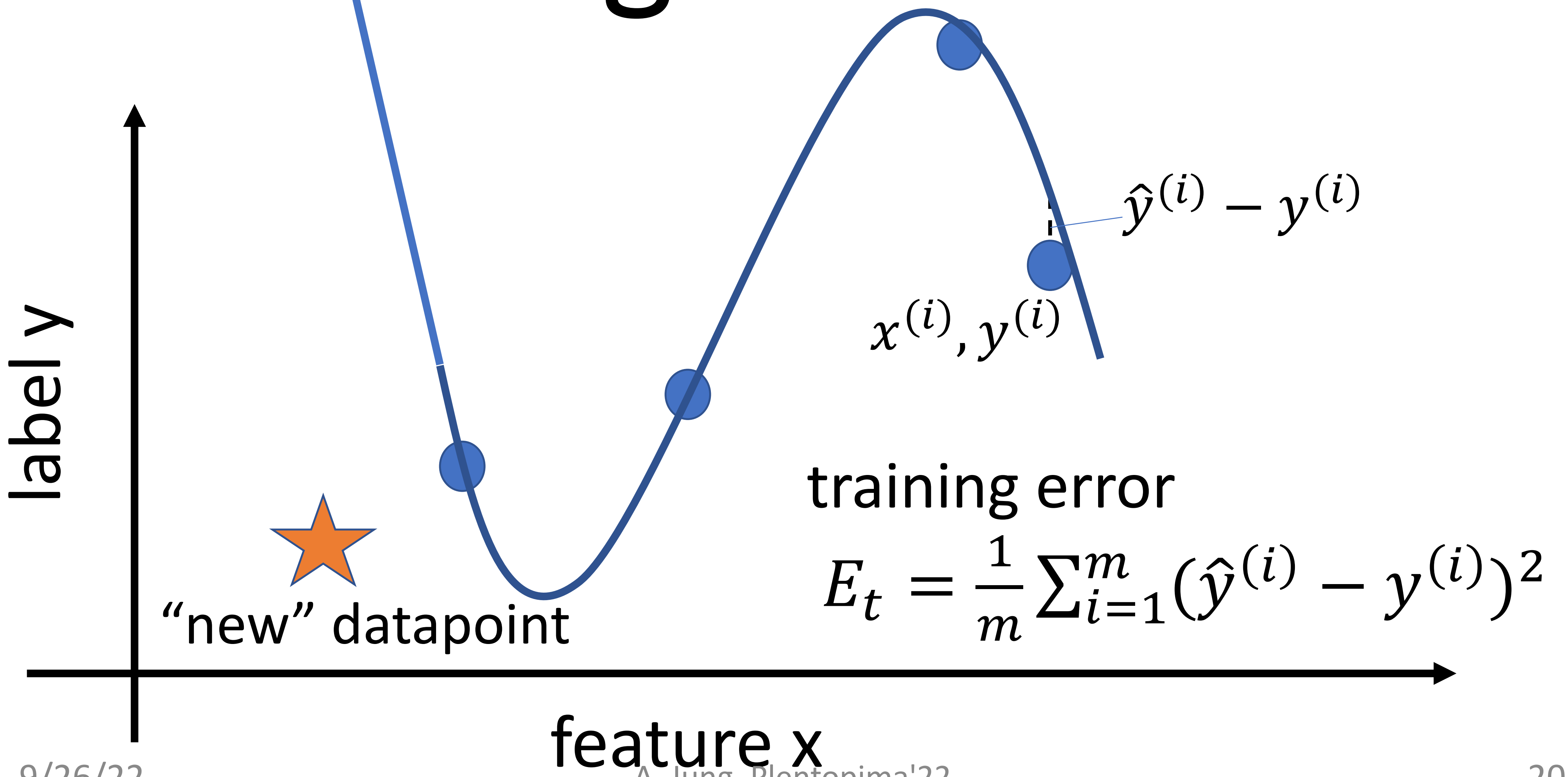
Train Error vs. ANN Layers



Train Error vs. Gradient Steps



Overfitting



small training error does not imply good performance on new data points!

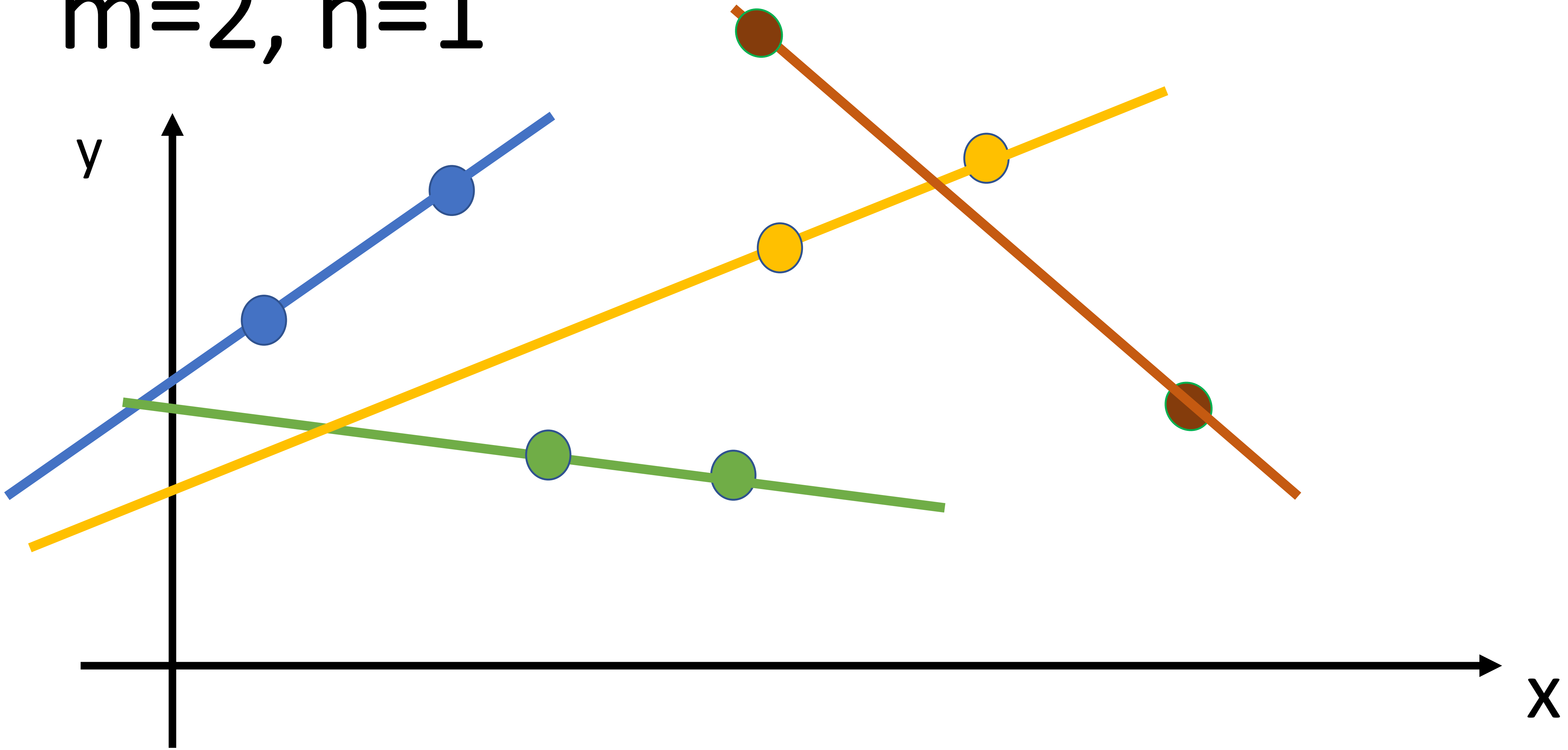
small training error merely indicates that training algorithm has been implemented correctly

A Case in Point

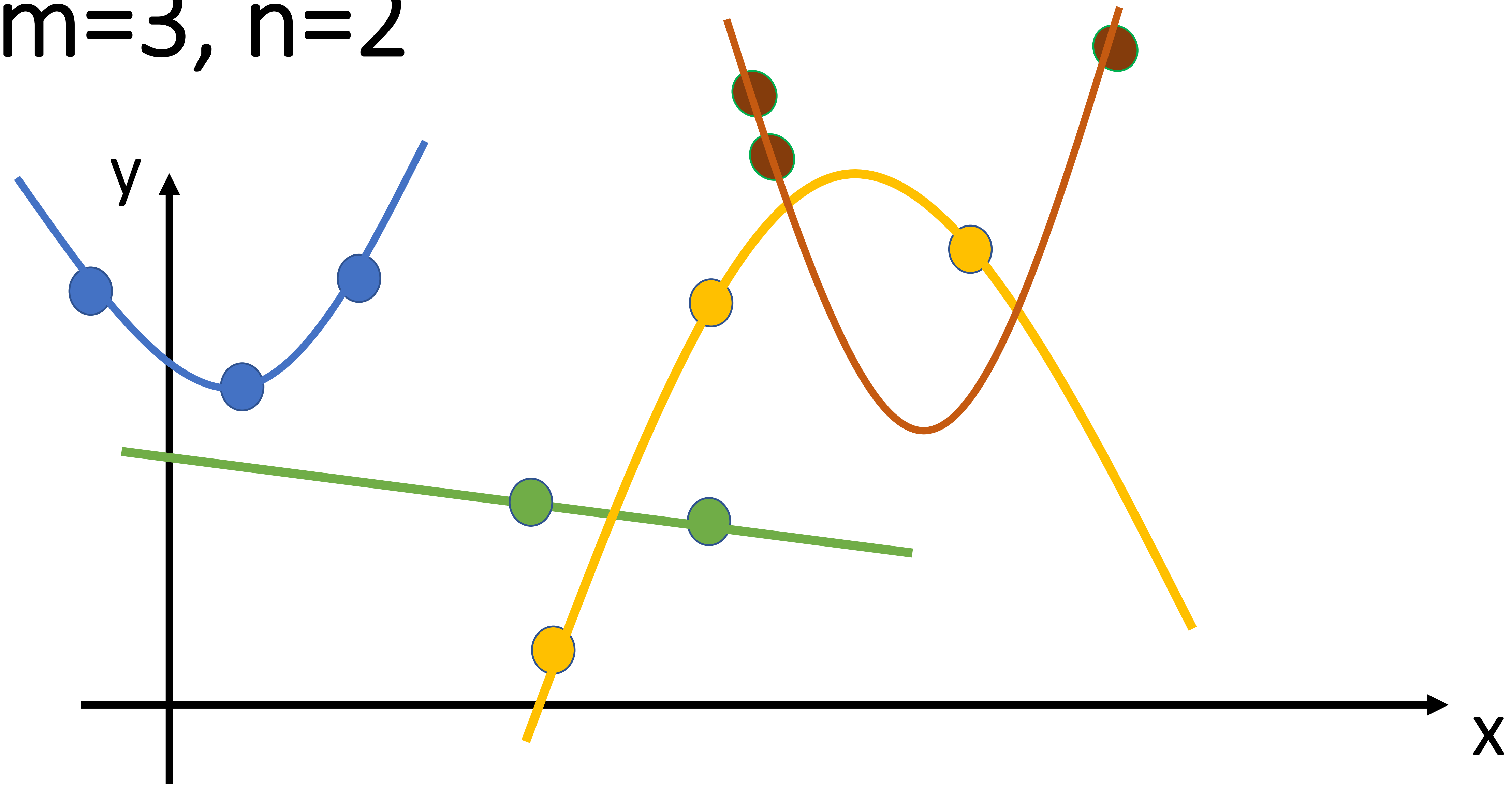
we can perfectly fit (almost) any m data points using polynomials of degree n as soon as

$$n \geq m-1$$

m=2, n=1



m=3, n=2



Reminder: Probabilistic Model

- data points are realizations of RVs
- joint pdf p(x,y) of features and label
- training set is a RV
- learnt hypothesis h(.) is a RV
- prediction h(x) is a RV

Why Can Train. Err. Mislead?

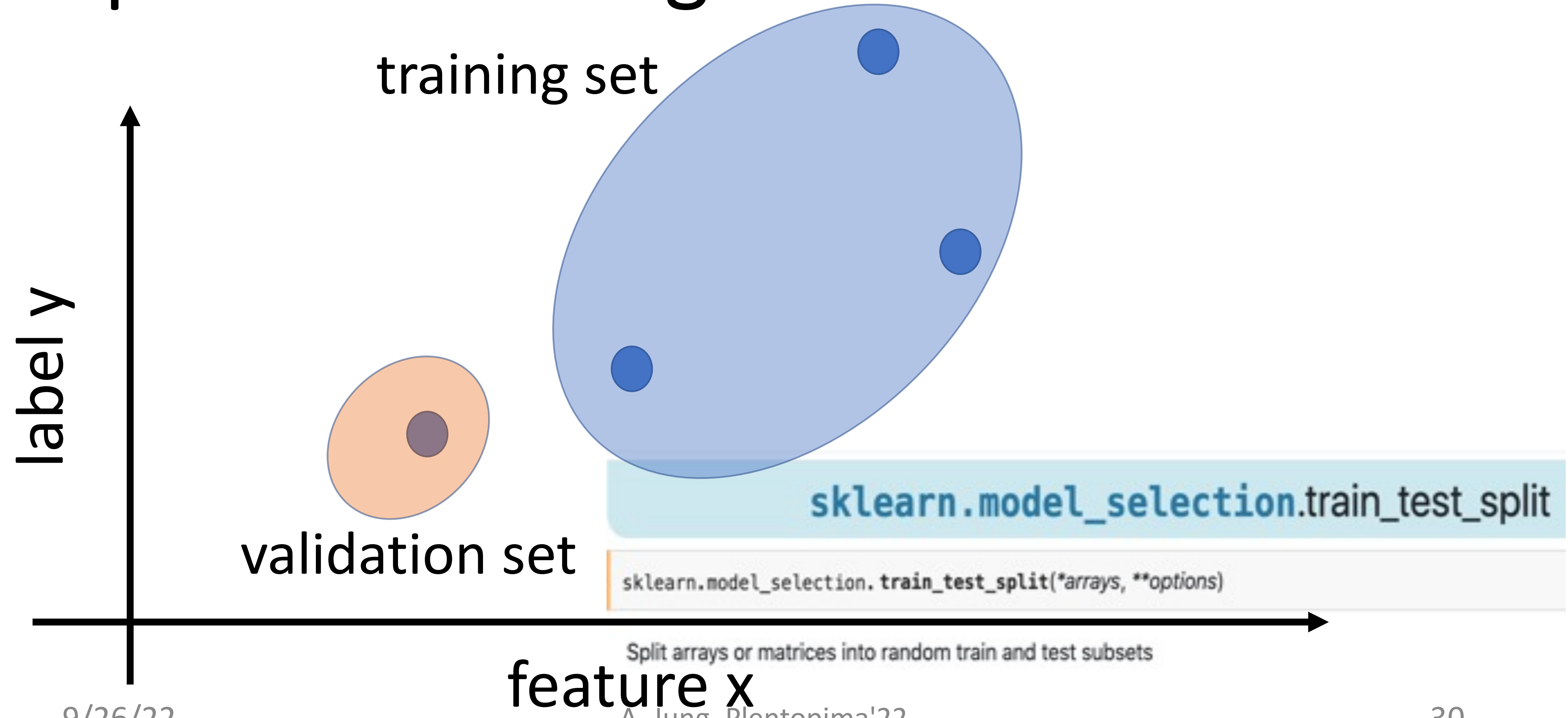
- consider expected loss of hypothesis
- estimate expectation using sample average
- this only works if hypothesis does not depends on data points used in average
- does not hold for training error

Model Validation

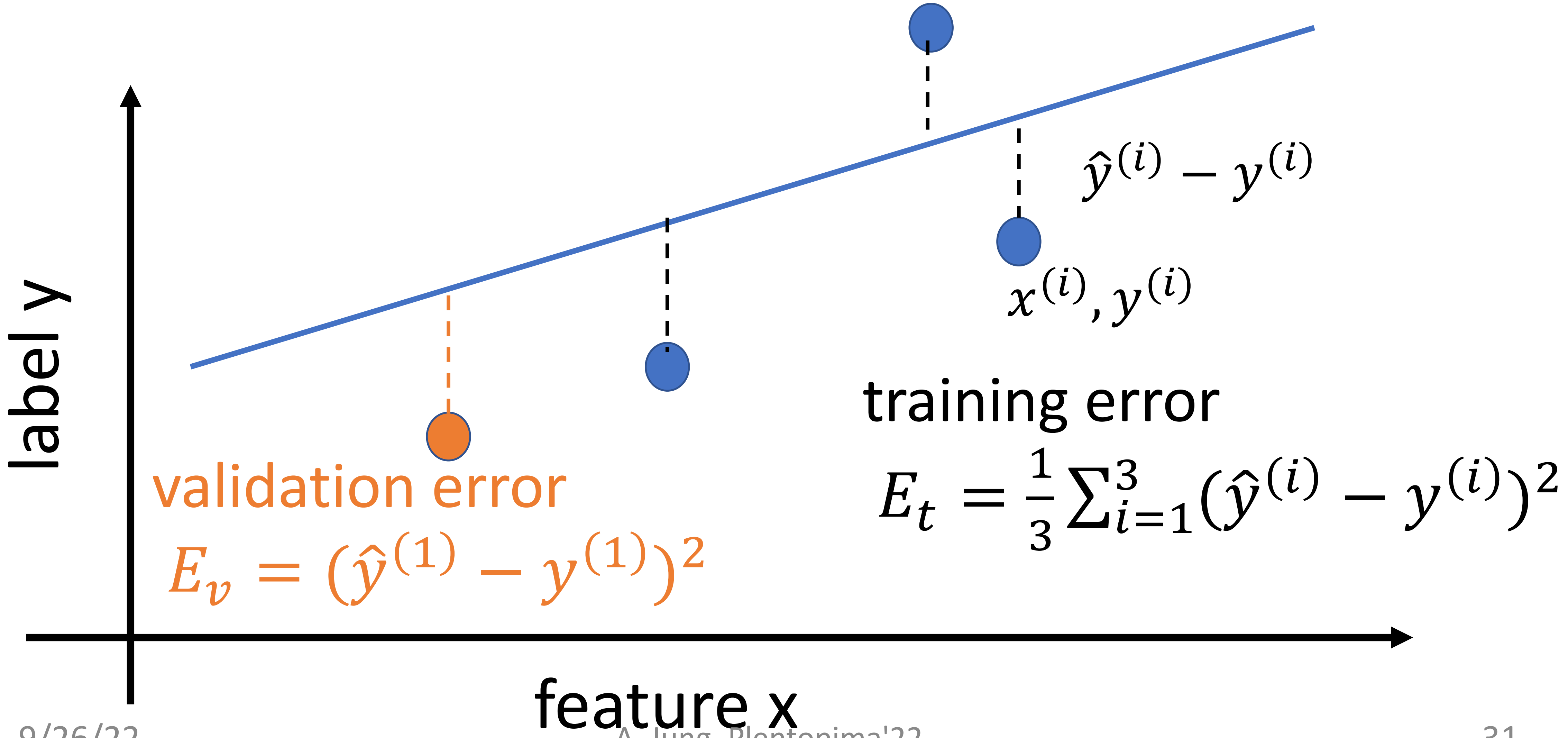
Basic Idea of Validation

- divide data points into two subsets
- use training set to learn predictor
- use validation set to estimate loss

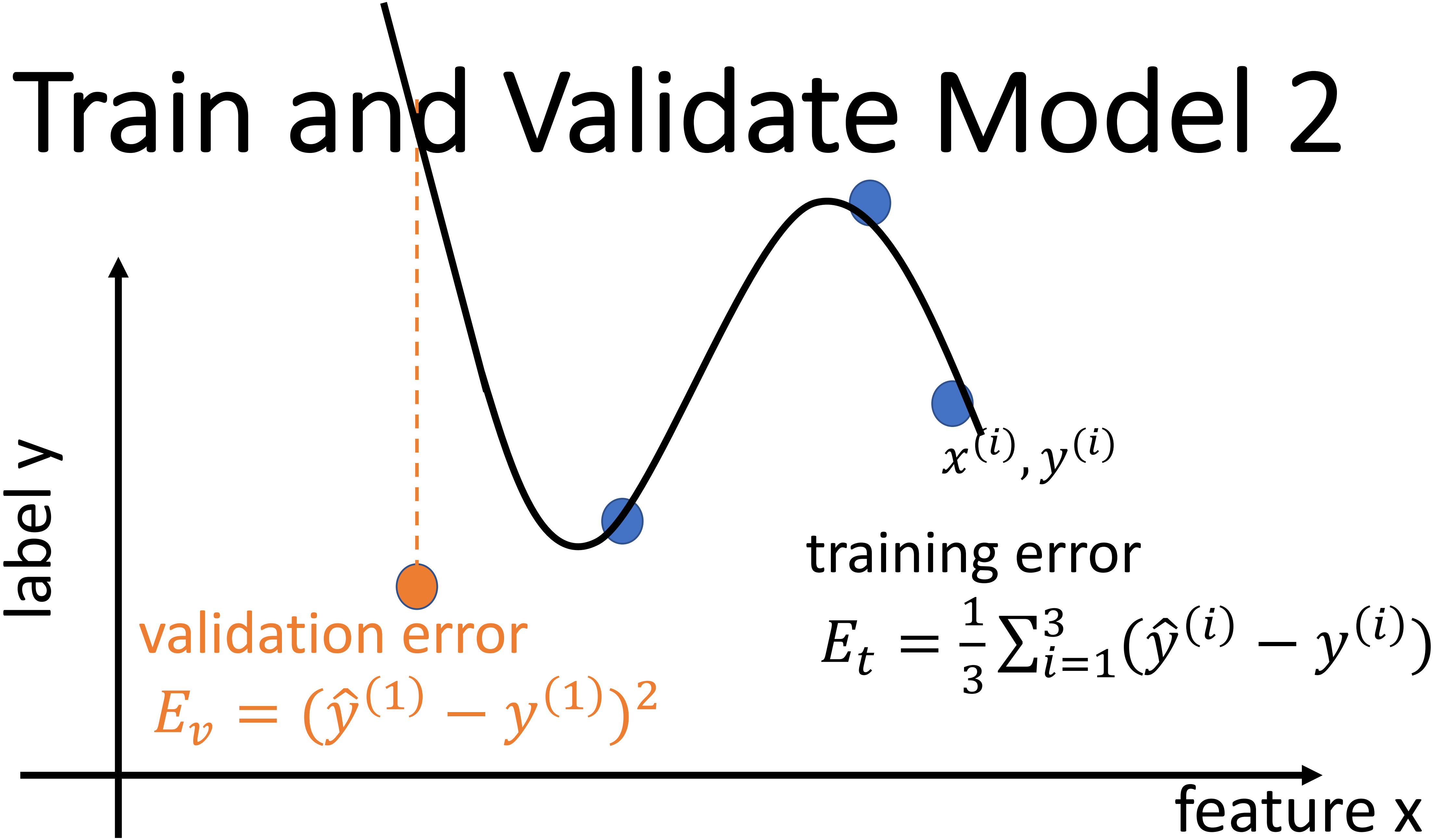
Split into Training and Validation Set



Train and Validate Model 1



Train and Validate Model 2



validation error

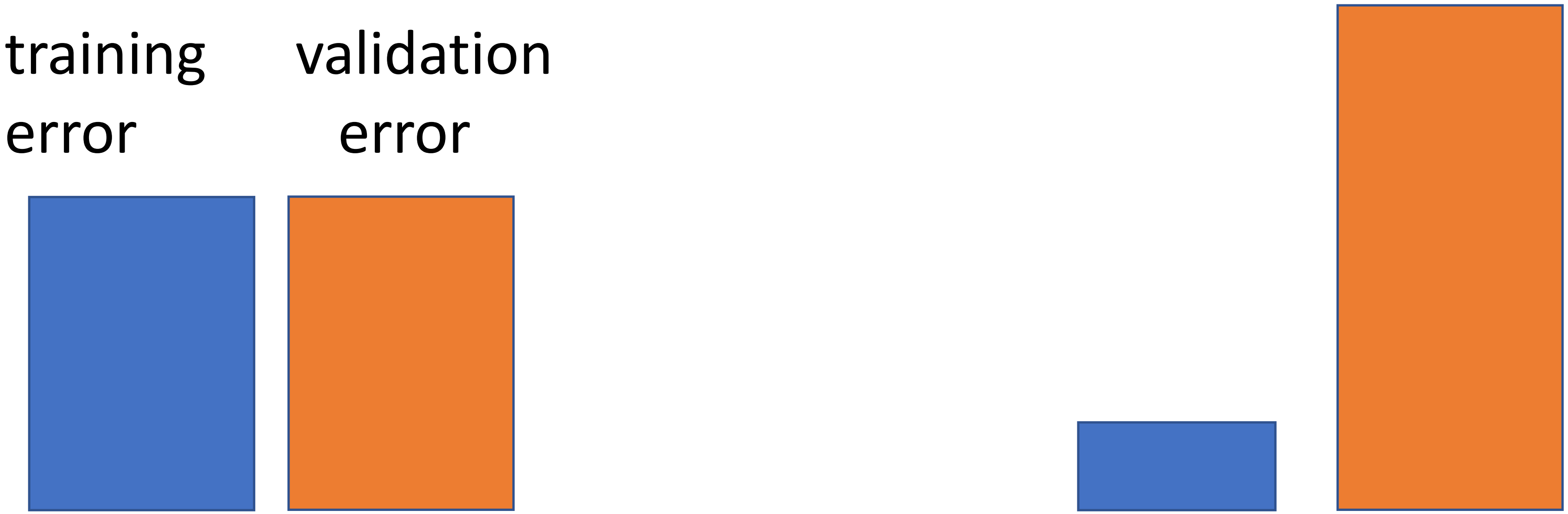
$$E_v = (\hat{y}^{(1)} - y^{(1)})^2$$

training error

$$E_t = \frac{1}{3}\sum_{i=1}^{3}(\hat{y}^{(i)} - y^{(i)})^2$$

Basic Idea of Model Selection

choose model via validation error

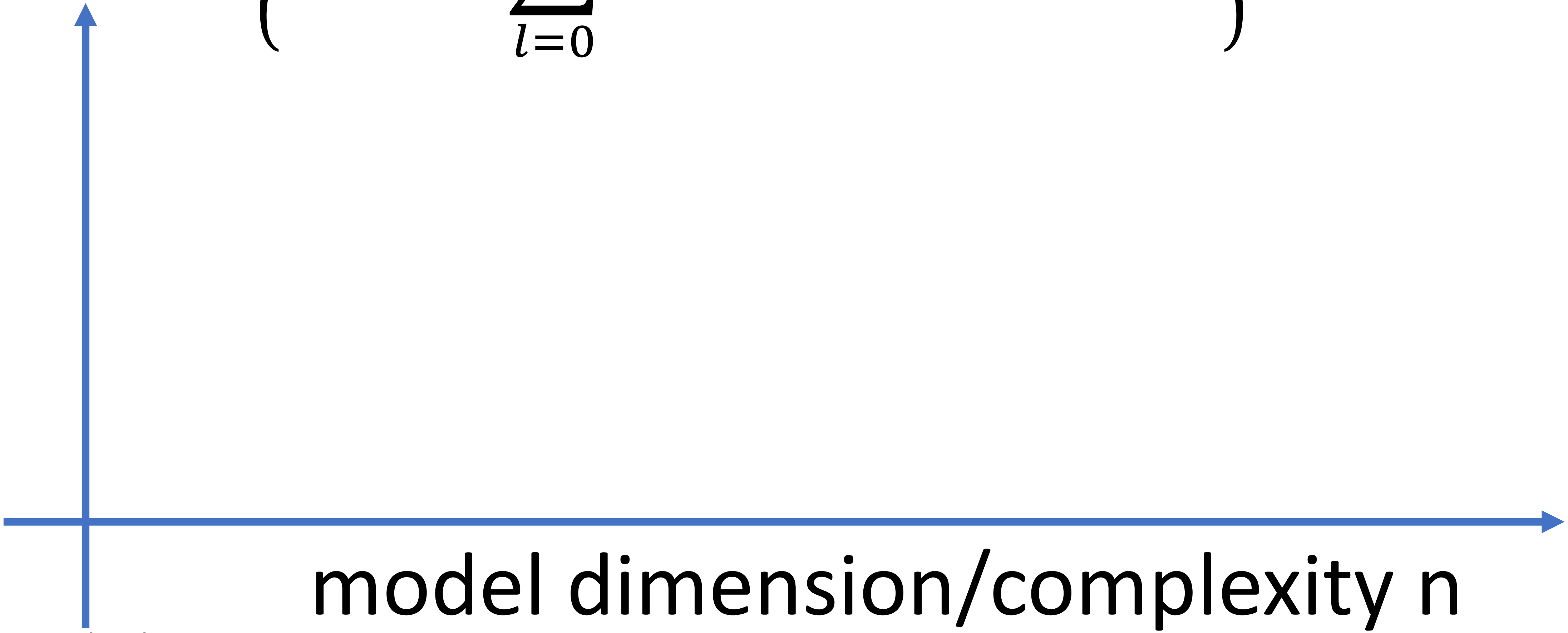


model 1: linear maps

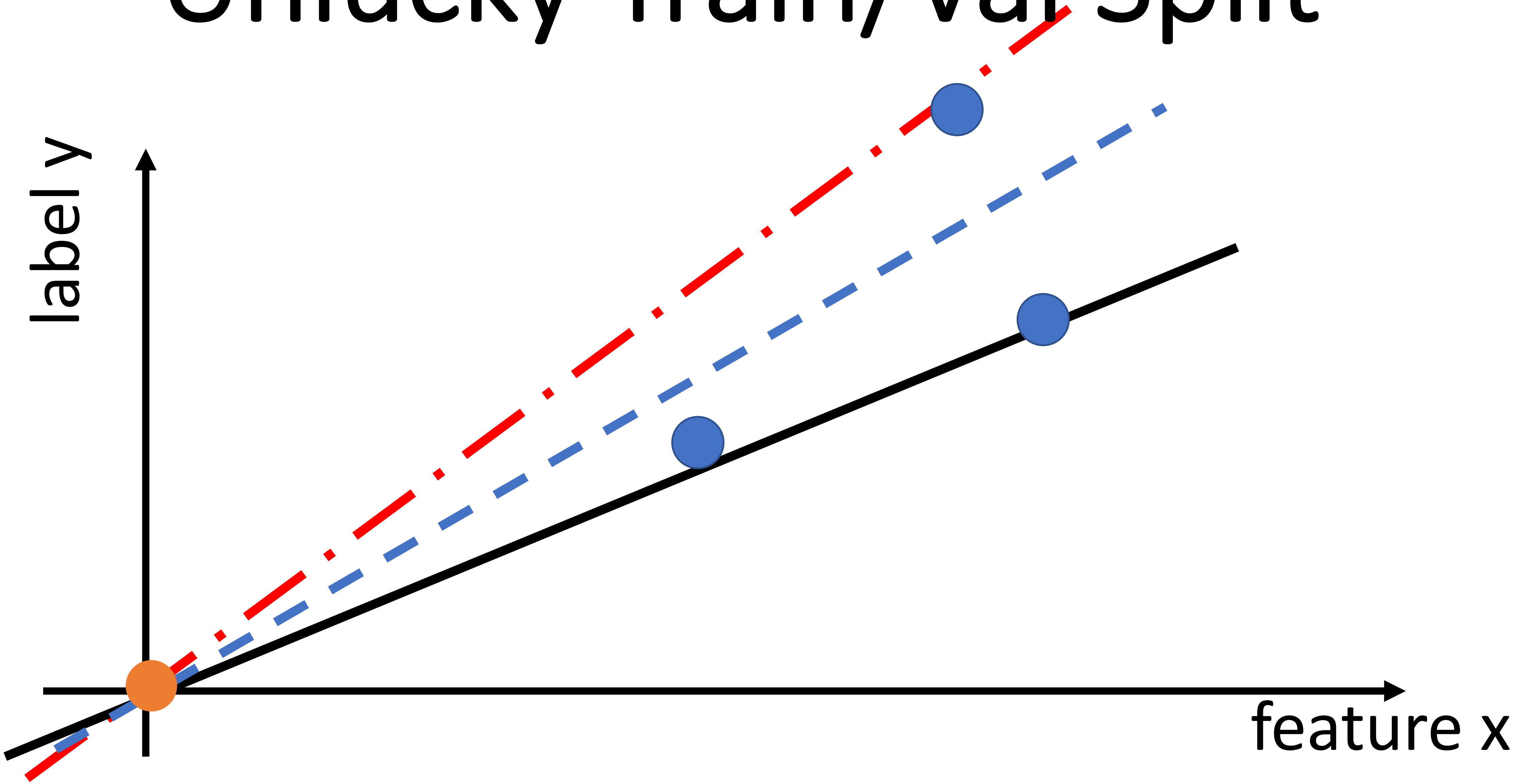
model 2: degree 3 polyn.

Train/Val Error vs Model Complexity

$$\mathcal{H}^{(n)} = \left\{ h(x) = \sum_{l=0}^{n-1} w_l x^l \text{ with } \textcolor{red}{\text{weights}}\ w_l \right\}$$



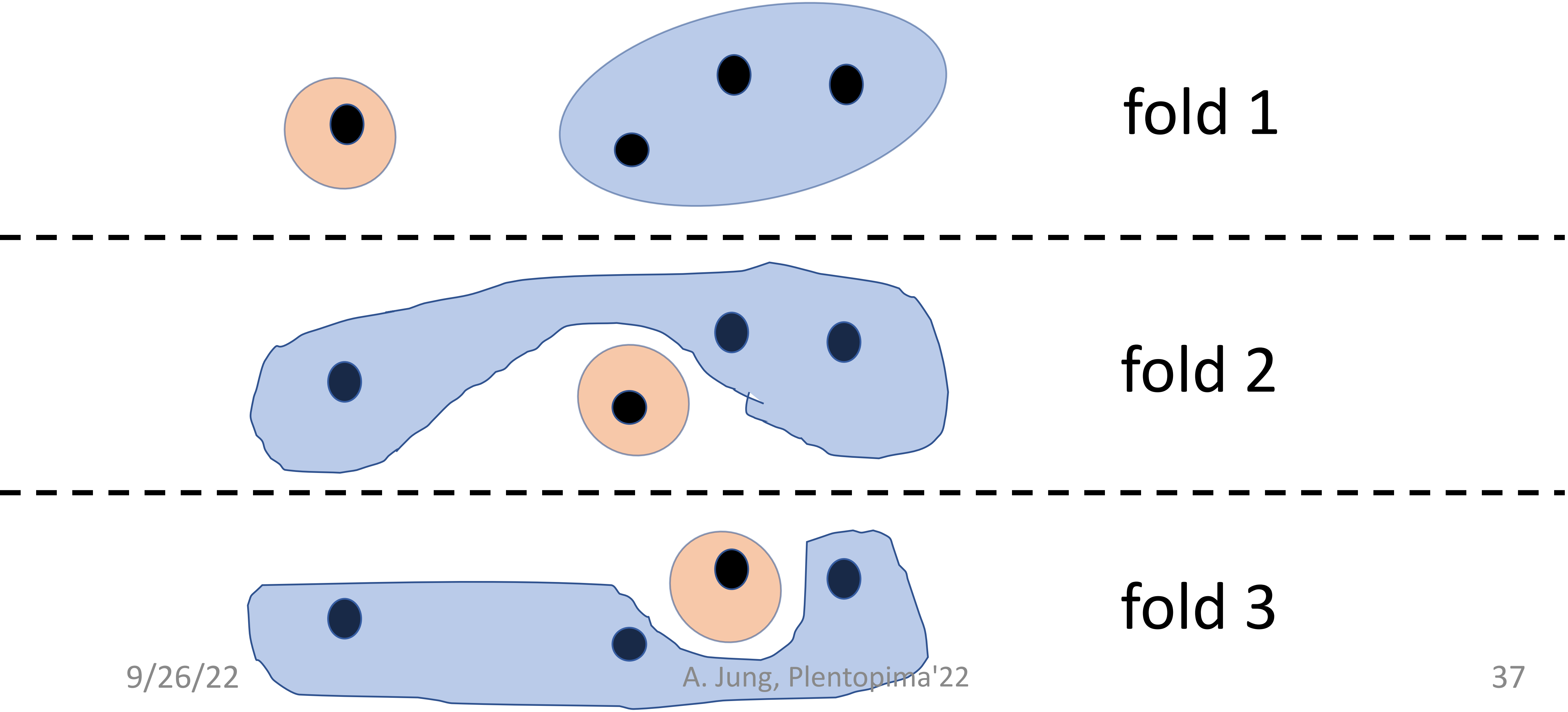
Unlucky Train/Val Split



k-Fold Cross Validation

- might be unlucky with train/val split
- problematic for small datasets
- IDEA: randomly split several times
- “average out” unlucky splits

K-Fold Cross Validation



k-Fold Cross Validation

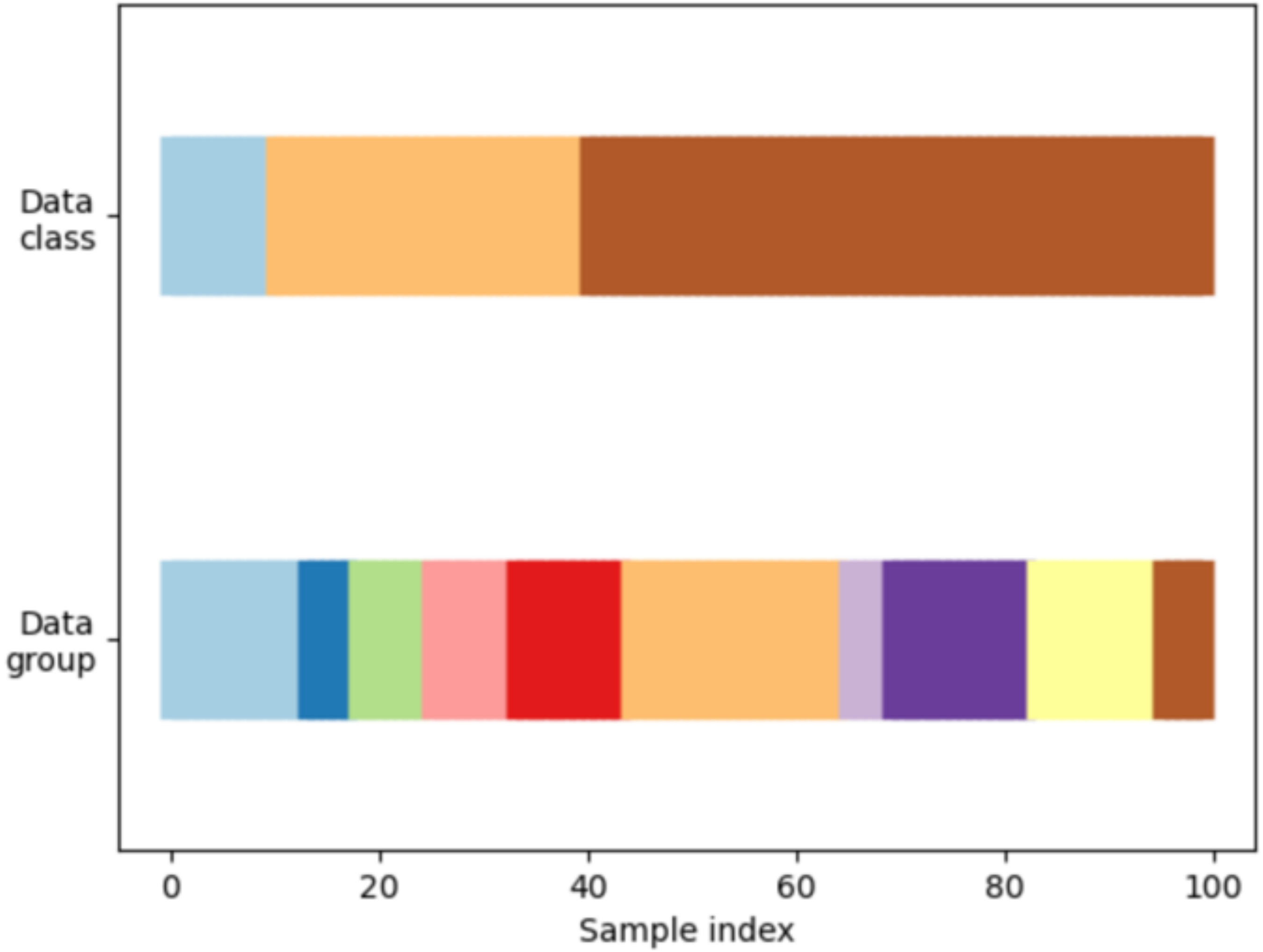
how to choose nr of folds (the “k” in k-fold CV) ?

- train fold should be sufficiently large (avoid overfitting)
- val folds should sufficiently large (to get reliable estimate of generalization)

CAUTION!

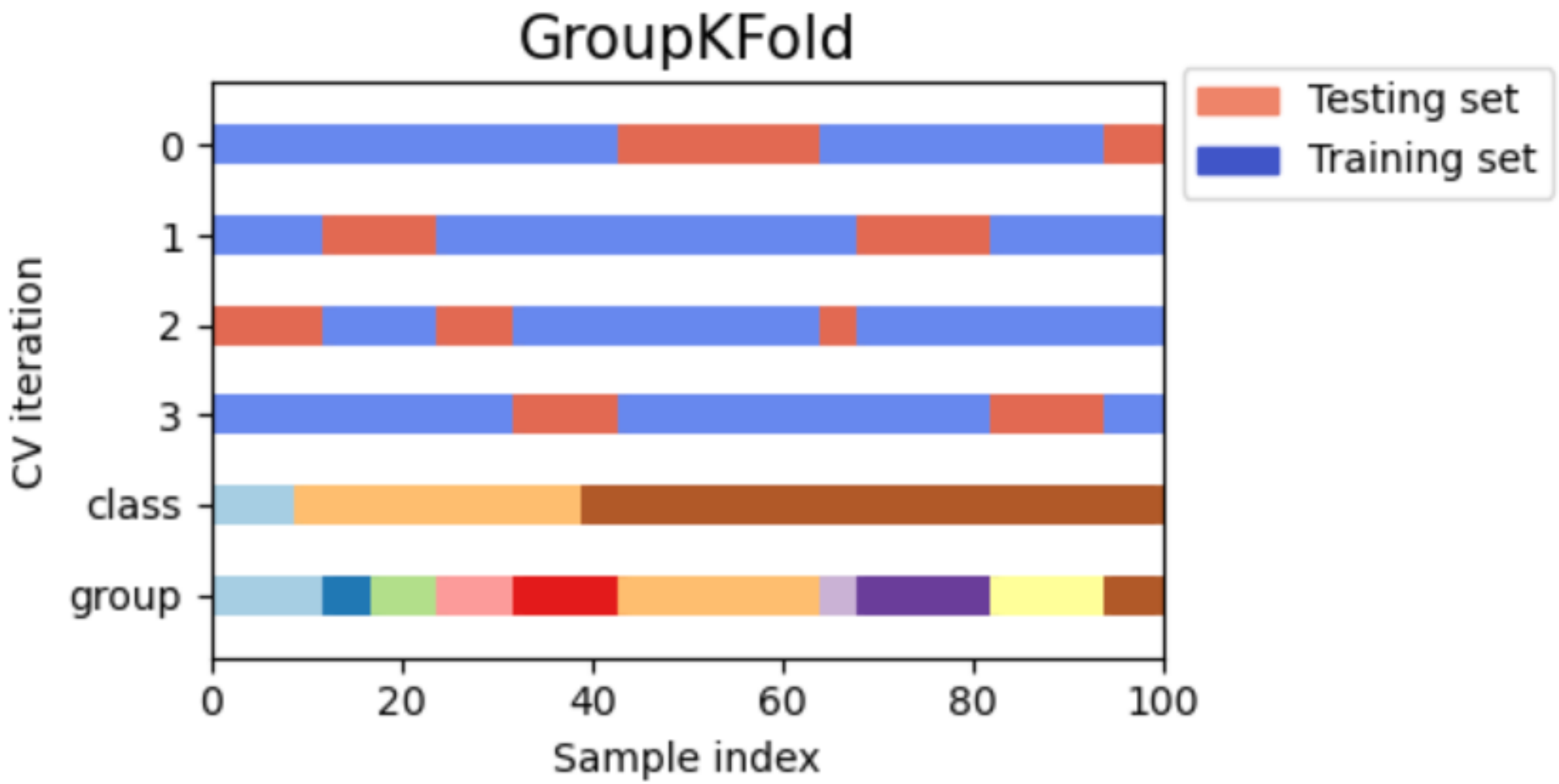
- k-fold CV requires a method to split into folds
- most basic method: evenly divide into k folds
- works if data is i.i.d. (“order of data points is arbitrary”)
- fails if data points are grouped or ordered

Imbalanced Classes and Group Structure



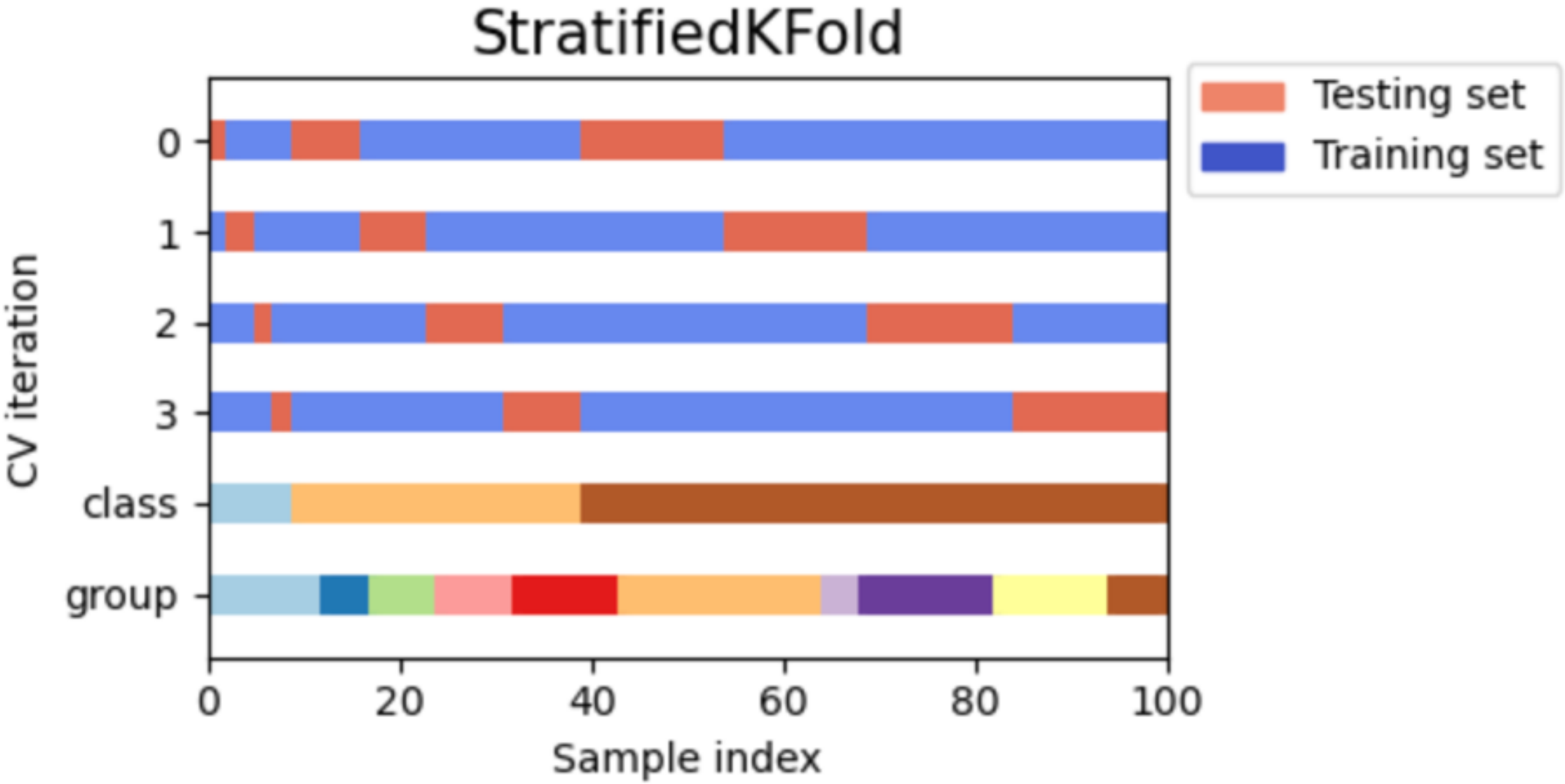
- e.g. data points with same label are contiguous blocks
- or data points are obtained at consecutive time instants (→ correlations)

Group-Preserving Splitting

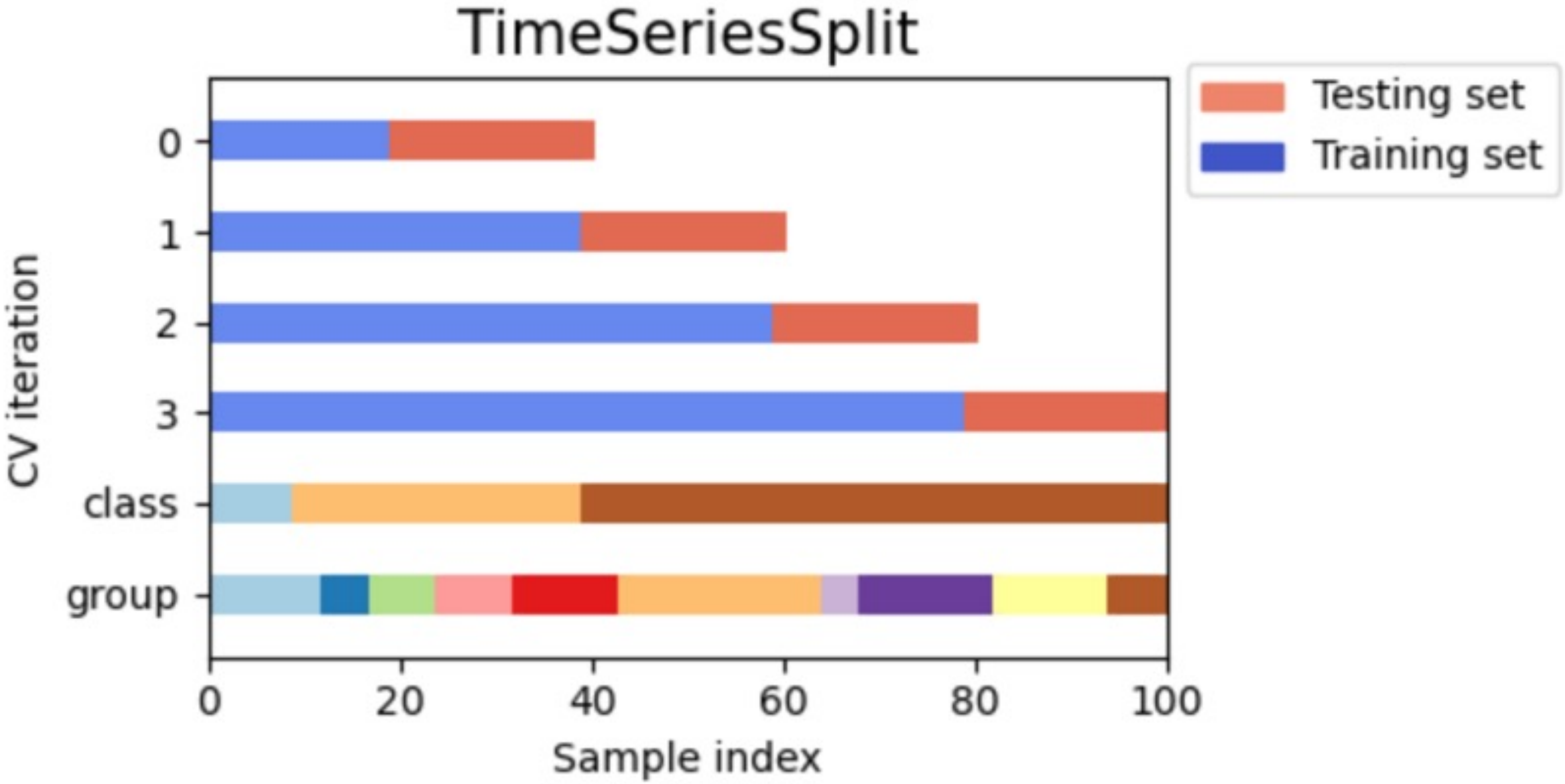


https://scikit-learn.org/stable/modules/generated/sklearn.model_selection.GroupKFold.html

Class-Ratio Preserving Splitting



Temporal Successive Splitting



source: https://scikit-learn.org/stable/

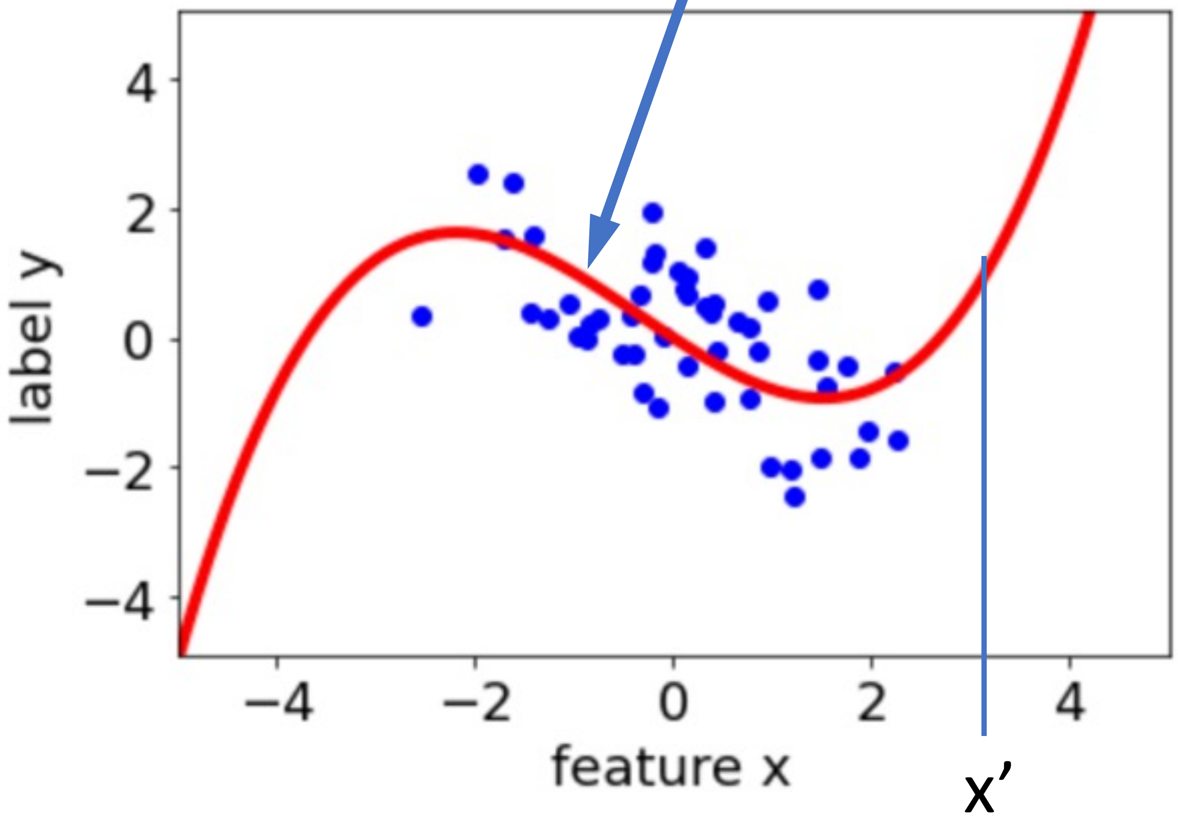
Bias and Variance Decomposition

“Bias” error component due to model being too small

“Variance” reflects error due to dataset being too small

Toy Data

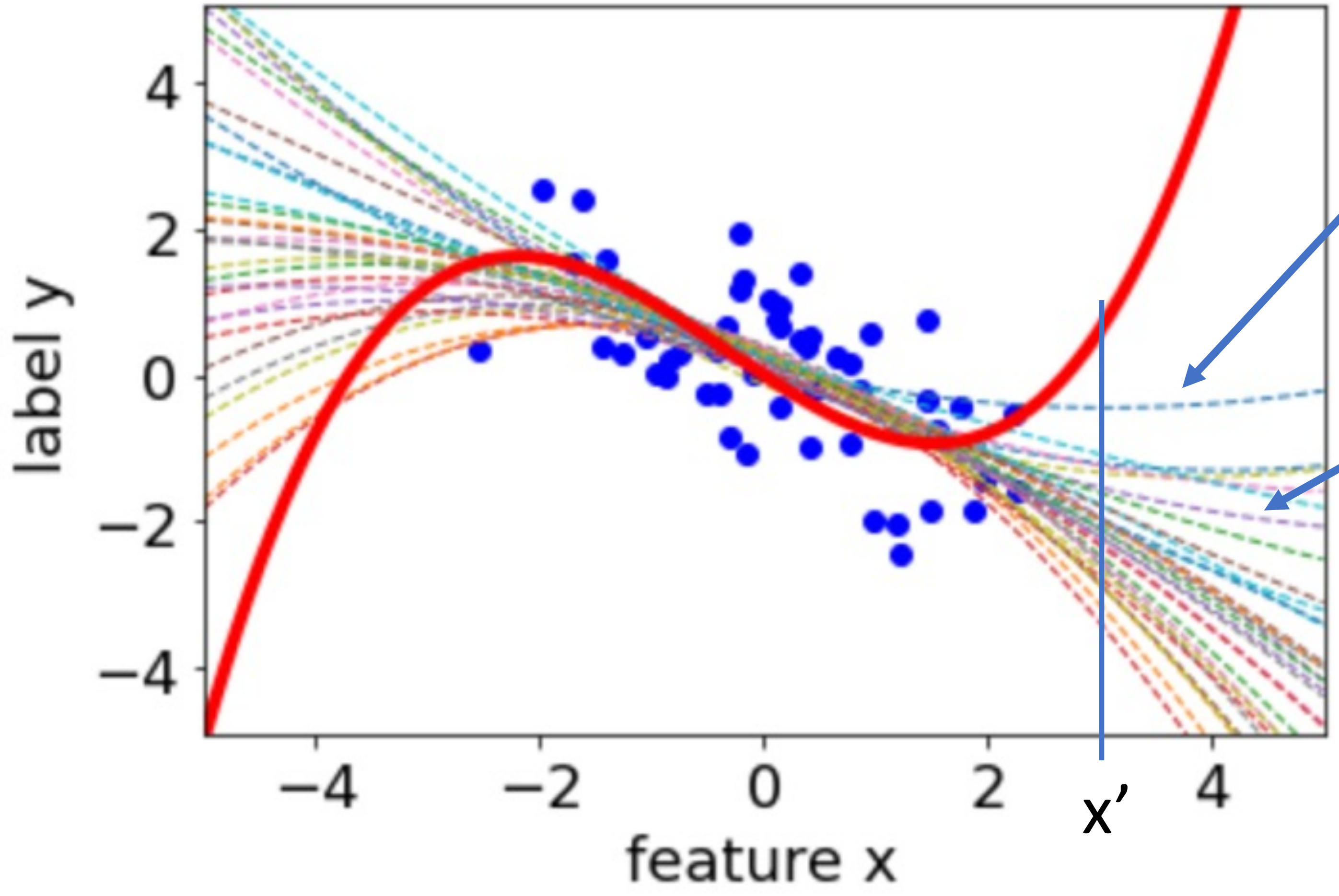
y = g(x) + ”noise”



learn hypothesis h(.) using a randomly selected training set

compute prediction h(x’) for a fixed feature value x’

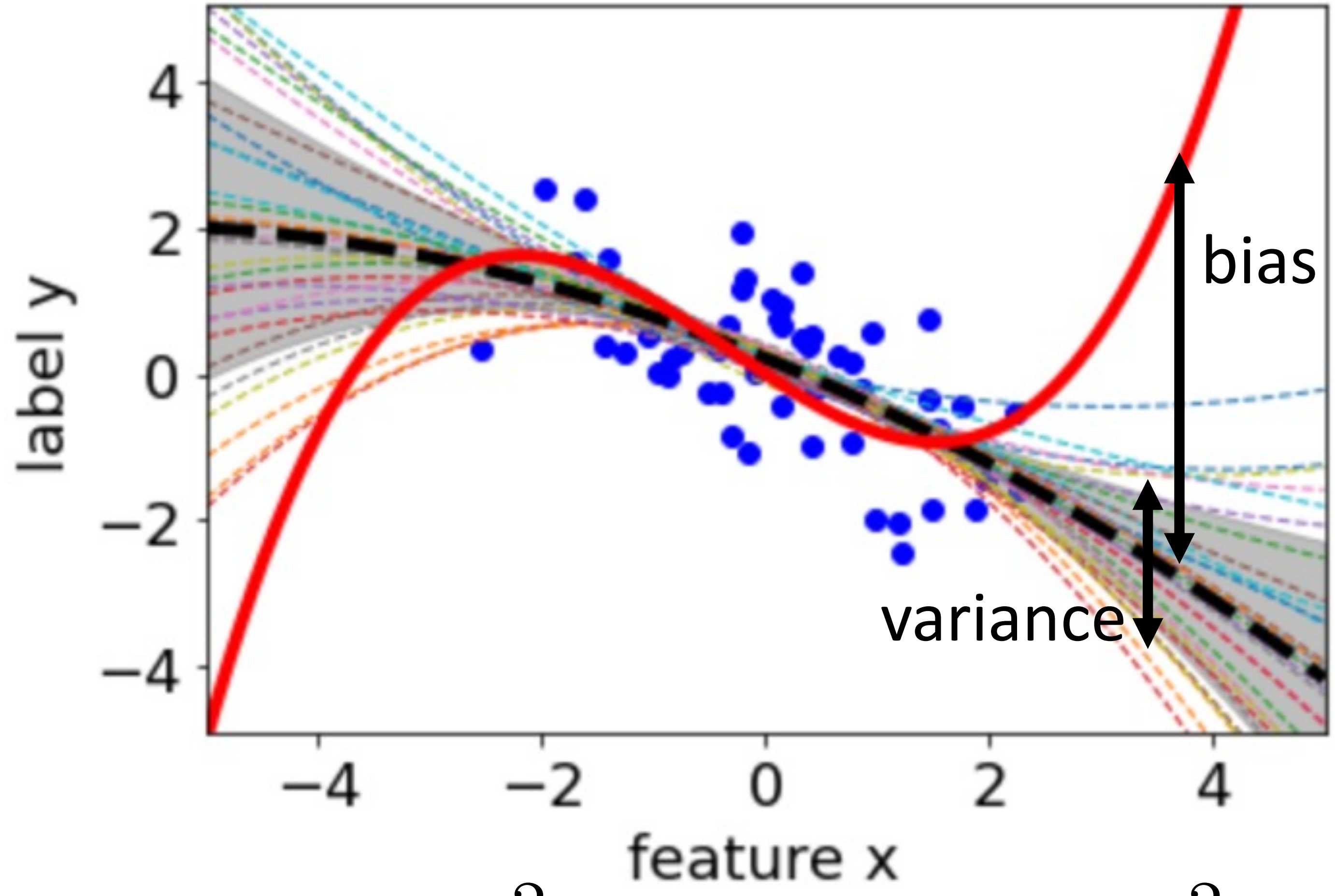
Ensemble of Learnt Hypotheses



hypothesis learn on train set #1

hypothesis learn on train set #2

Bias and Variance

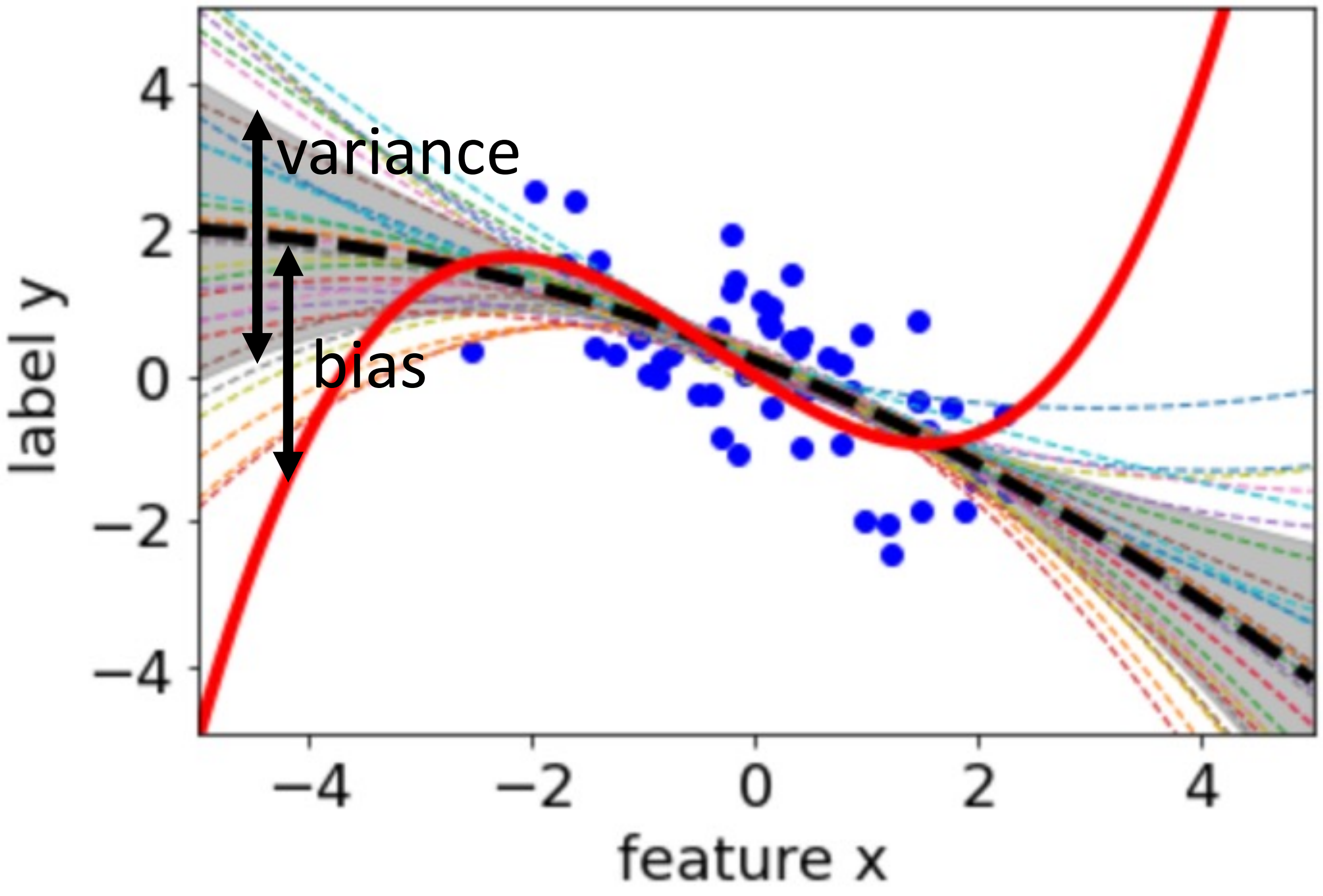


$$\hat{y} = h(x')$$

RV since obtained
from a randomly
selected training set

$$\mathrm{E}\{(\hat{y}-y)^2\} = (\mathrm{E}\{\hat{y}\}-y)^2 + \mathrm{E}\{(\hat{y}-\mathrm{E}\{\hat{y}\})^2\}$$

Bias and Variance Tradeoff

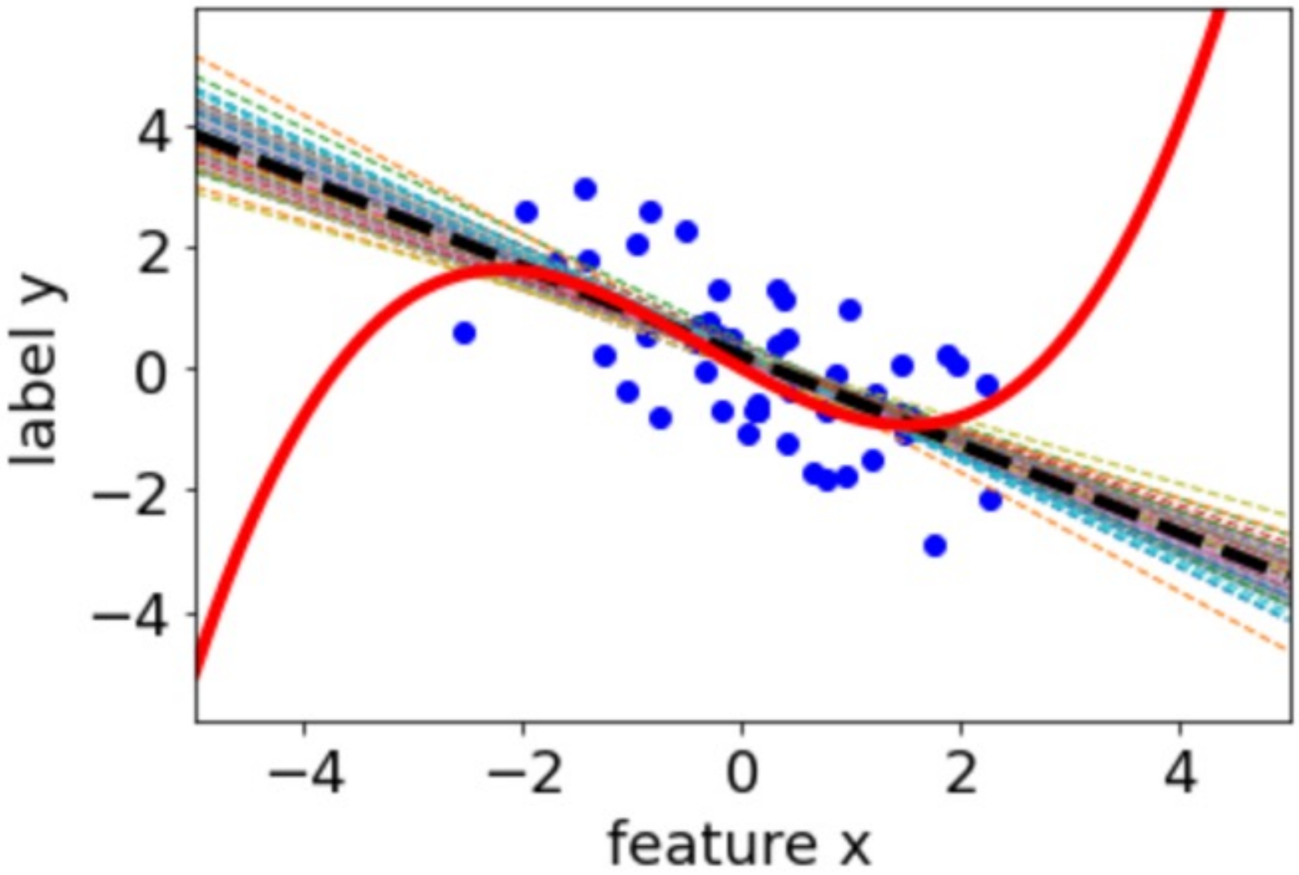


"Prediction Error = Bias + Variance"

bias reduction typically incurs variance increase and vice versa

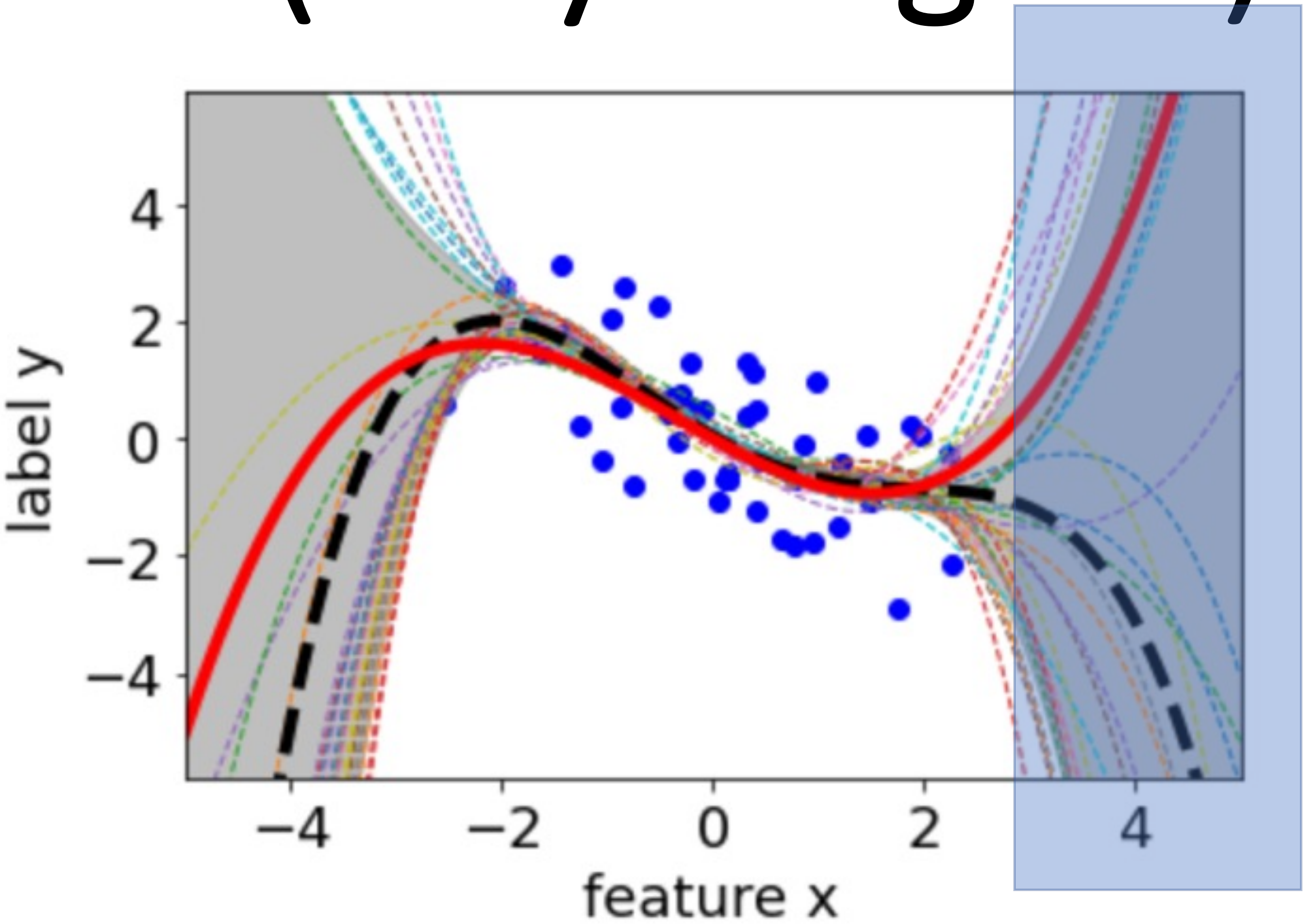
Smaller Model (Poly.Degree)

- small variance
- large bias

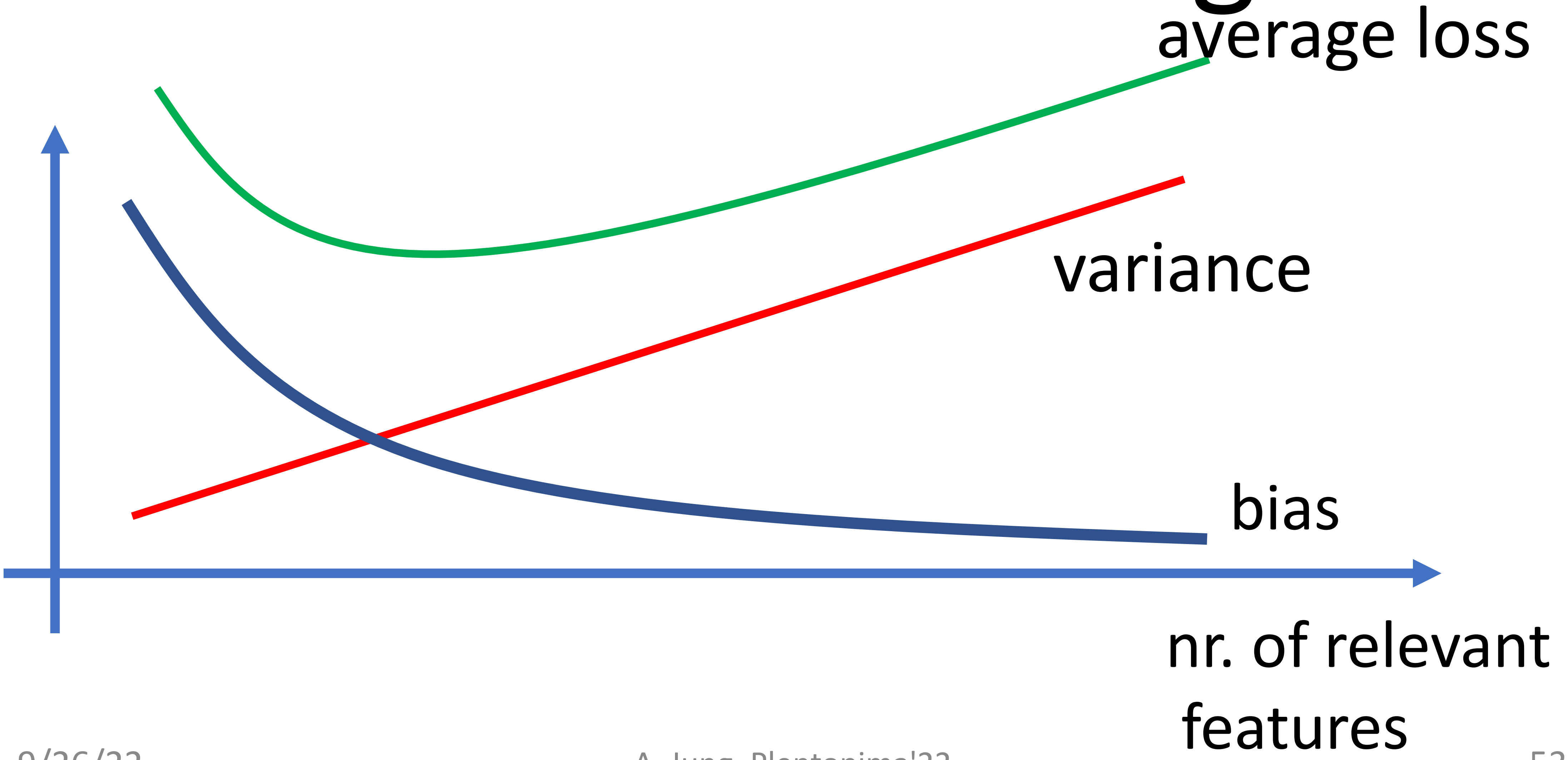


Larger Model (Poly. Degree)

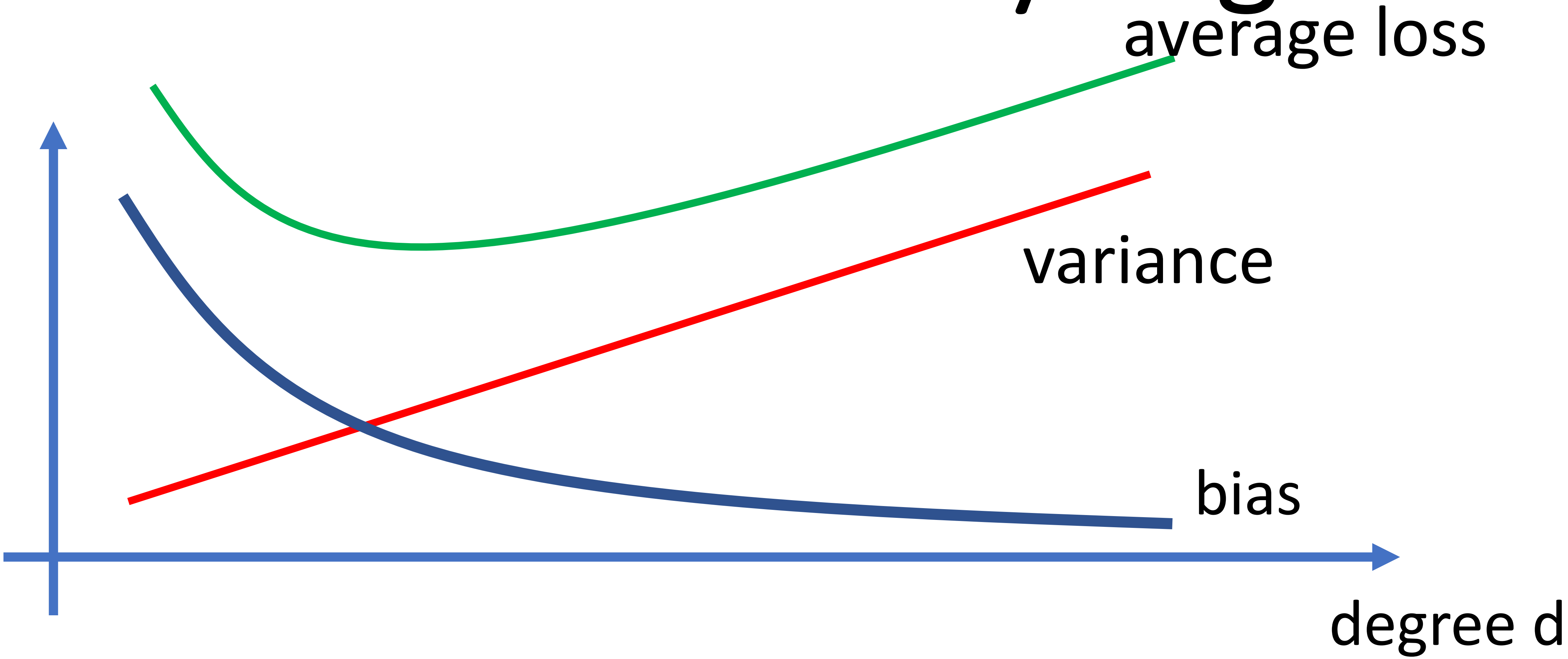
- large variance
- small bias



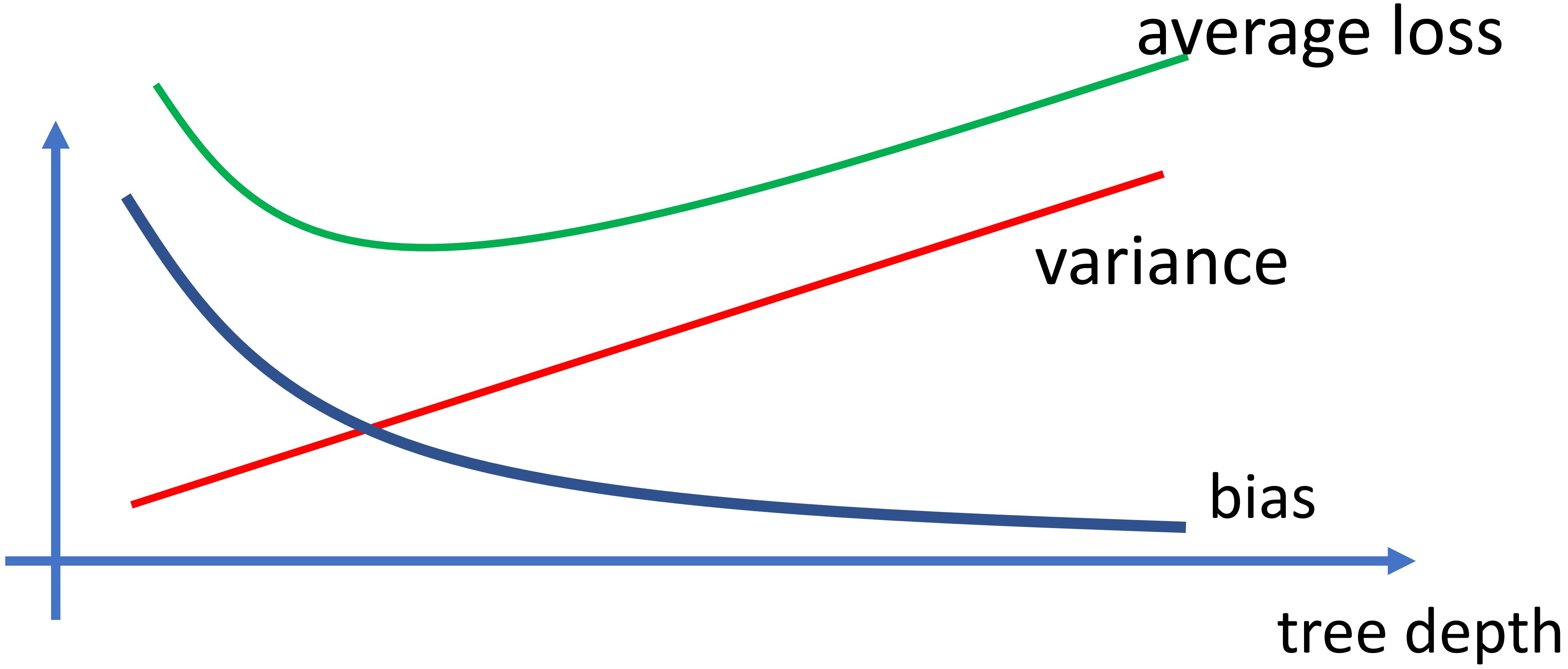
Bias vs. Variance Lin.Reg.



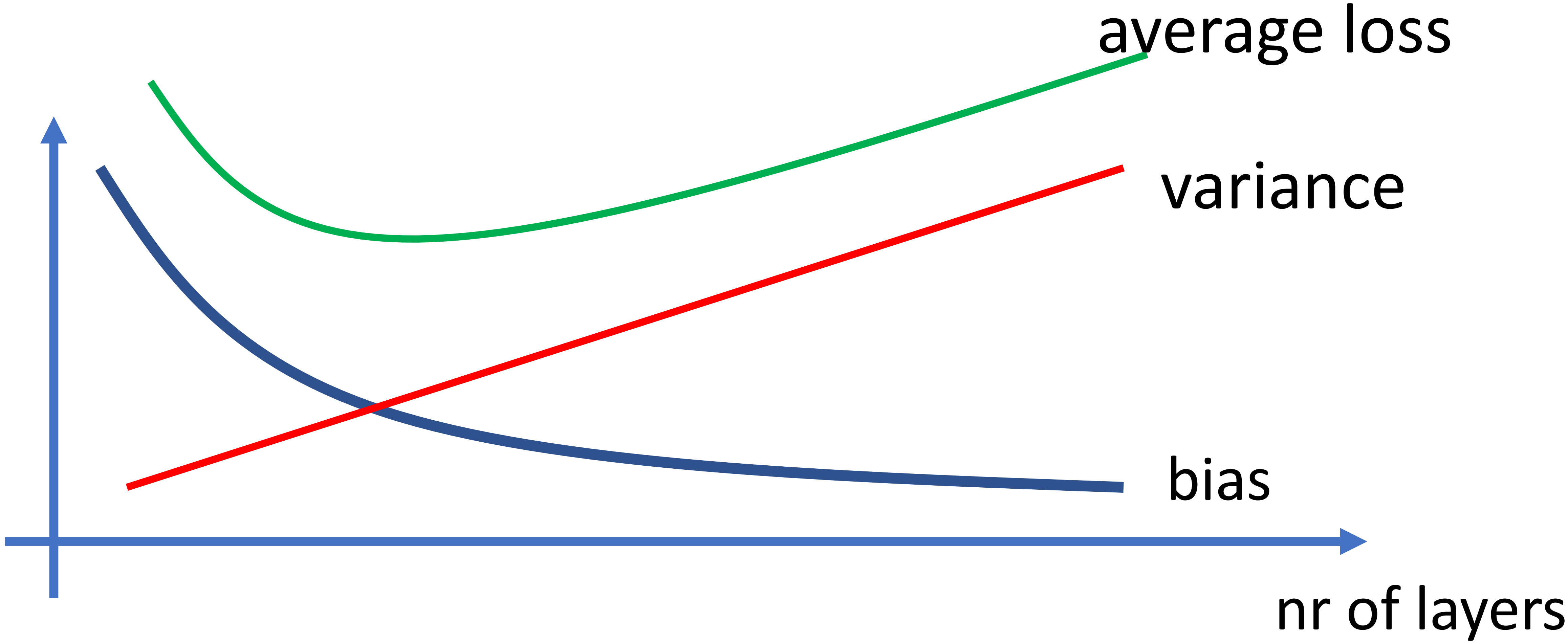
Bias vs. Variance Poly.Reg.



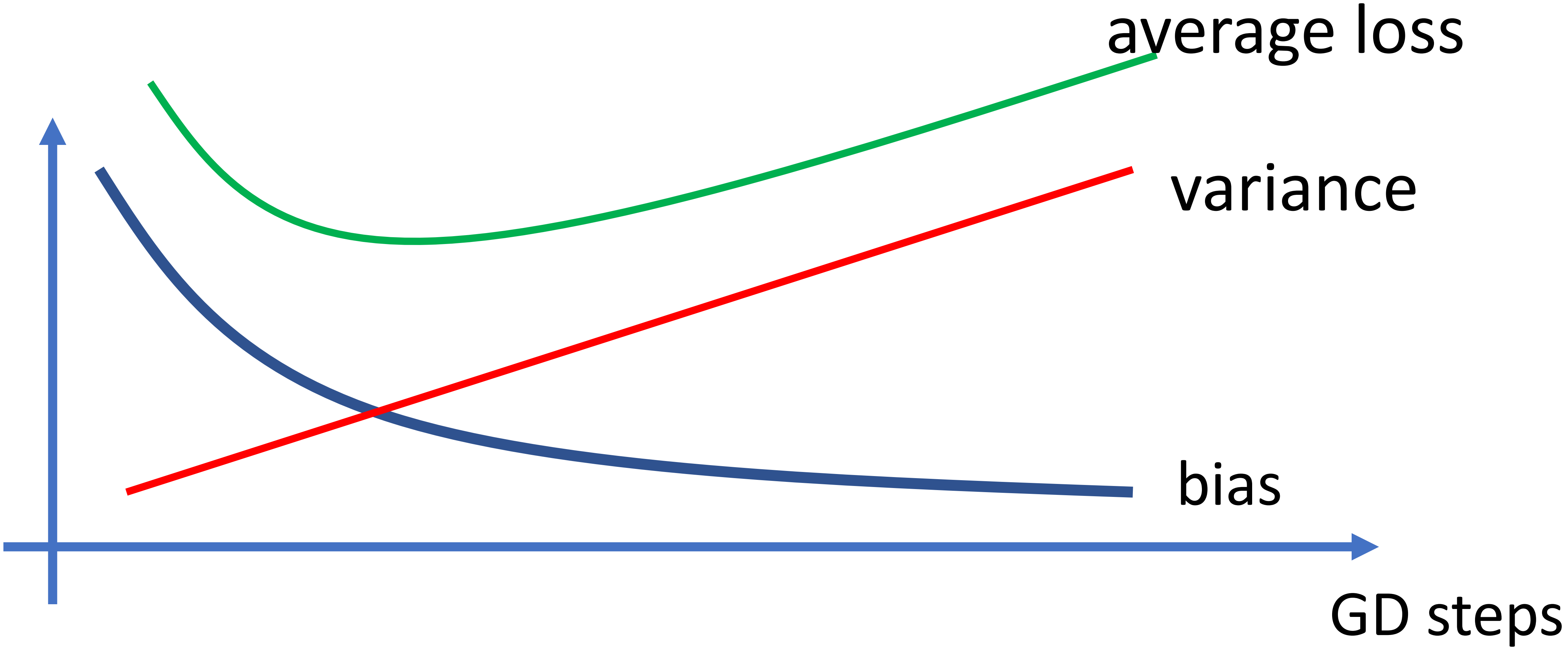
Bias vs. Variance Dec. Tree.



Bias vs. Variance Deep Learning

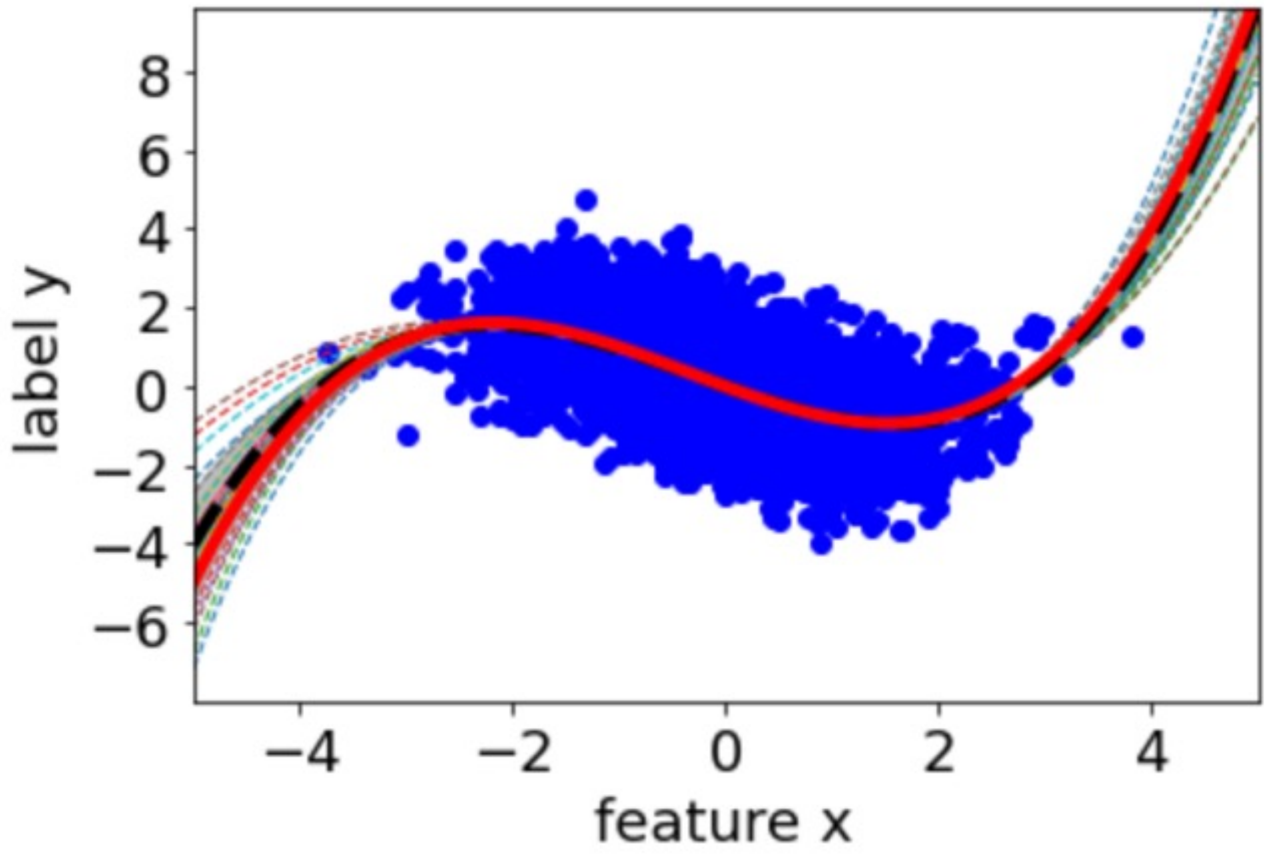


Bias vs. Variance Grad. Desc.



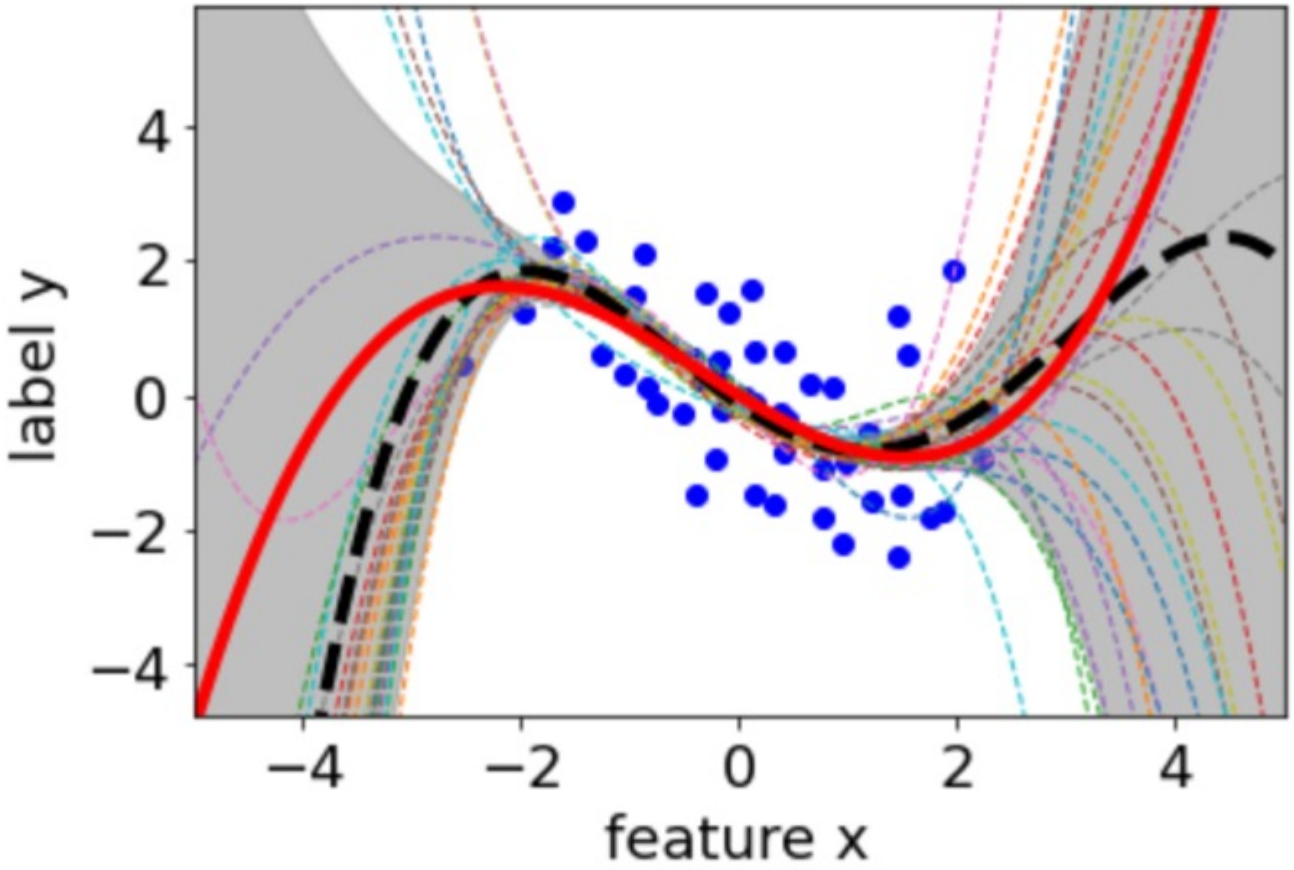
More Data

-> smaller variance

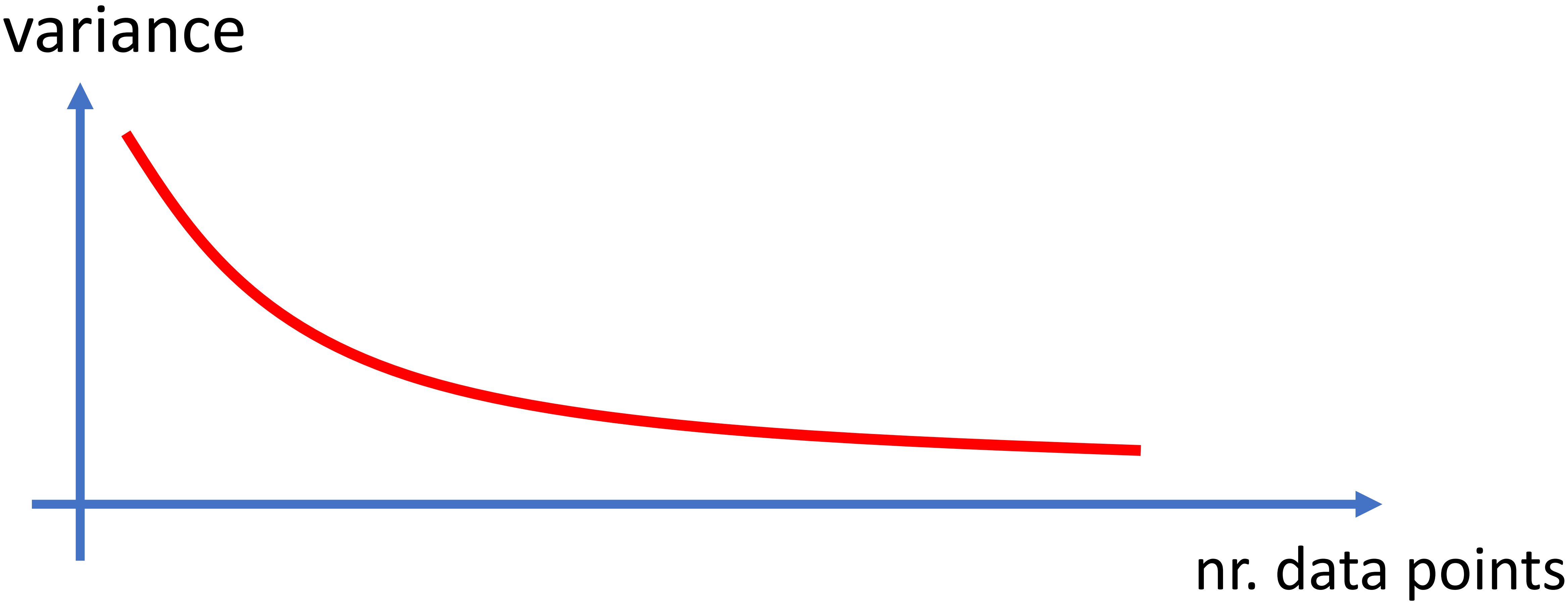


Less Data

-> larger variance



Learning Curve



Alex’ Rule of Thumb

effective number of training data points

>

10 * nr. tunable effective model parameters

stretch the term “effective” as much as possible !

ML Diagnosis

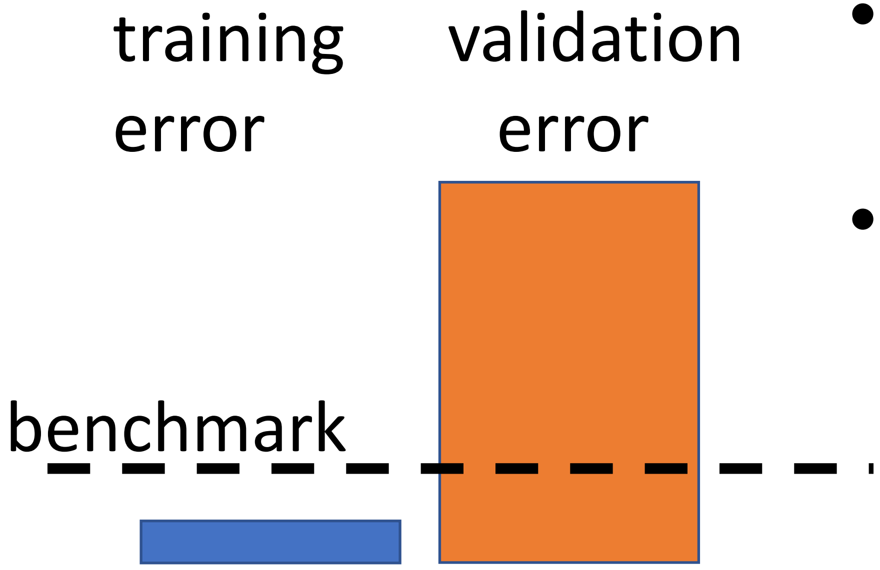
Simple Recipe

- consider ML method with some hypothesis space
- learn hypothesis by min. average loss on train.set
- training error = average loss of learnt hypothesis
- compute validation error
- compare val err, train err with a baseline

Benchmark/Baseline

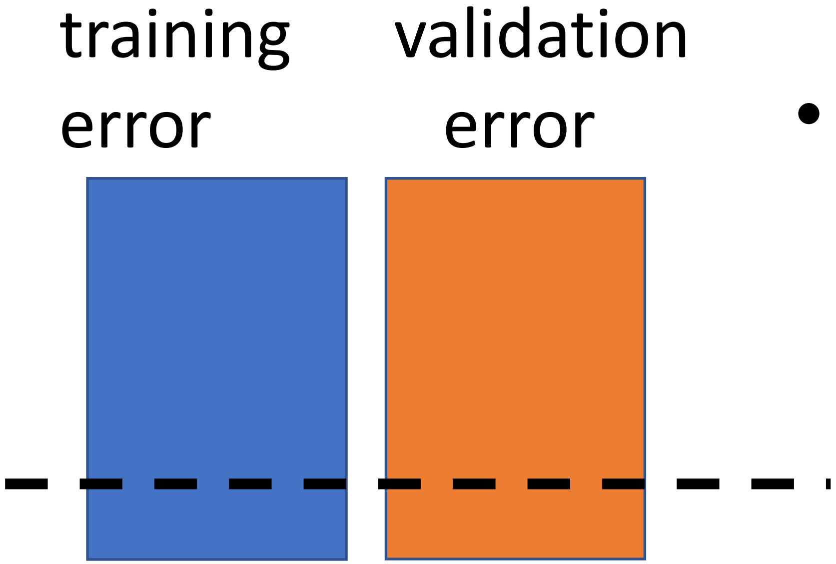
could be obtained from

- probabilistic models
- domain expertise
- existing ML methods
- human performance
- …

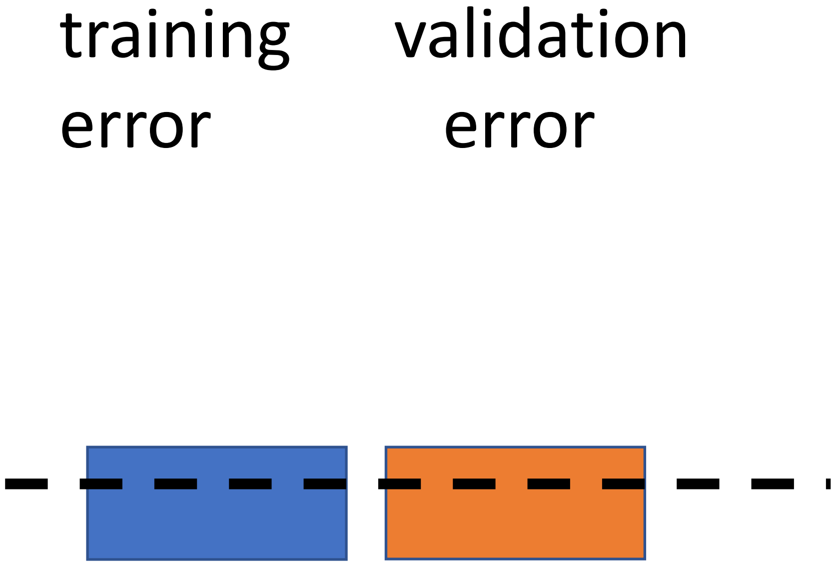


- small train error -> hypothesis space is large
- large val err -> overfitting

- Workaround ?



- large train error -> no good hypothesis found
- Workaround ?



- Case Solved !

Take Home Messages

- large models (e.g. deep nets) often overfit
- small training error does not mean much!
- diagnosis by comparing train/val err
- bias/variance analysis can guide model improvement

Thank You !