Applied Machine Learning

Some basic concepts

Siamak Ravanbakhsh

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	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

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

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

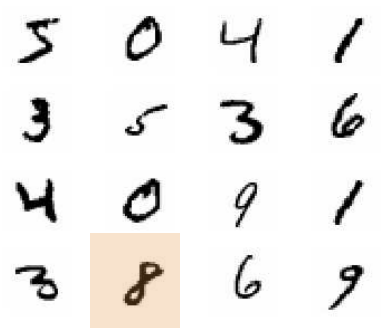
Let's focus on classification

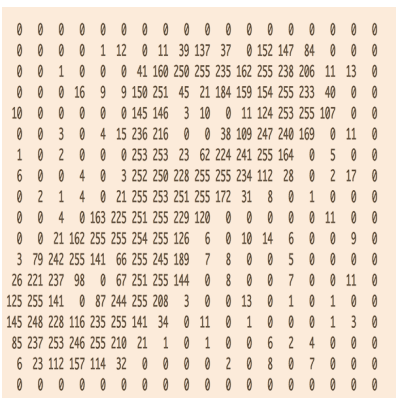
Learning =

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		

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

Digits dataset





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:

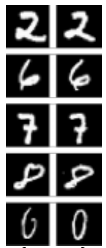
$x \to \text{vec}(x) \in \mathbb{R}^{784}$ input dimension **D**

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

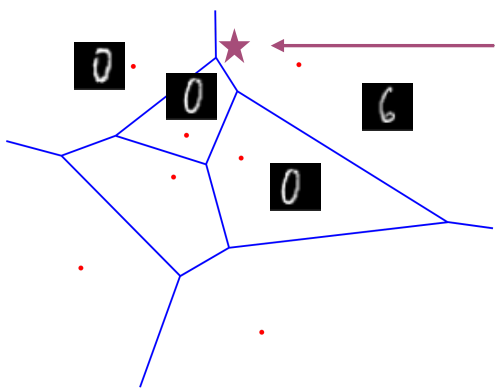


training: do nothing

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

need a measure of distance

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



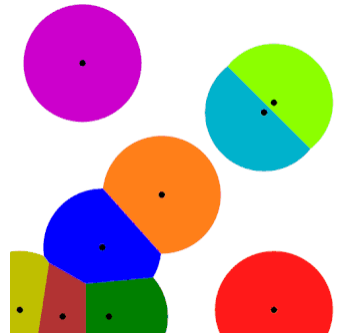
 test instance: will be classified as 6

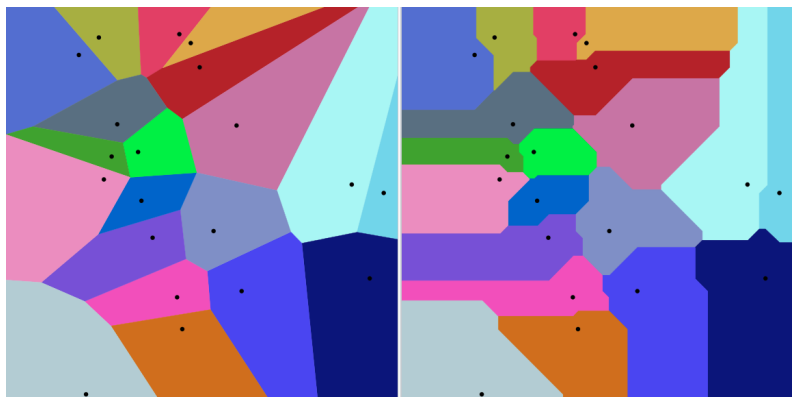
Voronoi diagram shows the decision boundaries

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

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

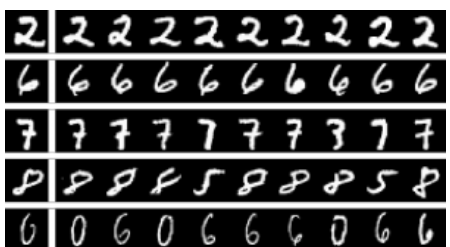
training: do nothing

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



closest instances

new test instance

$$p(y = 6 \mid \text{[image]}) = \frac{6}{9}$$

K- nearest neighbours

training: do nothing

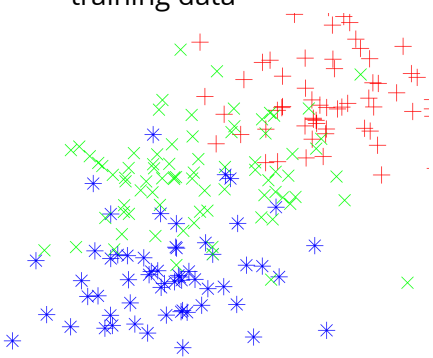
test: predict the lable by finding the **K** closest instances

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

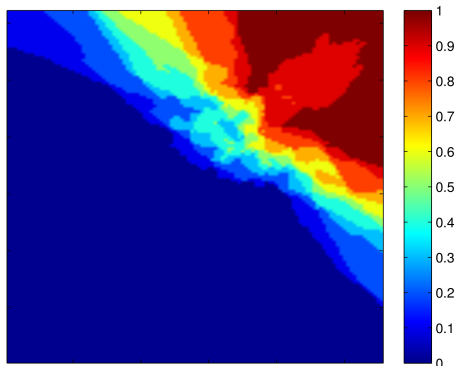
probability of class c — K-nearest neighbours

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

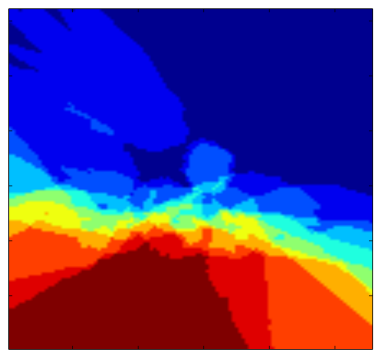
training data



prob. of class 1



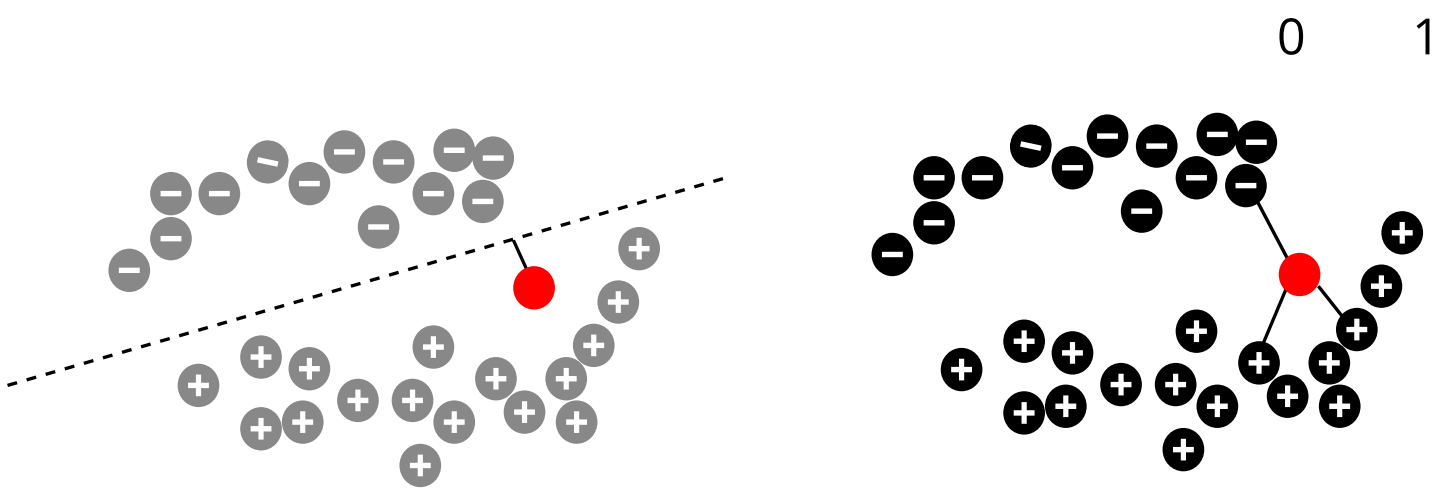
prob. of class 2



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

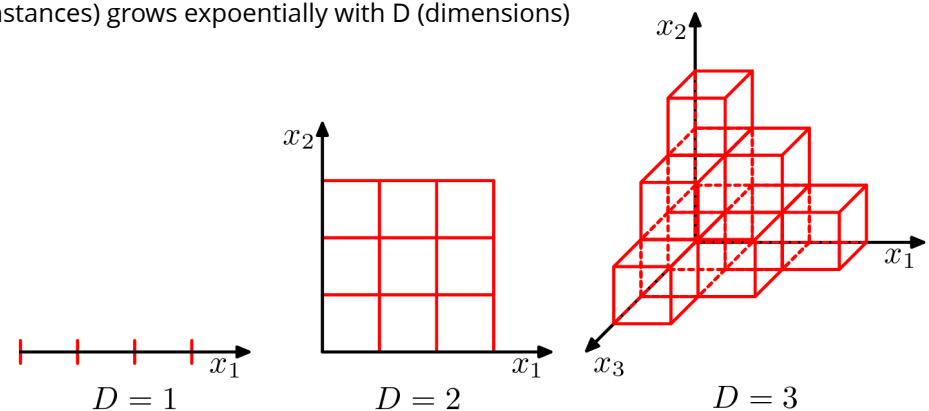
high dimensions are unintuitive!

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

- 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)



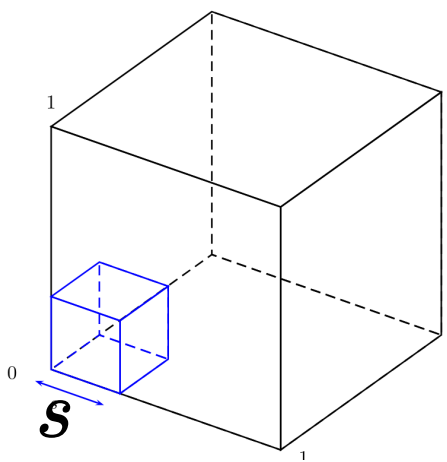
Curse of dimensionality

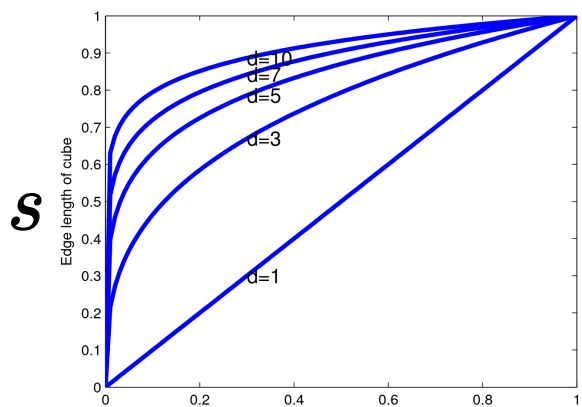
high dimensions are unintuitive!

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

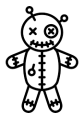
- need exponentially more instances for K-NN

  Another way to see this





fraction of data in the neighbourhood

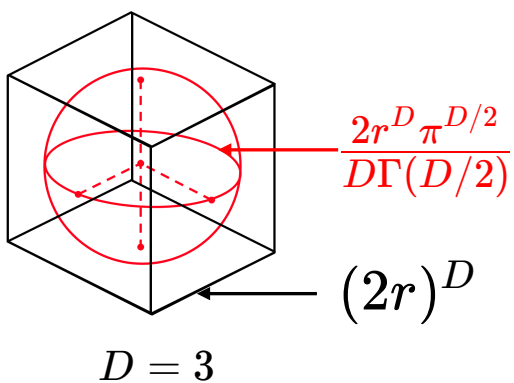


Curse of dimensionality

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

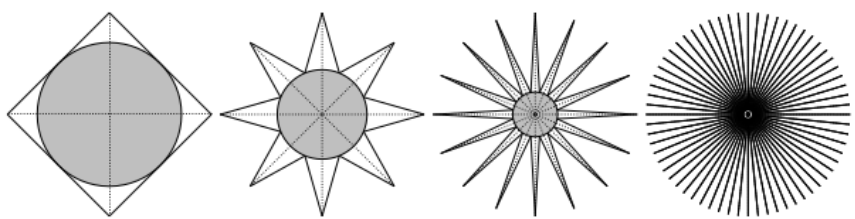
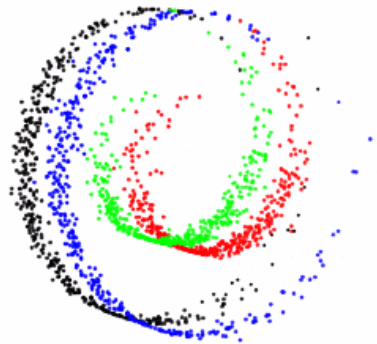


image: Zaki's book on Data Mining and Analysis

Manifold hypothesis

real-world data is often far from uniform

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



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

ambient (data) dimension: $D = 3$

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

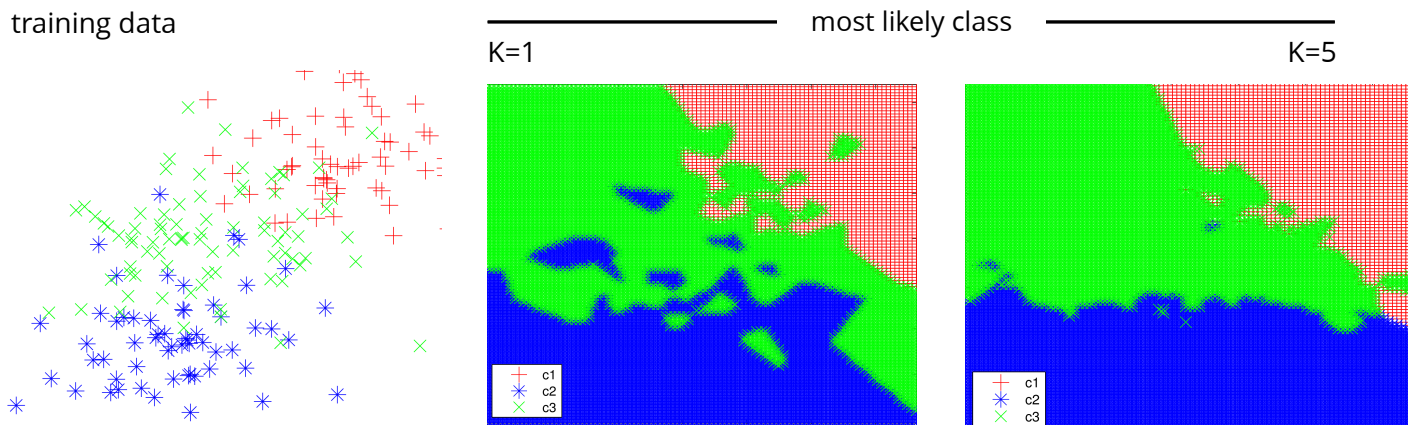
$D = 784$ is the number of pixels

manifold dimension ?

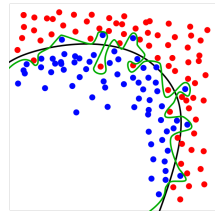
Model selection

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

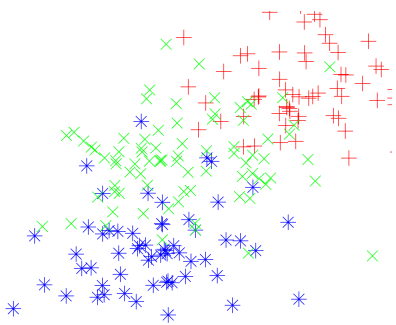
e.g., misclassification error $\sum_n \mathbb{I}(\arg\max_y p(y \mid x^{(n)}) \neq y^{(n)})$

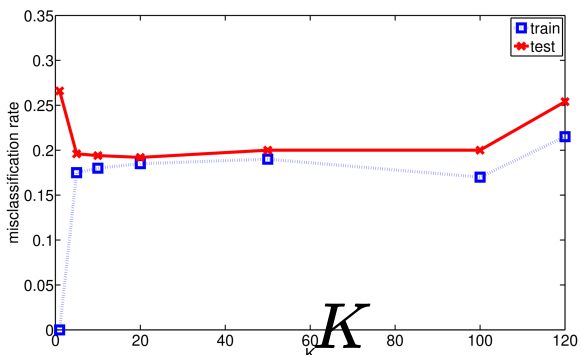
bad idea!

we can overfit the training data

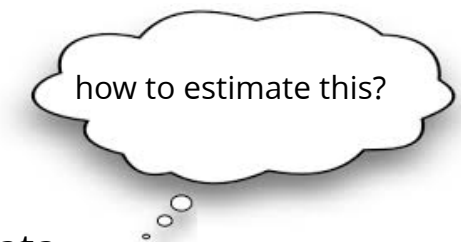
we can have bad performance on new instances

example





Generalization



what we care about is generalization

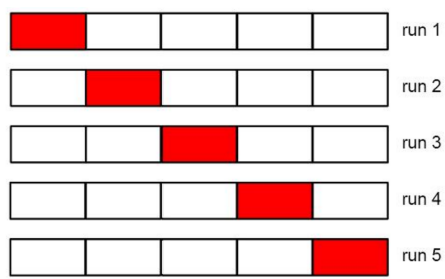
expected loss: performance of algorithm on unseen data

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

performance on validation set $\approx$ *expected error*

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



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:

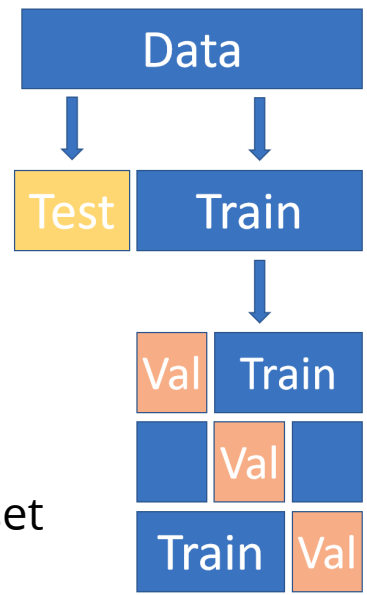
- for final evaluation

validation set (*aka* development set):

- for hyper-parameter tuning

training set:

- to train the model

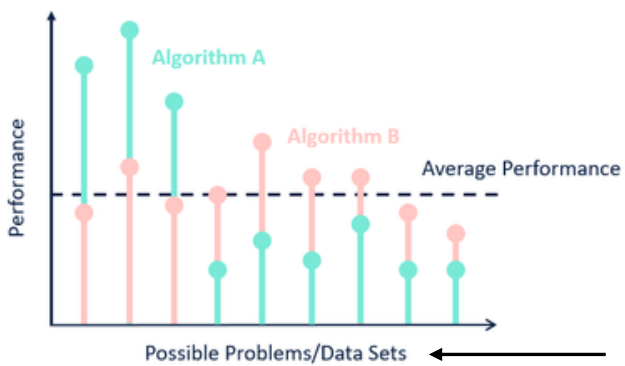


we can use k-fold *cross validation* with train+validation set

No free lunch

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

{ 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**

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