Large-Scale Nearest Neighbor Classification with Statistical Guarantees

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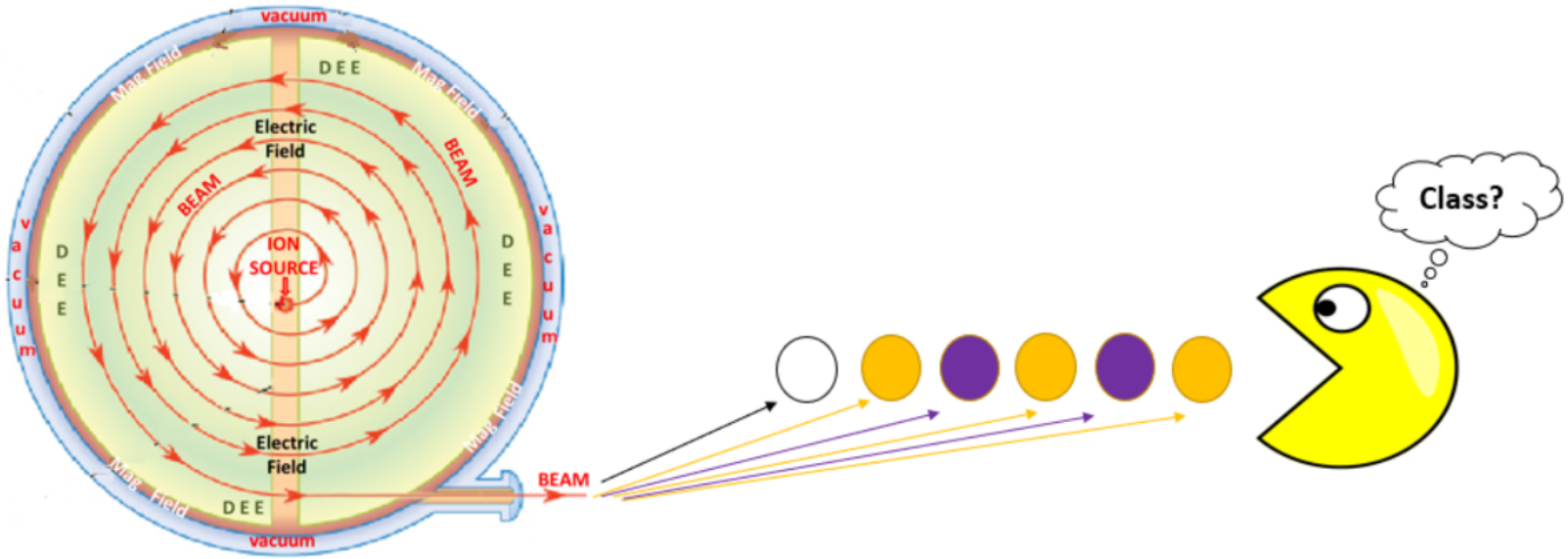
SUSY Data Set (UCI Machine Learning Repository)

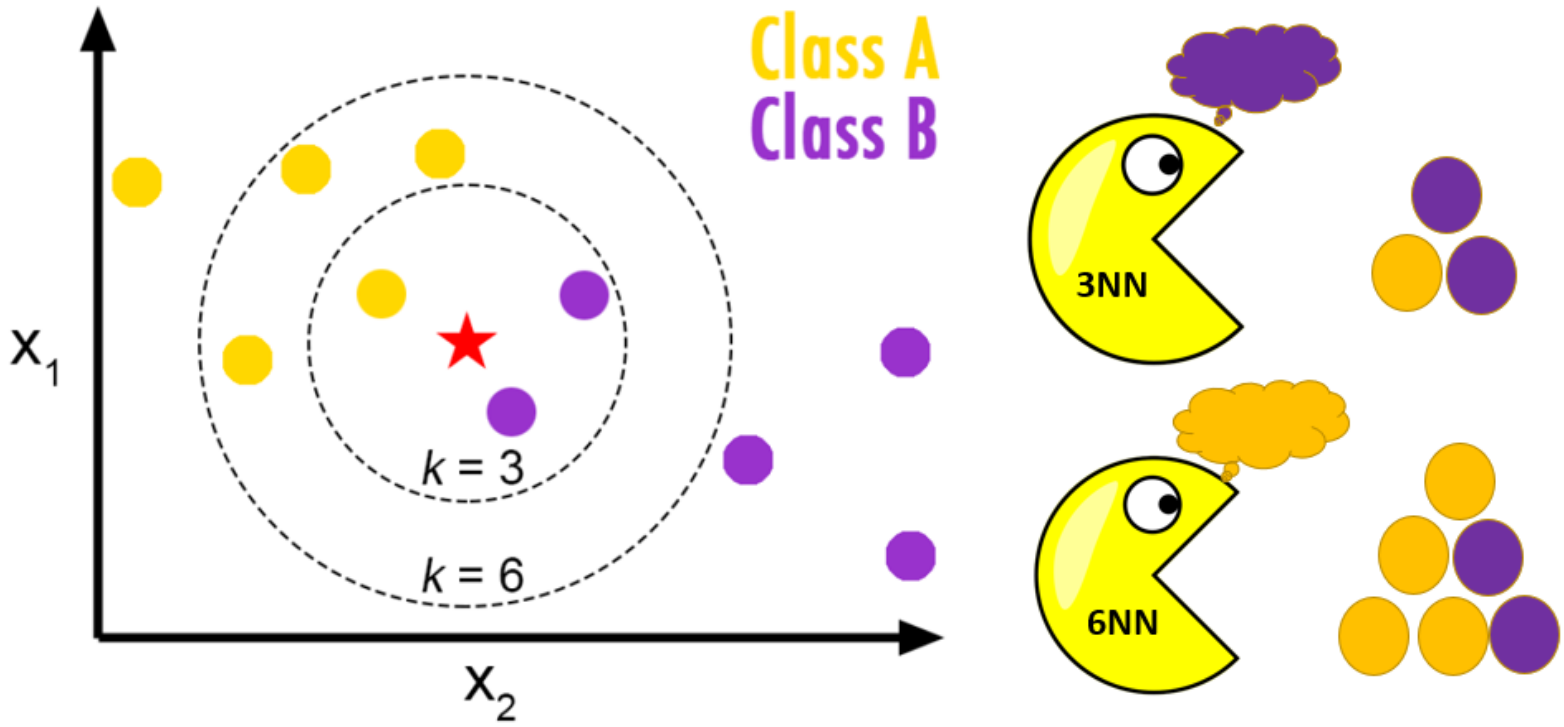
- Size: 5,000,000 particles from the accelerator
- Predictor variables: 18 (properties of the particles)
- Goal – Classification:

  distinguish between a signal process and a background process



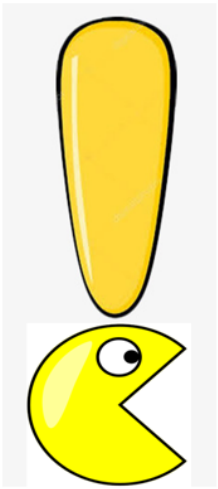
Nearest Neighbor Classification

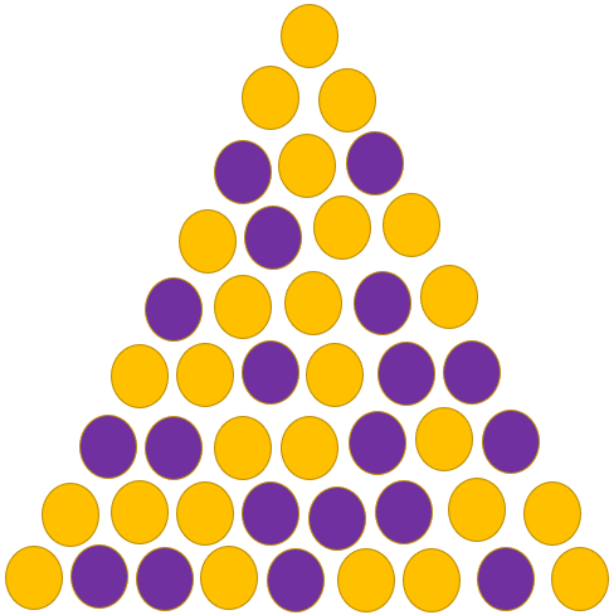
The kNN classifier predicts the class of $x \in \mathbb{R}^d$ to be the most frequent class of its k nearest neighbors (Euclidean distance).



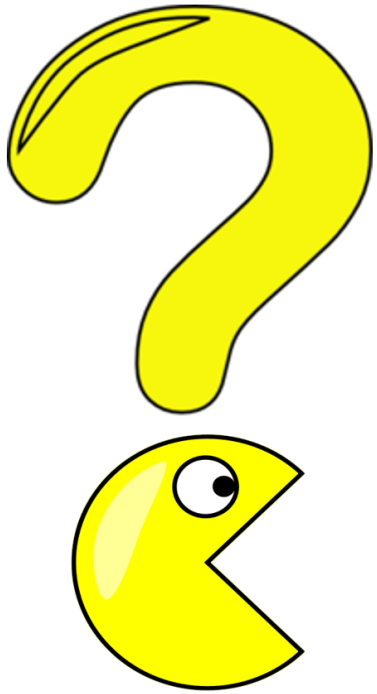
Computational/Space Challenges for kNN Classifiers

- Time complexity: $O(dN + Nlog(N))$
  - dN: computing distances from the query point to all N observations in $\mathbb{R}^d$
  - $Nlog(N)$: sorting N distances and selecting the k nearest distances
- Space complexity: $O(dN)$
- Here, N is the size of the entire dataset





How to Conquer "Big Data?"



Train the total data at one time: oracle kNN

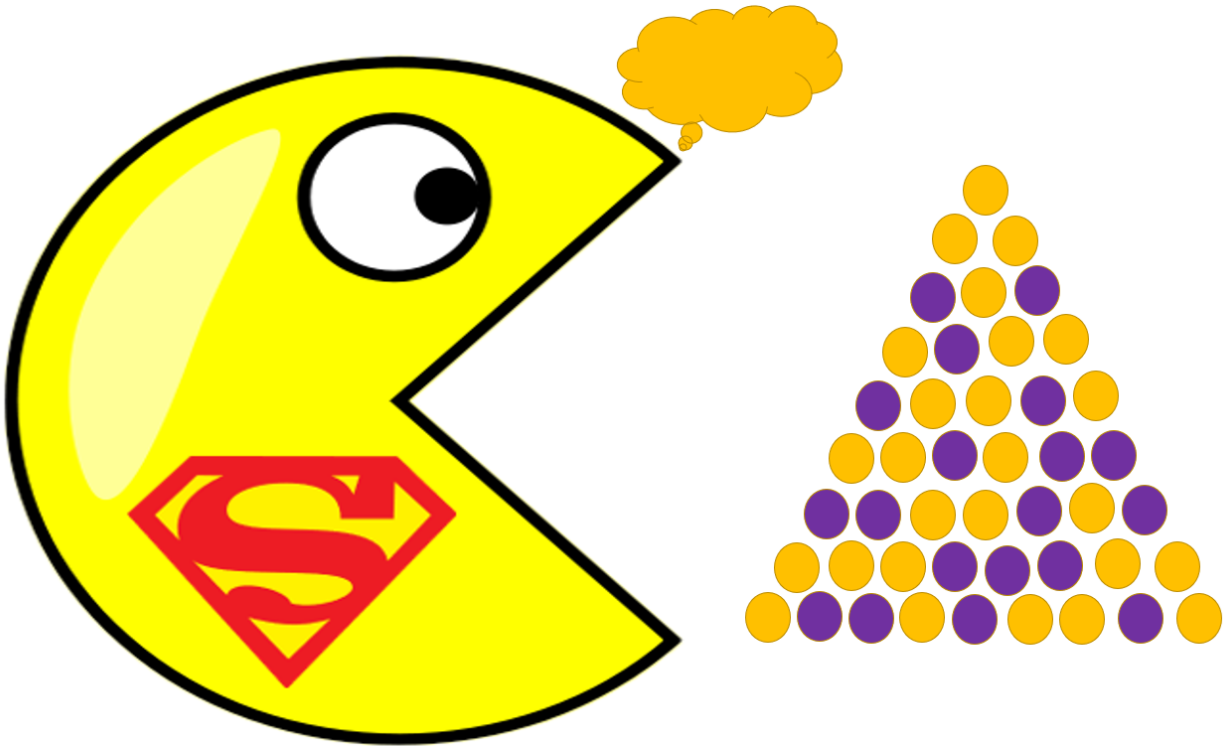
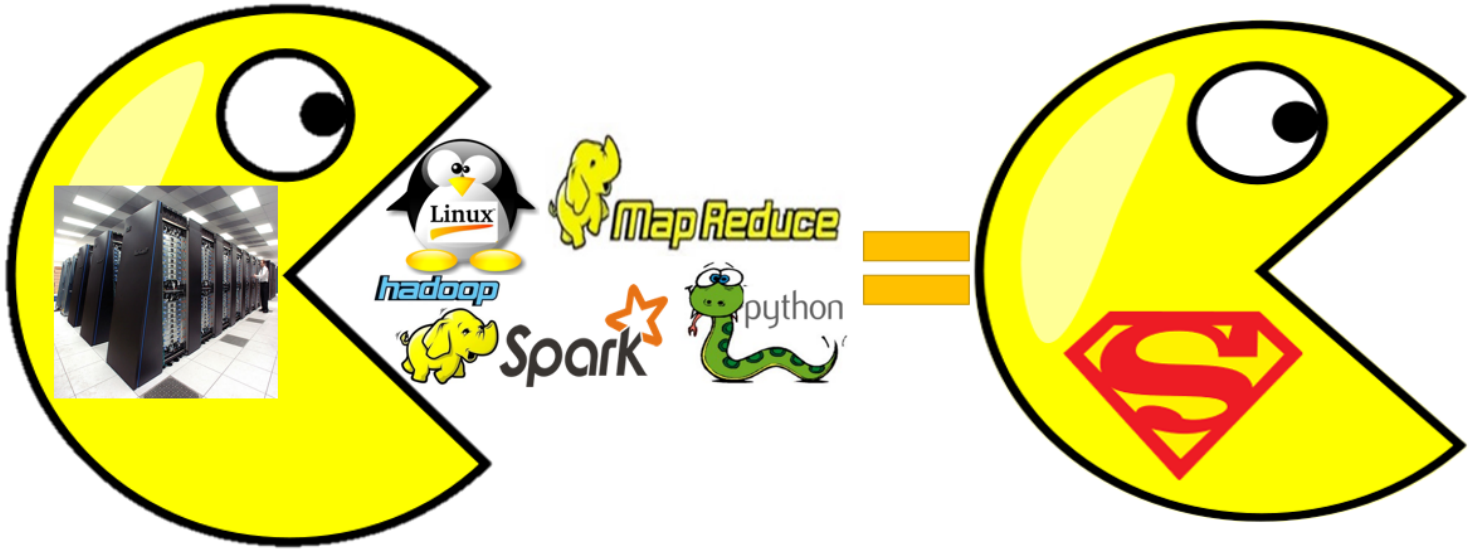


Figure: I'm Pac-Superman!

Construction of Pac-Superman



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- Expensive super-computer

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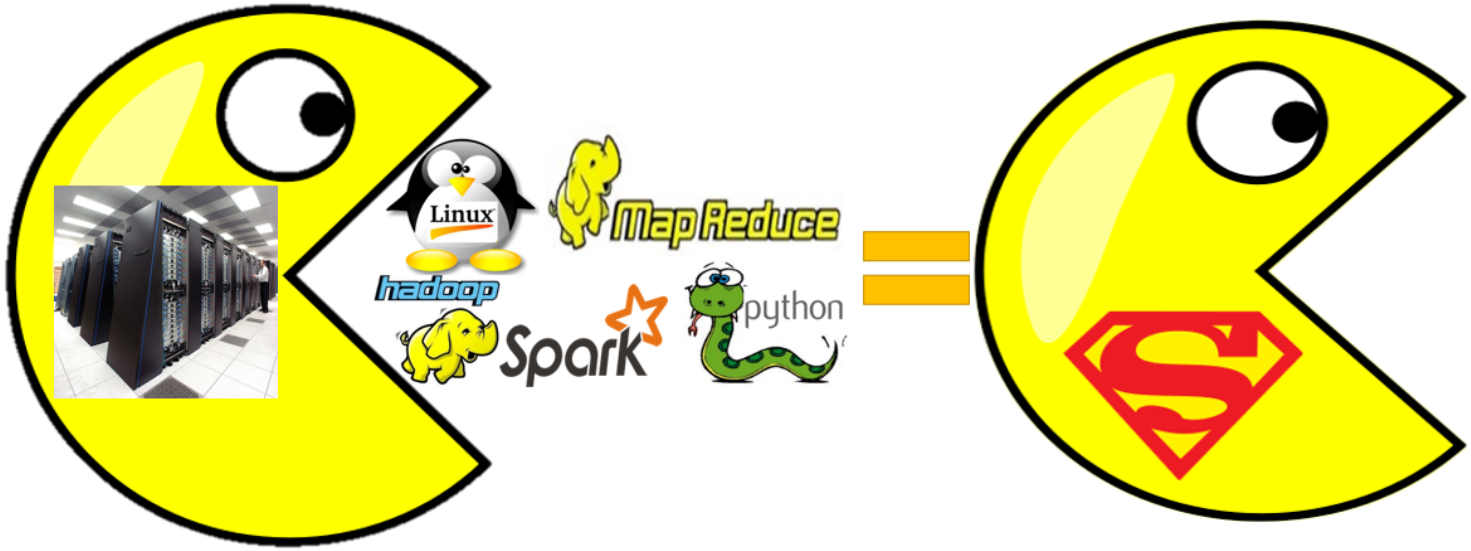

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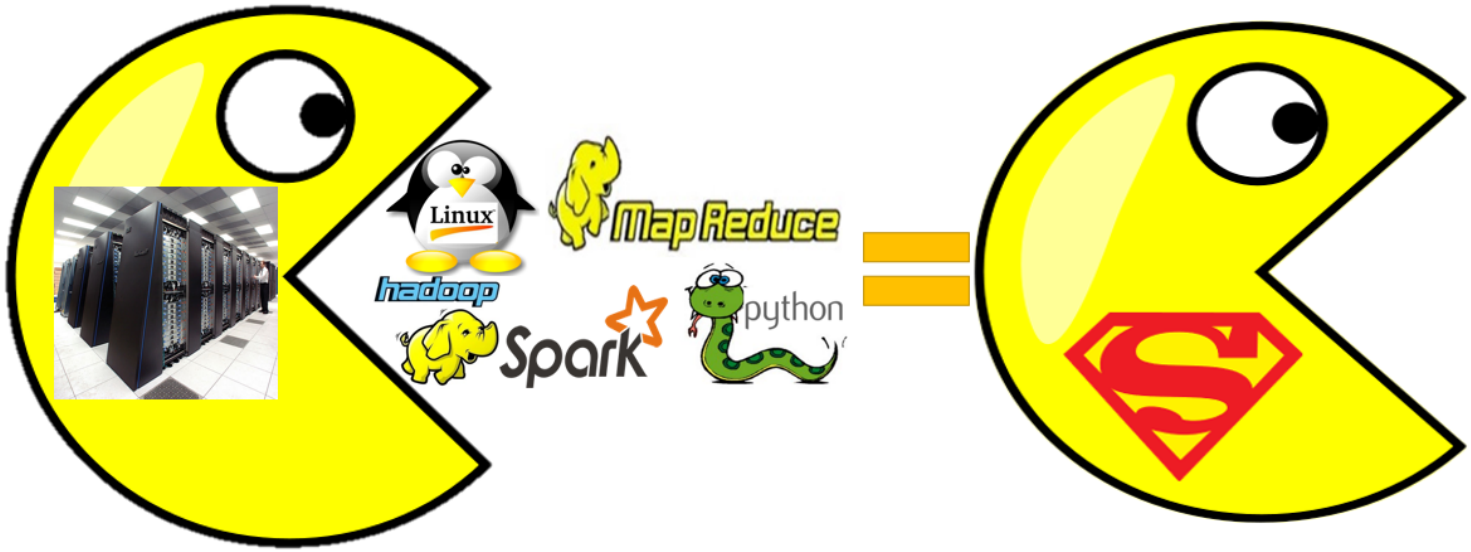

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- Statistical software designed for big data, e.g. Spark, Hadoop

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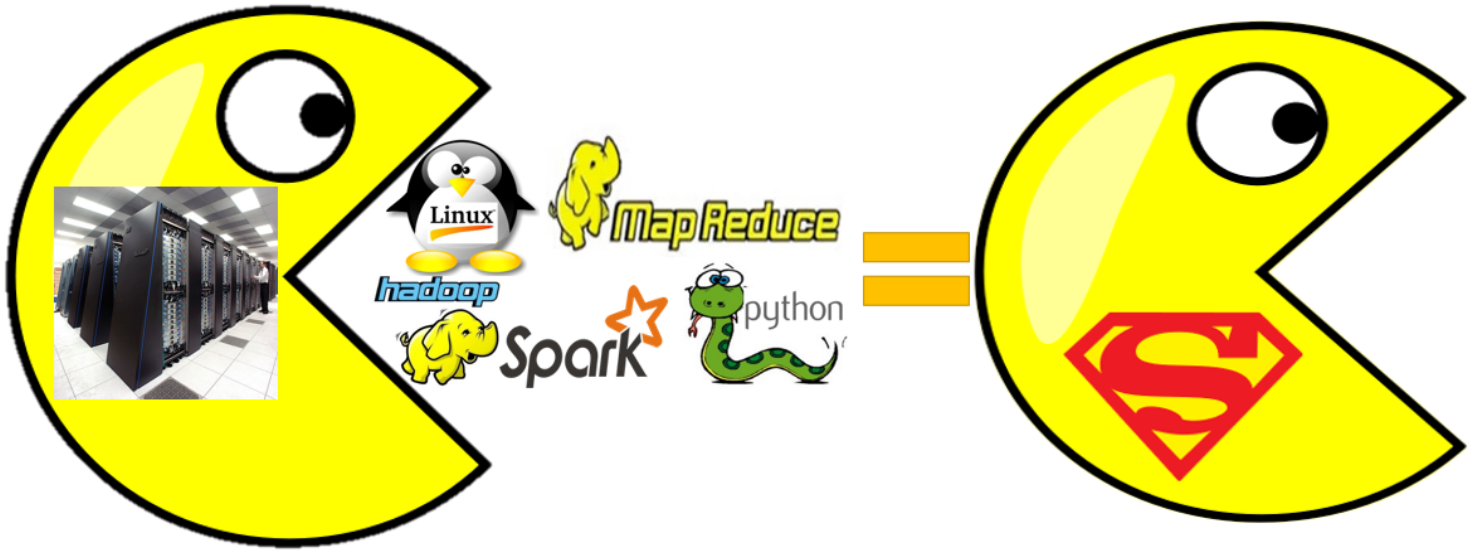


To build a Pac-superman for oracle-kNN, we need:

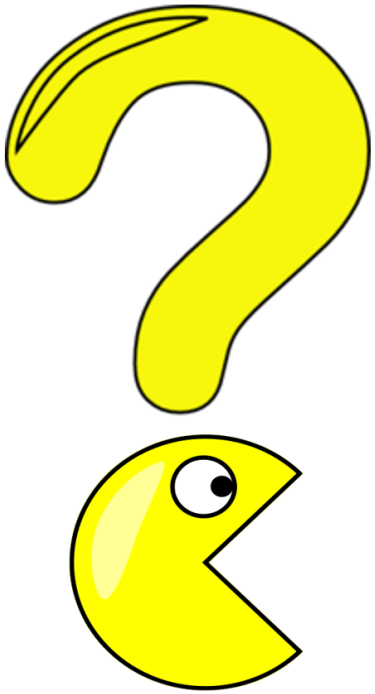
- Expensive super-computer
- Operation system, e.g. Linux
- Statistical software designed for big data, e.g. Spark, Hadoop
- Write complicated algorithms (e.g. MapReduce) with limited extendibility to other classification methods

Machine Learning Literature

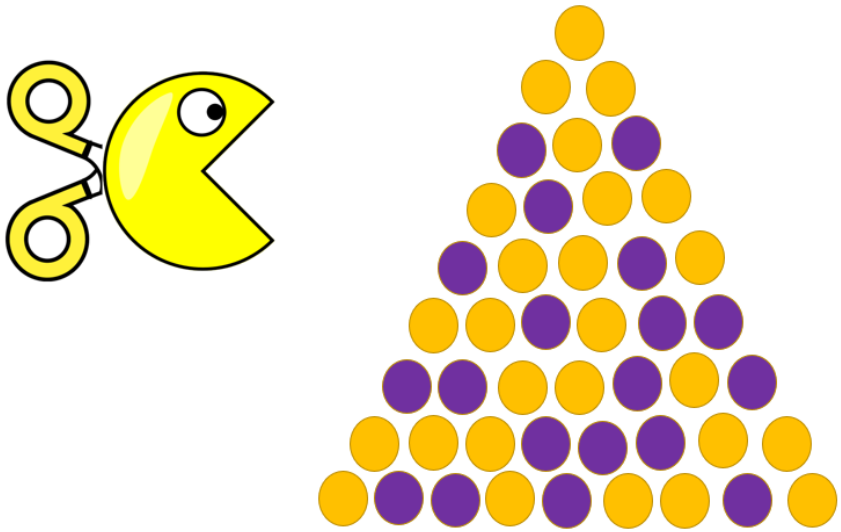
- In machine learning area, there are some nearest neighbor algorithms for big data already
  - Muja&Lowe(2014) designed an algorithm to search nearest neighbors for big data
  - Comments: complicated; without statistical gurantee; lack of extendibility
- We hope to design an algorithm framework:
  - Easy to implement
  - Strong statistical guarantee
  - More generic and expandable (e.g. easy to be applied to other classifiers (decision trees, SVM, etc)

If We Don't Have A Supercomputer...

What can we do?

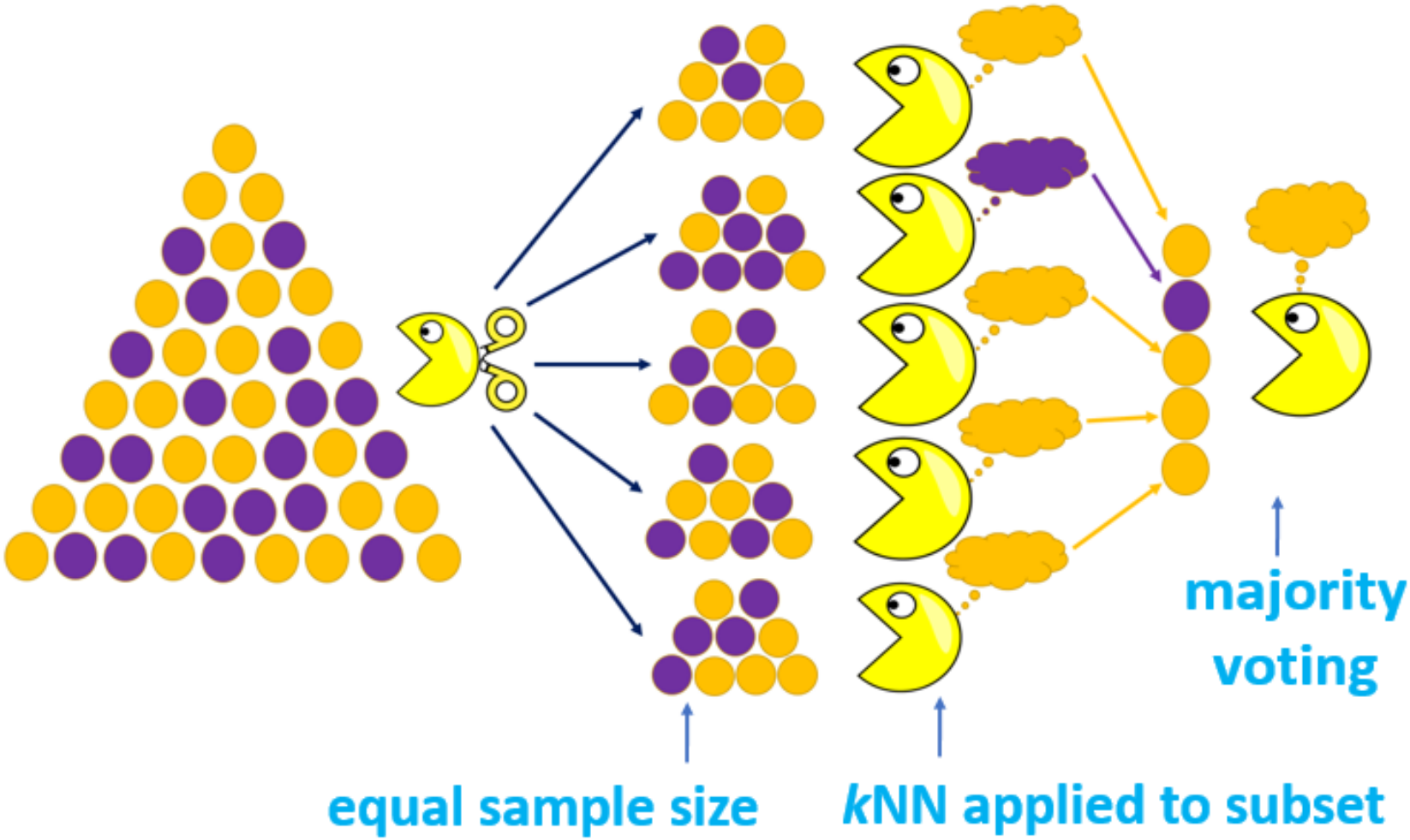


What about splitting the data?



Divide & Conquer (D&C) Framework

Goal: deliver *different* insights from regression problems.



Big-kNN for SUSY Data

- Oracle-kNN: kNN trained by the entire data
- Number of subsets: $s = N^{\gamma}$, $\gamma = 0.1, 0.2, \ldots 0.8$

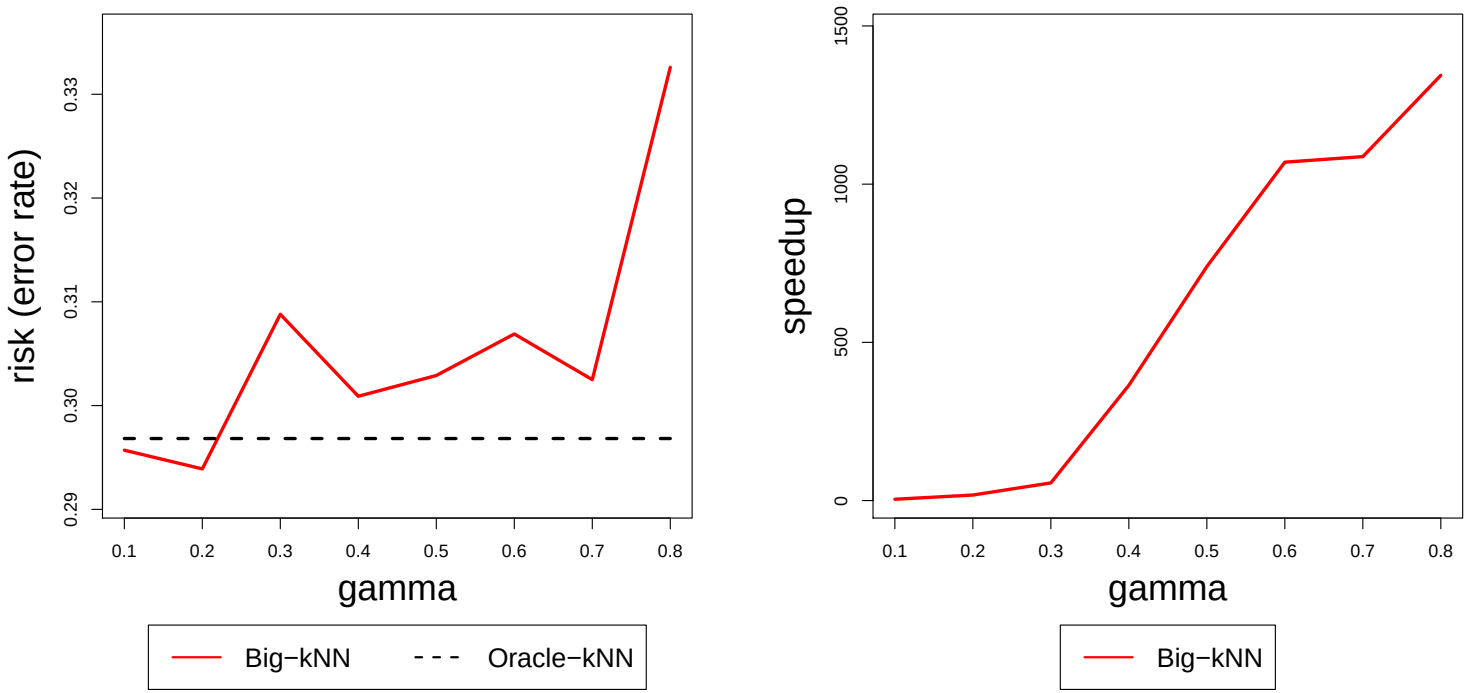
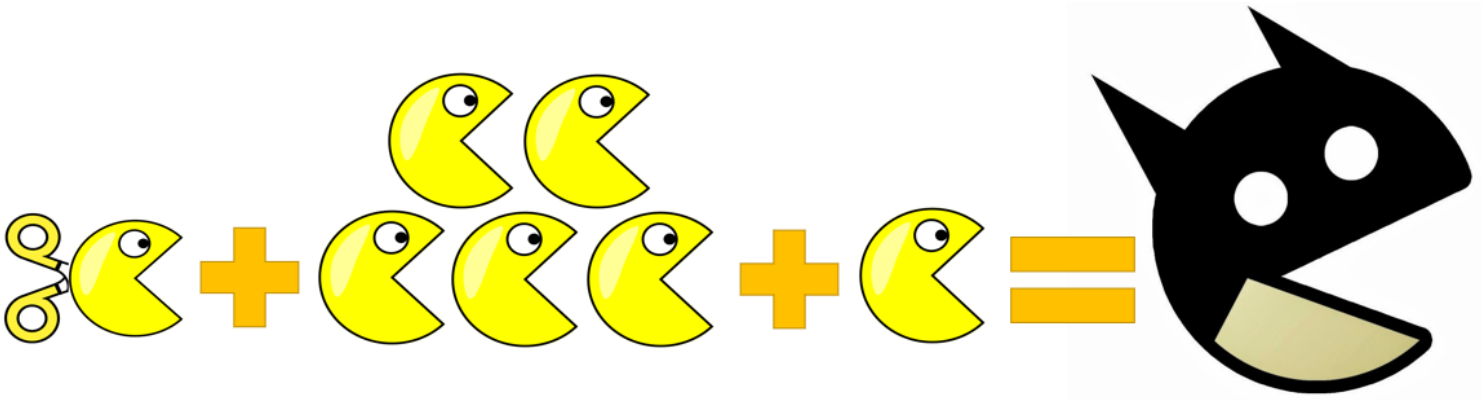


Figure: Risk and Speedup for Big-kNN.

- Risk of classifier ϕ: $R(\phi) = \mathbb{P}(\phi(X) \neq Y)$
- Speedup: running time ratio between Oracle-kNN & Big-kNN

Construction of Pac-Batman (Big Data)



We need a *statistical* understanding of Big-kNN....

Weighted Nearest Neighbor Classifiers (WNN)

Definition: WNN

In a dataset with size n, the WNN classifier assigns a weight w_{ni} on the i-th neighbor of x:

$$\widehat{\phi}_n^{w_n}(x) = \mathbb{1}\left\{\sum_{i=1}^{n} w_{ni}\mathbb{1}\{Y_{(i)} = 1\} \geq \frac{1}{2}\right\} \ s.t. \ \sum_{i=1}^{n} w_{ni} = 1,$$

When $w_{ni} = k^{-1}\mathbb{1}\{1 \leq i \leq k\}$, WNN reduces to kNN.

Construction of Big-WNN

In a big data set with size $N = sn$, the Big-WNN is constructed as:

$$\widehat{\phi}_{n,s}^{Big}(x) = \mathbb{1}\left\{ s^{-1} \sum_{j=1}^{s} \widehat{\phi}_{n}^{(j)}(x) \geq 1/2 \right\},$$

where $\widehat{\phi}_{n}^{(j)}(x)$ is the local WNN in j-th subset.

Statistical Guarantees: Classification Accuracy & Stability

- *Primary* criterion: accuracy
  - Regret=Expected Risk−Bayes Risk= $\mathbb{E}_{\mathcal{D}}\left[R(\widehat{\phi}_n)\right] - R(\phi^{\text{Bayes}})$
  - A small value of regret is preferred

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  - A small value of regret is preferred
- *Secondary* criterion: stability (Sun et al, 2016, *JASA*)

Definition: Classification Instability (CIS)

Define classification instability of a classification procedure Ψ as

$$\text{CIS}(\Psi) = \mathbb{E}_{\mathcal{D}_1,\mathcal{D}_2}\left[\mathbb{P}_X\left(\widehat{\phi}_{n1}(X) \neq \widehat{\phi}_{n2}(X)\right)\right],$$

where $\widehat{\phi}_{n1}$ and $\widehat{\phi}_{n2}$ are the classifiers trained from the same classification procedure Ψ based on $\mathcal{D}_1$ and $\mathcal{D}_2$ with the same distribution.

- A small value of CIS is preferred

Asymptotic Regret of Big-WNN

Theorem (Regret of Big-WNN)

Under regularity assumptions, with s upper bounded by the subset size n, we have as $n, s \to \infty$,

$$Regret\,(Big\text{-}WNN) \approx B_1 s^{-1} \sum_{i=1}^{n} w_{ni}^2 + B_2 \Big(\sum_{i=1}^{n} \frac{\alpha_i w_{ni}}{n^{2/d}} \Big)^2,$$

where $\alpha_i = i^{1+\frac{2}{d}} - (i-1)^{1+\frac{2}{d}}$, w_{ni} are the local weights. The constants B_1 and B_2 are distribution-dependent quantities.

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Variance part

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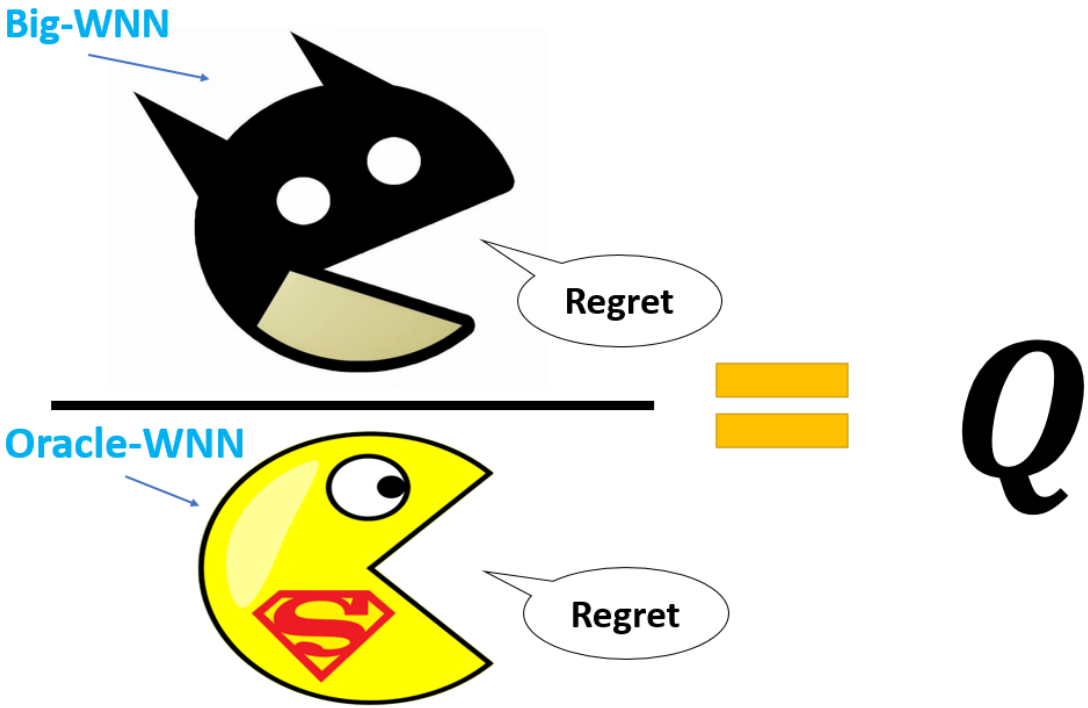
Variance part

Bias part

Asymptotic Regret Comparison



Round 1

Asymptotic Regret Comparison

Theorem (Regret Ratio of Big-WNN and Oracle-WNN)

Given an Oracle-WNN classifier, we can always design a Big-WNN by adjusting its weights according to those in the oracle version s.t.

$$\frac{Regret\left(Big\text{-}WNN\right)}{Regret\left(Oracle\text{-}WNN\right)} \to Q,$$

where $Q = \left(\frac{\pi}{2}\right)^{\frac{4}{d+4}}$ *and* $1 < Q < 2$.

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- E.g., in Big-kNN case, we set $k = \lfloor (\frac{\pi}{2})^{\frac{d}{d+4}} \frac{k^O}{s} \rfloor$ given the oracle k^O. We need a multiplicative constant $(\frac{\pi}{2})^{\frac{d}{d+4}}$!

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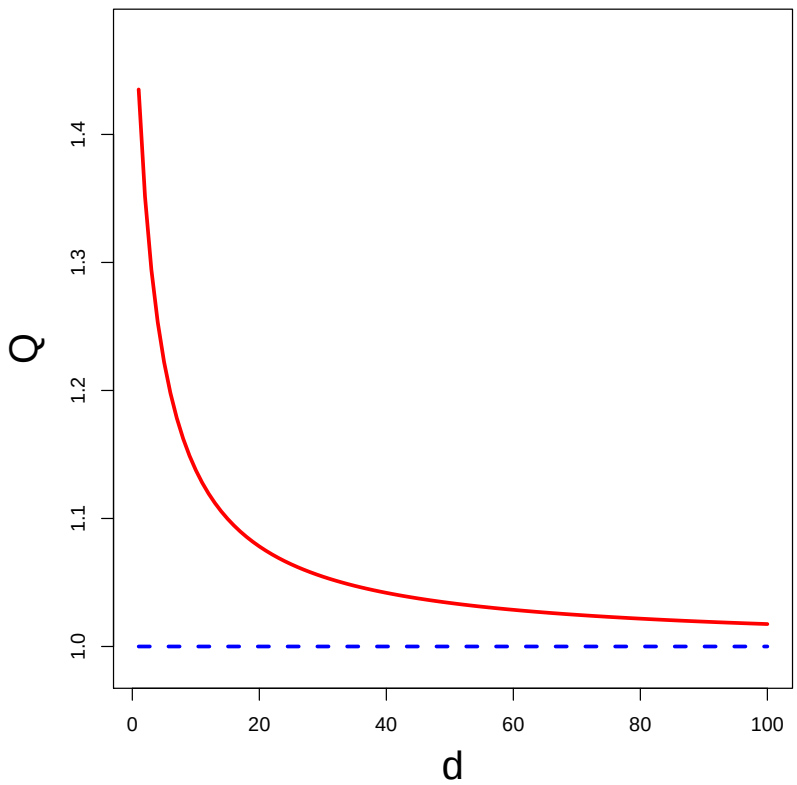
- We name Q the *Majority Voting (MV) Constant*.

Majority Voting Constant

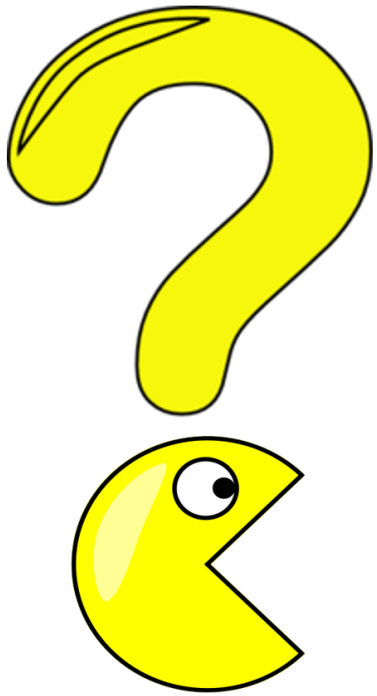
MV constant monotonically decreases to one as d increases



For example:

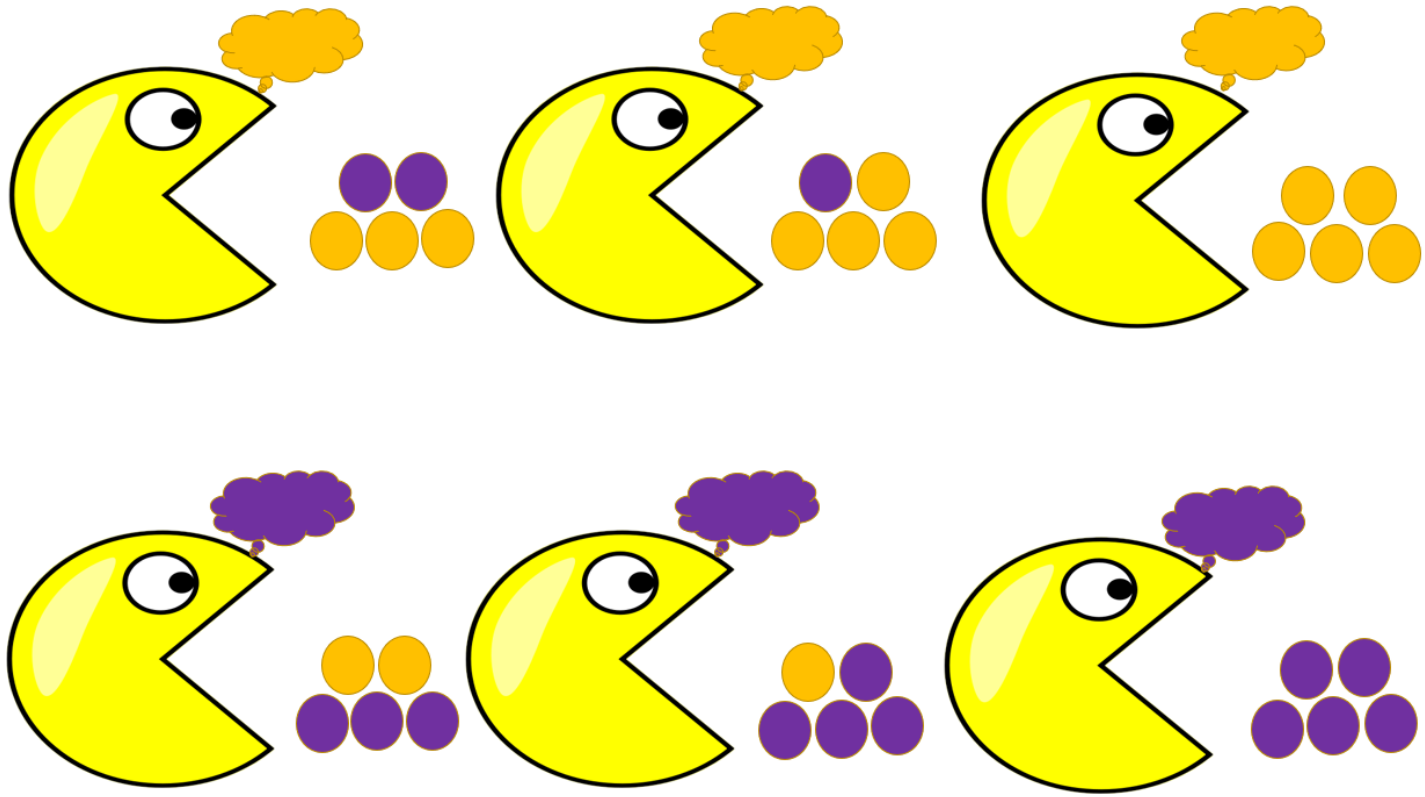
- d=1, Q=1.44
- d=2, Q=1.35
- d=5, Q=1.22
- d=10, Q=1.14
- d=20, Q=1.08
- d=50, Q=1.03
- d=100, Q=1.02

Why is there statistical accuracy loss?



Statistical Accuracy Loss due to Majority Voting

Accuracy loss due to the transformation from (continuous) percentage to (discrete) 0-1 label



Only one majority voting in oracle classifier

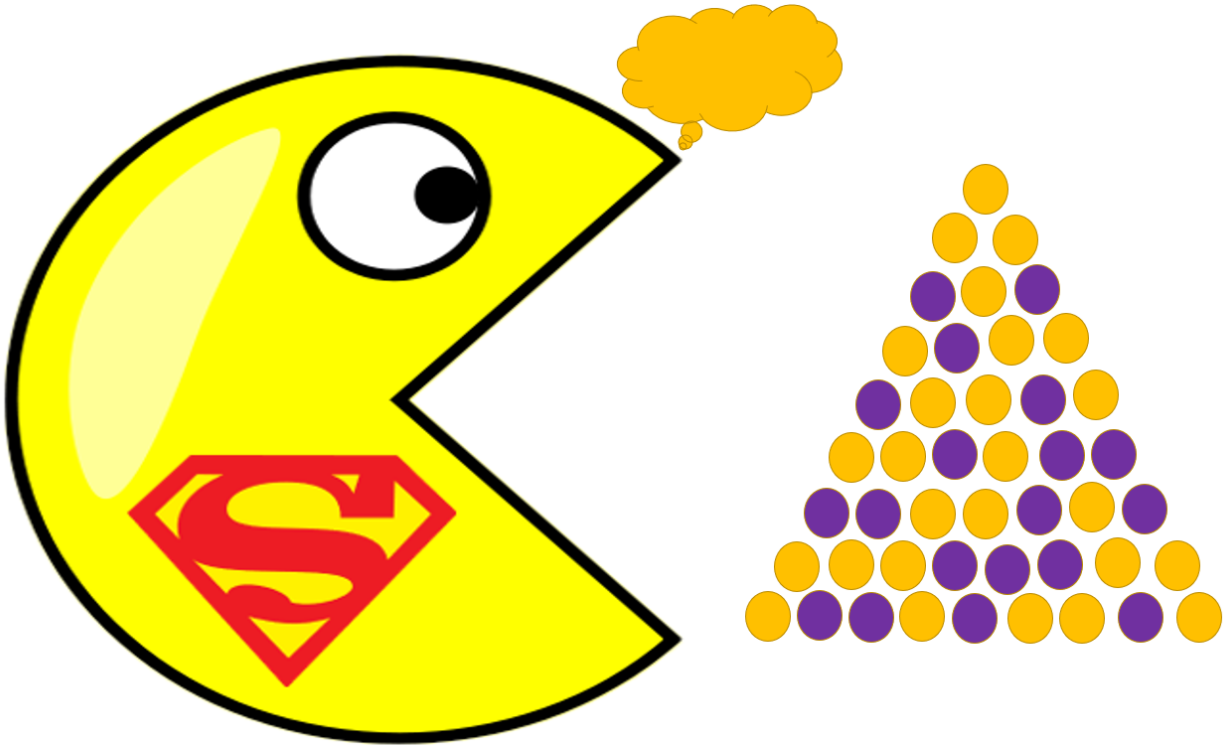
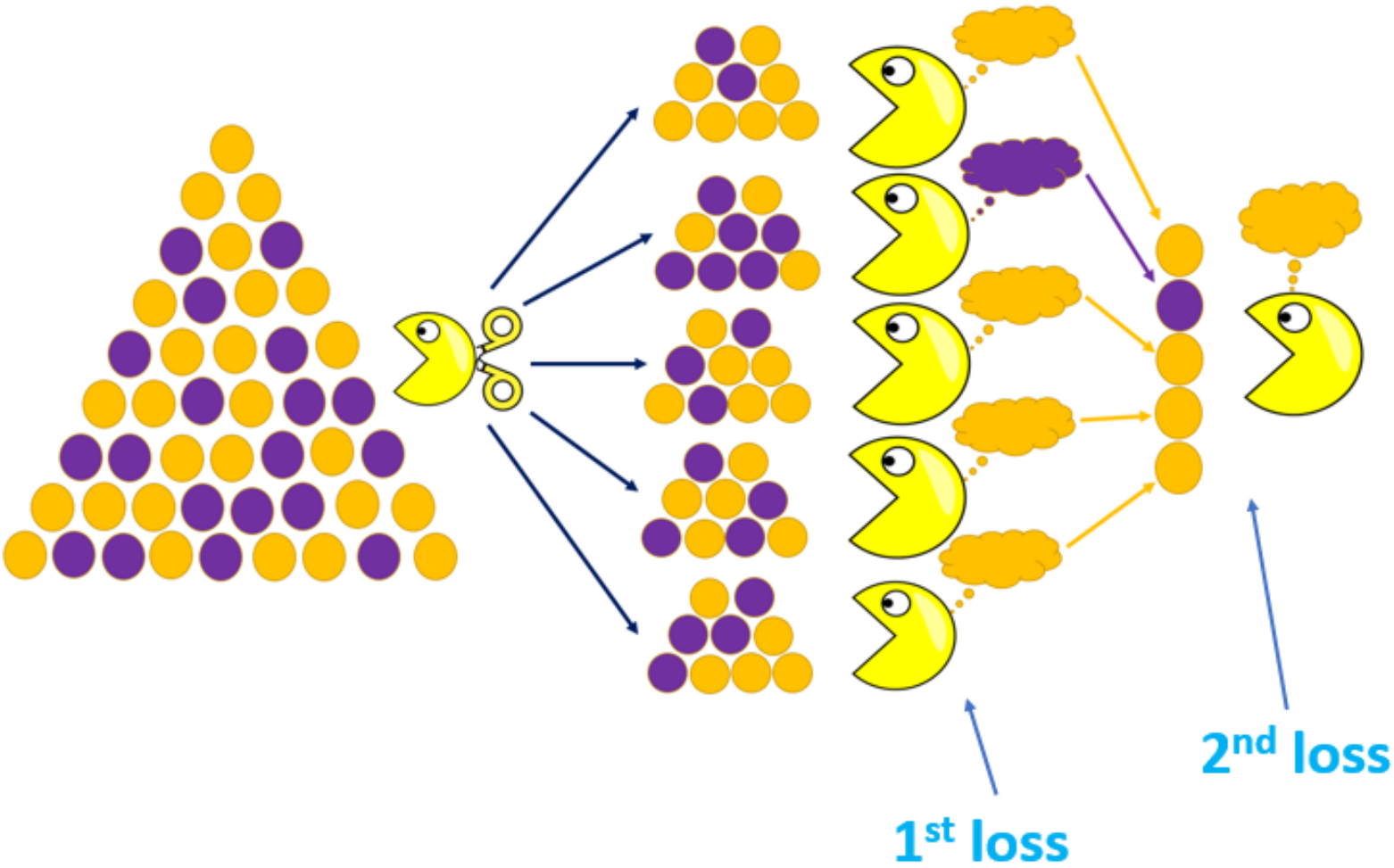
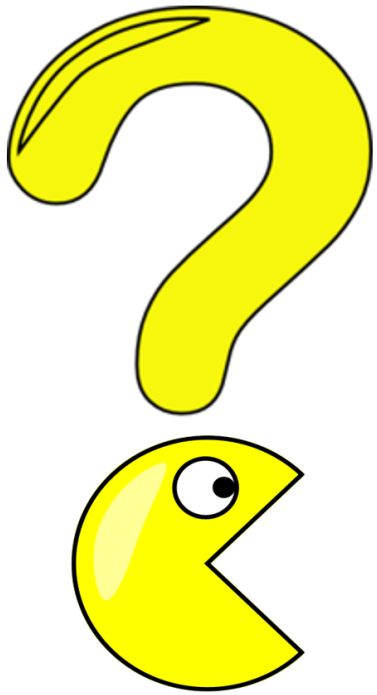


Figure: I'm Pac-Superman!

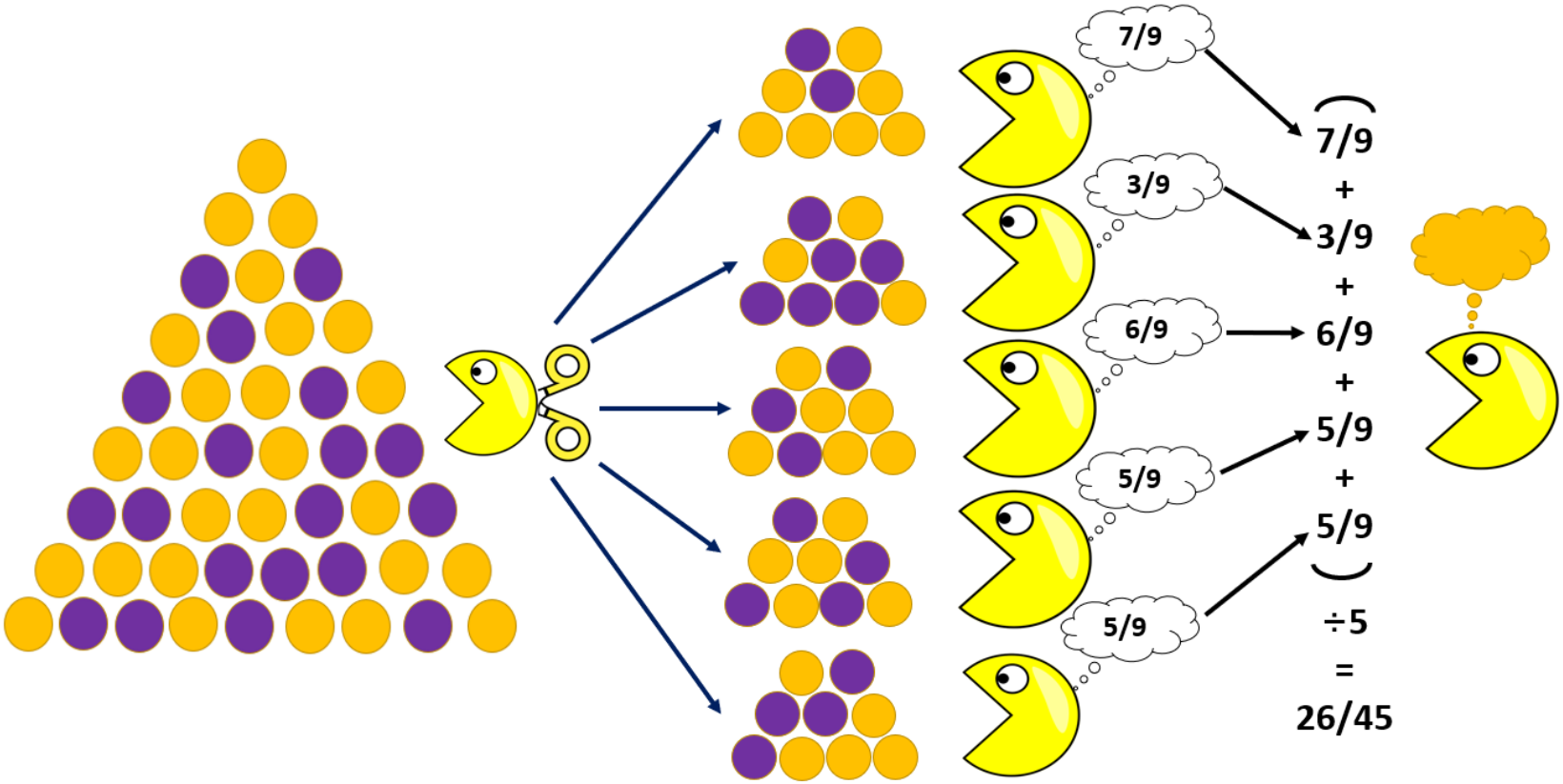
Majority Voting/Accuracy Loss Twice in D&C Framework



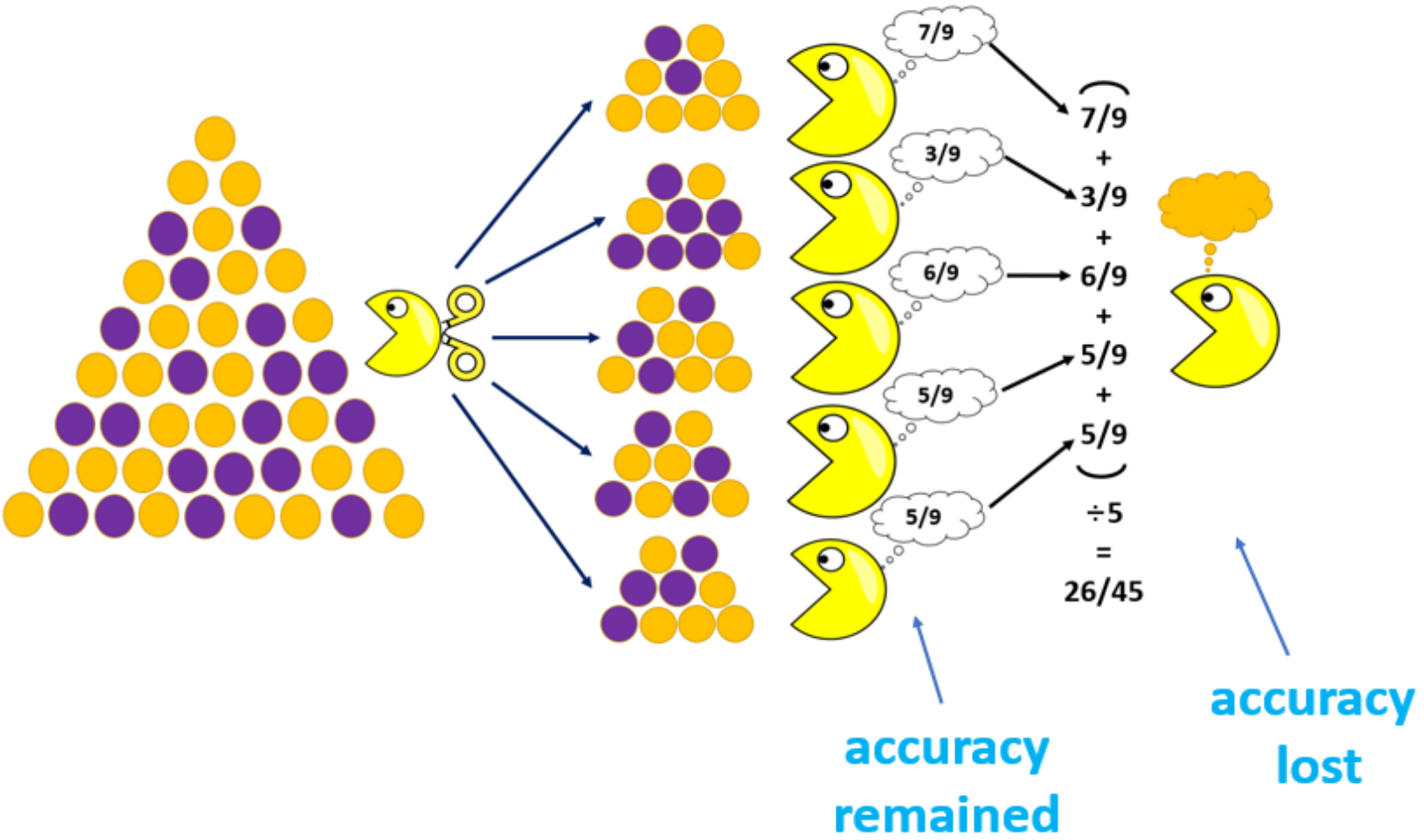
Is it possible to apply majority voting once in D&C?



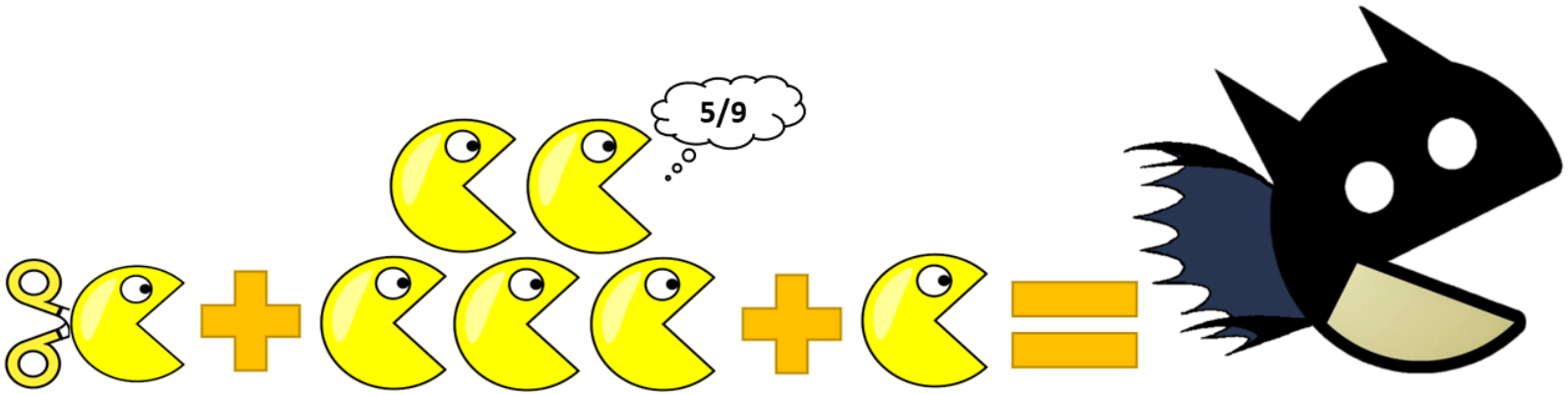
A Continuous Version of D&C Framework



Only Loss Once in the Continuous Version



Construction of Pac-**Bat**man (Continuous Version)



Continuous Version of Big-WNN (C-Big-WNN)

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$$\widehat{\phi}_{n,s}^{CBig}(x) = \mathbb{1}\left\{\frac{1}{s}\sum_{j=1}^{s}\widehat{S}_n^{(j)}(x) \geq 1/2\right\},$$

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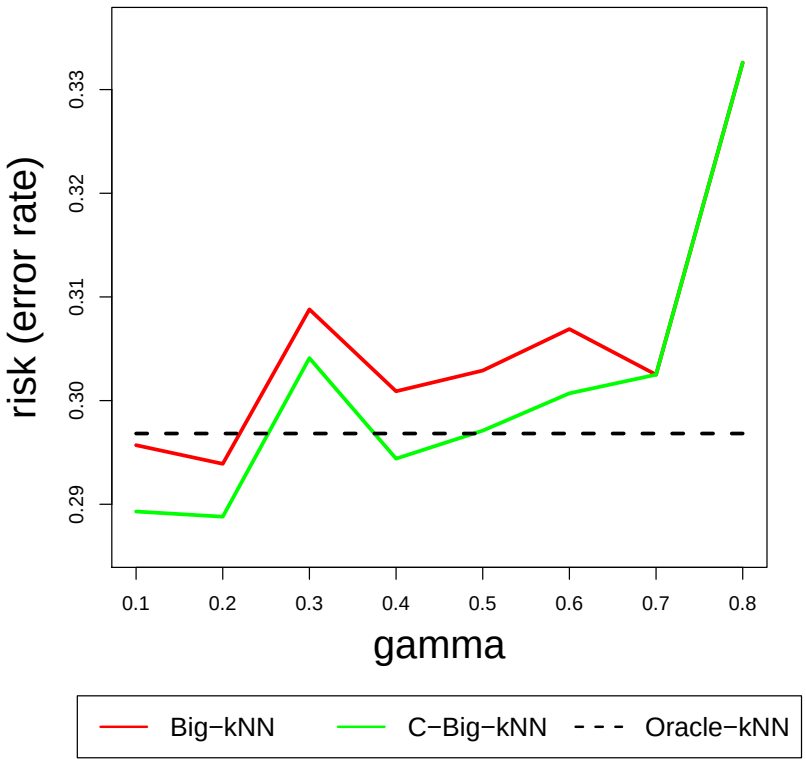
C-Big-kNN for SUSY Data



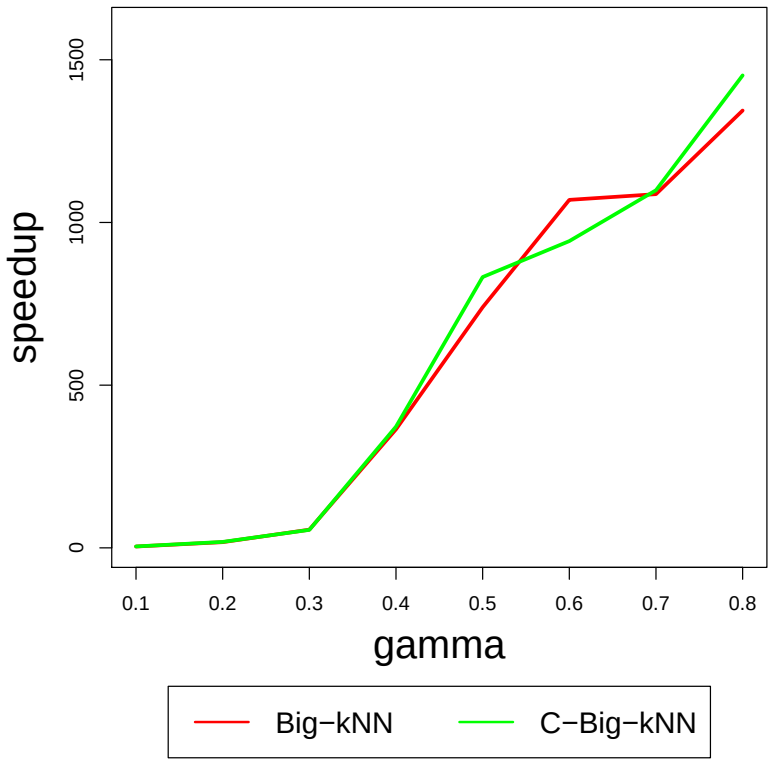
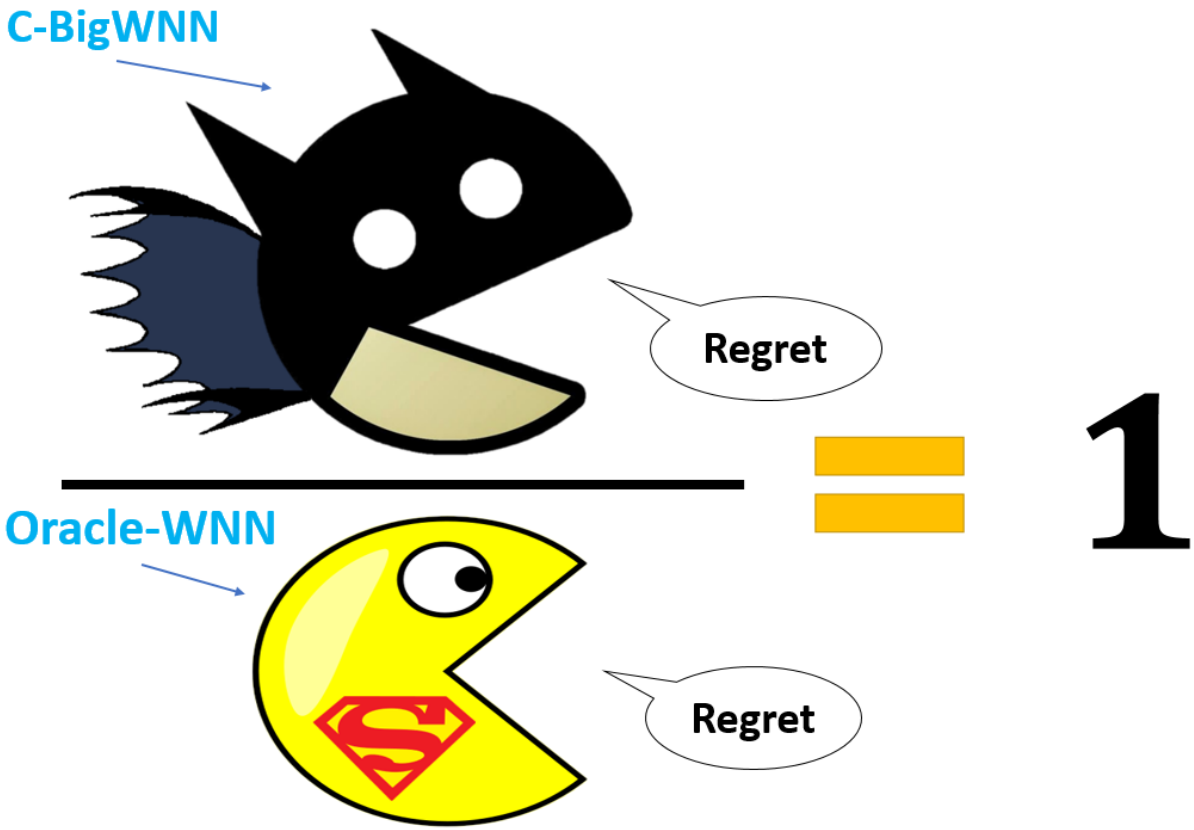


Figure: Risk and Speedup for Big-kNN and C-Big-kNN.

Asymptotic Regret Comparison



Round 2

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- E.g., in the C-Big-kNN case, we can set $k = \lfloor \frac{k^O}{s} \rfloor$ given the oracle k^O. There is no multiplicative constant!
- Note that this theorem can be directly applied to the optimally weighted NN (Samworth, 2012, *AoS*), i.e., OWNN, whose weights are optimized to lead to the minimal regret.

Practical Consideration: Speed vs Accuracy

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- It is time consuming to apply OWNN in each subset although it leads to the minimal regret
- Rather, it is more easier and faster to implement kNN in each subset (with accuracy loss, though)
- What is the statistical price (in terms of accuracy and stability) in order to trade accuracy with speed?

Theorem (Statistical Price)

We can design an optimal C-Big-kNN by setting its weights as $k = \lfloor \frac{k^{O,opt}}{s} \rfloor$ *s.t.*

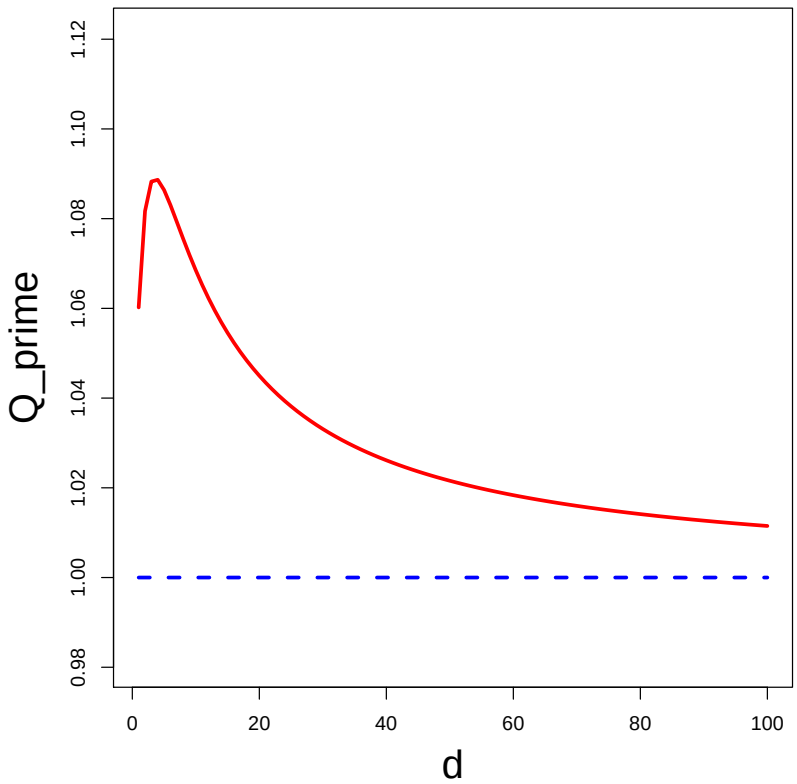
$$\frac{Regret(\,Optimal\ C\text{-}Big\text{-}kNN)}{Regret(\,Oracle\text{-}OWNN)} \to Q',$$

$$\frac{CIS(\,Optimal\ C\text{-}Big\text{-}kNN)}{CIS(\,Oracle\text{-}OWNN)} \to \sqrt{Q'},$$

where $Q' = 2^{-4/d+4}(\frac{d+4}{d+2})^{(2d+4)/(d+4)}$ *and* $1 < Q' < 2$. *Here,* $k^{O,opt}$ *minimizes the regret of Oracle-kNN.*

Interestingly, both Q and Q' only depend on data dimension!

Q' converges to one as d grows in a unimodal way



For example:

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- d=5, Q=1.08
- d=10, Q=1.07
- d=20, Q=1.04
- d=50, Q=1.02
- d=100, Q=1.01

The worst dimension is $d^* = 4 \Longrightarrow Q^* = 1.089$.

Simulation Analysis – kNN

Consider the classification problem for Big-kNN and C-Big-kNN:

- Sample size: $N = 27,000$
- Dimensions: $d = 6, 8$
- $P_0 \sim N(0_d, \mathbb{I}_d)$ and $P_1 \sim N(\frac{2}{\sqrt{d}} 1_d, \mathbb{I}_d)$
- Prior class probability: $\pi_1 = Pr(Y = 1) = 1/3$
- Number of neighbors in Oracle-kNN: $k^O = N^{0.7}$
- Number of subsamples in D&C: $s = N^\gamma$, $\gamma = 0.1, 0.2, \ldots 0.8$
- Number of neighbors in Big-kNN: $k^d = \lfloor (\frac{\pi}{2})^{\frac{d}{d+4}} \frac{k^O}{s} \rfloor$
- Number of neighbors in C-Big-kNN: $k^c = \lfloor \frac{k^O}{s} \rfloor$

Simulation Analysis – Empirical Risk

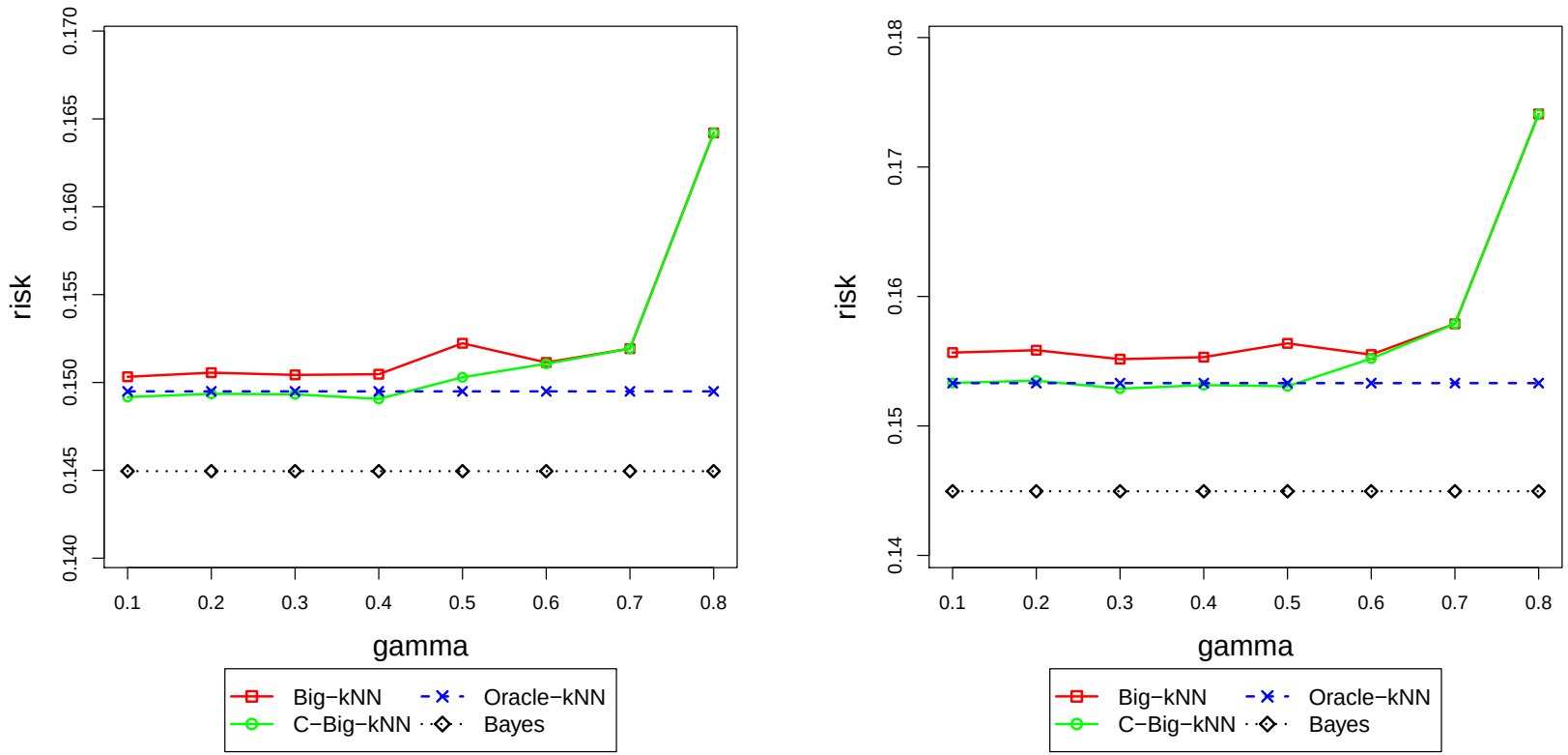


Figure: Empirical Risk (Testing Error). Left/Right: $d = 6/8$.

Simulation Analysis – Running Time

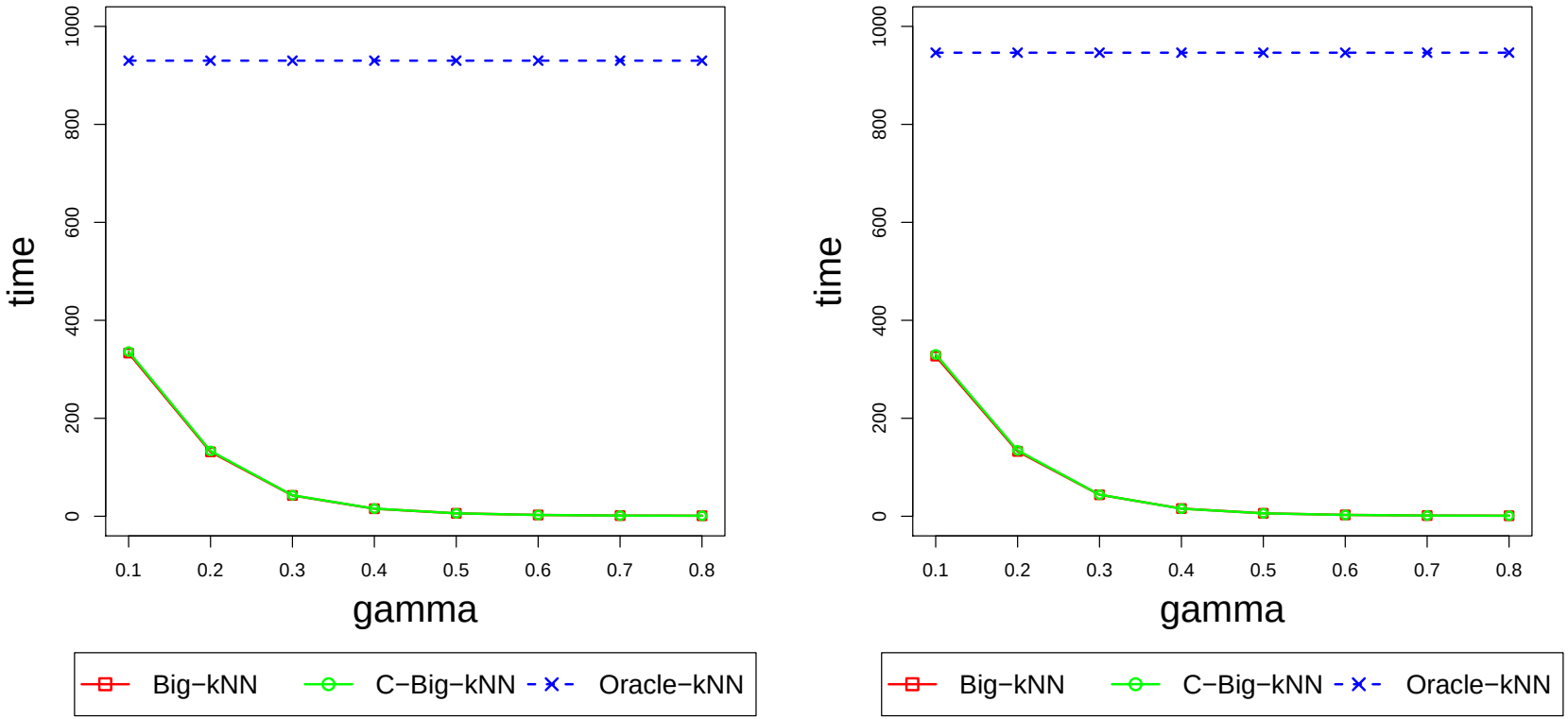


Figure: Running Time. Left/Right: $d = 6/8$.

Simulation Analysis – Empirical Regret Ratio

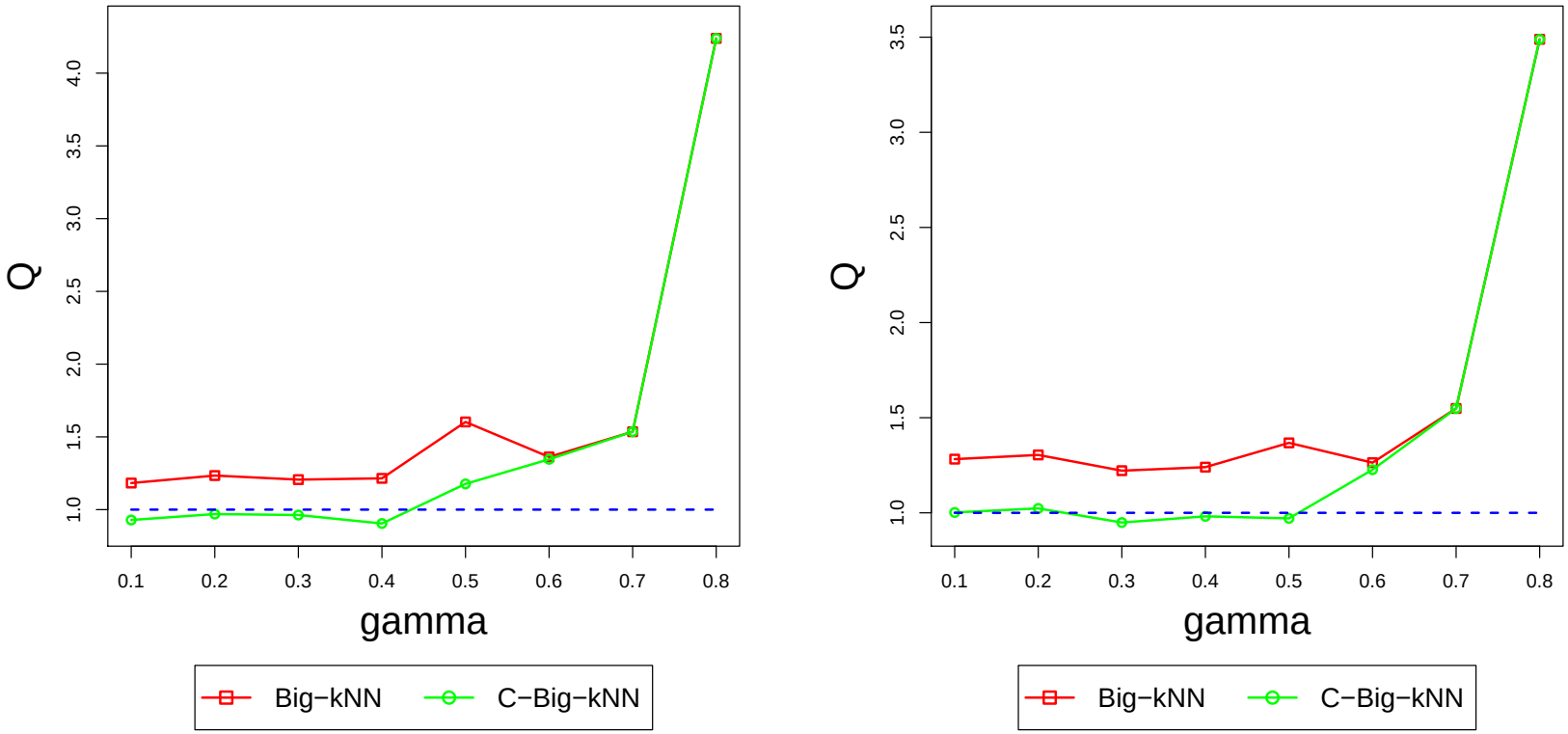


Figure: Empirical Ratio of Regret. Left/Right: $d = 6/8$.

- Q: Regret(Big-kNN)/Regret(Oracle-kNN) or Regret(C-Big-kNN)/Regret(Oracle-kNN)

Simulation Analysis – Empirical CIS

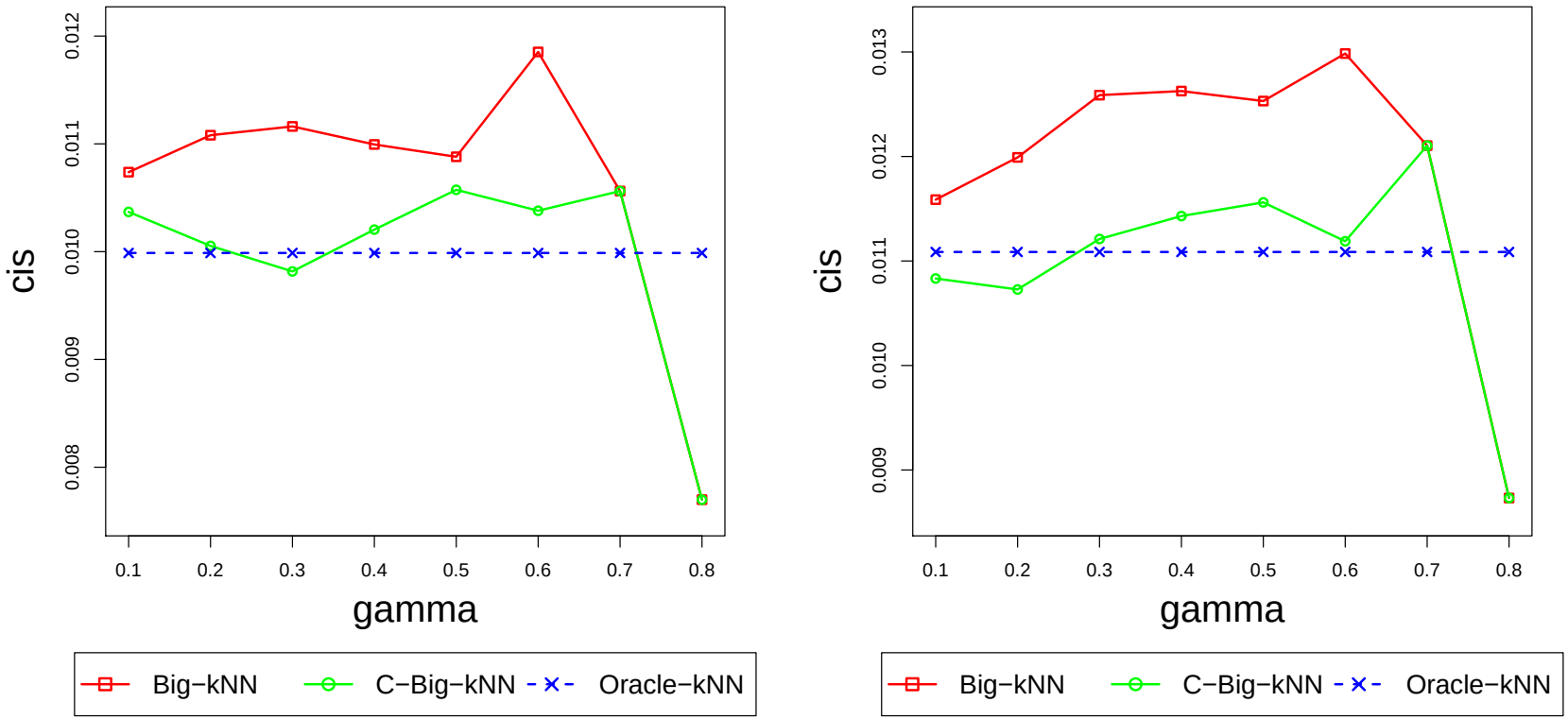
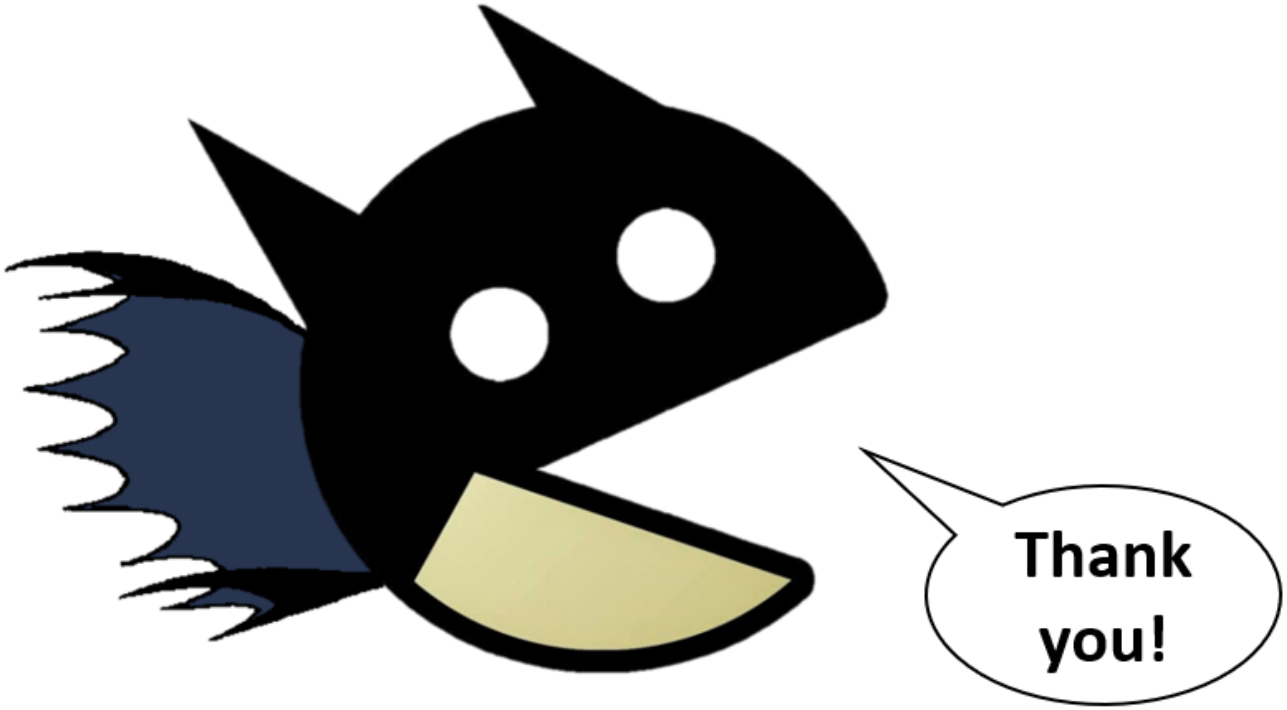


Figure: Empirical CIS. Left/Right: $d = 6/8$.

Real Data Analysis – UCI Machine Learning Repository

Data	Size	Dim	Big-kNN	C-Big-kNN	Oracle-kNN	Speedup
htru2	17898	8	3.72	3.36	**3.34**	21.27
gisette	6000	5000	12.86	**10.77**	10.78	12.83
musk1	476	166	36.43	**33.87**	35.71	3.6
musk2	6598	166	10.43	**9.98**	10.14	14.68
occup	20560	6	5.09	**4.87**	5.19	20.31
credit	30000	24	21.85	**21.37**	21.5	22.44
SUSY	5000000	18	30.66	30.08	**30.01**	68.45

Table: Test error (Risk): Big-kNN compared to Oracle-kNN in real datasets. Best performance is shown in bold-face. The speedup factor is defined as computing time of Oracle-kNN divided by the time of the slower Big-kNN method. Oracle $k = N^{0.7}$, number of subsets $s = N^{0.3}$.


Thank
you!