Applied Machine Learning

Generalization

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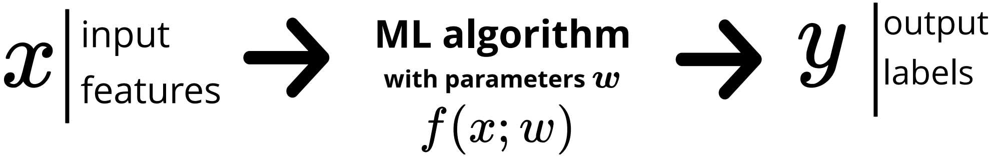
COMP 551 (Fall 2023)

Learning objectives

- generalization
- bias and variance trade-off
- validation and cross-validation
- evaluation

Generalization



x | input features → **ML algorithm** **with parameters w** $f(x; w)$ → y | output labels

training: parameter estimation

$$\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_{n=1}^{N}$$

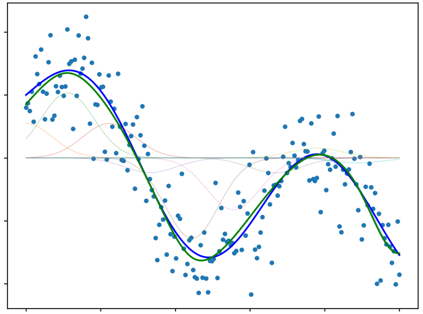
$$w^* = \arg\min_w J(w)$$

$$J(w) = \frac{1}{N}\sum_{n=1}^{N} l(y^{(n)}, f(x^{(n)}; w))$$

Example: Linear regression

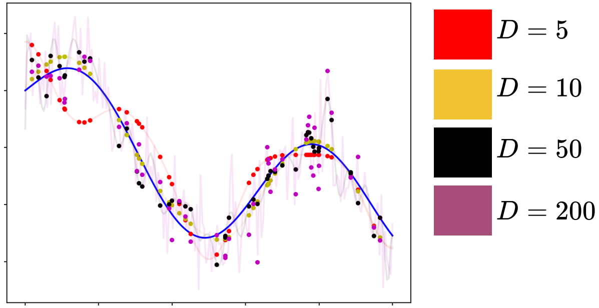
model: $\hat{y} = f_w(x) = w^\top x \ : \mathbb{R}^D \to \mathbb{R}$

cost function: $J_w = \frac{1}{N}\sum_n \frac{1}{2}(y^{(n)} - \hat{y}^{(n)})^2$



inference: $\hat{y} = f(x; w^*)$

on unseen data for which we haven't seen the label



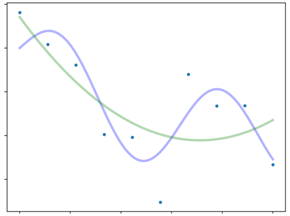
does the trained model generalizes to unseen data?
how accurate is the model in general?

Generalization and model complexity

simple models cannot fit the data

- large training error due to underfitting

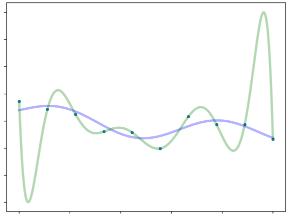
bias



expressive models can overfit the data

- small training error
- large test error due to overfitting

variance



regularization can help us trade-off between bias and variance

we want to see how these two terms contribute to the **generalization error**

Generalization and model complexity

example

columns: a different type of model $g(x)$

rows: different datasets

datasets are from the same distribution

$$x^{(n)}, y^{(n)} \sim p(x,y)$$

$F(x)$ the best possible model

higher variance

the complex model varies more with the dataset
it may not generalize well for this reason

higher bias

the simple model is biased to a particular type of data
it underfits, but it has a low variance

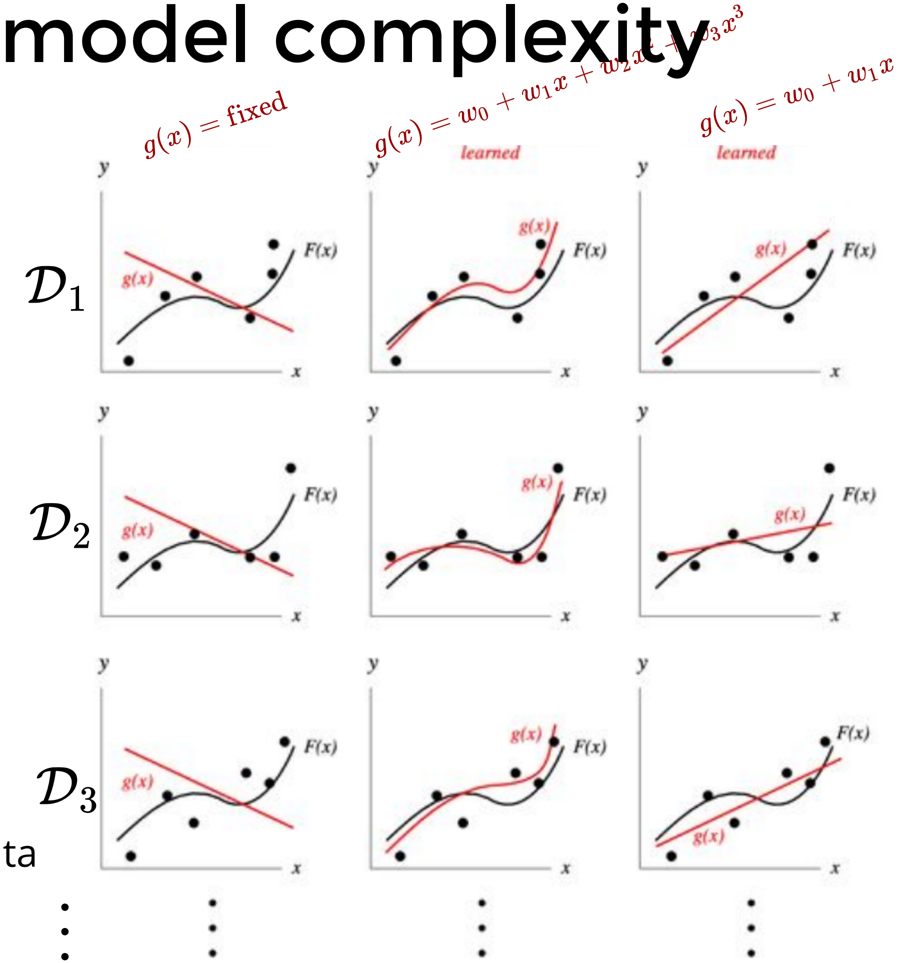


image:Duda, R. O., Hart, P. E., & Stork, D. G. (2012). *Pattern classification*.

Bias-variance decomposition: Setup

decompose the generalization error to see the effect of bias and variance (for L2 loss)

assume a true distribution $p(x, y)$

best prediction given L2 loss $f(x) = \mathbb{E}_p[y|x]$

assume that a dataset $\mathcal{D} = \{(x^{(n)}, y^{(n)})\}_n$ is sampled from $p(x, y)$

let $\hat{f}_{\mathcal{D}}$ be our model based on the dataset

what we care about is the generalization error (aka expected loss, expected risk)

$$\mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - y)^2]$$

all blue items are random variables

Bias-variance decomposition

what we care about is the generalization error

$$\mathbb{E}[(\underbrace{\hat{f}_{\mathcal{D}}(x)}_{\hat{f}_{\mathcal{D}}(x) + \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)]} - \underbrace{y}_{f(x) + \epsilon})^2] \quad = \mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)] - y + \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2]$$

add and subtract a term

above simplifies to the following (the remaining terms are going to be zero)

$$= \underbrace{\mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2]}_{\text{variance}} + \underbrace{\mathbb{E}[(f(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2]}_{\text{bias^2}} \quad + \underbrace{\mathbb{E}[\epsilon^2]}_{\text{unavoidable noise error}}$$

Bias-variance decomposition

the expected loss is decomposed to:

$$= \mathbb{E}[(\hat{f}_{\mathcal{D}}(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2] + \mathbb{E}[(f(x) - \mathbb{E}_{\mathcal{D}}[\hat{f}_{\mathcal{D}}(x)])^2] + \mathbb{E}[\epsilon^2]$$

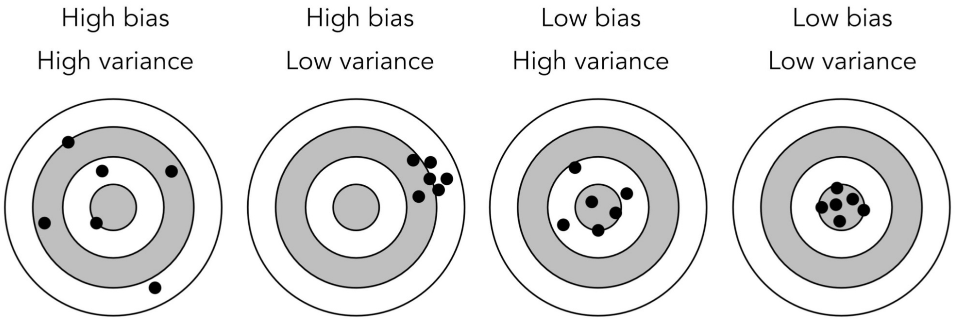
variance: how change of dataset affects the prediction

bias: how average over all datasets differs from the regression function

noise error: the error even if we used the true model $f(x)$

different models vary in their trade off between error due to bias and variance

- simple models: often more biased
- complex models: often have more variance



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Bias vs. variance

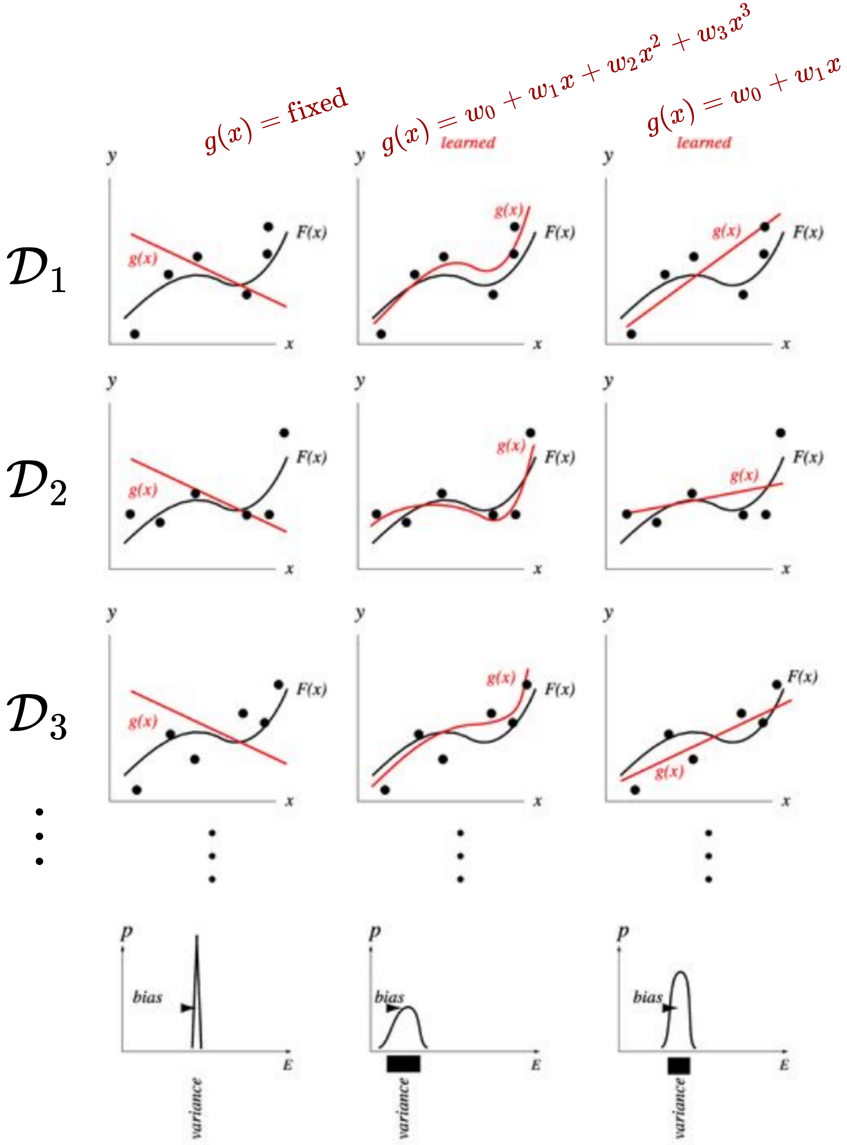
example

distribution of error (cost) due to randomness of dataset

we care about the expected error

bias causes a high error for all choices of dataset

higher variance also increases the expected error



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Example: bias vs. variance

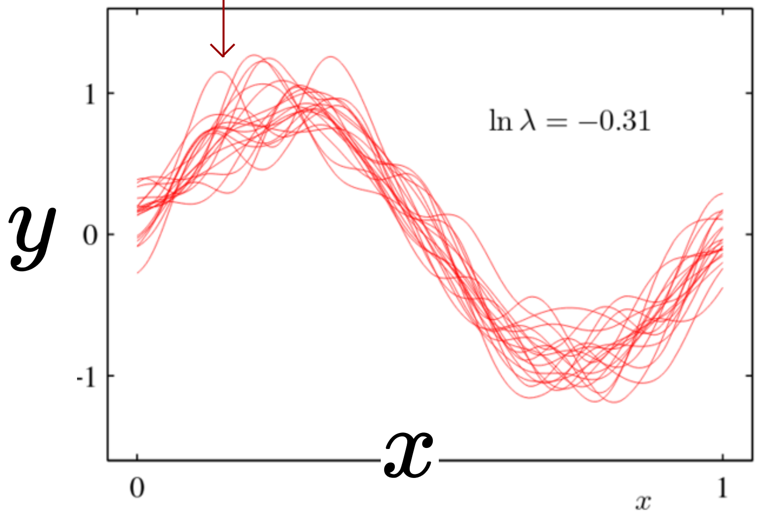
models for different datasets $\hat{f}_{\mathcal{D}}$

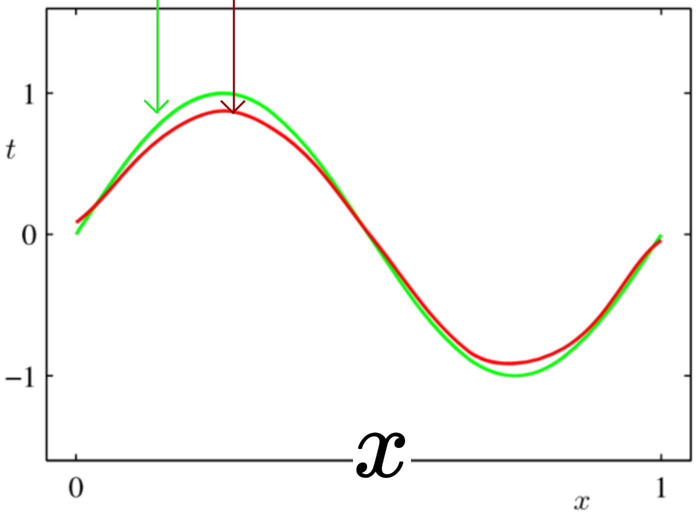
using Gaussian bases

true model f

their average $\mathbb{E}[\hat{f}_{\mathcal{D}}]$

random datasets of size N=25 instances are not shown

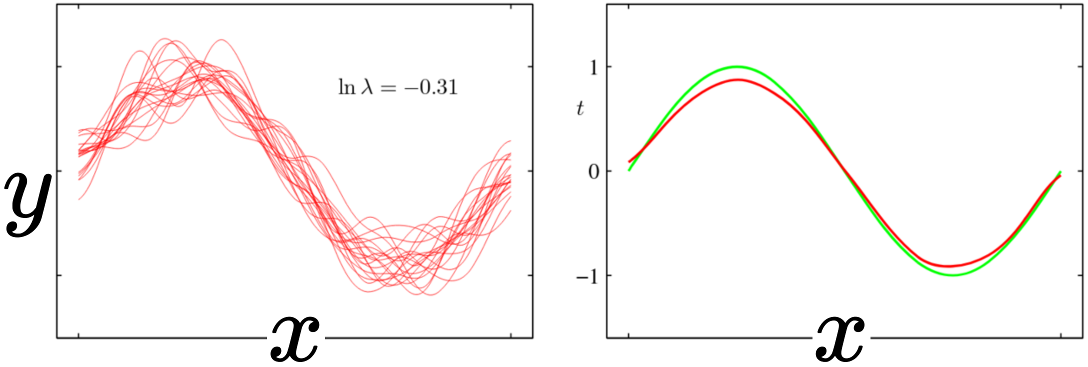




variance is the average difference (in squared L2 norm) between these curves and their average

bias is the difference (in L2 norm) between two curves

Example: bias vs. variance

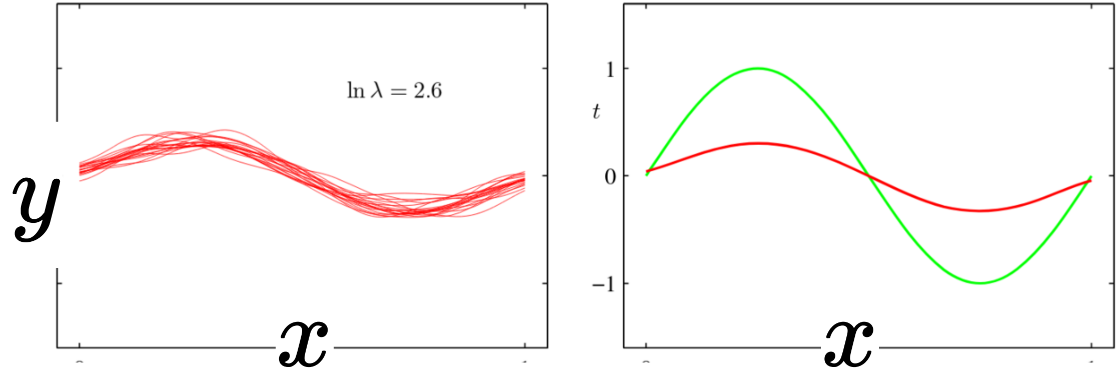


side note

the average fit is very good, despite high variance

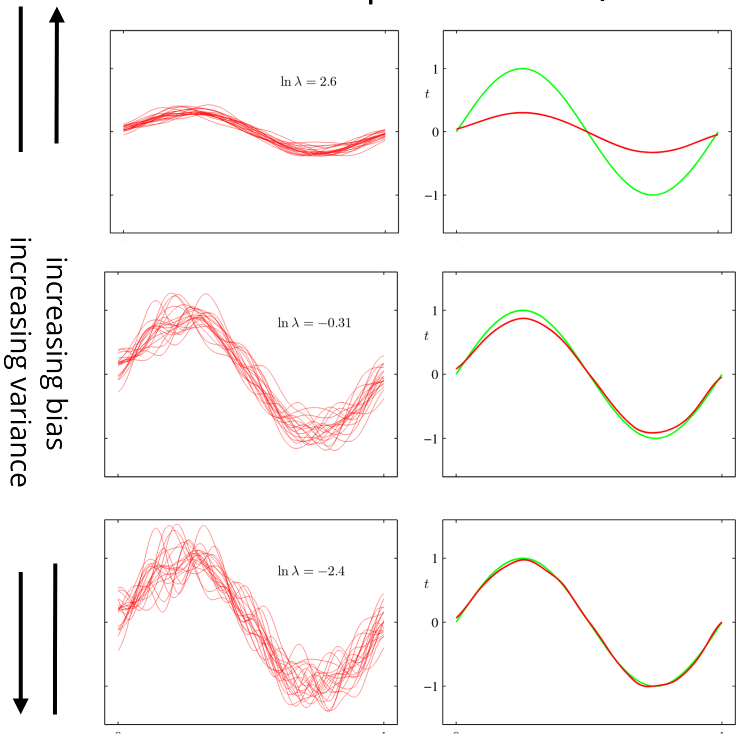
model averaging: uses "average" prediction of expressive models to prevent overfitting

using larger regularization penalty: higher bias - lower variance



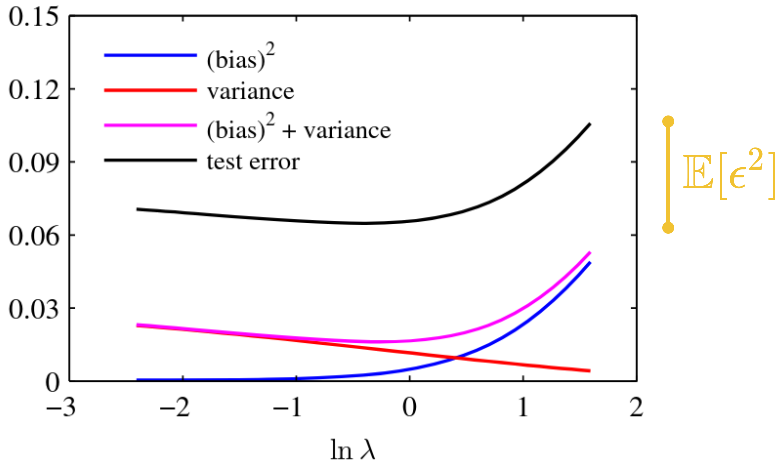
Example: bias vs. variance

the lowest expected loss (test error) is somewhere between the two extremes



increasing bias

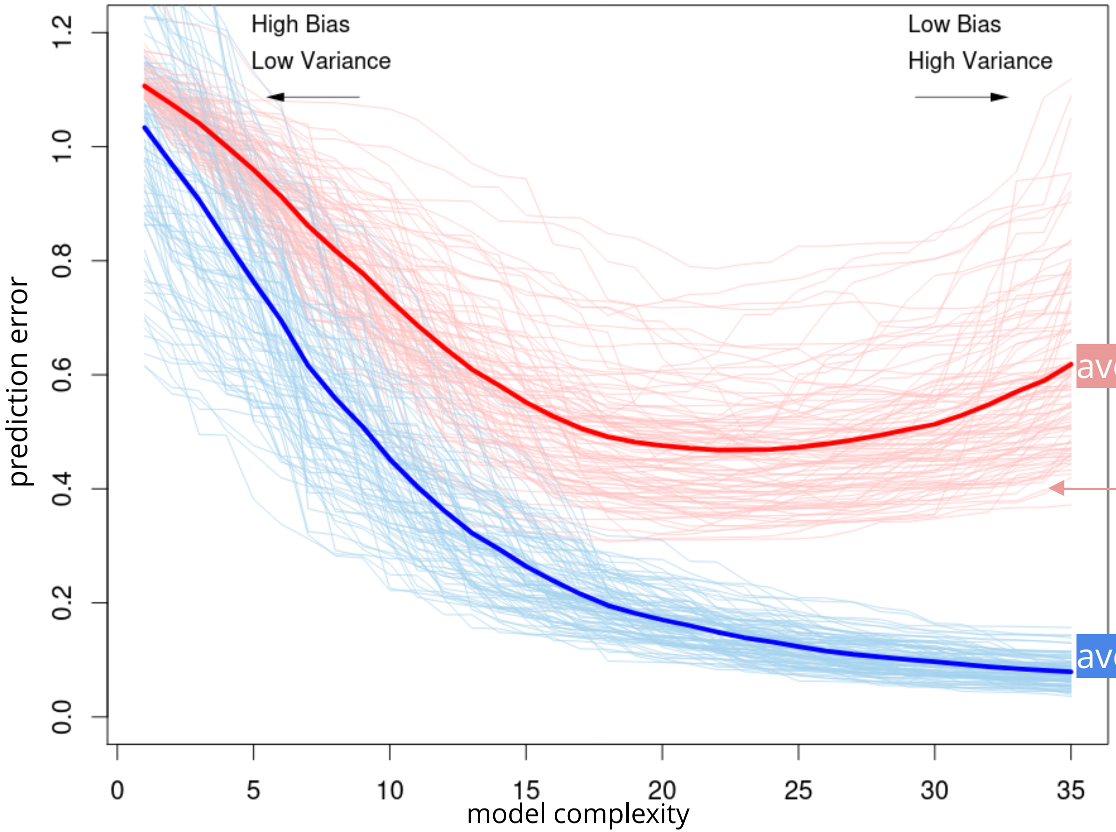
increasing variance



in practice, how to decide which model to use?

Effect on training and test error

high bias in simplistic models means that training error can be high



average test error

error for random dataset $\mathcal{D}$

average training error

high variance in more complex models means that test and training error can be very different

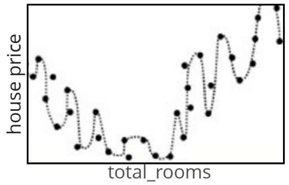
Model selection

many ML algorithms have hyper-parameters

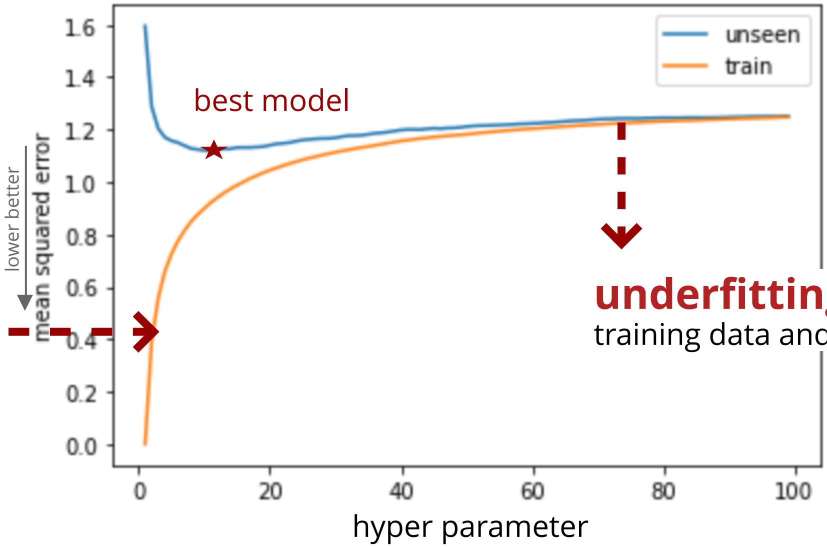
(e.g., the number of nonlinear basis to use)

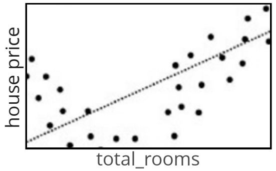
how should we select the best hyper-parameter?

example performance of a regression model on *California Housing Dataset*



overfitting to the training data
bad performance on unseen data





underfitting the model can more closely fit the training data and still get good test error

Model selection

what if unseen data is completely different from training data?

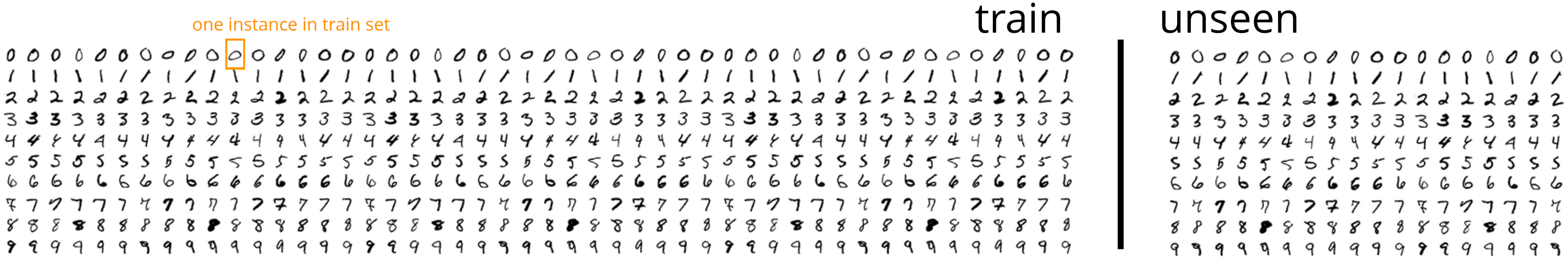
no point in learning!

assumption: training data points are samples from an unknown distribution

*independent identically distributed (**IID**)*

$$x^{(n)}, y^{(n)} \sim p(x, y)$$

unseen data comes from the same distribution.



Loss, cost and generalization

assume we have a **model** $f : x \mapsto y$ for example $f :$ $\mapsto 3$

and we have a **loss function** that measures the error in our prediction $\ell : y, \hat{y} \to \mathbb{R}$

for example

$$\left| \begin{array}{ll} \ell(y, \hat{y}) = (y - \hat{y})^2 & \text{for regression} \\ \ell(y, \hat{y}) = \mathbb{I}(y \neq \hat{y}) & \text{for classification} \end{array} \right.$$

we train our models to minimize **the cost function**:

$$J = \frac{1}{|\mathcal{D}_{\text{train}}|} \sum_{x,y \in \mathcal{D}_{\text{train}}} \ell(y, f(x))$$

We can drop this, why?

how to estimate this?

what we really care about is the **generalization error:** $\mathbb{E}_{x,y \sim p}\, \ell(y, f(x))$

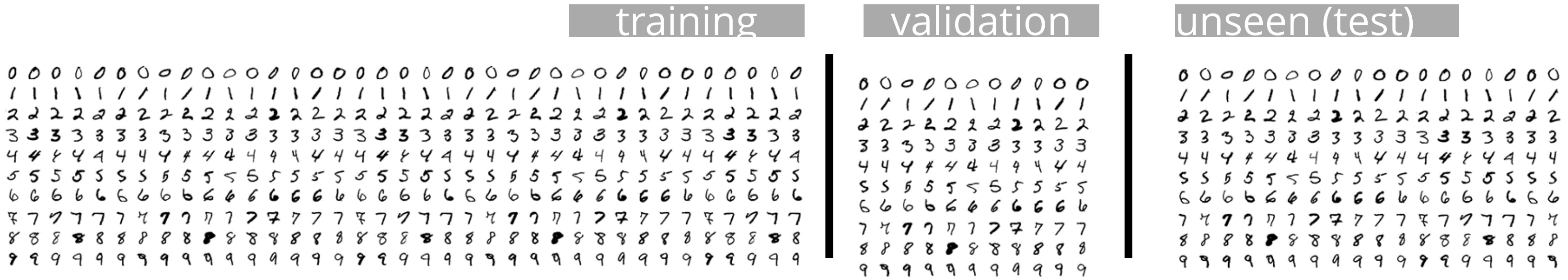
we can not measure this, why?

we can set aside part of the given data and use it to estimate generalization error how to estimate this?

Validation set

what we really care about is the **generalization error:** $\mathbb{E}_{x,y\sim p}\,\ell(y, f(x))$

we can set aside part of the training data and use it to **estimate** the generalization error

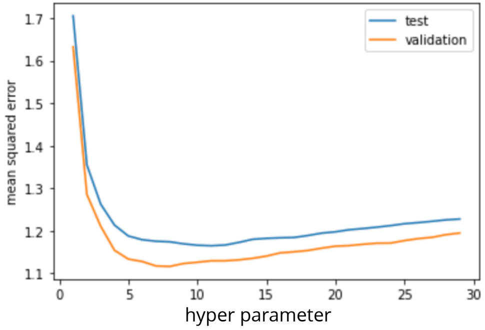


pick a hyper-parameter that gives us the best **validation error**

at the very end, we report the error on **test set**

validation and test error could be different

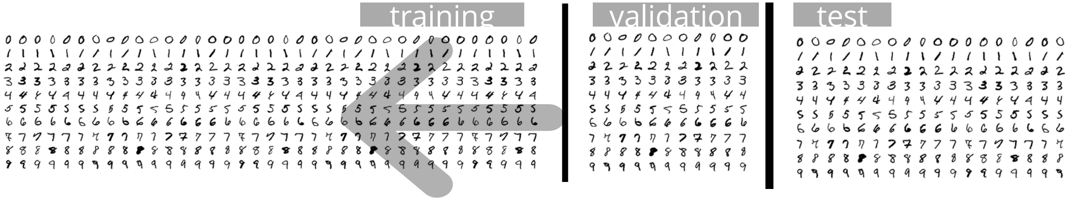
because they use limited amount of data



Cross validation

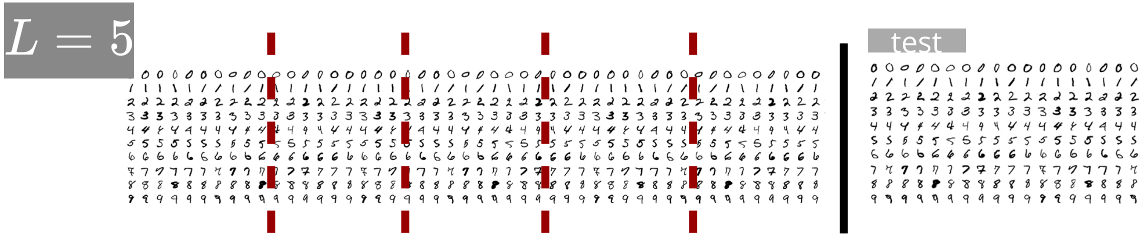
how to get a better estimate of generalization error?

increase the size of the validation set? *this reduces the training set*



Cross-validation helps us in getting better estimates + uncertainty measure

- divide the (training + validation) data into L parts
- use one part for validation and L-1 for training



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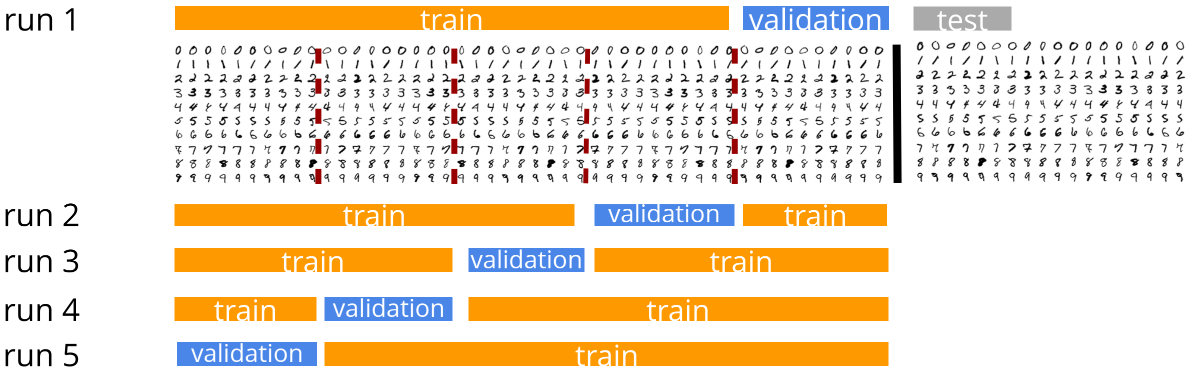

- use the **average** validation error and its variance (uncertainty) to pick the best model
- report the test error for the final model

this is called **L-fold** cross-validation

in **leave-one-out** cross-validation L=N (only one instance is used for validation)

Cross validation

- divide the (training + validation) data into L parts
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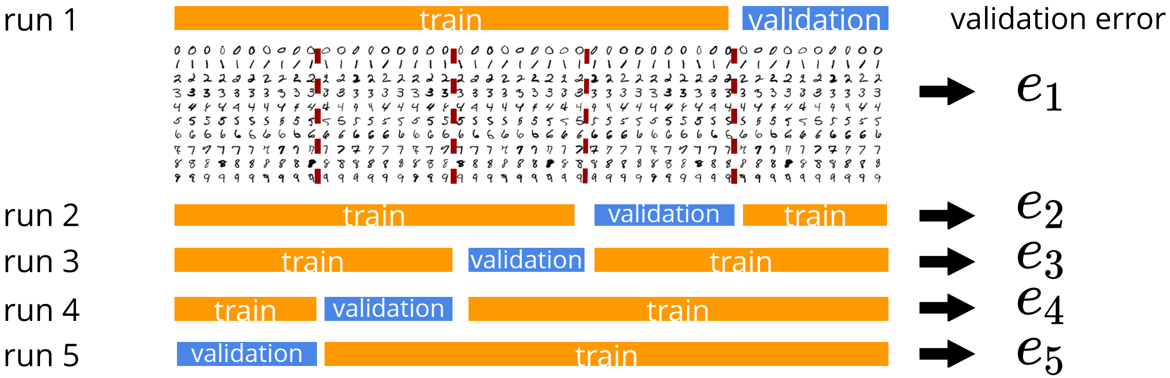
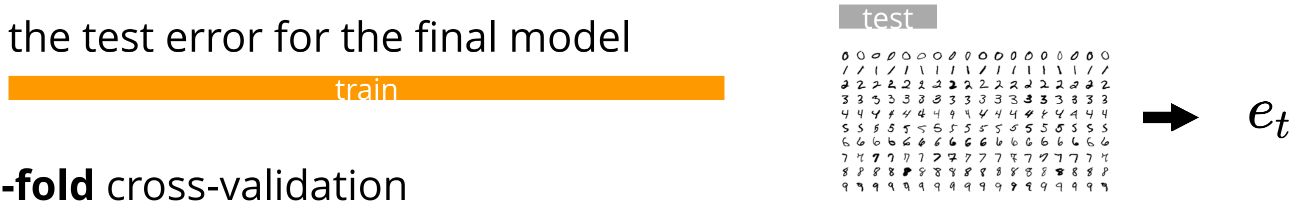


- use the **average** validation error and its variance (uncertainty) to pick the best model

$$\bar{e} = \frac{1}{5} \sum_{i=1}^{5} e_i$$

- report the test error for the final model

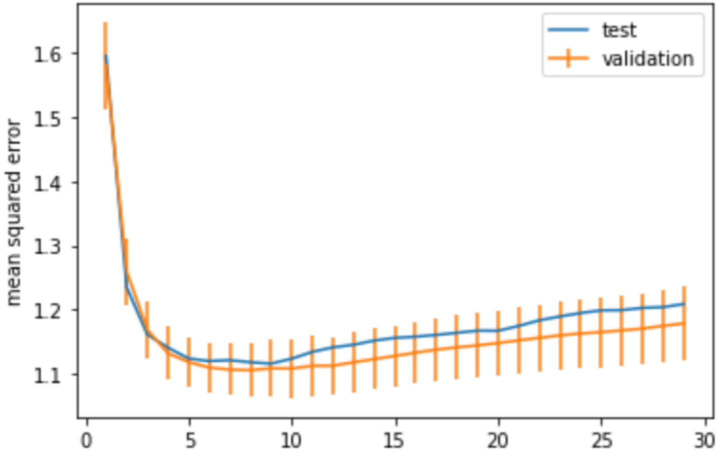


this is called **L-fold** cross-validation

in **leave-one-out** cross-validation L=N (only one instance is used for validation)

Cross validation

example the plot of the mean and standard deviation in 10 fold cross-validation



hyper parameter

test error is plotted only to show its agreement with the validation error; in practice we don't look at the test set for hyper-parameter tunning

a rule of thumb: pick the simplest model within one std of the model with lowest validation error

Performance metrics for classification

Not all errors are the same

In particular in classification, we have different types of mistakes

false positive (type I) and false negative (type II)

example:

patient does not have disease but received positive diagnostic (Type I error)
patient has disease but it was not detected (Type II error)

a message that is not spam is assigned to the spam folder (Type I error)

a message that is spam appears in the regular folder (Type II error)

Performance metrics for classification

binary classification results:

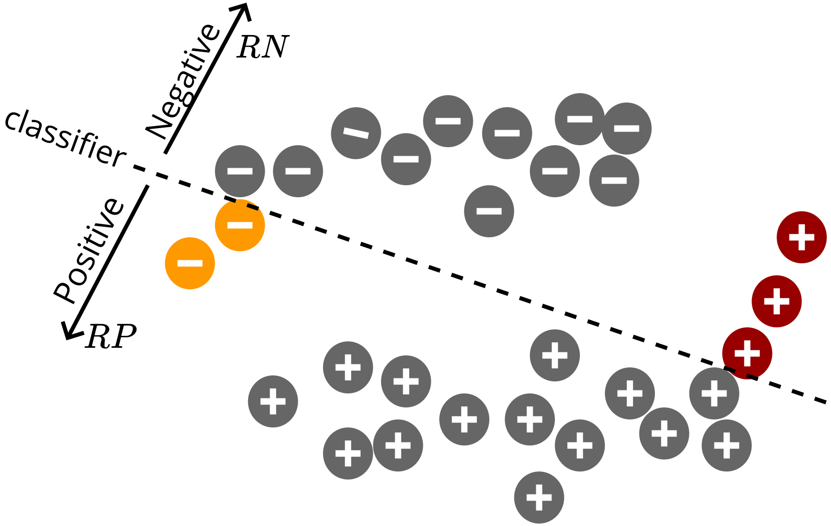
FP false positive (type I)
FN false negative (type II)
TP true positive
TN true negative

confusion matrix	Truth		Σ
Result	TP	FP	RP
	FN	TN	RN
Σ	P	N	

marginals

$$RP = TP + FP$$
$$RN = TN + FN$$
$$P = TP + FN$$
$$N = TN + FP$$

$$TN + TP + FN + FP = ?$$



example:	Truth		Σ
Result	14	2	16
	3	11	14
Σ	17	13	

Performance metrics for classification

confusion matrix

	Truth		Σ
Result	TP	FP	RP
	FN	TN	RN
Σ	P	N	

example:

	Truth		Σ
Result	14	2	16
	3	11	14
Σ	17	13	

$$Precision = \frac{TP}{RP} = \frac{14}{16}$$

$$Recall = \frac{TP}{P} = \frac{14}{17}$$

$$\frac{1}{F_\beta score} = \frac{1}{1+\beta^2}\frac{1}{Precision} + \frac{\beta^2}{1+\beta^2}\frac{1}{Recall}$$

$$Accuracy = \frac{TP+TN}{P+N}$$

$$Precision = \frac{TP}{RP}$$

$$Recall = \frac{TP}{P}$$ sensitivity

$$F_1 score = 2\frac{Precision \times Recall}{Precision + Recall}$$ {Harmonic mean}

$$F_\beta score = (1+\beta^2)\frac{Precision \times Recall}{\beta^2 Precision + Recall}$$

recall is β times more important compared to precision

less common

$$Miss\ rate = \frac{FN}{P}$$

$$Fallout = \frac{FP}{N}$$ false positive rate

$$False\ discovery\ rate = \frac{FP}{RP}$$

$$Selectivity = \frac{TN}{N}$$ specificity

$$False\ omission\ rate = \frac{FN}{RN}$$

$$Negative\ predictive\ value = \frac{TN}{RN}$$

Trade-off between precision and recall

How many false positives do we tolerate?

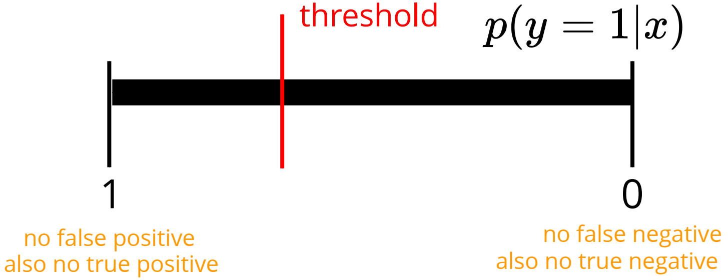
How important are false negatives?

e.g. spam in inbox v.s. negative test for cancer test

We can often control the trade-off between type I & type II error

e.g. by changing the threshold of $p(y=1|x)$ if we produce class score (probability)

Most ML algorithm produces class score or probability



threshold

$p(y=1|x)$

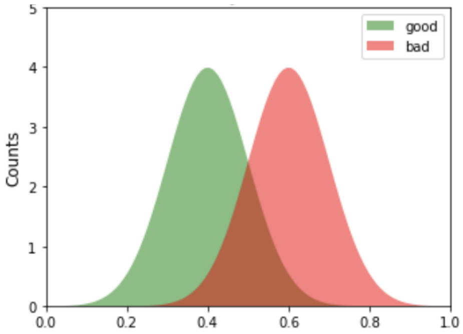
1

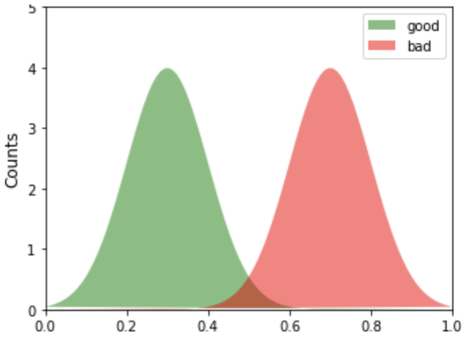
0

no false positive
also no true positive

no false negative
also no true negative

goal: evaluate class scores/probabilities (independent of choice of threshold)





Trade-off between precision and recall

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goal: evaluate class scores/probabilities (independent of choice of threshold)

Receiver Operating Characteristic **ROC curve,** a function of threshold t

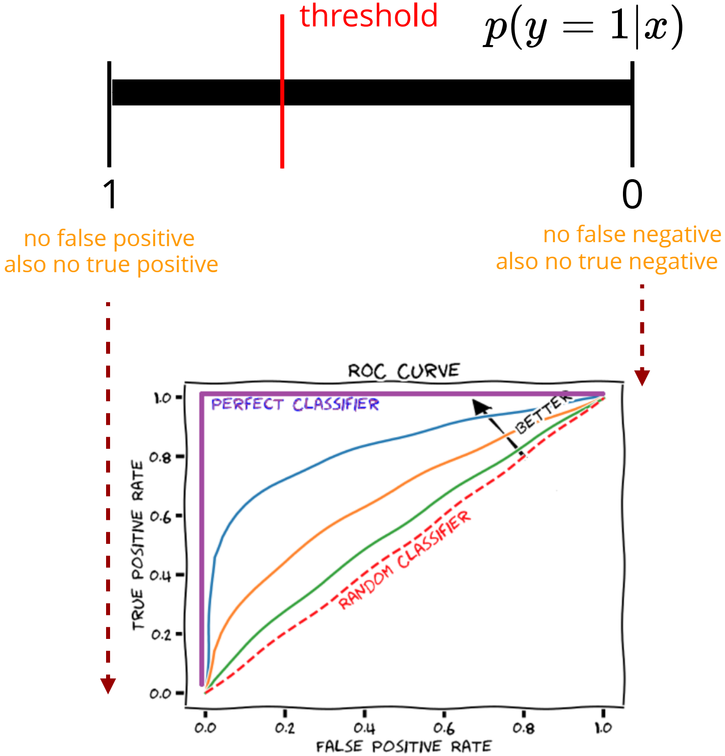
TPR(t) = TP(t)/P (**recall**, sensitivity at t, hit rate)

FPR(t) = FP(t)/N (**fallout**, false alarm at t, type I error rate)

Area Under the Curve (**AUC**) is used as a threshold independent measure of quality of the classifier

$AUC = \sum_t TPR(t)(FPR(t) - FPR(t-1))$, box-rule approximation

Most ML algorithm produces class score or probability



threshold

$p(y=1|x)$

1

0

no false positive
also no true positive

no false negative
also no true negative

what is the maximum value for AUC? what is AUC of a random classifier?

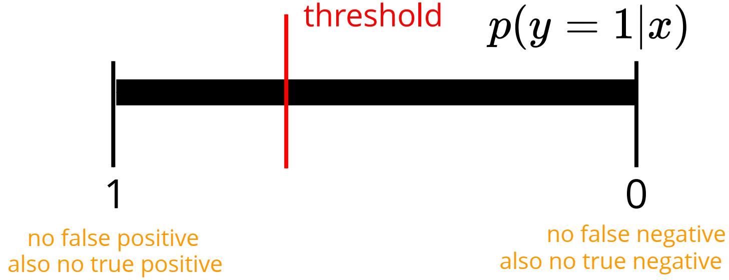
Precision-recall curves

Similar to ROC curve but more helpful in some situation

- when size of negative set is also a model parameter, e.g. in information retrieval
- when there is class imbalance, e.g. in fraud detection when $N \gg P$), since *ROC curves are insensitive to class imbalance*

Instead we curve Precision vs Recall for different thresholds

Most ML algorithm produces class score or probability



threshold

$p(y = 1|x)$

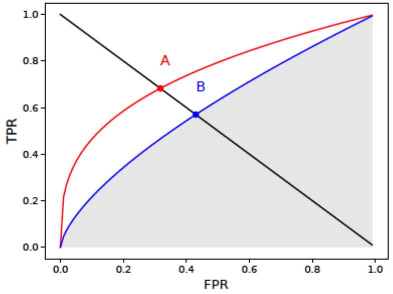
1

no false positive
also no true positive

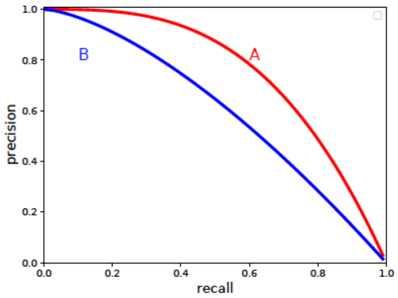
0

no false negative
also no true negative

ROC



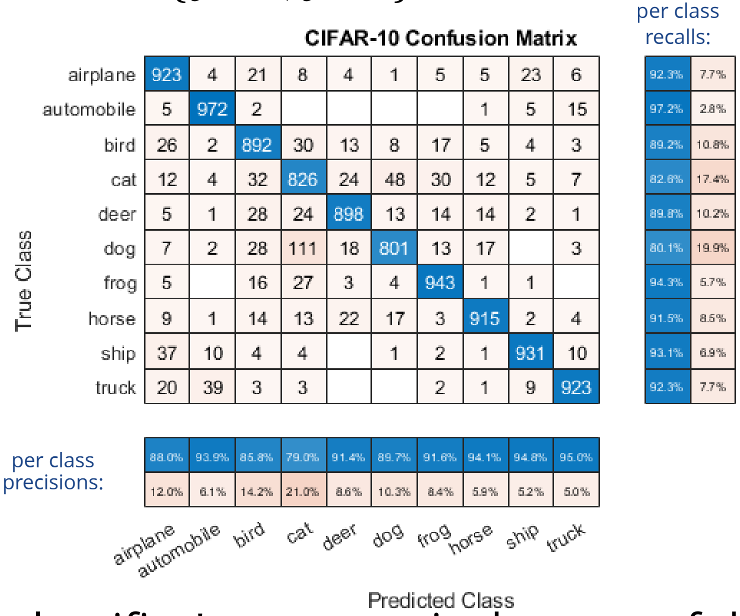
Precision-Recall



Confusion Matrix for multiclass classification

A CxC table that shows how many samples of each class are classified as belonging to another class

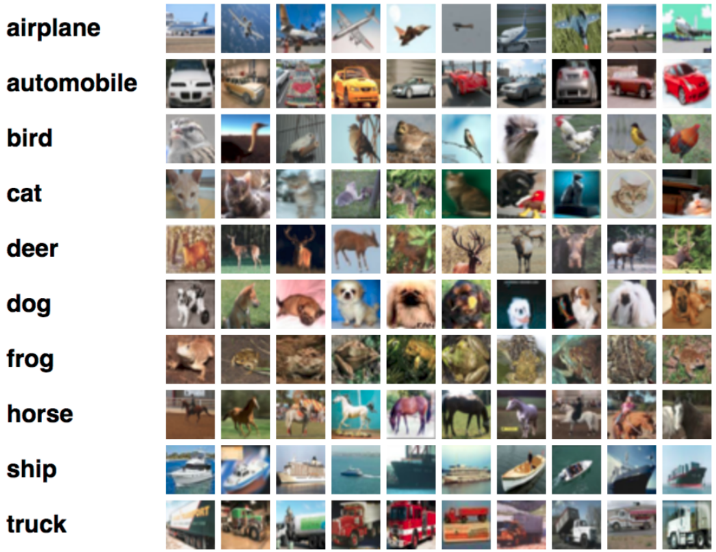
$$M_{rc} = N\{\hat{y} = r, y = c\}$$



CIFAR-10 Confusion Matrix

	airplane	automobile	bird	cat	deer	dog	frog	horse	ship	truck	per class recalls:	
airplane	923	4	21	8	4	1	5	5	23	6	92.3%	7.7%
automobile	5	972	2					1	5	15	97.2%	2.8%
bird	26	2	892	30	13	8	17	5	4	3	89.2%	10.8%
cat	12	4	32	826	24	48	30	12	5	7	82.6%	17.4%
deer	5	1	28	24	898	13	14	14	2	1	89.8%	10.2%
dog	7	2	28	111	18	801	13	17		3	80.1%	19.9%
frog	5		16	27	3	4	943	1	1		94.3%	5.7%
horse	9	1	14	13	22	17	3	915	2	4	91.5%	8.5%
ship	37	10	4	4		1	2	1	931	10	93.1%	6.9%
truck	20	39	3	3			2	1	9	923	92.3%	7.7%
per class precisions:	88.0%	93.9%	85.8%	79.0%	91.4%	89.7%	91.6%	94.1%	94.8%	95.0%		
	12.0%	6.1%	14.2%	21.0%	8.6%	10.3%	8.4%	5.9%	5.2%	5.0%		

sample images from Cifar-10 dataset



classifier's accuracy is the sum of diagonal divided by the sum-total of the matrix,

you can also report the average of the F_1 scores per class (macro), or weight the average by class sizes

when evaluating a classifier it is useful to look at the confusion matrix

Bias and Fairness Challenge

The model learns from the distribution of the input data
{train, validation, test are still sampled based on some process}

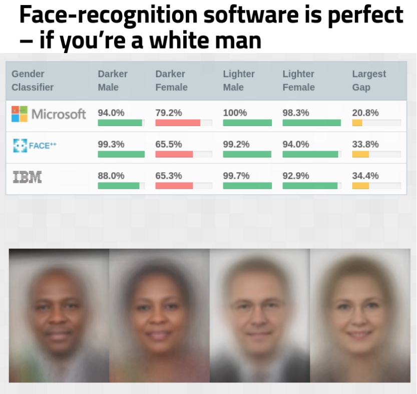
the demographic and phenotypic composition of training and benchmark datasets are important

Growing use, growing concerns

- Amazon's hiring algorithm decides not to invite women to interview, read it here
- Google's online ad algorithm decides to show high-income jobs to men much more often than to women, read about it here
- A machine learning algorithm denies you credit based on race or gender, read it here
- Health care algorithm offers less care to black patients, read it here, and here
- Florida risk score algorithm used in courts assign higher risk to black defendants, read it here

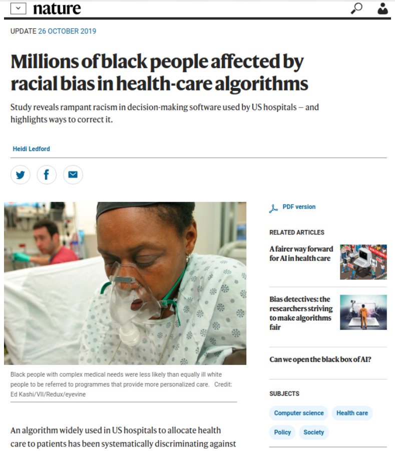
How can we factor these in the evaluation of models?

Many recent works, for example see this book on fairness & ML, here, read this article on bias detectives, or this course on data ethics



Face-recognition software is perfect – if you're a white man

Gender Classifier	Darker Male	Darker Female	Lighter Male	Lighter Female	Largest Gap
Microsoft	94.0%	79.2%	100%	98.3%	20.8%
FACE++	99.3%	65.5%	99.2%	94.0%	33.8%
IBM	88.0%	65.3%	99.7%	92.9%	34.4%



nature

UPDATE 26 OCTOBER 2019

Millions of black people affected by racial bias in health-care algorithms

Study reveals rampant racism in decision-making software used by US hospitals – and highlights ways to correct it.

Heidi Ledford

Black people with complex medical needs were less likely than equally ill white people to be referred to programmes that provide more personalized care. Credit: Ed Kashi/VII/Redux/eyevine

An algorithm widely used in US hospitals to allocate health care to patients has been systematically discriminating against

PDF version

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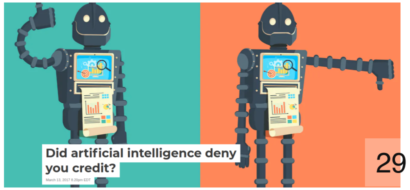
A fairer way forward for AI in health care

Bias detectives: the researchers striving to make algorithms fair

Can we open the black box of AI?

SUBJECTS

Computer science · Health care · Policy · Society



Did artificial intelligence deny you credit?

Inductive bias

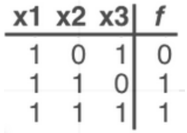
learning algorithms make implicit assumptions learning or inductive bias

e.g., we are often biased towards **simplest explanations** of our data

Occam's razor between two models (explanations) we should prefer the simpler one

example

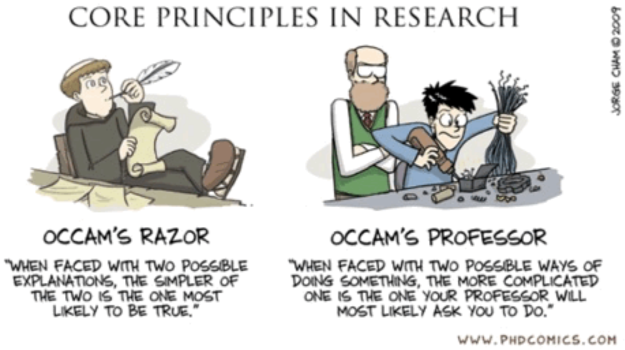
both of the following models perfectly fit the data



x1	x2	x3	f
1	0	1	0
1	1	0	1
1	1	1	1

$\hat{f}(x) = x_2$ this one is simpler

$\hat{f}(x) = x_1 \wedge x_2$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OCCAM'S PROFESSOR
"WHEN FACED WITH TWO POSSIBLE WAYS OF DOING SOMETHING, THE MORE COMPLICATED ONE IS THE ONE YOUR PROFESSOR WILL MOST LIKELY ASK YOU TO DO."
WWW.PHDCOMICS.COM

why does is make sense for learning algorithms to be biased?

- the world is not random
- there are regularities, and induction is possible (why do you think the sun will rise in the east tomorrow morning?

what are some of the inductive biases in using linear regression?

optional

Curse of dimensionality

learning in **high dimensions** can be difficult since the volume of space grows exponentially fast with the dimension

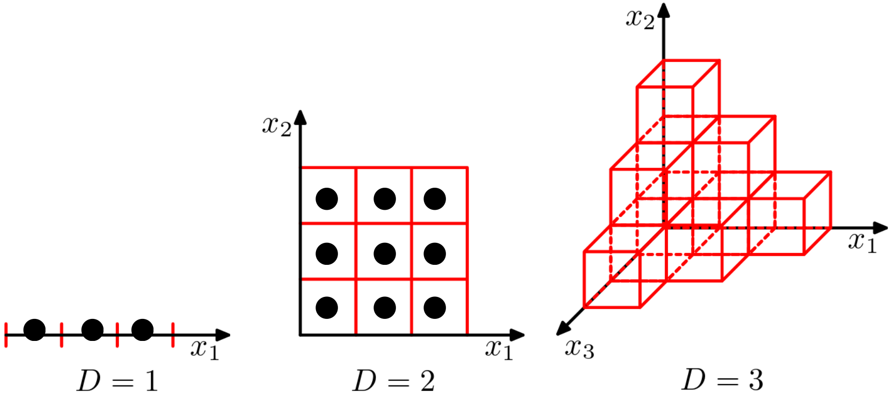
example:

suppose our data is uniformly distributed in some range, say $x \in [0,3]^D$

predict the label by counting labels in the same unit of the grid

to have at least one example per unit, we need 3^D training examples

for D=180 we need more training examples than the number of particles in the universe

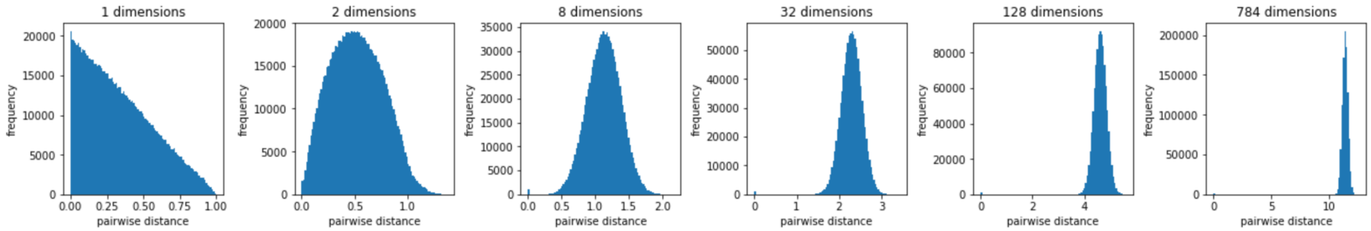


optional

Curse of dimensionality

in high dimensions most points have similar distances!

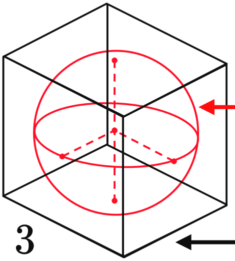
histogram of pairwise distance of 1000 points with random features of D dimensions



as we increase dimension, distances become "similar"!

Q. why are most distances similar?

A. in high dimensions most of the volume is close to the corners!



$$\frac{2r^D \pi^{D/2}}{D\Gamma(D/2)}$$

$$D = 3$$

$$(2r)^D$$

$$\lim_{D\to\infty} \frac{\text{volum}(\circ)}{\text{volum}(\square)} = 0$$

a "conceptual" visualization of the same idea

# corners and the mass in the corners grow quickly with D

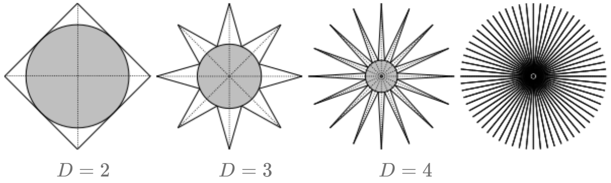


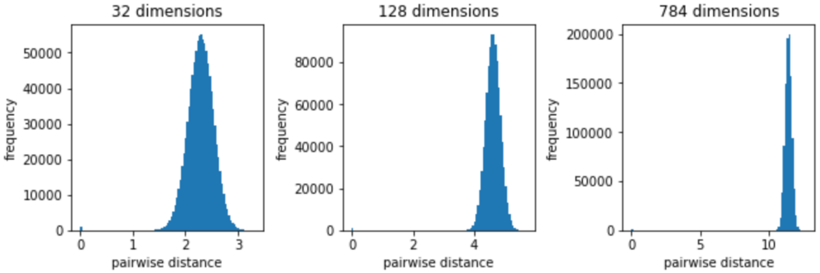
image: Zaki's book on Data Mining and Analysis

optional

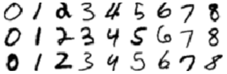
Real-word vs. randomly generated data

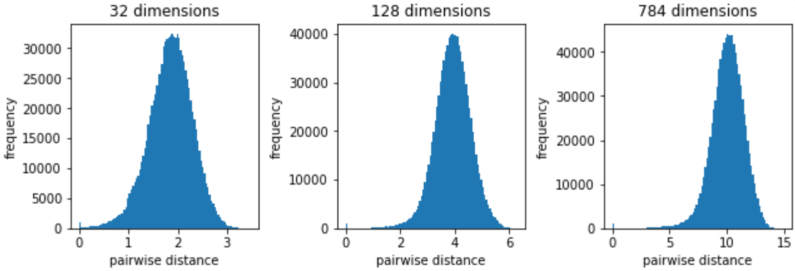
how come ML methods work for image data (D=number of pixels)?

pairwise distance for random data



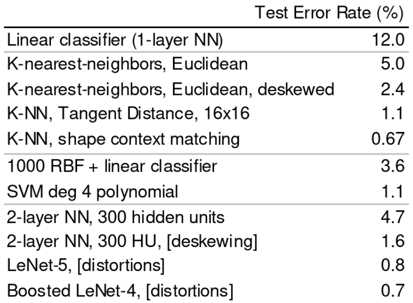
pairwise distance for D pixels of MNIST digits





the statistics do not match that of random high-dimensional data!

in fact KNN works well for image classification



	Test Error Rate (%)
Linear classifier (1-layer NN)	12.0
K-nearest-neighbors, Euclidean	5.0
K-nearest-neighbors, Euclidean, deskewed	2.4
K-NN, Tangent Distance, 16x16	1.1
K-NN, shape context matching	0.67
1000 RBF + linear classifier	3.6
SVM deg 4 polynomial	1.1
2-layer NN, 300 hidden units	4.7
2-layer NN, 300 HU, [deskewing]	1.6
LeNet-5, [distortions]	0.8
Boosted LeNet-4, [distortions]	0.7

see here for more results on MNIST

optional

Manifold hypothesis

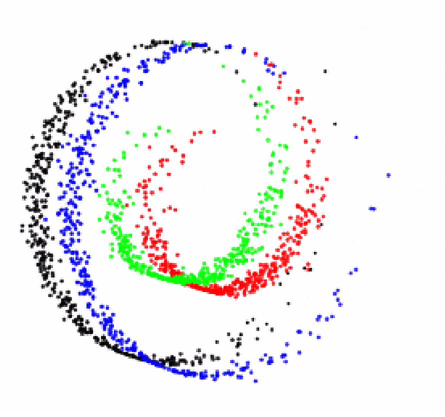
real-world data is often far from uniformly random

manifold hypothesis: real data lies close to the surface of a *manifold*

example

data dimension: $D = 3$

manifold dimension: $\hat{D} = 2$



example

data dimension: D = number of pixels (64x64)

manifold dimension: $\hat{D} = 2$

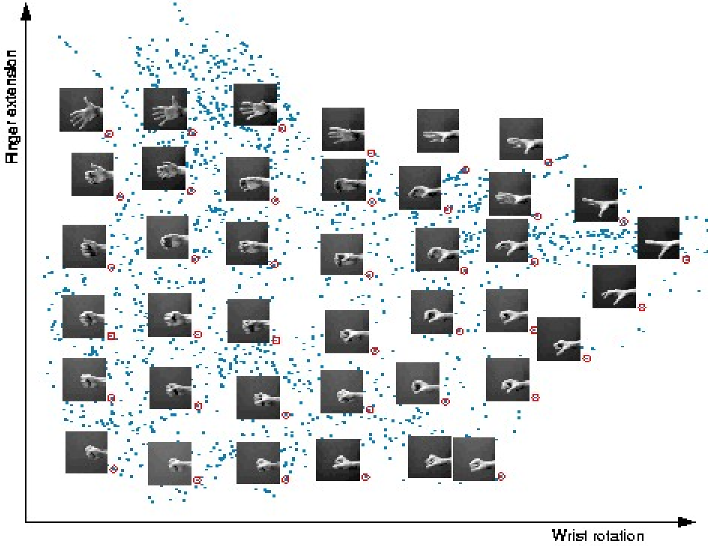
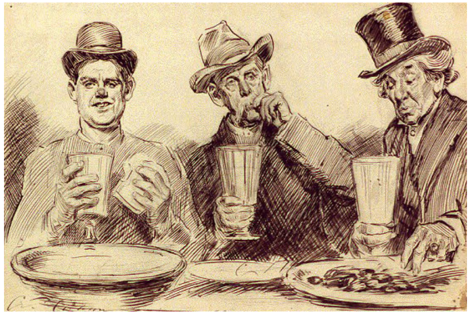


image from here

optional

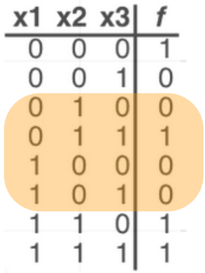
No free lunch



read more here

consider the binary classification task:

suppose this is our dataset ⟶



x1	x2	x3	*f*
0	0	0	1
0	0	1	0
0	1	0	0
0	1	1	1
1	0	0	0
1	0	1	0
1	1	0	1
1	1	1	1

there are $2^4 = 16$ binary functions that perfectly fit our dataset

our **learning algorithm** can produce one of these as our classifier $\hat{f} : \{0,1\}^3 \rightarrow \{0,1\}$

the same algorithm cannot perform well for all possible class of problems (f) no free lunch

each ML algorithm is biased to perform well on some class of problems

there is no single algorithm that performs well on all class of problems

Summary

- complex models can have very different training and test error (*generalization gap*)
- regularization bounds this gap by penalizing model complexity
- bias-variance trade off:
    - formalizes the relation between
        - training error (bias)
        - complexity (variance) and
        - and the test error (bias + variance)
    - not so elegant beyond L2 loss
- what we care about is the **generalization** of ML algorithms
    - **overfitting**: good performance on the training set doesn't mean the same for the test set
    - **underfitting**: we don't even have a good performance on the training set
- estimated using a **validation set** or better, we could use **cross-validation**