Applied Machine Learning

Some basic concepts

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COMP 551 **(winter 2020)**

Objectives

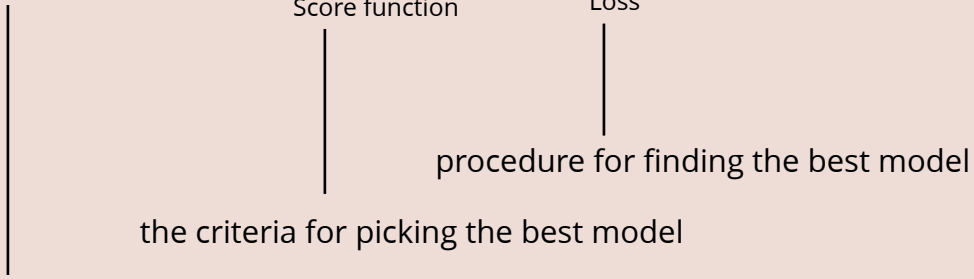
- learning as representation, evaluation and optimization
- k-nearest neighbors for classification
- curse of dimensionality
- manifold hypothesis
- overfitting & generalization
- cross validation
- no free lunch theorem
- inductive bias

A useful perspective on ML

Let's focus on classification

Learning = **Representation** + **Evaluation** + **Optimization**

- **Representation**: Model, Hypothesis space
- **Evaluation**: Objective function, Cost function, Score function
- **Optimization**: Objective, Cost, Loss



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

Let's focus on classification

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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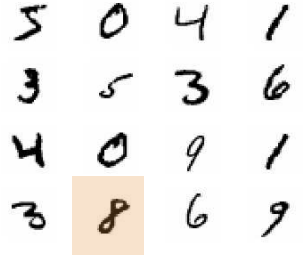
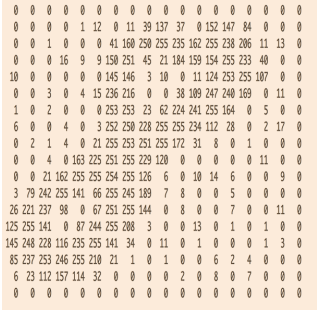
Digits dataset

MNIST





white → black

input $x^{(n)} \in \{0, \dots, 255\}^{28 \times 28}$ size of the input image in pixels

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

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

sometime we drop (n)

vectorization:

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

pretending intensities are real numbers

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

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

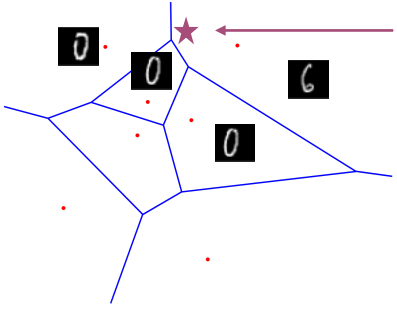
Nearest neighbour classifier

training: do nothing

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

need a measure of distance

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



test instance: will be classified as 6

Voronoi diagram shows the decision boundaries

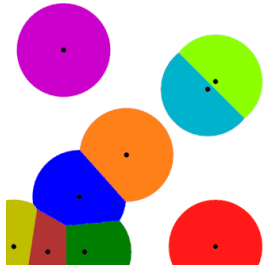
(this example D=2, can't visualize D=784)

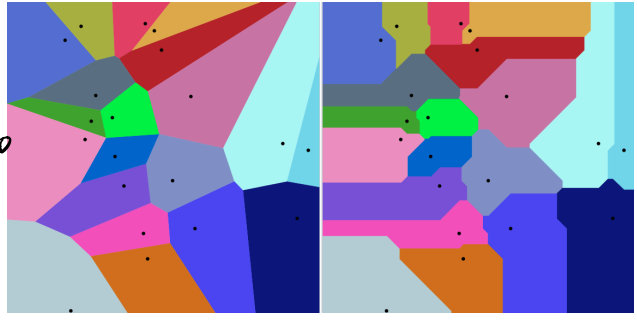
KNN is a nonlinear classifier

The decision boundaries of KNN are locally linear segments, but in general have a complex shape that is not equivalent to a line in 2D or a hyperplane in higher dimensions.

the Voronoi Diagram

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





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

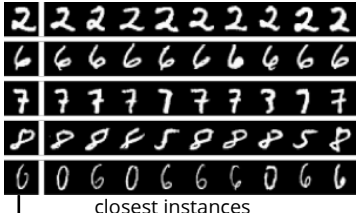
training: do nothing

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



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

K- nearest neighbours

training: do nothing

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

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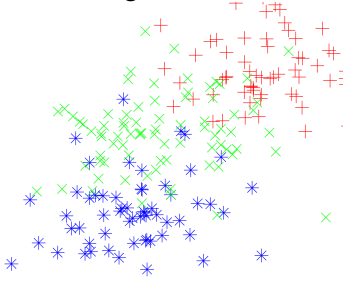
probability of class c

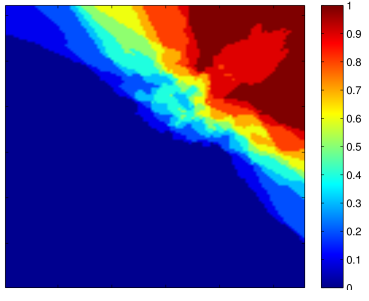
K-nearest neighbours

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

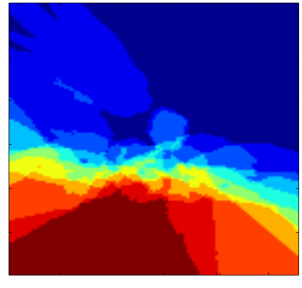
training data



prob. of class 1



prob. of class 2



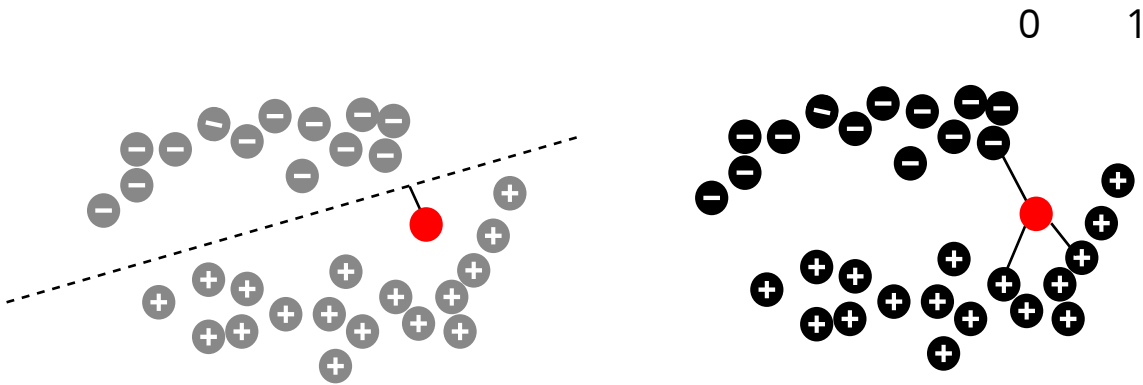
doesn't mean that the model completely lack parameters but that the number and nature of the parameters are flexible and not fixed in advance.

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!

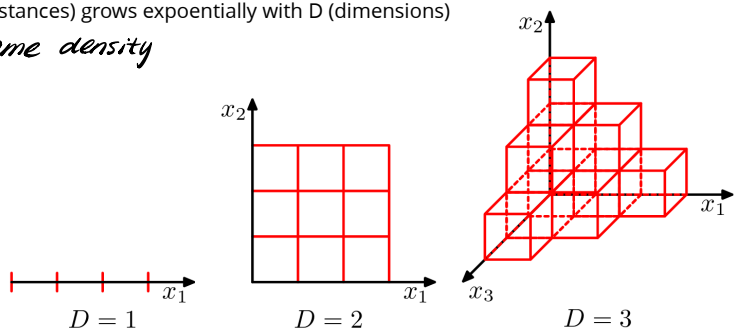
assuming a uniform distribution $x \in [0,1]^D$

- need exponentially more instances for K-NN (more sparse)

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

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

to remain same density



Curse of dimensionality

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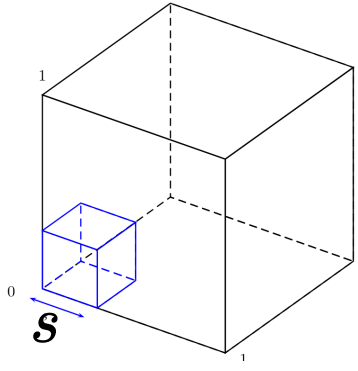
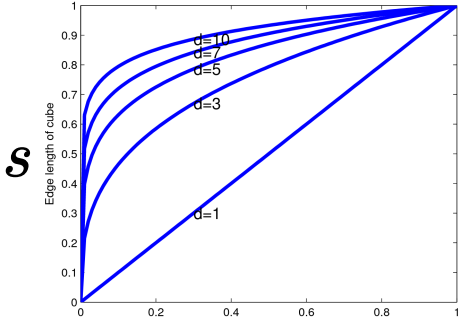
assuming a uniform distribution $x \in [0,1]^D$

- need exponentially more instances for K-NN

Another way to see this





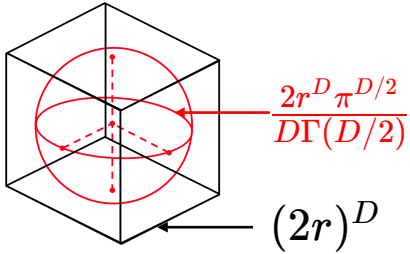
fraction of data in the neighbourhood

Curse of dimensionality

high dimensions are unintuitive!

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

- need exponentially more instances for K-NN
- all instances have similar distances



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

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
- all instances have similar distances

a "conceptual" visualization of the same example

- # corners and the mass in the corners grows quickly

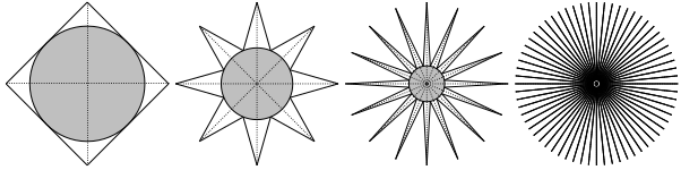


image: Zaki's book on Data Mining and Analysis

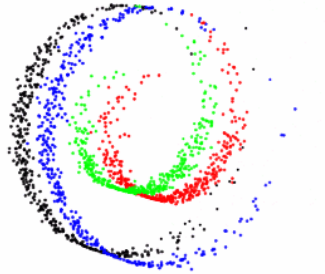
Manifold hypothesis

real-world data is often far from uniform

assumption

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

fix dimensionality curse



ambient (data) dimension: $D = 3$

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

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

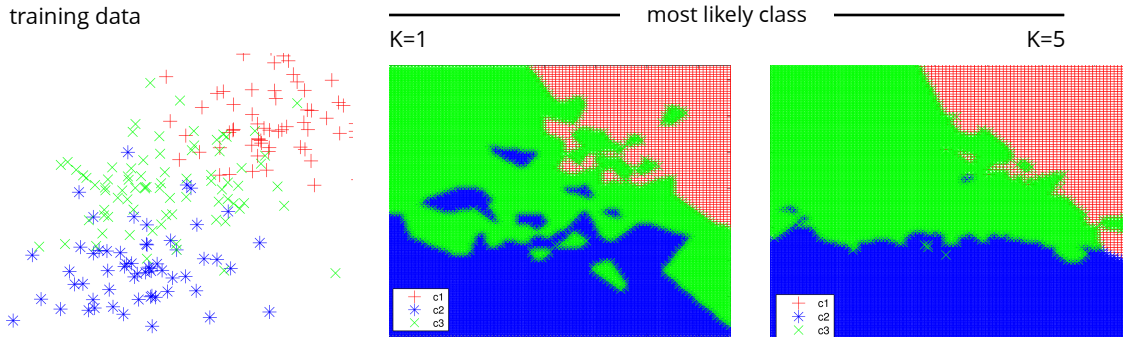
$D = 784$ is the number of pixels

manifold dimension ?

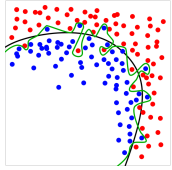
Model selection

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

example



Overfitting



how to pick the best K?

first attempt pick K that gives "best results" on the training set $K=1$

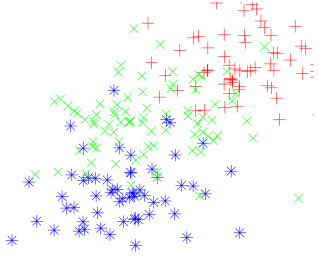
e.g., misclassification error $\sum_n \mathbb{I}(\arg\max_y p(y \mid x^{(n)}) \neq y^{(n)})$

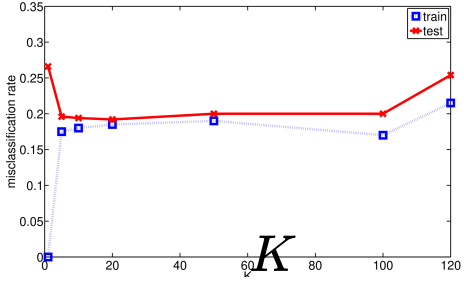
bad idea!

we can overfit the training data

we can have bad performance on new instances

example





Generalization

how to estimate this?

what we care about is generalization

expected loss: performance of algorithm on unseen data

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

performance on validation set ≈ *expected error*

minimize

⇒ minimize validation error

k-fold cross validation(CV)

find hyper-parameter

- partition the data into k *folds* (start from scratch
- use k-1 for training, and 1 for validation every time)
- average the validation error over all folds

leave-one-out CV: extreme case of k=N (most reliable)

Train-validation-test split

We often use a 3-way split of the data

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

test set:

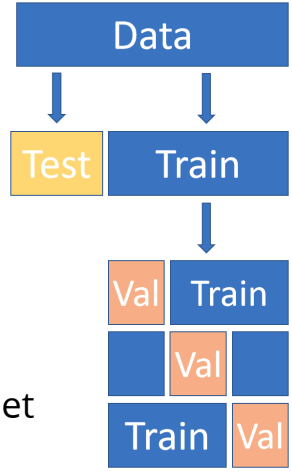
- for final evaluation

validation set (*aka* development set):

- for hyper-parameter tuning

training set:

- to train the model



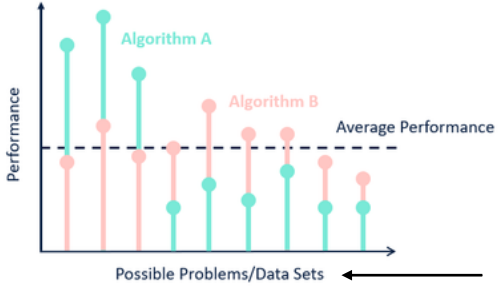
we can use k-fold *cross validation* with train+validation set

$x \in \{0,1\}^2$
$y \in \{0,1\}$
$\rightarrow 4$

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

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

Inductive Bias

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

how is learning possible at all?

because world is not random, there are regularities, induction is possible!

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

reduce more dim

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

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

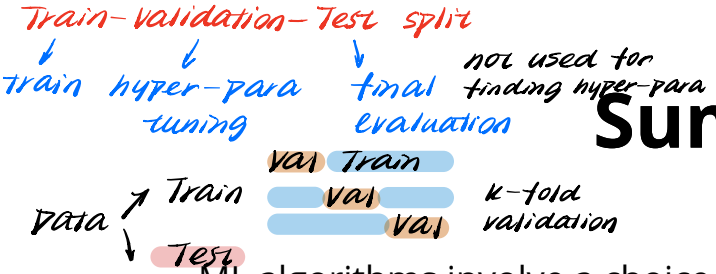
examples

manifold hypothesis in KNN (and many other methods)

close to linear dependencies in linear regression

conditional independence and causal structure in probabilistic graphical models

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



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