Applied Machine Learning

Some core concepts

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Learning objectives

understanding the following concepts

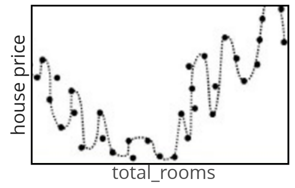
- overfitting & generalization
- validation and cross-validation
- curse of dimensionality
- no free lunch
- inductive bias of a learning algorithm

Model selection

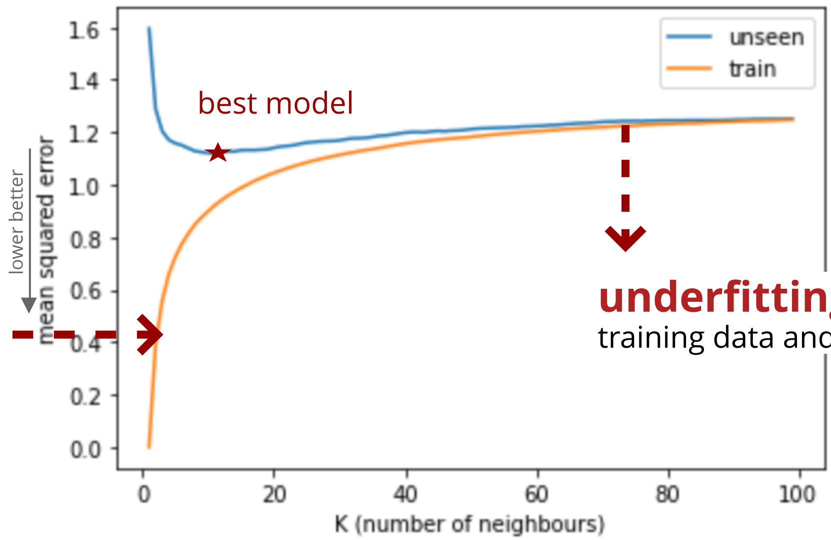
many ML algorithms have hyper-parameters
(e.g., K in K-nearest neighbors, max-depth of decision tree, etc)

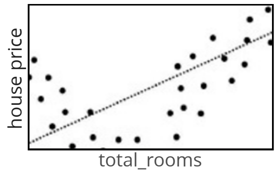
how should we select the best hyper-parameter?

example performance of KNN regression 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?

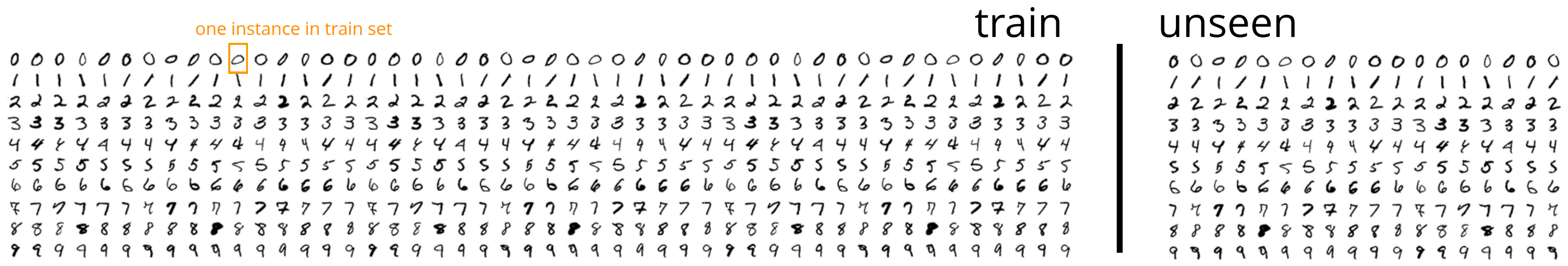
no point in learning!

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

$$\ell(y, \hat{y}) = (y - \hat{y})^2 \quad \text{for regression}$$

$$\ell(y, \hat{y}) = \mathbb{I}(y \neq \hat{y}) \quad \text{for classification}$$

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:** $\mathbb{E}_{x,y \sim p}\, \ell(y, f(x))$

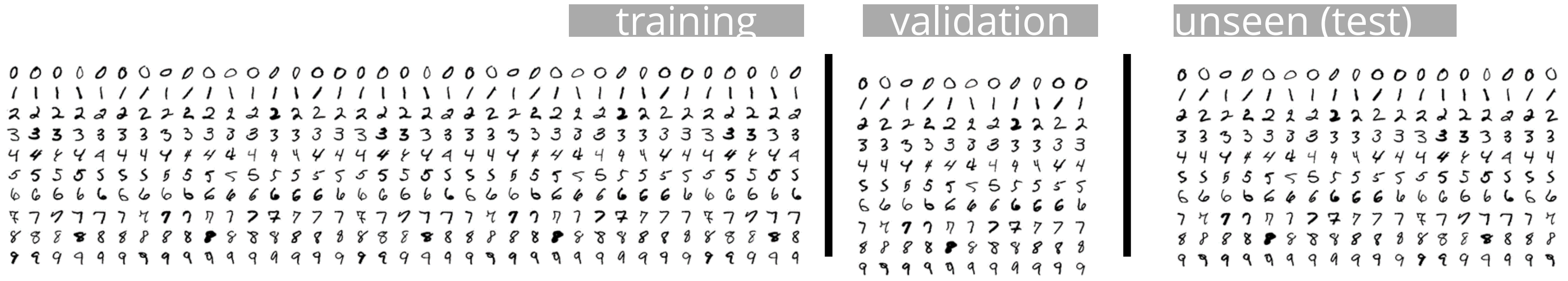
we can not measure this, why?

we can set aside part of the training 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

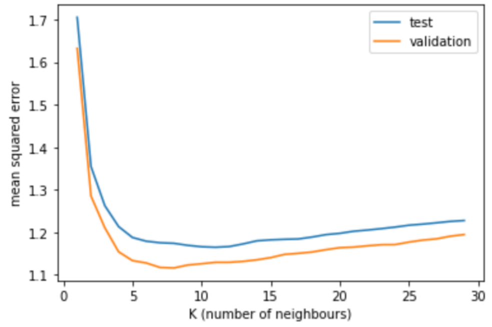


pick a hyper-parameter that gives us the best **validation error**

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

validation and test error could be different

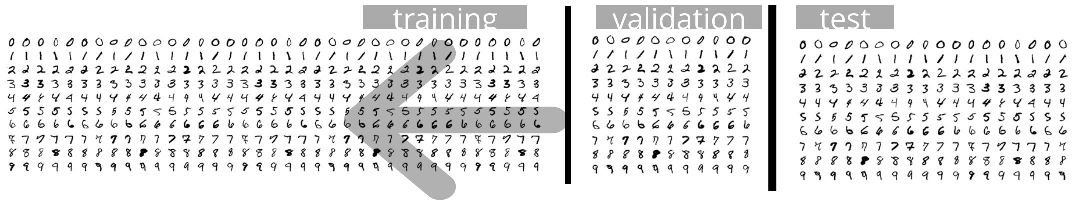
because they use limited amount of data



Cross validation

how to get a better estimate of generalization error?

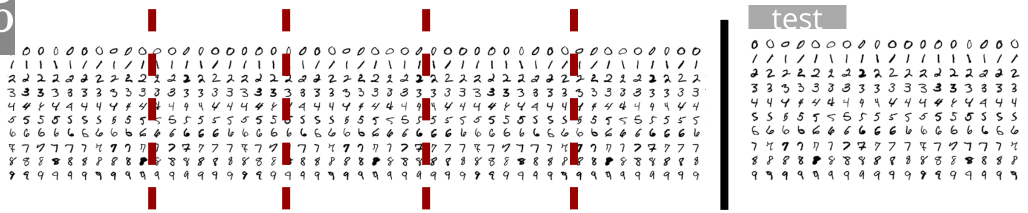
increase the size of the validation set? *this reduces the training set*



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

$L = 5$



Cross validation

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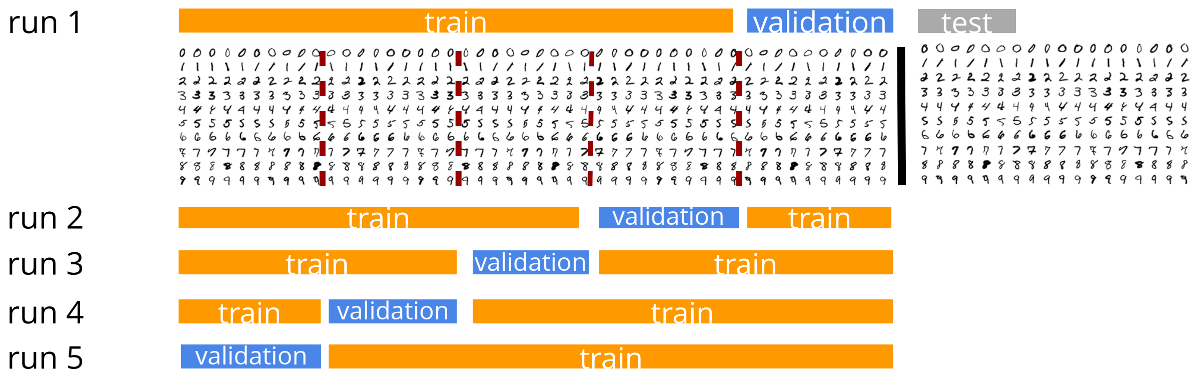


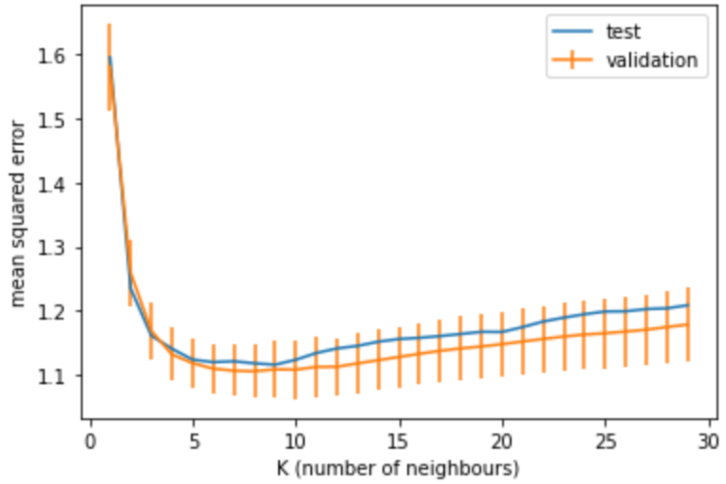
- use the **average** validation error and its variance (uncertainty) to pick the best model
- report the test error for the final model

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

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

Cross validation

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



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

Generalization 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

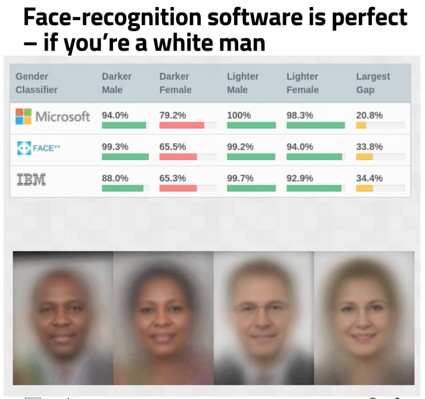
Bias and Fairness Challenge

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

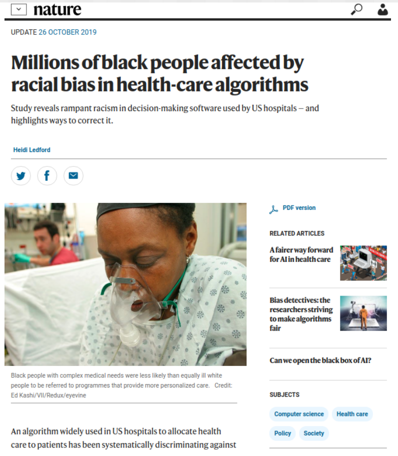
How can we factor these in the evaluation of models?

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



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

PDF version

RELATED ARTICLES

A fairer way forward for AI in health care

Bias detectives: the researchers striving to make algorithms fair

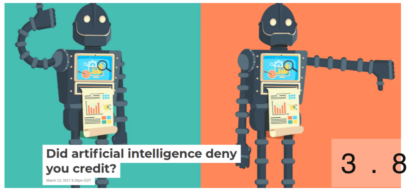
Can we open the black box of AI?

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

SUBJECTS

Computer science · Health care · Policy · Society

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



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)

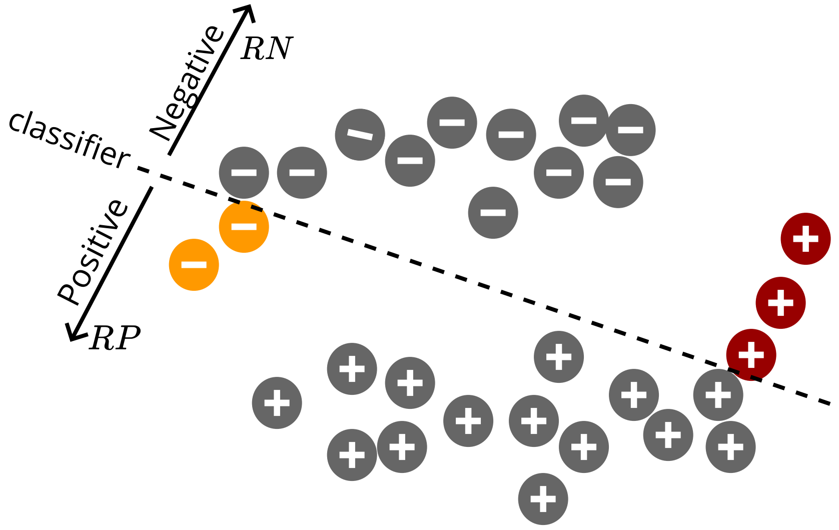
Performance metrics for classification

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	

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

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

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

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

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

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

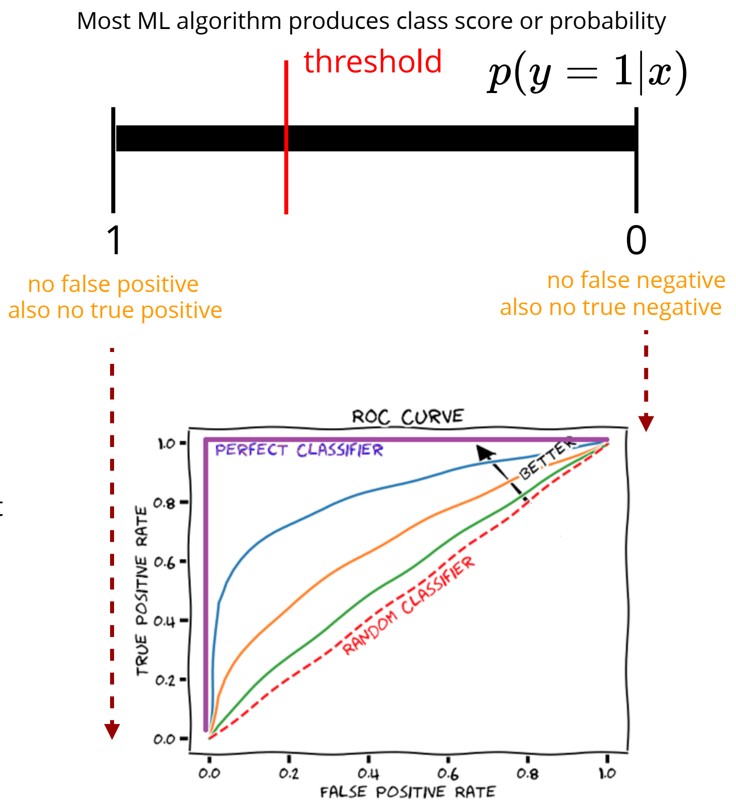
Receiver Operating Characteristic **ROC curve,** a function of threshold t

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

FPR(t) = FP(t)/N (**fallout**, false alarm at t)

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

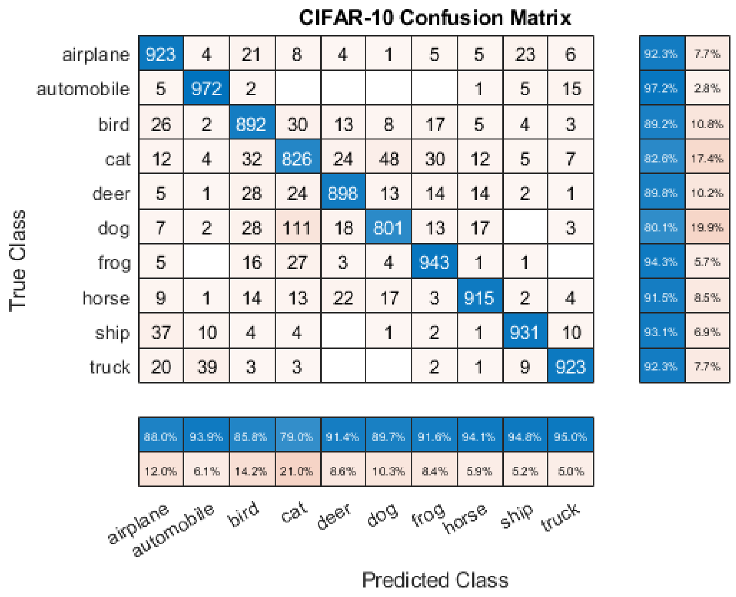
$AUC = \sum_t TPR(t)(FPR(t) - FPR(t-1))$, box-rule approximation



Confusion Matrix for multiclass classification

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

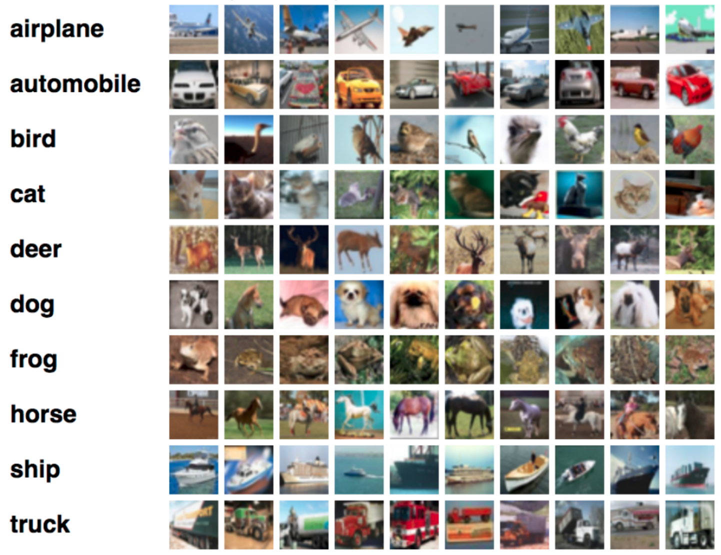
$$M_{rc} = N\{\hat{y} = r, y = c\}$$



CIFAR-10 Confusion Matrix

True Class \ Predicted Class	airplane	automobile	bird	cat	deer	dog	frog	horse	ship	truck		
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%
	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
when evaluating a classifier it is useful to look at the confusion matrix

Curse of dimensionality

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

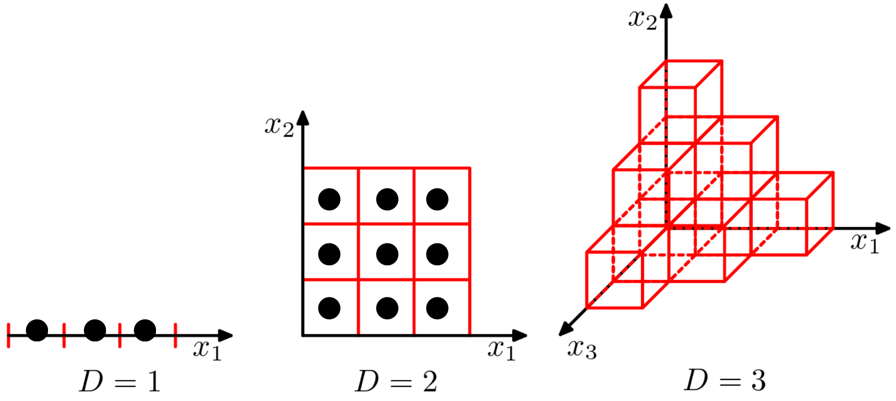
example:

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 (similar to KNN)

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

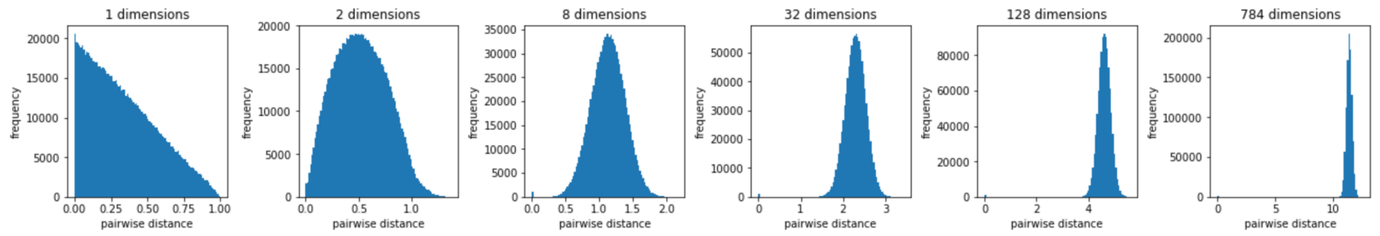
for D=180 we need more training examples than the number of particles in the universe



Curse of dimensionality

in high dimensions most points have similar distances!

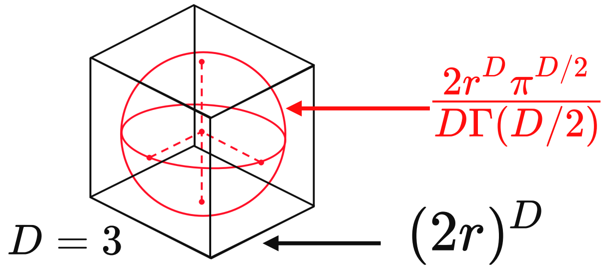
histogram of pairwise distance of 1000 points with random features of D dimensions



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!



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

a "conceptual" visualization of the same idea

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

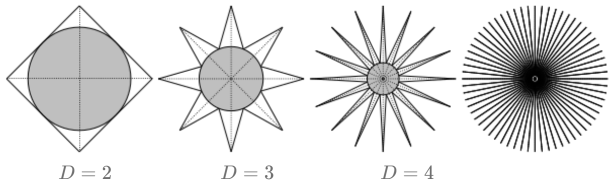
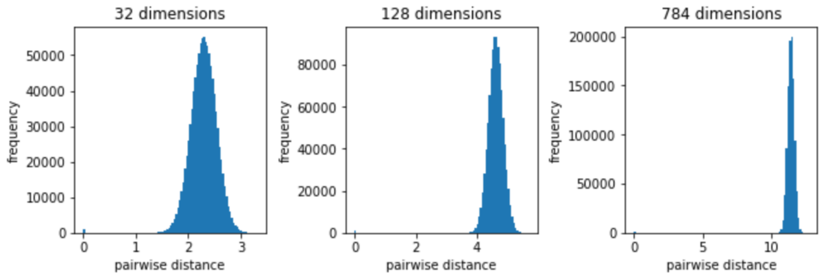


image: Zaki's book on Data Mining and Analysis

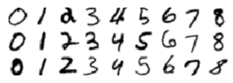
Real-word vs. randomly generated data

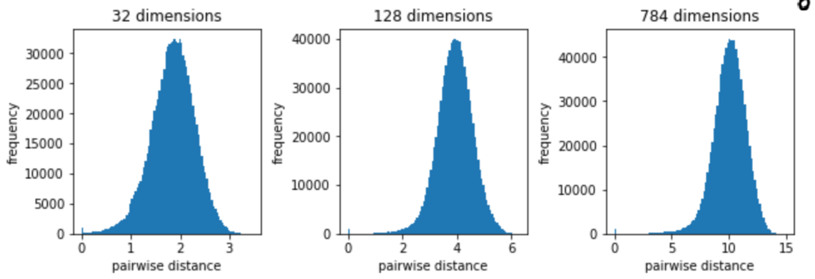
how come ML methods work for image data (D=number of pixels)?

pairwise distance for random data



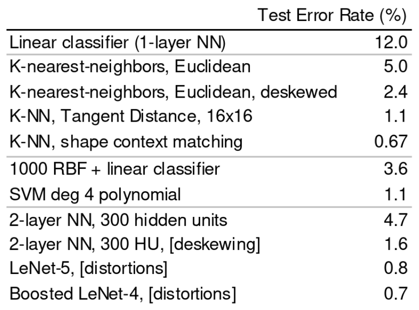
pairwise distance for D pixels of MNIST digits





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

Manifold hypothesis

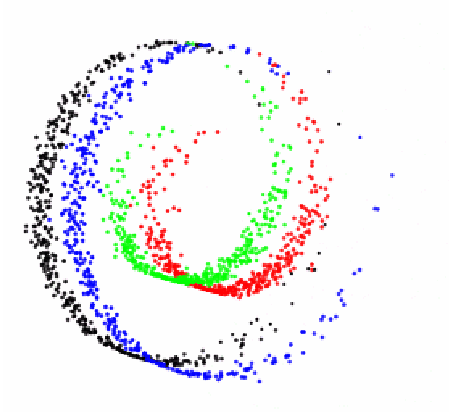
real-world data is often far from uniformly random

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: $\hat{D} = 2$

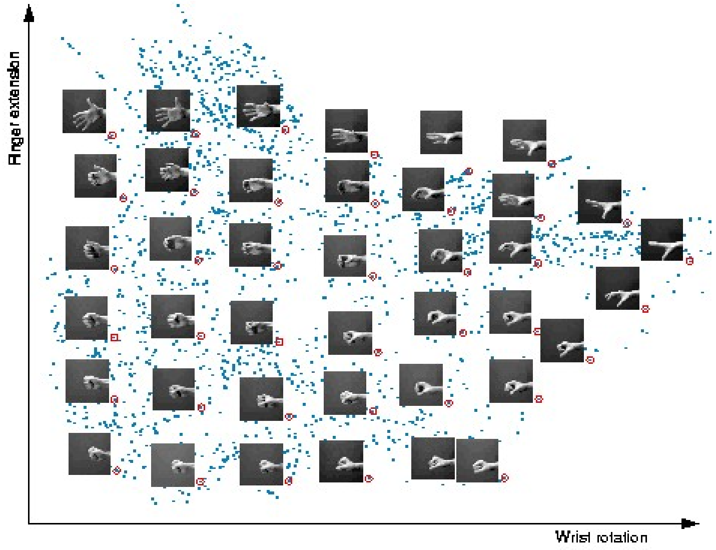
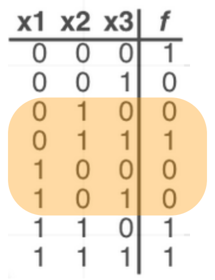


image from here

No free lunch

consider the binary classification task:

suppose this is our dataset $\longrightarrow$



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

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

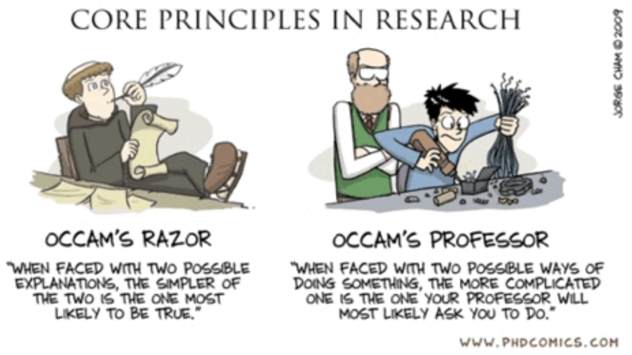
example

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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"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."
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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 K-NN?

Summary

- **curse of dimensionality**: exponentially more data needed in higher dimensions
- the **manifold hypothesis** to the rescue!
- 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**
- no algorithm can perform well on all problems, **no free lunch**
- learning algorithms make assumptions about the data (**inductive biases**)
- strength and correctness of those assumptions about the data affects their performance