K-Nearest Neighbors

K Sri Rama Murty

IIT Hyderabad

ksrm@ee.iith.ac.in

• Classification is a supervised learning problem

- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$

- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$
- Given a set of labeled data $[\mathbf{x}_n, y_n]$, $n = 1, 2, \dots, N$ for training, classify a new instance \mathbf{x}_0

- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$
- Given a set of labeled data $[\mathbf{x}_n, y_n]$, $n = 1, 2, \dots, N$ for training, classify a new instance \mathbf{x}_0
- KNN classification algorithm

- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$
- Given a set of labeled data $[\mathbf{x}_n, y_n]$, $n = 1, 2, \dots, N$ for training, classify a new instance \mathbf{x}_0
- KNN classification algorithm
 - Evaluate distance of \mathbf{x}_0 to all points \mathbf{x}_n , $n = 1, 2, \dots N$ in training set

$$d_n = ||\mathbf{x}_n - \mathbf{x}_0||_p$$

$$d_n = 1 - \frac{\mathbf{x}_n^\mathsf{T} \mathbf{x}_0}{||\mathbf{x}_n|| \ ||\mathbf{x}_0||}$$

- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$
- Given a set of labeled data $[\mathbf{x}_n, y_n]$, $n = 1, 2, \dots, N$ for training, classify a new instance \mathbf{x}_0
- KNN classification algorithm
 - Evaluate distance of \mathbf{x}_0 to all points \mathbf{x}_n , $n=1,2,\cdots N$ in training set

$$d_n = ||\mathbf{x}_n - \mathbf{x}_0||_p$$

$$d_n = 1 - \frac{\mathbf{x}_n^\mathsf{T} \mathbf{x}_0}{||\mathbf{x}_n|| \ ||\mathbf{x}_0||}$$

ullet Sort the distances and identify K nearest neighbors - X_{NN}

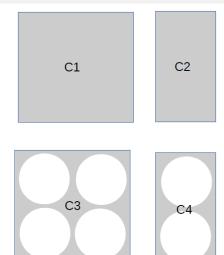
- Classification is a supervised learning problem
- In classification, the target variable admits a discrete set of values. eg. $[(x_1=6 \text{ ft}, x_2=65 \text{ kg}), y=A], [(x_1=3.4 \text{ ft}, x_2=18 \text{ kg}), y=K]$
- Given a set of labeled data $[\mathbf{x}_n, y_n]$, $n = 1, 2, \dots, N$ for training, classify a new instance \mathbf{x}_0
- KNN classification algorithm
 - Evaluate distance of \mathbf{x}_0 to all points \mathbf{x}_n , $n=1,2,\cdots N$ in training set

$$d_n = ||\mathbf{x}_n - \mathbf{x}_0||_p$$

$$d_n = 1 - \frac{\mathbf{x}_n^\mathsf{T} \mathbf{x}_0}{||\mathbf{x}_n|| \ ||\mathbf{x}_0||}$$

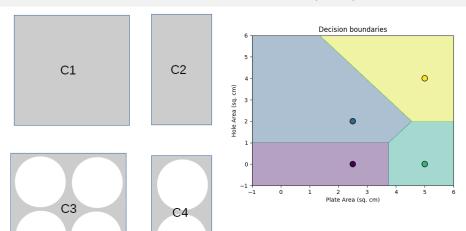
- Sort the distances and identify K nearest neighbors X_{NN}
- Assign output label y_0 for test point \mathbf{x}_0 from labels of y_{NN} Voting

Geometry of KNN Decision Boundaries (k=1)



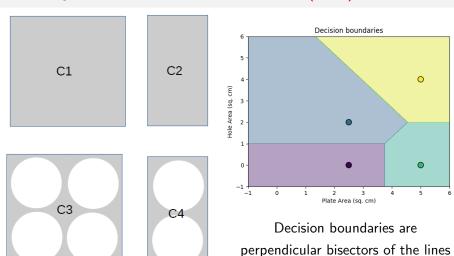
Steel-plate classification

Geometry of KNN Decision Boundaries (k=1)



Steel-plate classification

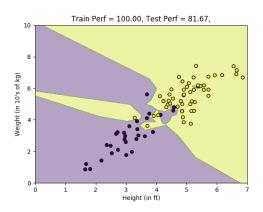
Geometry of KNN Decision Boundaries (k=1)

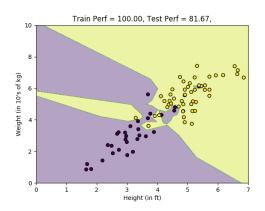


Steel-plate classification

4□ > 4個 > 4 ≥ > 4 ≥ > ≥ 90

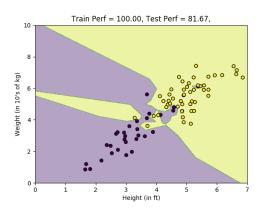
joining nearest competitors!



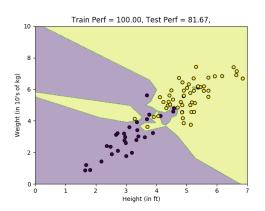


• 50 points from adult-class and 30 points from kid-class

K Sri Rama Murty (IITH)

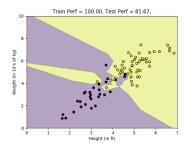


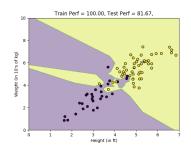
- 50 points from adult-class and 30 points from kid-class
- ullet Big difference between train and test performances (k=1 is a overfit)

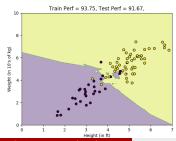


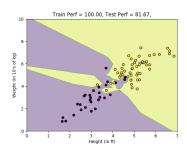
- 50 points from adult-class and 30 points from kid-class
- ullet Big difference between train and test performances (k=1 is a overfit)
- In a KNN-classifier, the decision regions are typically nonconvex

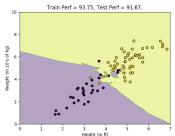
4/21

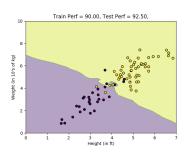


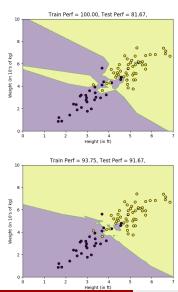


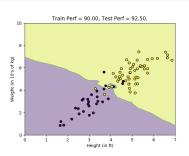


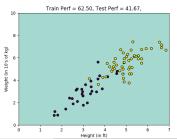


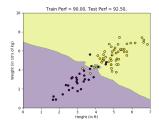


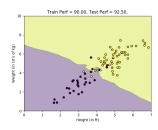


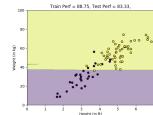


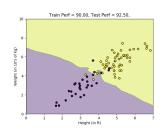


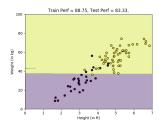






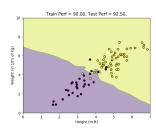


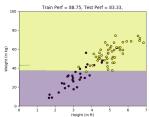




Distance between two points x and y is

$$d_{xy} = \sqrt{(x_h - y_h)^2 + (x_w - y_w)^2}$$

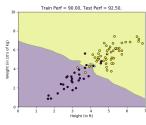


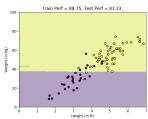


Distance between two points x and y is

$$d_{xy} = \sqrt{(x_h - y_h)^2 + (x_w - y_w)^2}$$

 Contribution of a dimension to distance is proportional to its variance

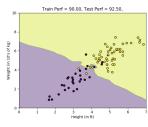


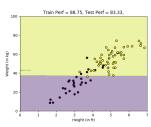


Distance between two points x and y is

$$d_{xy} = \sqrt{(x_h - y_h)^2 + (x_w - y_w)^2}$$

- Contribution of a dimension to distance is proportional to its variance
- When weight is in kg, distance is dominated by it (horizontal boundary)





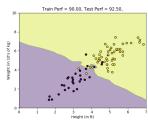
Distance between two points x and y is

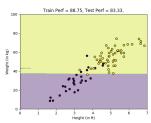
$$d_{xy} = \sqrt{(x_h - y_h)^2 + (x_w - y_w)^2}$$

- Contribution of a dimension to distance is proportional to its variance
- When weight is in kg, distance is dominated by it (horizontal boundary)
- Normalize each dim. to unit variance

$$\tilde{x}_{w} = \frac{x_{w} - \mu_{w}}{\sigma_{w}}$$

$$\sigma_w^2 = \frac{1}{N} \sum_{n=1}^{N} (x_{nw} - \mu_w)^2 \quad \mu_w = \frac{1}{N} \sum_{n=1}^{N} x_{nw}$$





• Distance between two points **x** and **y** is

$$d_{xy} = \sqrt{(x_h - y_h)^2 + (x_w - y_w)^2}$$

- Contribution of a dimension to distance is proportional to its variance
- When weight is in kg, distance is dominated by it (horizontal boundary)
- Normalize each dim. to unit variance

$$\tilde{x}_{w} = \frac{x_{w} - \mu_{w}}{\sigma_{w}}$$

$$\sigma_w^2 = \frac{1}{N} \sum_{n=1}^{N} (x_{nw} - \mu_w)^2 \quad \mu_w = \frac{1}{N} \sum_{n=1}^{N} x_{nw}$$

• This process is called data whitening

• Regression is a supervised learning problem

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
у	58	53	63	65	60	50	52	55	61	49	?

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
У	58	53	63	65	60	50	52	55	61	49	?

• Average of the *k*-nearest neighbors in the training data.

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
У	58	53	63	65	60	50	52	55	61	49	?

- Average of the *k*-nearest neighbors in the training data.
- (k = 1) NN $\{(5.7, 65)\}$: $y_{11} = 65$ (overfit high variance)

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
У	58	53	63	65	60	50	52	55	61	49	?

- Average of the *k*-nearest neighbors in the training data.
- (k = 1) NN $\{(5.7, 65)\}$: $y_{11} = 65$ (overfit high variance)
- (k = 3) NN $\{(5.7, 65), (5.8, 63), (5.4, 60)\}$: $y_{11} = 62.66$

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
У	58	53	63	65	60	50	52	55	61	49	?

- Average of the *k*-nearest neighbors in the training data.
- (k = 1) NN $\{(5.7, 65)\}$: $y_{11} = 65$ (overfit high variance)
- (k = 3) NN $\{(5.7, 65), (5.8, 63), (5.4, 60)\}$: $y_{11} = 62.66$
- ullet (k=10) assigns average weight irrespective of test height (high bias)

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
У	58	53	63	65	60	50	52	55	61	49	?

- Average of the *k*-nearest neighbors in the training data.
- (k = 1) NN $\{(5.7, 65)\}$: $y_{11} = 65$ (overfit high variance)
- (k = 3) NN $\{(5.7, 65), (5.8, 63), (5.4, 60)\}$: $y_{11} = 62.66$
- \bullet (k=10) assigns average weight irrespective of test height (high bias)
- KNN-regression gives equal importance to all neighbors

- Regression is a supervised learning problem
- In regression, the target variable admits continuous values

S.No	1	2	3	4	5	6	7	8	9	10	t
X	5.2	4.8	5.8	5.7	5.4	5.1	4.9	5.3	5.9	4.5	5.6
у	58	53	63	65	60	50	52	55	61	49	?

- Average of the *k*-nearest neighbors in the training data.
- (k = 1) NN $\{(5.7, 65)\}$: $y_{11} = 65$ (overfit high variance)
- (k = 3) NN $\{(5.7, 65), (5.8, 63), (5.4, 60)\}$: $y_{11} = 62.66$
- \bullet (k=10) assigns average weight irrespective of test height (high bias)
- KNN-regression gives equal importance to all neighbors
- Assign higher weightage to closer neighbors

$$y_{t} = \frac{\sum_{n=0}^{N} k(x_{n}, x_{t}) y_{n}}{\sum_{n=0}^{N} k(x_{n}, x_{t})}$$

• Weighted k-NN regression: the unknown quantity y_t is estimated as

$$y_{t} = \frac{\sum_{n=0}^{N} k(x_{n}, x_{t}) y_{n}}{\sum_{n=0}^{N} k(x_{n}, x_{t})}$$

• $k(x_n, x_t)$ denotes similarity between x_n and x_t

$$y_t = \frac{\sum\limits_{n=0}^{N} k(x_n, x_t) y_n}{\sum\limits_{n=0}^{N} k(x_n, x_t)}$$

- $k(x_n, x_t)$ denotes similarity between x_n and x_t
- Similarity (or inverse distance) as weight to give preference to NNs

$$y_{t} = \frac{\sum_{n=0}^{N} k(x_{n}, x_{t}) y_{n}}{\sum_{n=0}^{N} k(x_{n}, x_{t})}$$

- $k(x_n, x_t)$ denotes similarity between x_n and x_t
- Similarity (or inverse distance) as weight to give preference to NNs
- (k = 3) NN {(10, 65), (5, 63), (5, 60)}: $y_{11} = 63.25$

$$y_{t} = \frac{\sum_{n=0}^{N} k(x_{n}, x_{t}) y_{n}}{\sum_{n=0}^{N} k(x_{n}, x_{t})}$$

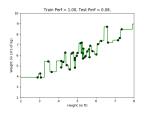
- $k(x_n, x_t)$ denotes similarity between x_n and x_t
- Similarity (or inverse distance) as weight to give preference to NNs
- (k = 3) NN {(10, 65), (5, 63), (5, 60)}: $y_{11} = 63.25$
- Number of neighbors k is not very critical.

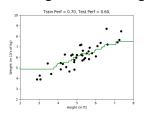
$$y_{t} = \frac{\sum_{n=0}^{N} k(x_{n}, x_{t}) y_{n}}{\sum_{n=0}^{N} k(x_{n}, x_{t})}$$

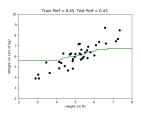
- $k(x_n, x_t)$ denotes similarity between x_n and x_t
- Similarity (or inverse distance) as weight to give preference to NNs
- (k = 3) NN $\{(10, 65), (5, 63), (5, 60)\}$: $y_{11} = 63.25$
- Number of neighbors k is not very critical.
- Similarity measure $k(x_n, x_t)$ is an important design choice

KNN-Regression Illustration

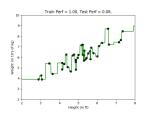
Uniform weights for the neighbors

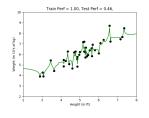


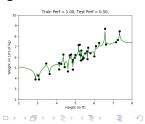




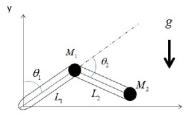
Inverse distance wights for the neighbors



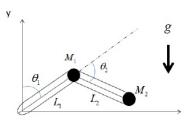




Robotic Arm Control - ME Approach



Robotic Arm Control - ME Approach

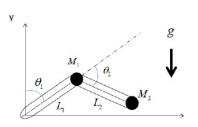


Solving for the forces:

$$\begin{split} F_{\theta_1} &= ((M_1 + M_2)L_1^2 + M_2L_2^2 + 2M_2L_1L_2cos\theta_2)\ddot{\theta}_1 \\ &+ (M_2L_2^2 + M_2L_1L_2cos\theta_2)\ddot{\theta}_2 - M_2L_1L_2sin\theta_2(2\dot{\theta}_1\dot{\theta}_2 + \dot{\theta}_2^2) \\ &- (M_1 + M_2)gL_1sin\theta_1 - M_2gL_2sin(\theta_1 + \theta_2)\gamma \end{split}$$

$$\begin{split} F_{\theta_2} &= (M_2 L_2^2 + M_2 L_1 L_2 cos \theta_2) \ddot{\theta}_1 + M_2 L_2^2 \ddot{\theta}_2 \\ - M_2 L_1 L_2 sin(\theta_2) \dot{\theta}_1 \dot{\theta}_2 - M_2 g L_2 sin(\theta_1 + \theta_2) \end{split}$$

Robotic Arm Control - ME Approach



Solving for the forces:

$$\begin{split} F_{\theta_1} &= ((M_1 + M_2)L_1^2 + M_2L_2^2 + 2M_2L_1L_2cos\theta_2)\ddot{\theta}_1 \\ &+ (M_2L_2^2 + M_2L_1L_2cos\theta_2)\ddot{\theta}_2 - M_2L_1L_2sin\theta_2(2\dot{\theta}_1\dot{\theta}_2 + \dot{\theta}_2^2) \\ &- (M_1 + M_2)gL_1sin\theta_1 - M_2gL_2sin(\theta_1 + \theta_2)\gamma \end{split}$$

 $F_{\theta_2} = (M_2 L_2^2 + M_2 L_1 L_2 \cos \theta_2) \ddot{\theta}_1 + M_2 L_2^2 \ddot{\theta}_2$ $-M_2 L_1 L_2 \sin(\theta_2) \dot{\theta}_1 \dot{\theta}_2 - M_2 g L_2 \sin(\theta_1 + \theta_2)$

- Force applied on robotic arm needs to be controlled
- Error between current and desired positions determine the forces
- F_{θ_1} and F_{θ_2} can be computing by solving Lagrangian using kinetic and potential energies
- Too complicated, and may not work
- However, we can conclude that

$$F = g(\theta_1, \theta_2, \dot{\theta_1}, \dot{\theta_2}, \ddot{\theta_1}, \ddot{\theta_2})$$

Robotic Arm Control - KNN Approach

θ_1	θ_2	$\dot{ heta_1}$	$\dot{\theta_2}$	$\ddot{ heta_1}$	$\ddot{\theta_2}$	F_{θ_1}	F_{θ_2}

- From the current and desired positions, estimate the angles and their derivatives.
- Look for the k(=1)-nearest match in the table, and pick forces.
- If succeeded in pitching, append the current configuration to the table
- As the table size increases, the robot skill improves!

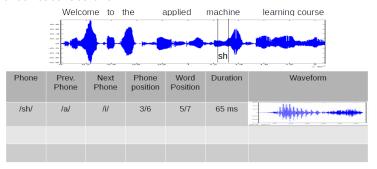
Robot Training - Testing

Speech Synthesis (Unit Selection)

- Regress speech waveform from the sequence of words
- Create a table of phonemes and their waveform from training data
- During synthesis, retrieve the waveforms for the sequence of phones, and concatenate them

Speech Synthesis (Unit Selection)

- Regress speech waveform from the sequence of words
- Create a table of phonemes and their waveform from training data
- During synthesis, retrieve the waveforms for the sequence of phones, and concatenate them



Pros

- Simple to implement
- Flexible to feature/distance function choices (no differentiability)
- Naturally handles multiclass data
- Does well even on complex tasks with enough data

Pros

- Simple to implement
- Flexible to feature/distance function choices (no differentiability)
- Naturally handles multiclass data
- Does well even on complex tasks with enough data

- Needs to access entire training data for every inference
- Computational complexity grows linearly with training data O(ND)

Pros

- Simple to implement
- Flexible to feature/distance function choices (no differentiability)
- Naturally handles multiclass data
- Does well even on complex tasks with enough data

- Needs to access entire training data for every inference
- Computational complexity grows linearly with training data O(ND)
- Distance function has to be chosen carefully
- The choice of k is empirical (no theoretical guidelines)

Pros

- Simple to implement
- Flexible to feature/distance function choices (no differentiability)
- Naturally handles multiclass data
- Does well even on complex tasks with enough data

- Needs to access entire training data for every inference
- Computational complexity grows linearly with training data O(ND)
- Distance function has to be chosen carefully
- The choice of k is empirical (no theoretical guidelines)
- Nonconvex decision regions
- Cannot naturally ignore noninformative dimensions

Pros

- Simple to implement
- Flexible to feature/distance function choices (no differentiability)
- Naturally handles multiclass data
- Does well even on complex tasks with enough data

- Needs to access entire training data for every inference
- Computational complexity grows linearly with training data O(ND)
- Distance function has to be chosen carefully
- The choice of k is empirical (no theoretical guidelines)
- Nonconvex decision regions
- Cannot naturally ignore noninformative dimensions
- Does not consider all the data at once, and hence, it cannot model the underlying process responsible for the observed data

Homework - Data Generation Models

Let the distribution of human height be given by

$$X \sim \mathcal{N}(5.3, 1)$$

Let the relationship between height and weight be given by

$$Y = 10X + 5 + \epsilon$$

where $\epsilon \sim \mathcal{N}(0,3)$. Evaluate the joint density function $p_{XY}(x,y)$, marginal density functions $p_X(x)$ & $p_Y(y)$, conditional density functions p(x/y) & p(y/x), and their corresponding expectations.

Homework

 Let the joint density function of human heights and weights follow a multivariate Gaussian given by

$$[X, Y] \sim \mathcal{N}(\boldsymbol{\mu}, \boldsymbol{\Sigma})$$

where $\mu \in \mathbb{R}^2$ is the mean vector and $\Sigma \in \mathbb{R}^{2 \times 2}$ is the covariance matrix. Evaluate the joint density function $p_{XY}(x,y)$, marginal density functions $p_X(x)$ & $p_Y(y)$, conditional density functions p(x/y) & p(y/x), and their corresponding expectations.

• Is it related to the earlier model?

Homework

ullet Let V be a 2-D random vector drawn from a standard Gaussian, i.e.,

$$\boldsymbol{V} \sim \mathcal{N}(\boldsymbol{\mathcal{O}}, \boldsymbol{I})$$

Let height and weight be obtained by an affine transformation of ${f V}$ as

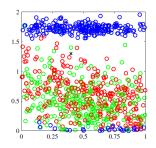
$$\left[\begin{array}{c} X \\ Y \end{array}\right] = \left[\begin{array}{cc} a & b \\ c & d \end{array}\right] \mathbf{V} + \left[\begin{array}{c} \mu_X \\ \mu_Y \end{array}\right]$$

Evaluate the joint density function $p_{XY}(x, y)$, marginal density functions $p_X(x)$ & $p_Y(y)$, conditional density functions p(x/y) & p(y/x), and their corresponding expectations.

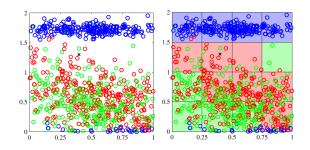
Is it related to two earlier models?

◄□▶◀圖▶◀불▶◀불▶ 불 ∽Q♡

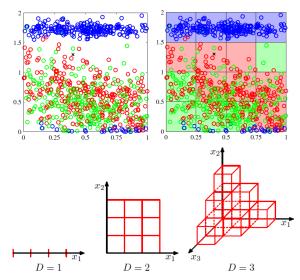
Curse of Dimensionality

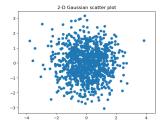


Curse of Dimensionality

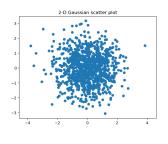


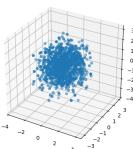
Curse of Dimensionality

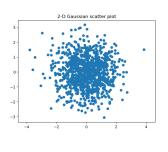


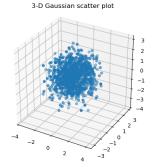




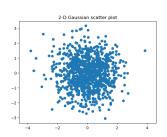


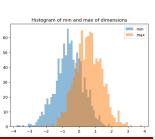




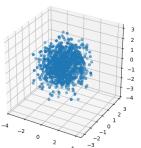


1000-D Gaussian



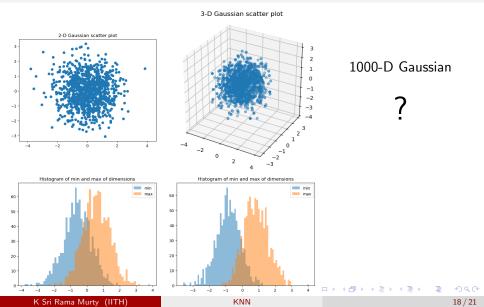


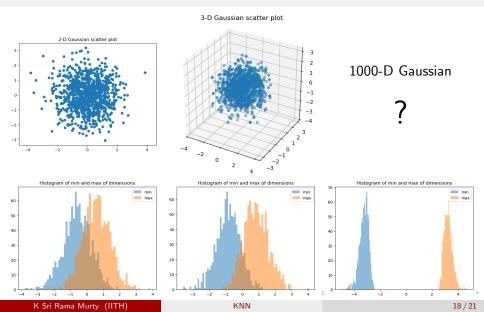




1000-D Gaussian

?





Gaussian in High Dimensional Space

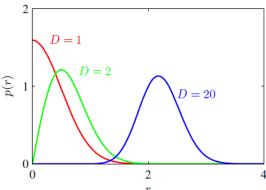
 The probability mass of a Gaussian distribution is concentrated in a thin shell

$$p(r)\Delta r = P\left[r - \frac{\Delta r}{2} < R < r + \frac{\Delta r}{2}\right]$$

Gaussian in High Dimensional Space

 The probability mass of a Gaussian distribution is concentrated in a thin shell

$$p(r)\Delta r = P\left[r - \frac{\Delta r}{2} < R < r + \frac{\Delta r}{2}\right]$$



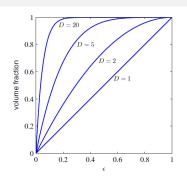
Thank You!

 Most of the volume of a sphere is concentrated in thin shell near the surface.

$$\frac{V_D(1) - V_D(1 - \epsilon)}{V_D(1)} = 1 - (1 - \epsilon)^D$$

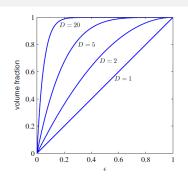
 Most of the volume of a sphere is concentrated in thin shell near the surface.

$$\frac{V_D(1) - V_D(1 - \epsilon)}{V_D(1)} = 1 - (1 - \epsilon)^D$$



 Most of the volume of a sphere is concentrated in thin shell near the surface.

$$\frac{V_D(1) - V_D(1 - \epsilon)}{V_D(1)} = 1 - (1 - \epsilon)^D$$



 The probability mass of a Gaussian distribution is concentrated in a thin shell

$$p(r)\Delta r = P\left[r - \frac{\Delta r}{2} < R < r + \frac{\Delta r}{2}\right]$$

 Most of the volume of a sphere is concentrated in thin shell near the surface.

$$\frac{V_D(1) - V_D(1 - \epsilon)}{V_D(1)} = 1 - (1 - \epsilon)^D$$

 The probability mass of a Gaussian distribution is concentrated in a thin shell

$$p(r)\Delta r = P\left[r - \frac{\Delta r}{2} < R < r + \frac{\Delta r}{2}\right]$$

