Applied Machine Learning

Some basic concepts

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COMP 551 (winter 2020)

Objectives

- learning as representation, evaluation and optimization
- k-nearest neighbors for classification
- curse of dimensionality
- manifold hypothesis
- overfitting & generalization
- cross validation
- no free lunch theorem
- inductive bias

A useful perspective on ML

Let's focus on classification

Learning = Representation + Evaluation + Optimization

from: Domingos, Pedro M. "A few useful things to know about machine learning." *Commun. acm* 55.10 (2012): 78-87.

A useful perspective on ML

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Learning = Representation + Evaluation + Optimization

Model

Hypothesis space

the space of functions to choose from is determined by how we represent/define the learner

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A useful perspective on ML

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Learning = Representation + Evaluation + Optimization

Representation	Evaluation	Optimization
Model	Objective function	
Hypothesis space	Cost function	
	Score function	

the criteria for picking the best model

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A useful perspective on ML

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Learning = Representation + Evaluation + Optimization

Representation	Evaluation	Optimization
Model	Objective function	Objective
Hypothesis space	Cost function	Cost
	Score function	Loss

procedure for finding the best model

the criteria for picking the best model

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Learning =

Representation	Evaluation	Optimization
Instances	Accuracy/Error rate	Combinatorial optimization
K-nearest neighbor	Precision and recall	Greedy search
Support vector machines	Squared error	Beam search
Hyperplanes	Likelihood	Branch-and-bound
Naive Bayes	Posterior probability	Continuous optimization
Logistic regression	Information gain	Unconstrained
Decision trees	K-L divergence	Gradient descent
Sets of rules	Cost/Utility	Conjugate gradient
Propositional rules	Margin	Quasi-Newton methods
Logic programs		Constrained
Neural networks		Linear programming
Graphical models		Quadratic programming
Bayesian networks		
Conditional random fields		

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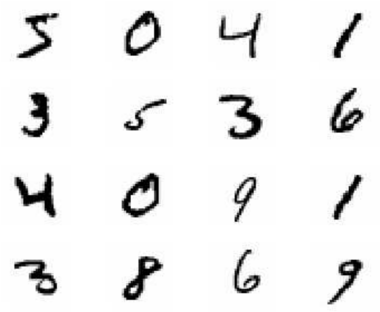
Digits dataset



input $x^{(n)} \in \{0, \ldots, 255\}^{28\times 28}$

label $y^{(n)} \in \{0, \ldots, 9\}$

$n \in \{1, \ldots, N\}$ indexes the training instance

sometime we drop (n)

image:https://medium.com/@rajatjain0807/machine-learning-6ecde3bfd2f4

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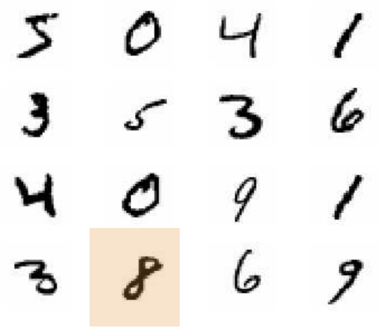

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	12	0	11	39	137	37	0	152	147	84	0	0	0
0	0	1	0	0	0	41	160	250	255	235	162	255	238	206	11	13	0
0	0	0	16	9	9	150	251	45	21	184	159	154	255	233	40	0	0
10	0	0	0	0	0	145	146	3	10	0	11	124	253	255	107	0	0
0	0	3	0	4	15	236	216	0	0	38	109	247	240	169	0	11	0
1	0	2	0	0	0	253	253	23	62	224	241	255	164	0	5	0	0
6	0	0	4	0	3	252	250	228	255	255	234	112	28	0	2	17	0
0	2	1	4	0	21	255	253	251	255	172	31	8	0	1	0	0	0
0	0	4	0	163	225	251	255	229	120	0	0	0	0	0	11	0	0
0	0	21	162	255	255	254	255	126	6	0	10	14	6	0	0	9	0
3	79	242	255	141	66	255	245	189	7	8	0	0	5	0	0	0	0
26	221	237	98	0	67	251	255	144	0	8	0	0	7	0	0	11	0
125	255	141	0	87	244	255	208	3	0	0	13	0	1	0	1	0	0
145	248	228	116	235	255	141	34	0	11	0	1	0	0	0	1	3	0
85	237	253	246	255	210	21	1	0	1	0	0	6	2	4	0	0	0
6	23	112	157	114	32	0	0	0	0	2	0	8	0	7	0	0	0
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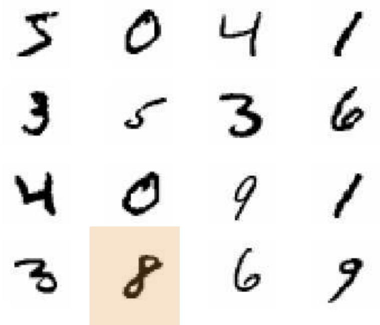

0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0
0	0	0	0	1	12	0	11	39	137	37	0	152	147	84	0	0	0
0	0	1	0	0	0	41	160	250	255	235	162	255	238	206	11	13	0
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sometime we drop (n)

vectorization:

$x \rightarrow \mathrm{vec}(x) \in \mathbb{R}^{784}$ input dimension **D**

pretending intensities are real numbers

image:https://medium.com/@rajatjain0807/machine-learning-6ecde3bfd2f4

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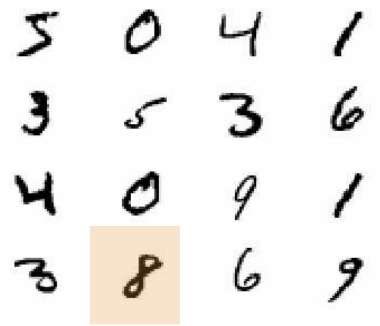

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vectorization:

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input dimension **D**

pretending intensities are real numbers

note: this ignores the spatial arrangement of pixels, but good enough for now

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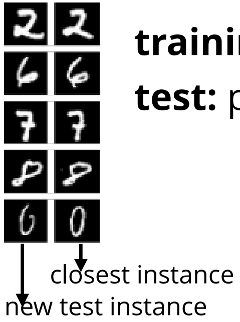
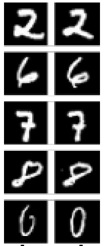
Nearest neighbour classifier



training: do nothing

test: predict the lable by finding the closest image in the training set and

Nearest neighbour classifier



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need a measure of distance

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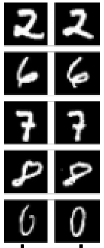

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e.g., Euclidean distance $||x - x'||_2 = \sqrt{\sum_{d=1}^{D}(x_d - x'_d)^2}$

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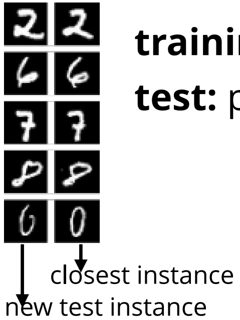

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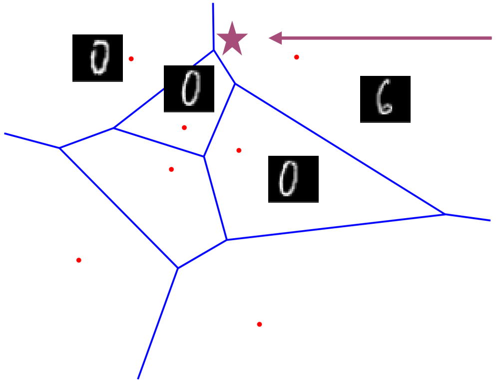


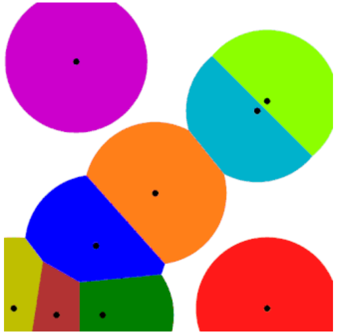
test instance: will be classified as 6

Voronoi diagram shows the decision boundaries

(this example D=2, can't visualize D=784)

the Voronoi Diagram

each colour shows all points closer to the corresponding training instance than to any other instance



images from wiki

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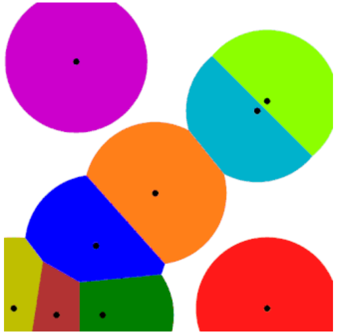
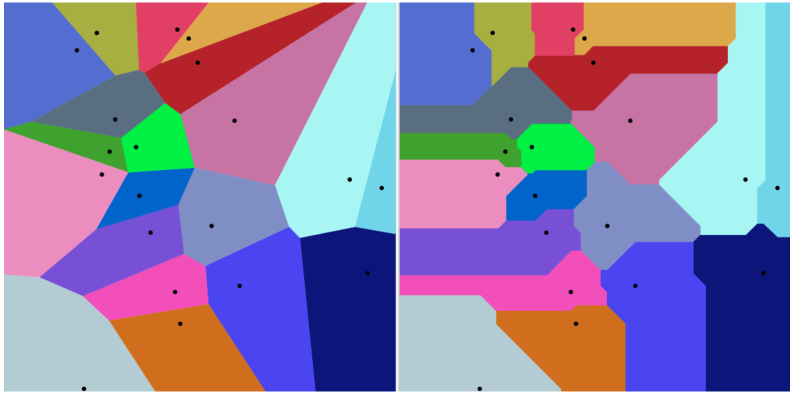




Euclidean distance

$$||x - x'||_2 = \sqrt{\sum_{d=1}^{D}(x_d - x'_d)^2}$$

Manhattan distance

$$||x - x'||_1 = \sum_{d=1}^{D}|x_d - x'_d|$$

images from wiki

K- nearest neighbours

training: do nothing

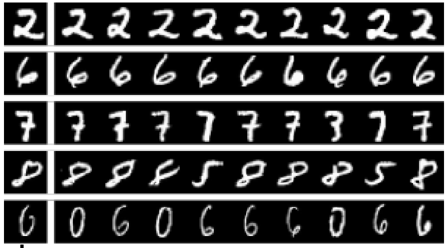
test: predict the lable by finding the **K** closest instances

$$p(y^{new} = c \mid x_{new}) = \frac{1}{K} \sum_{x' \in \mathrm{KNN}(x^{new})} \mathbb{I}(y' = c)$$

probability of class c

K-nearest neighbours

example K = 9



closest instances

new test instance

$p(y = 6 |$  $) = \frac{6}{9}$

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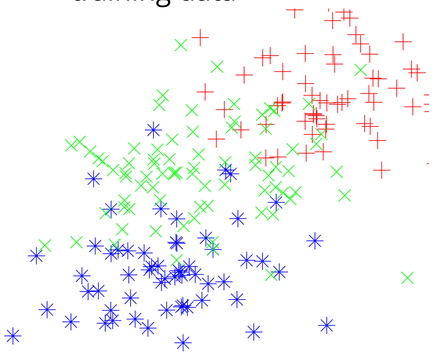
example C=3, D=2, K=10

training data



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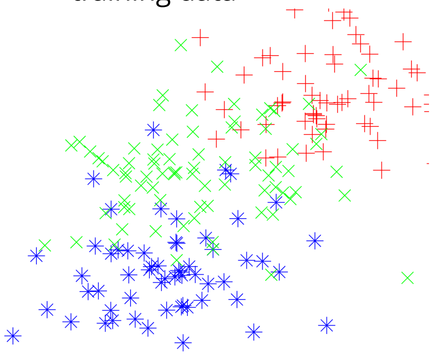
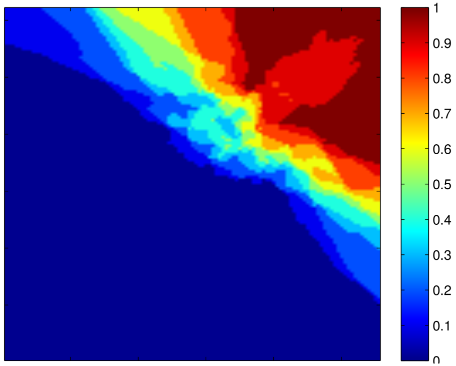


prob. of class 1



K- nearest neighbours

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K-nearest neighbours

example

C=3, D=2, K=10

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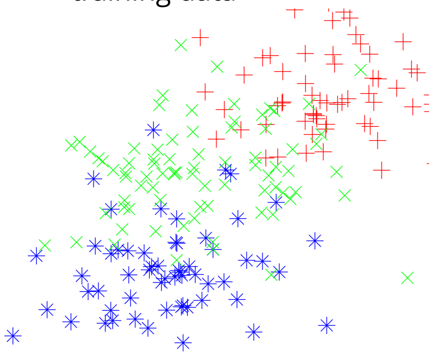

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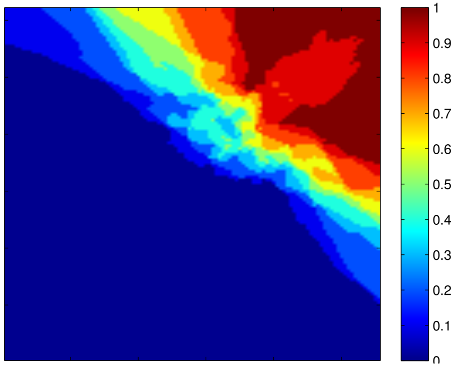
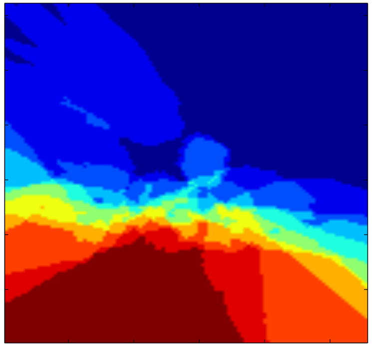


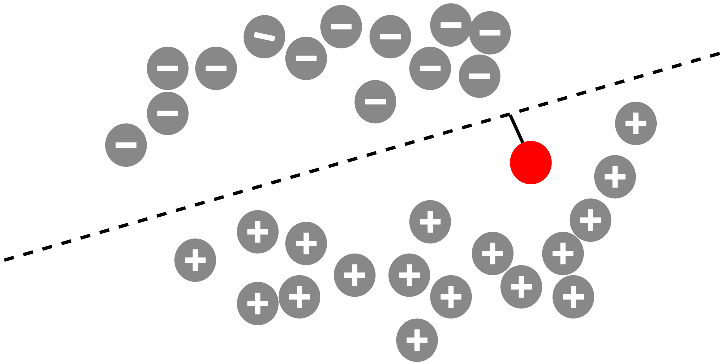
prob. of class 2

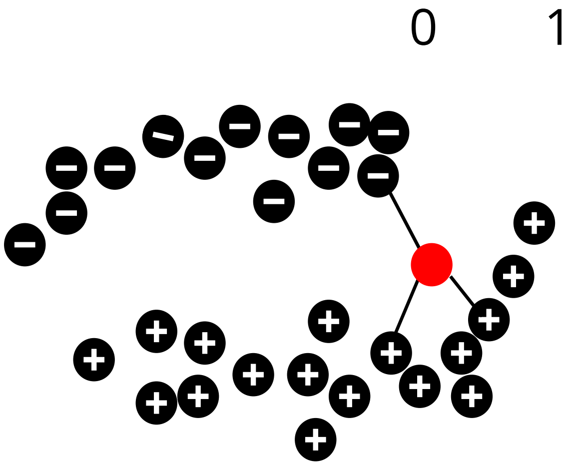


K- nearest neighbours

a **non-parametric method (misnomer)**: the number of model parameters grows with the data

a **lazy-learner**: no training phase, locally estimate when a query comes
useful for fast-changing datasets





Curse of dimensionality

high dimensions are unintuitive!

assuming a uniform distribution $x \in [0,1]^D$

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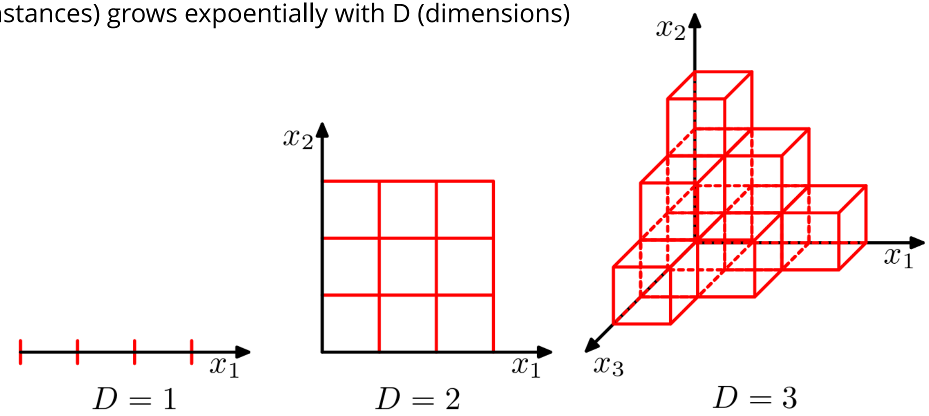
- need exponentially more instances for K-NN

suppose we want to maintain #samples per sub-cube of side 1/3

N (total #training instances) grows expoentially with D (dimensions)



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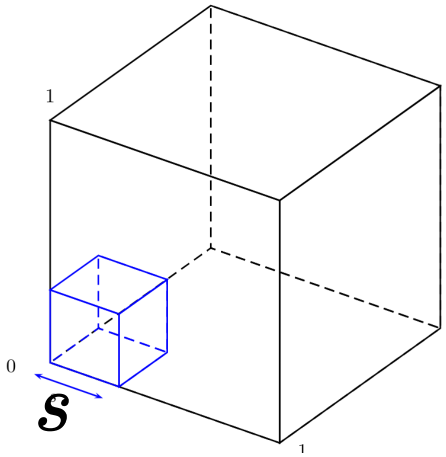
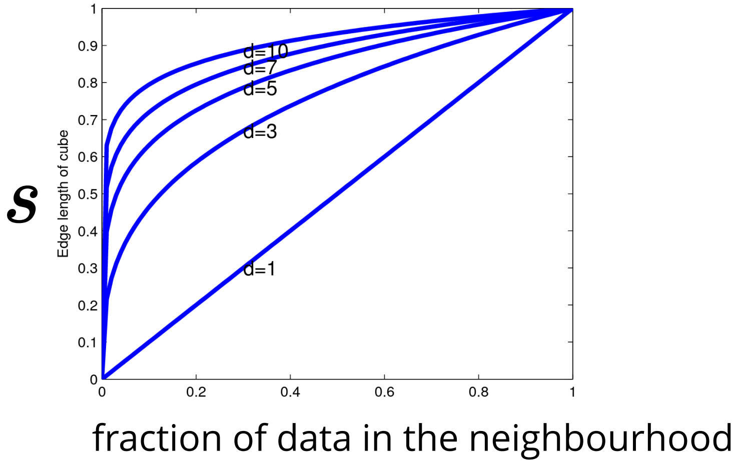
Another way to see this





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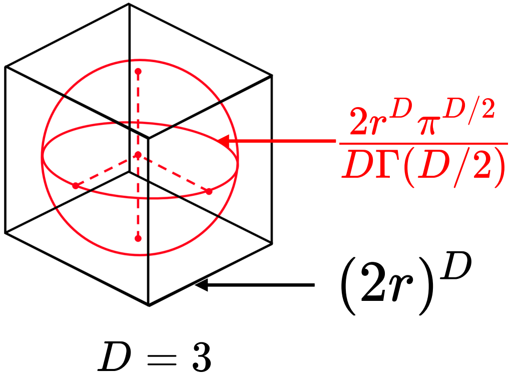

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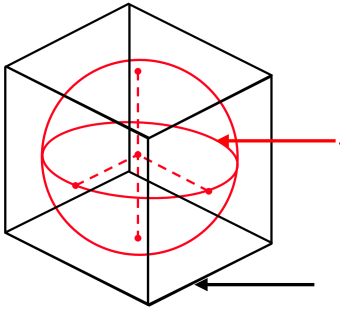

$$\frac{2r^D \pi^{D/2}}{D\Gamma(D/2)}$$

$$(2r)^D$$

$$D = 3$$

$$\lim_{D \to \infty} \frac{\mathrm{volum}(\bigcirc)}{\mathrm{volum}(\square)} = 0$$

most of the volume is close to the corners

most pairwise disstances are similar

Curse of dimensionality

high dimensions are unintuitive!

assuming a uniform distribution $x \in [0,1]^D$

- need exponentially more instances for K-NN
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a "conceptual" visualization of the same example

- # corners and the mass in the corners grows quickly

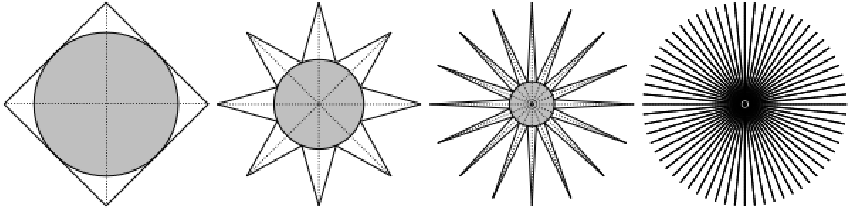

image: Zaki's book on Data Mining and Analysis

Manifold hypothesis

real-world data is often far from uniform

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

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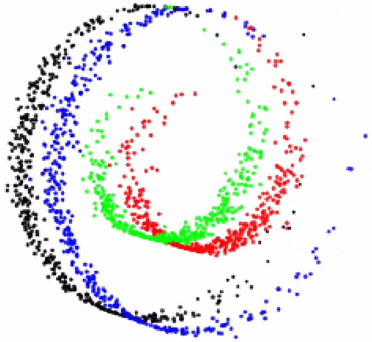

ambient (data) dimension: $D = 3$

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

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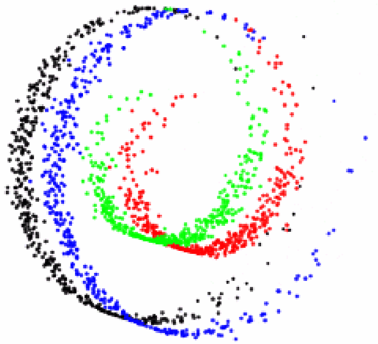

ambient (data) dimension: $D = 3$

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MNIST digit classification results

for K-NN the manifold dimension matters

so K-NN can be competitive

	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

$D = 784$ is the number of pixels

manifold dimension ?

Model selection

K is a **hyper-parameter**: a model parameter that is not learned by the algorithm

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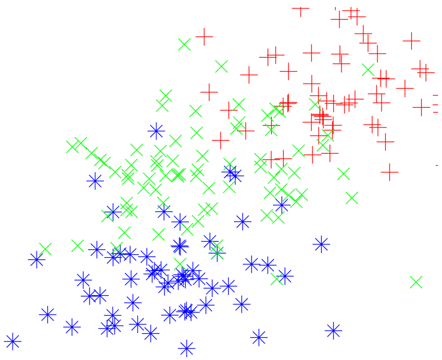
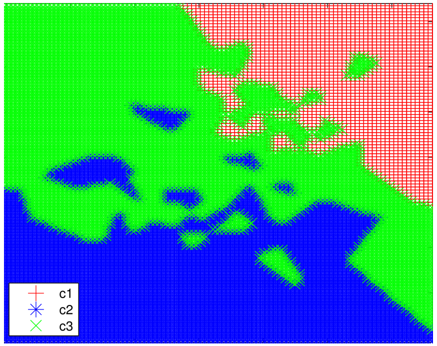
example

training data



K=1

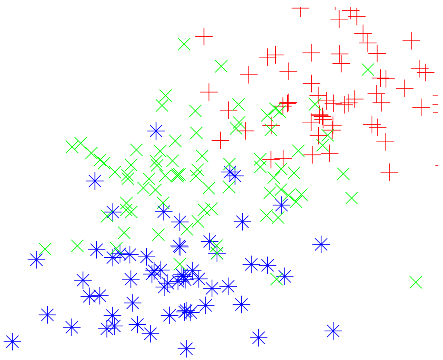


Model selection

K is a **hyper-parameter**: a model parameter that is not learned by the algorithm

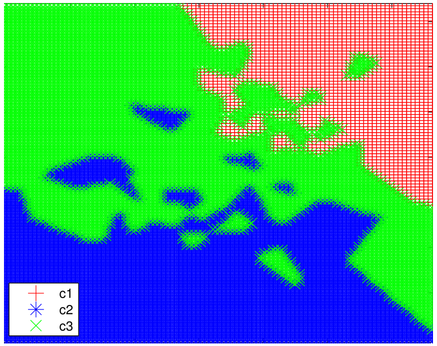
example

training data

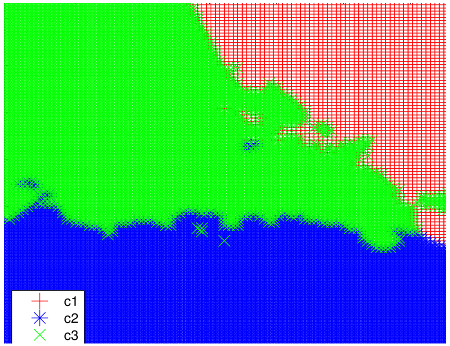


most likely class

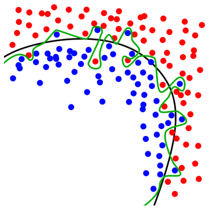
K=1



K=5

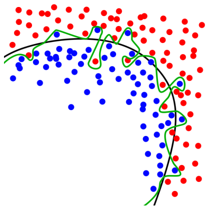


Overfitting



how to pick the best K?

Overfitting



how to pick the best K?

first attempt pick K that gives "best results" on the training set

e.g., misclassification error $\sum_n \mathbb{I}(\arg\max_y p(y \mid x^{(n)}) \neq y^{(n)})$

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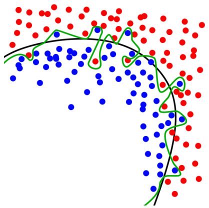

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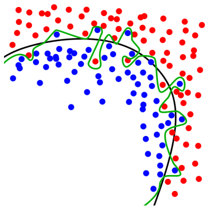
we can have bad performance on new instances



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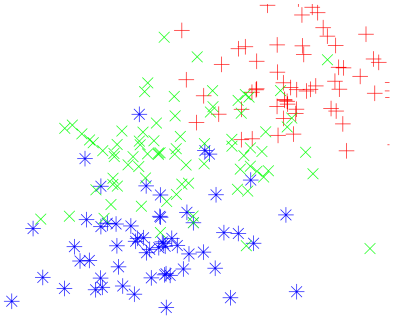
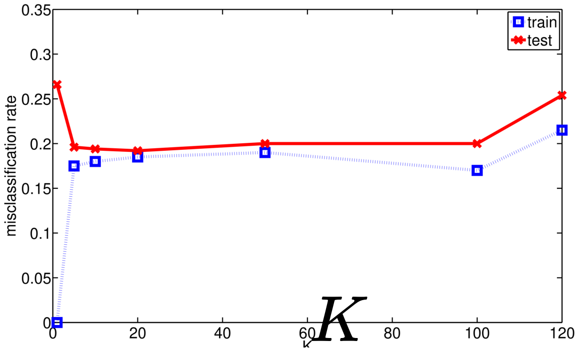
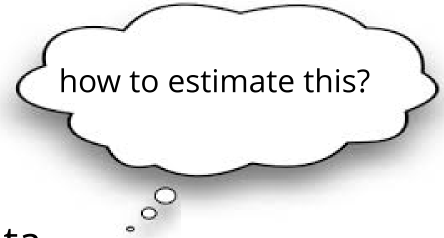




Generalization

what we care about is generalization

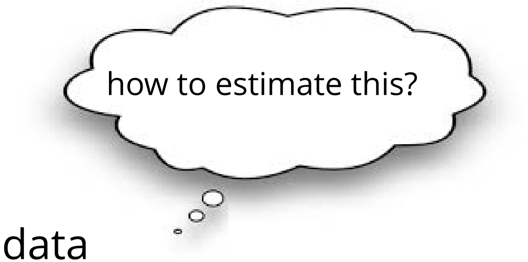
Generalization



what we care about is generalization

expected loss: performance of algorithm on unseen data

Generalization



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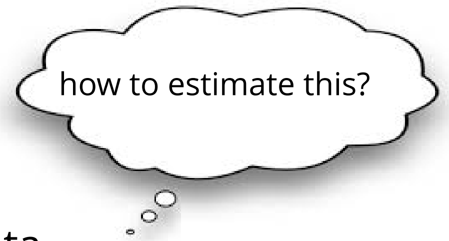
expected loss: performance of algorithm on unseen data

validation set: a subset of available data not used for training

$$\textit{performance on validation set} \approx \textit{expected error}$$

Generalization



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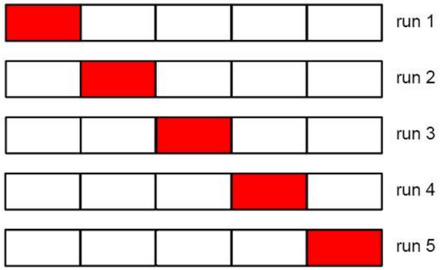
k-fold cross validation(CV)

- partition the data into k *folds*
- use k-1 for training, and 1 for validation
- average the validation error over all folds



Generalization

how to estimate this?

what we care about is generalization

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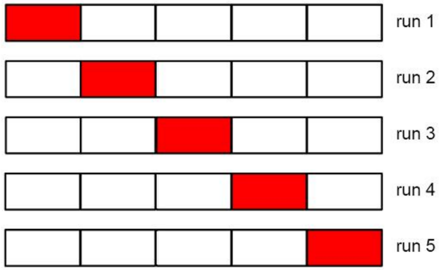


leave-one-out CV: extreme case of k=N

Train-validation-test split

We often use a 3-way split of the data

(e.g., 80%-10%-10% split)

test set:

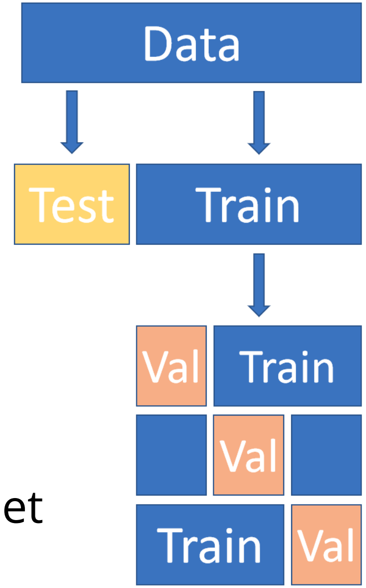
- for final evaluation

validation set (*aka* development set):

- for hyper-parameter tuning

training set:

- to train the model



we can use k-fold *cross validation* with train+validation set

No free lunch

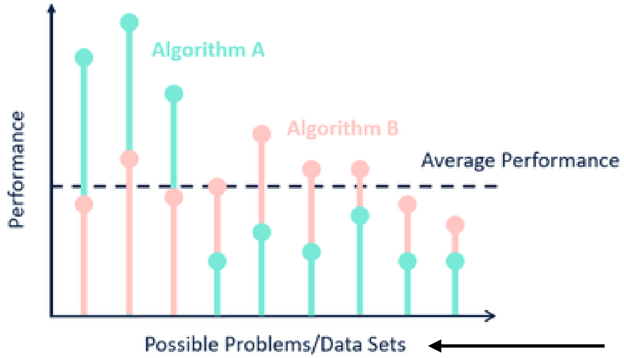
there is no single algorithm that performs well on all class of problems

image: https://community.alteryx.com/t5/Data-Science-Blog/There-is-No-Free-Lunch-in-Data-Science/ba-p/347402

No free lunch

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

consider **any** two binary classifiers (**A** and **B**)
they have the same average performance (test accuracy) on *all possible problems*



produce labels using a random (binary) function

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Inductive Bias

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ML algorithms need to make assumptions about the problem **inductive bias**

strength and **correctness** of assumptions are important in having good performance

related to bias - variance trade off that we will discuss later

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examples

manifold hypothesis in KNN (and many other methods)
close to linear dependencies in linear regression
conditional independence and causal structure in probabilistic graphical models

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Summary

ML algorithms involve a choice of **model**, **objective** and **optimization**

we saw **K-NN** method for classification

curse of dimensionality: exponentially more data needed in higher dims.

manifold hypothesis to the rescue!

what we care about is **generalization** of ML algorithms

estimated using **cross validation**

there ain't no such thing as a **free lunch**

the choice of **inductive bias** is important for good generalization