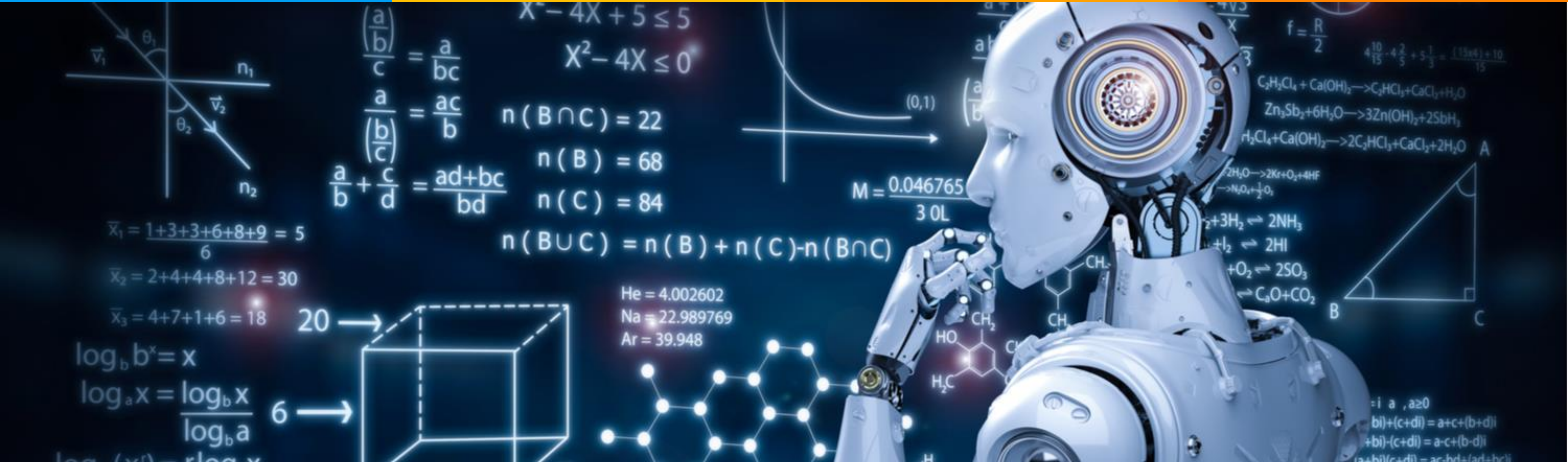
Duration: 120 min | Srikanth Shenoy | AML 5102 | M.E. AI & ML

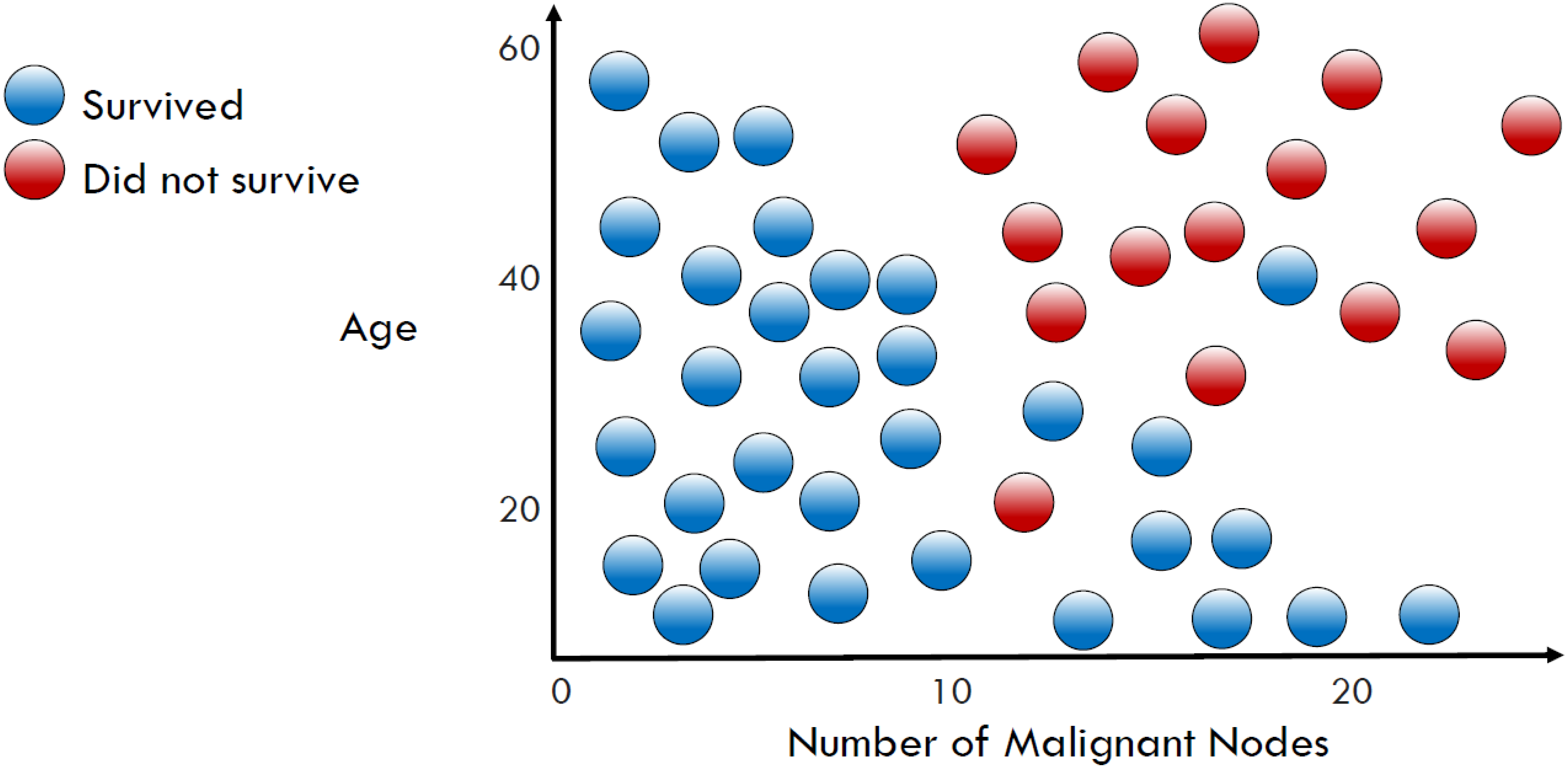


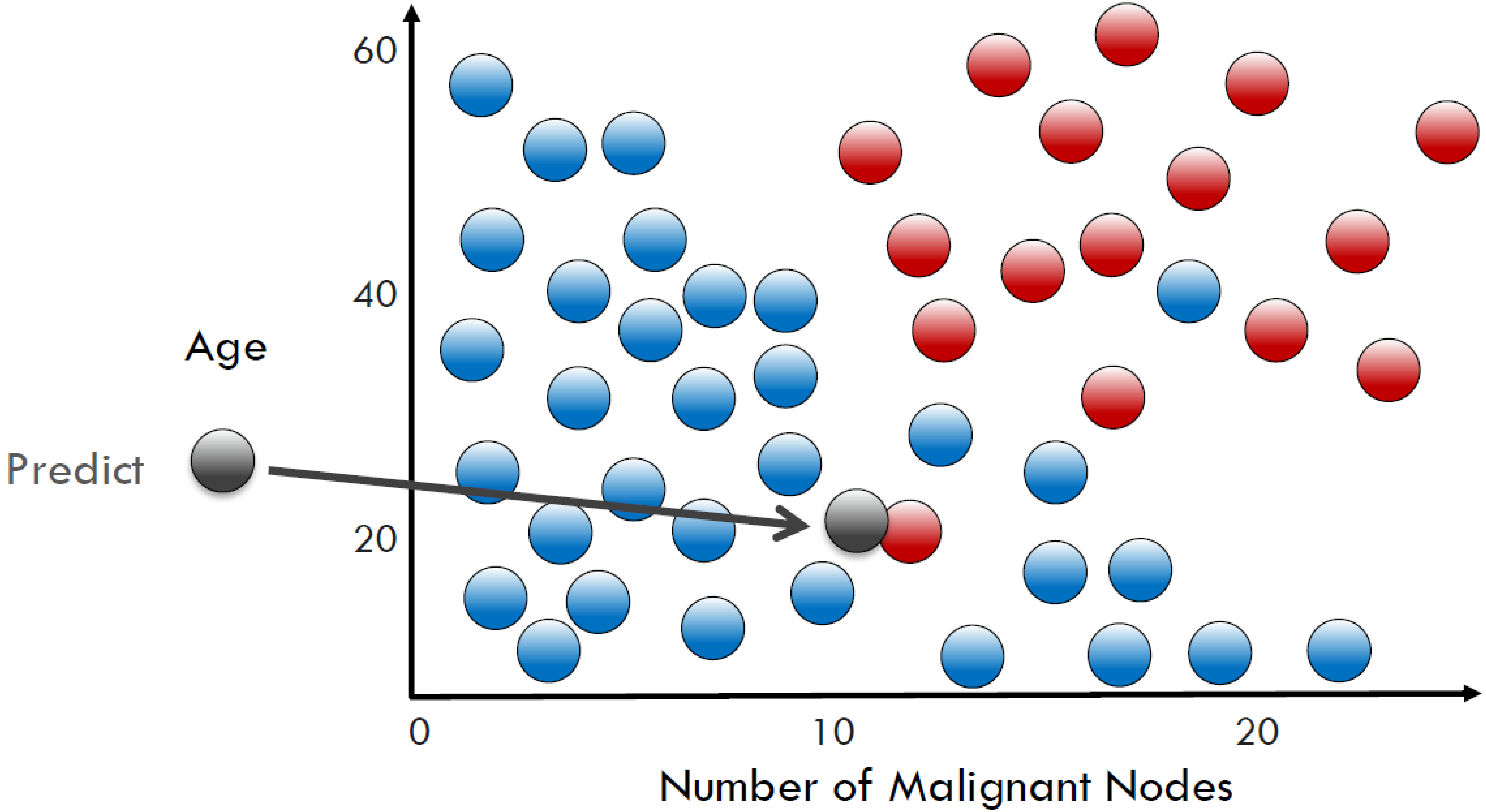
Lecture 6 & 7: KNN

Recap

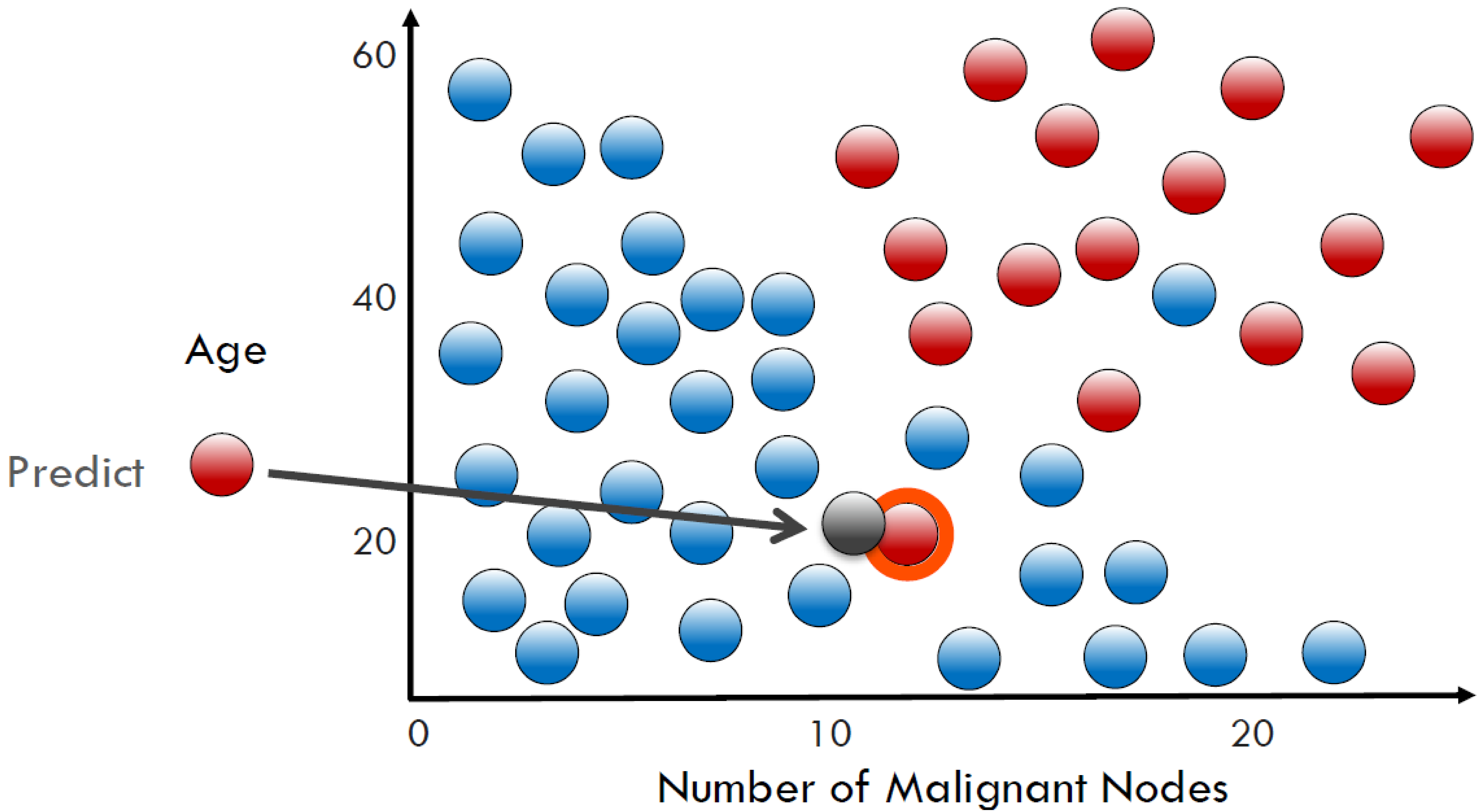
- Classifiers are better understood geometrically
- Decision boundary for most $w^T x + b = 0$
- Non linear classifiers use kernels or transform space
- First primitive classifier – Nearest Centroid
- View clustering geometrically

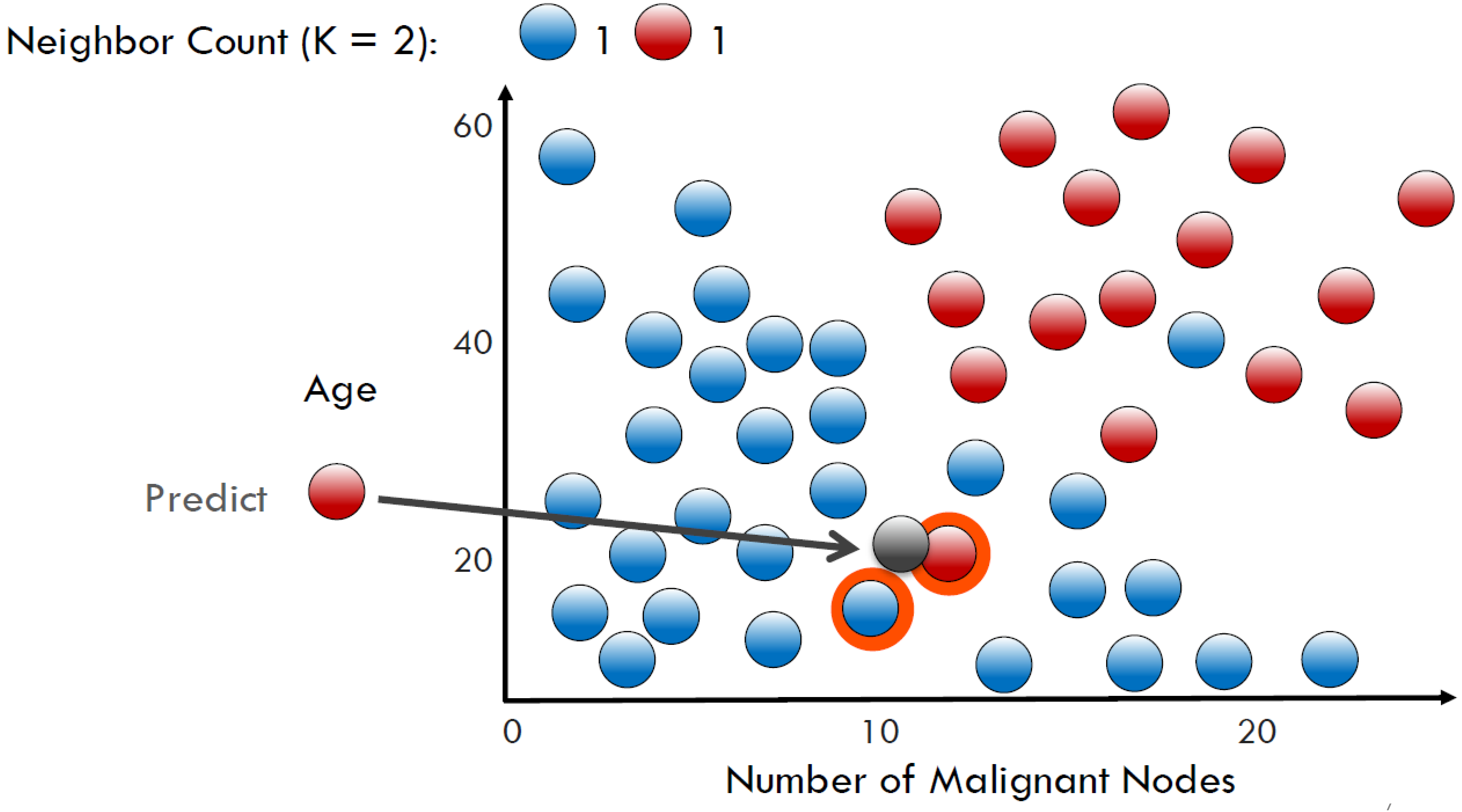

LOVE YOUR
NEIGHBOR


Survived
Did not survive
Age
60
40
20
0
10
20
Number of Malignant Nodes


60
40
20
Age
Predict
0
10
20
Number of Malignant Nodes

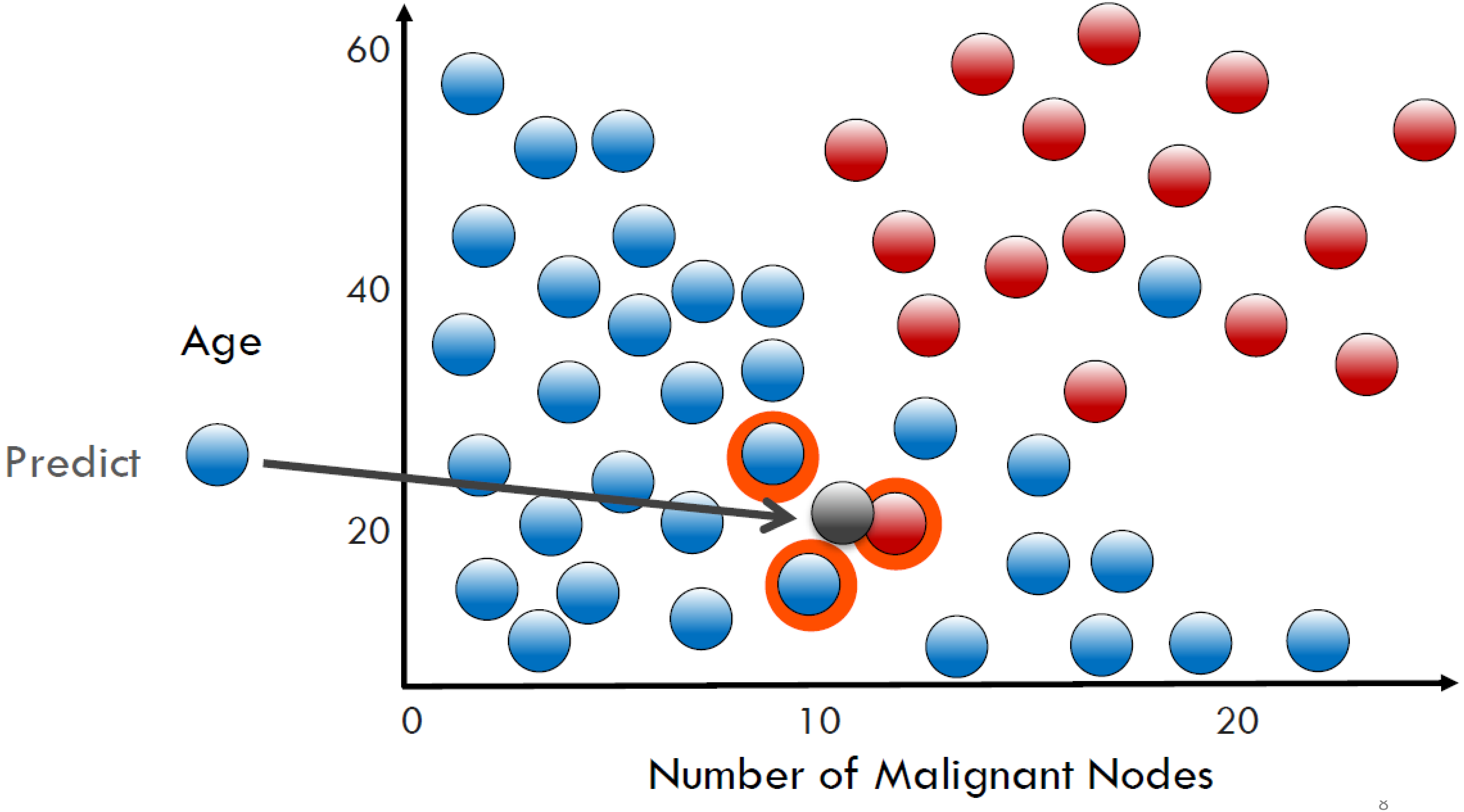
Neighbor Count (K = 1): 0 1

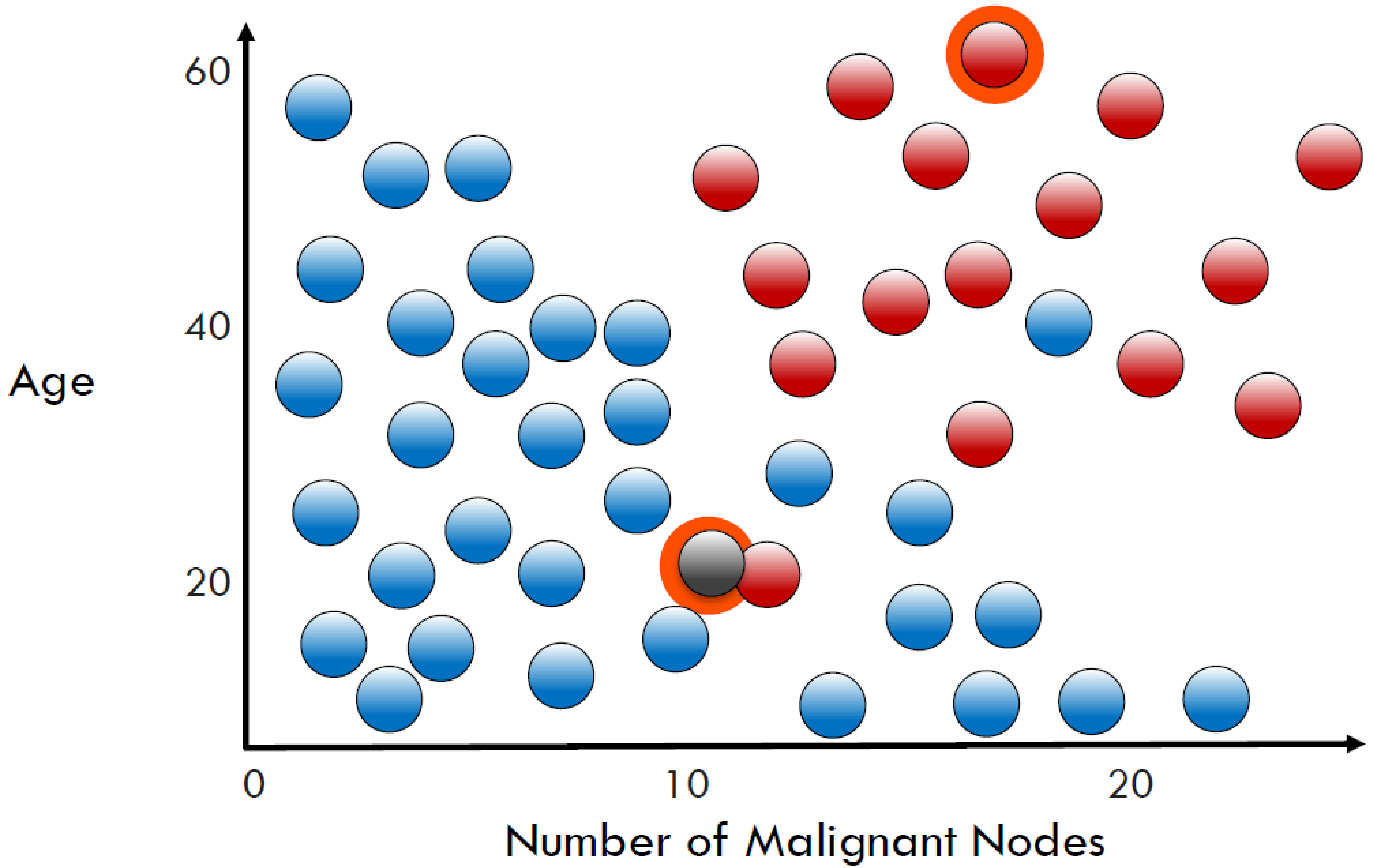




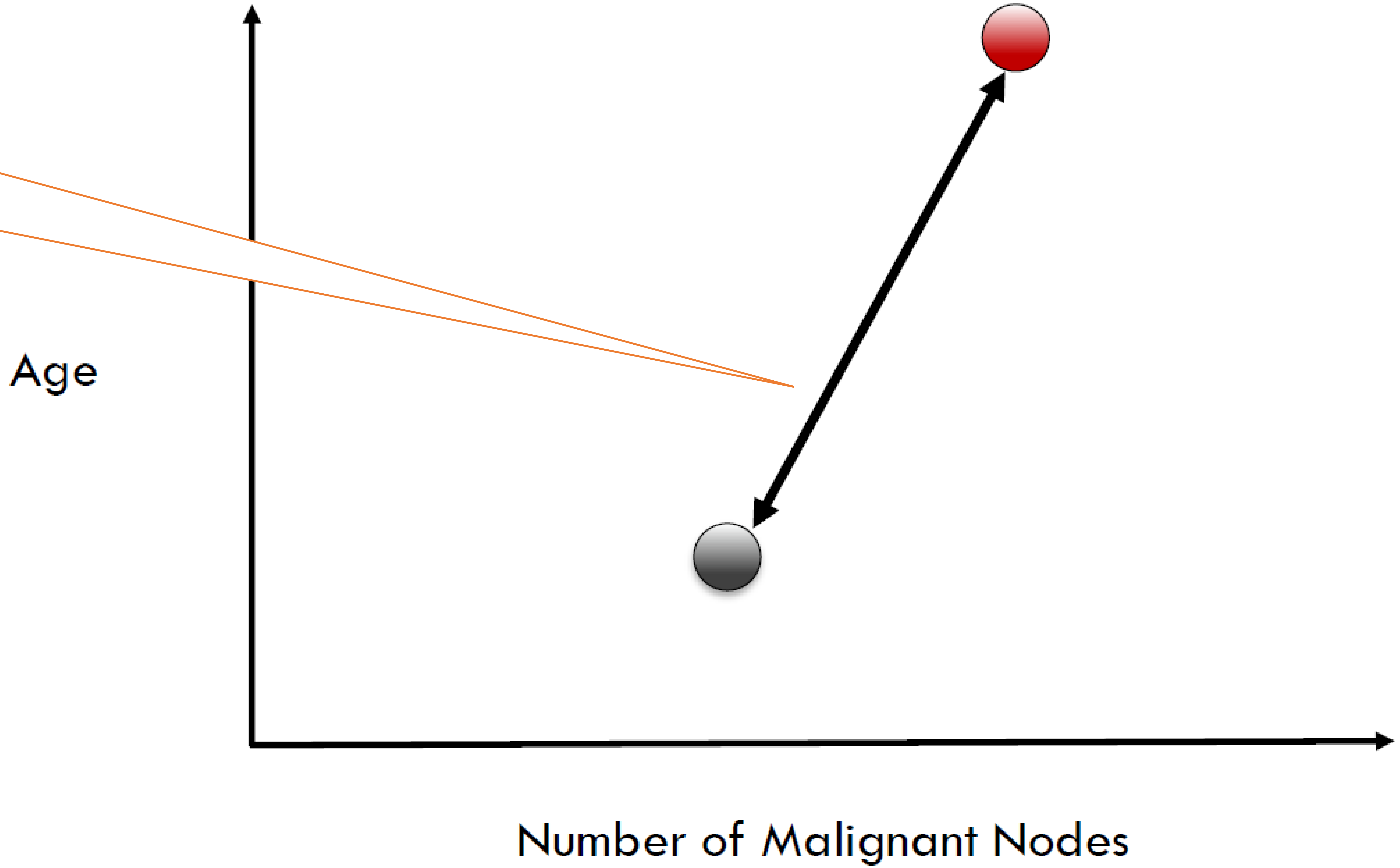
Neighbor Count (K = 2):
1
1
60
40
20
Age
Predict
0
10
20
Number of Malignant Nodes

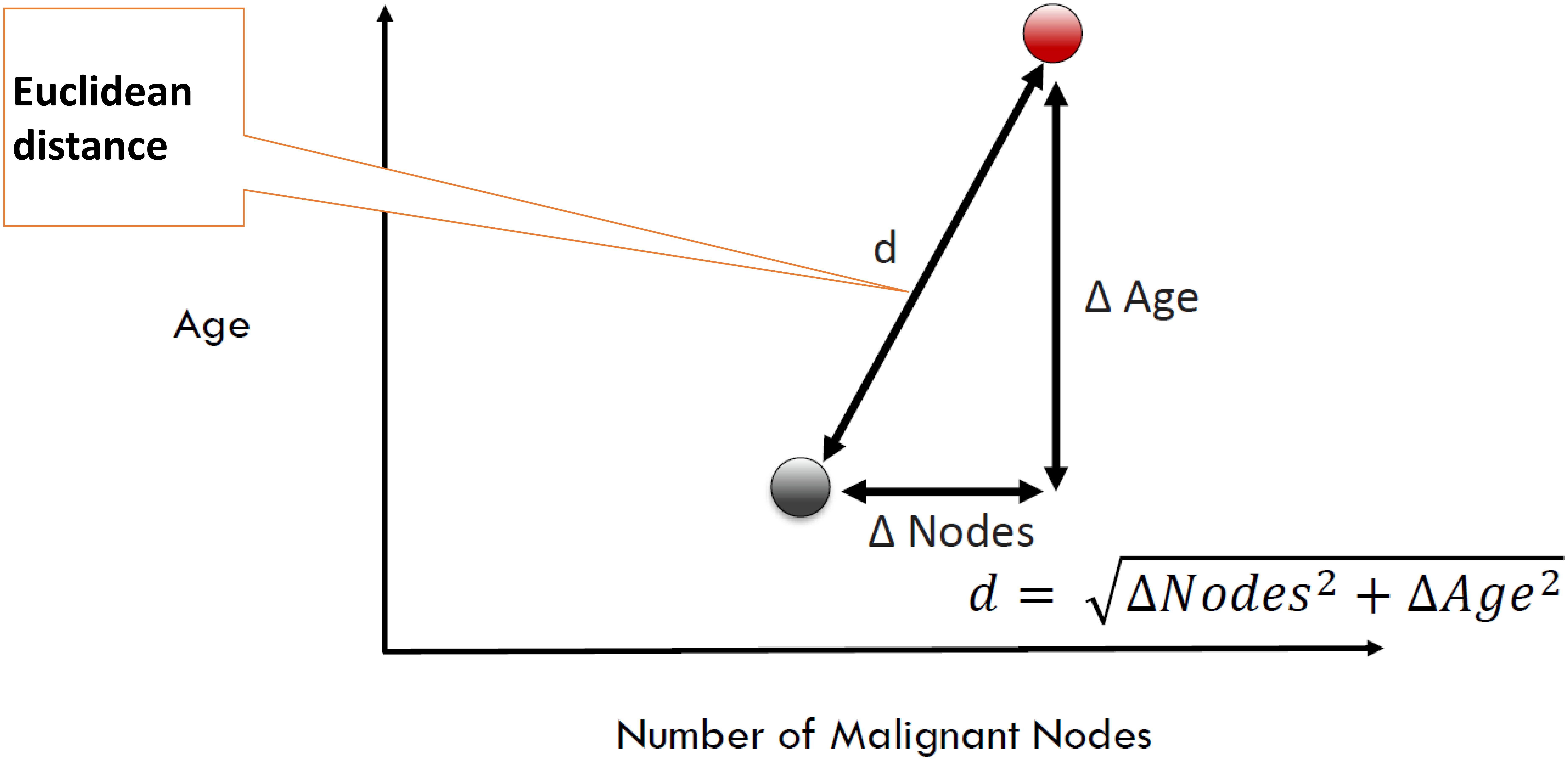
Neighbor Count (K = 3): 2 1

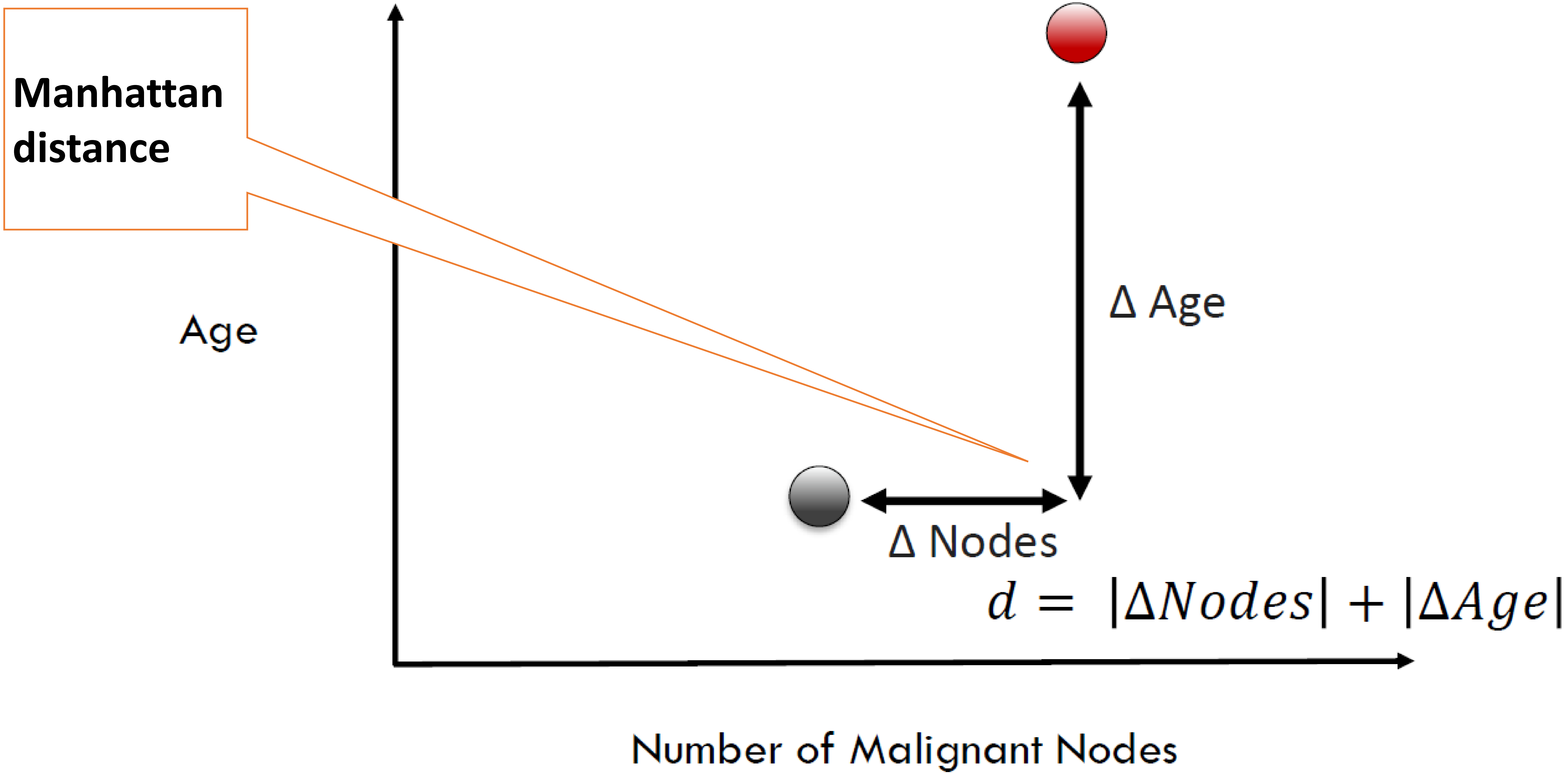


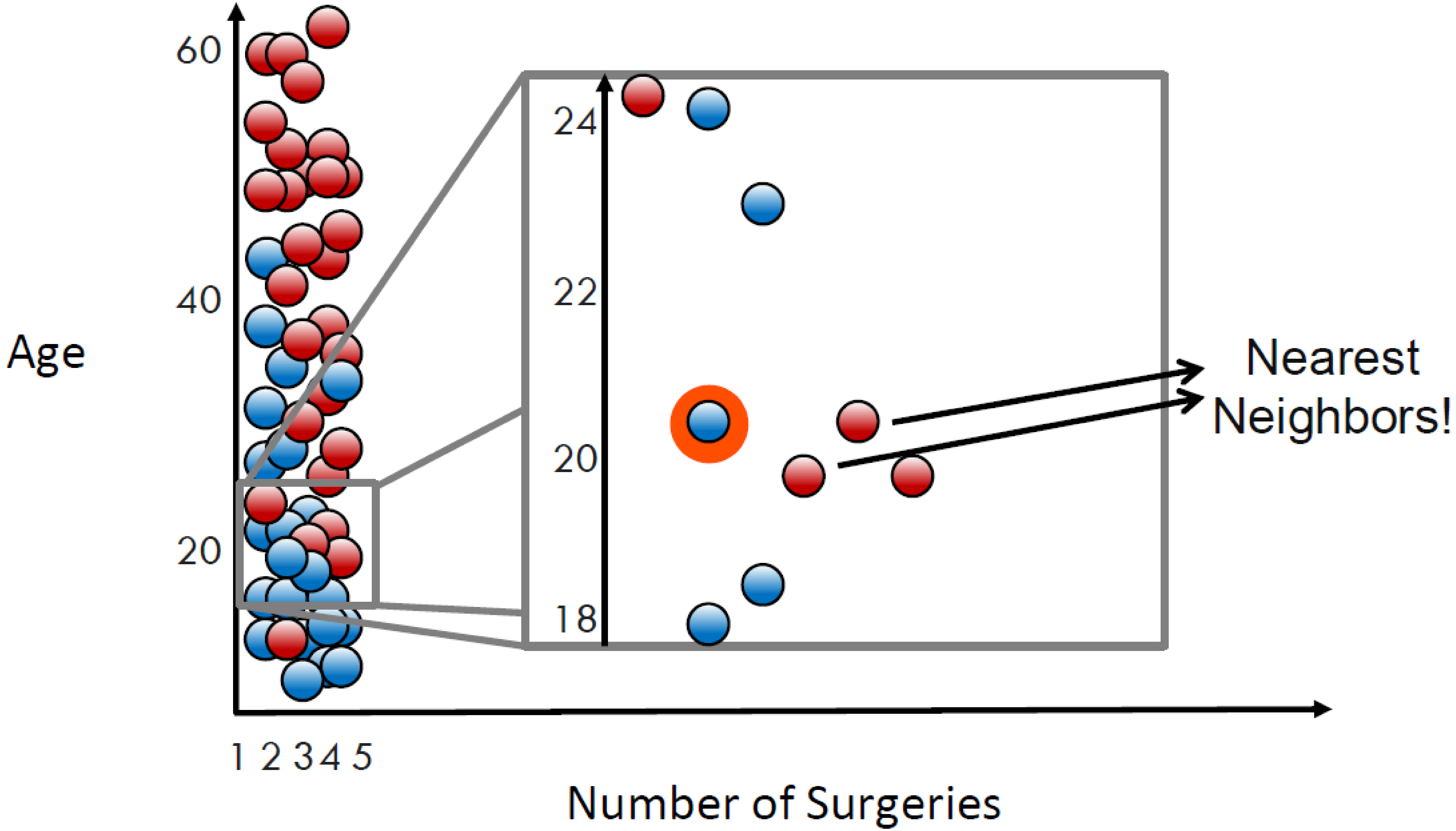

60
40
20
Age
0
10
20
Number of Malignant Nodes

How to find distance between 2 points

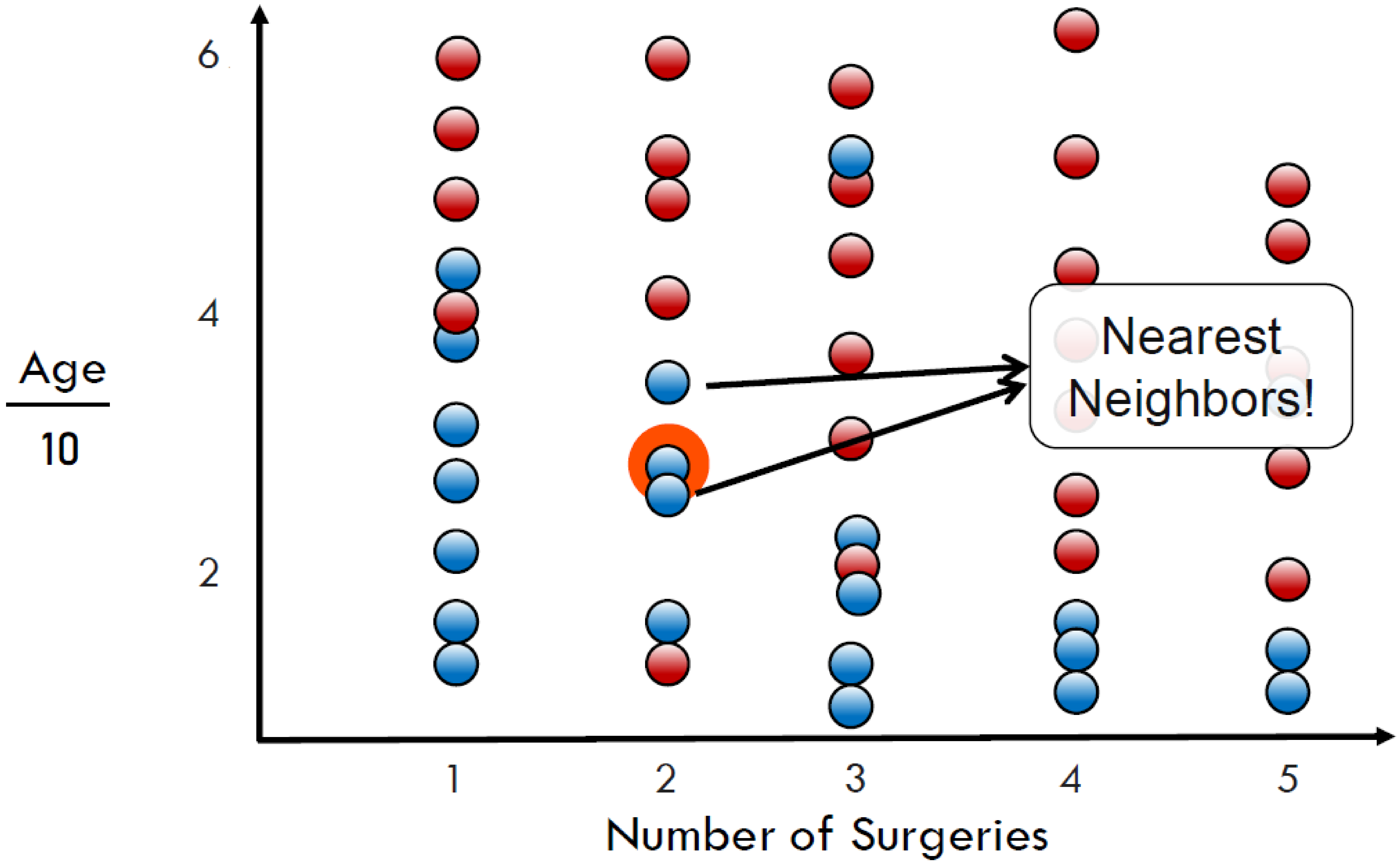



Euclidean distance
Age
d
Δ Age
Δ Nodes
$d = \sqrt{\Delta Nodes^2 + \Delta Age^2}$
Number of Malignant Nodes


Manhattan distance
Age
Δ Age
Δ Nodes
$d = |\Delta Nodes| + |\Delta Age|$
Number of Malignant Nodes



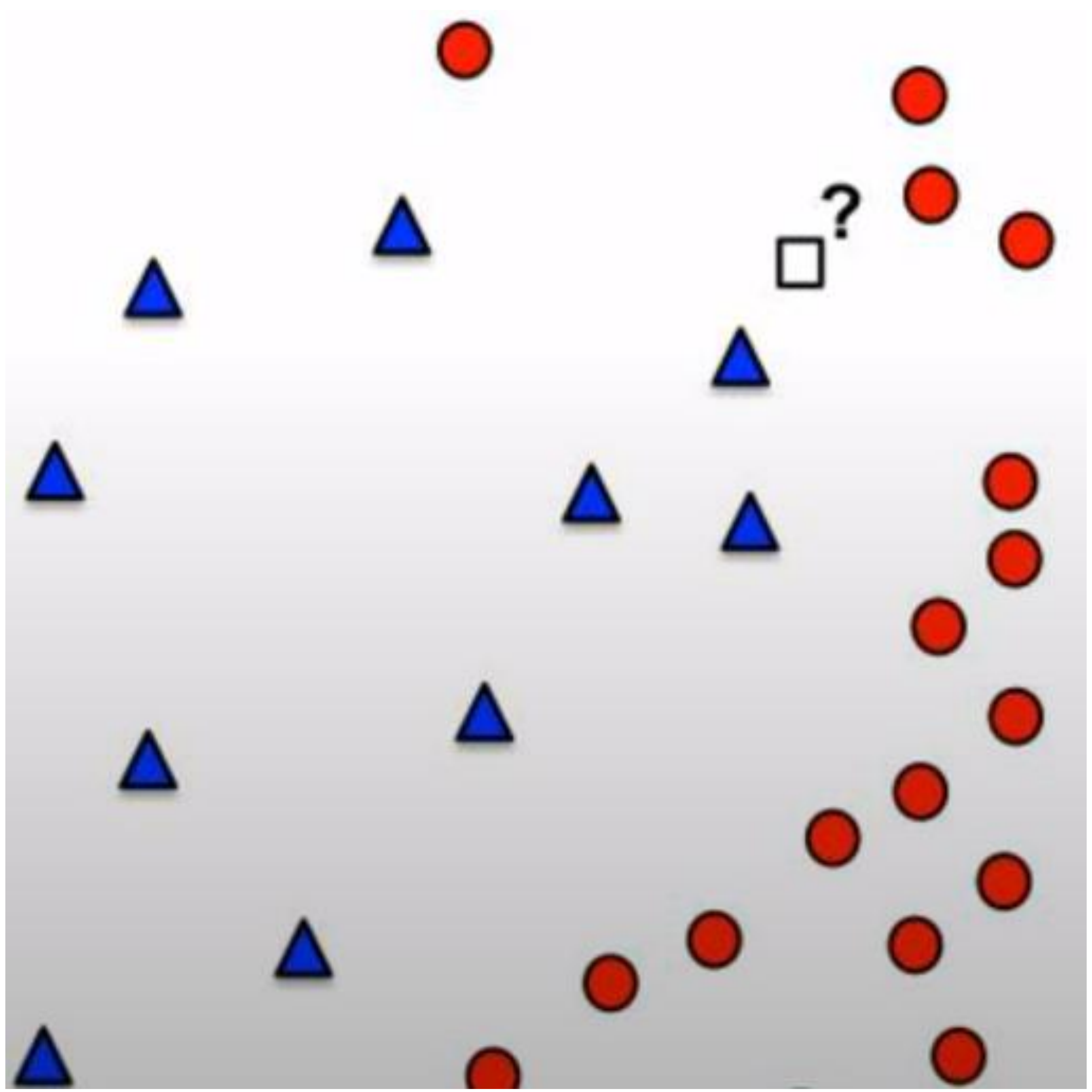
Age
60
40
20
24
22
20
18
Nearest Neighbors!
1 2 3 4 5
Number of Surgeries

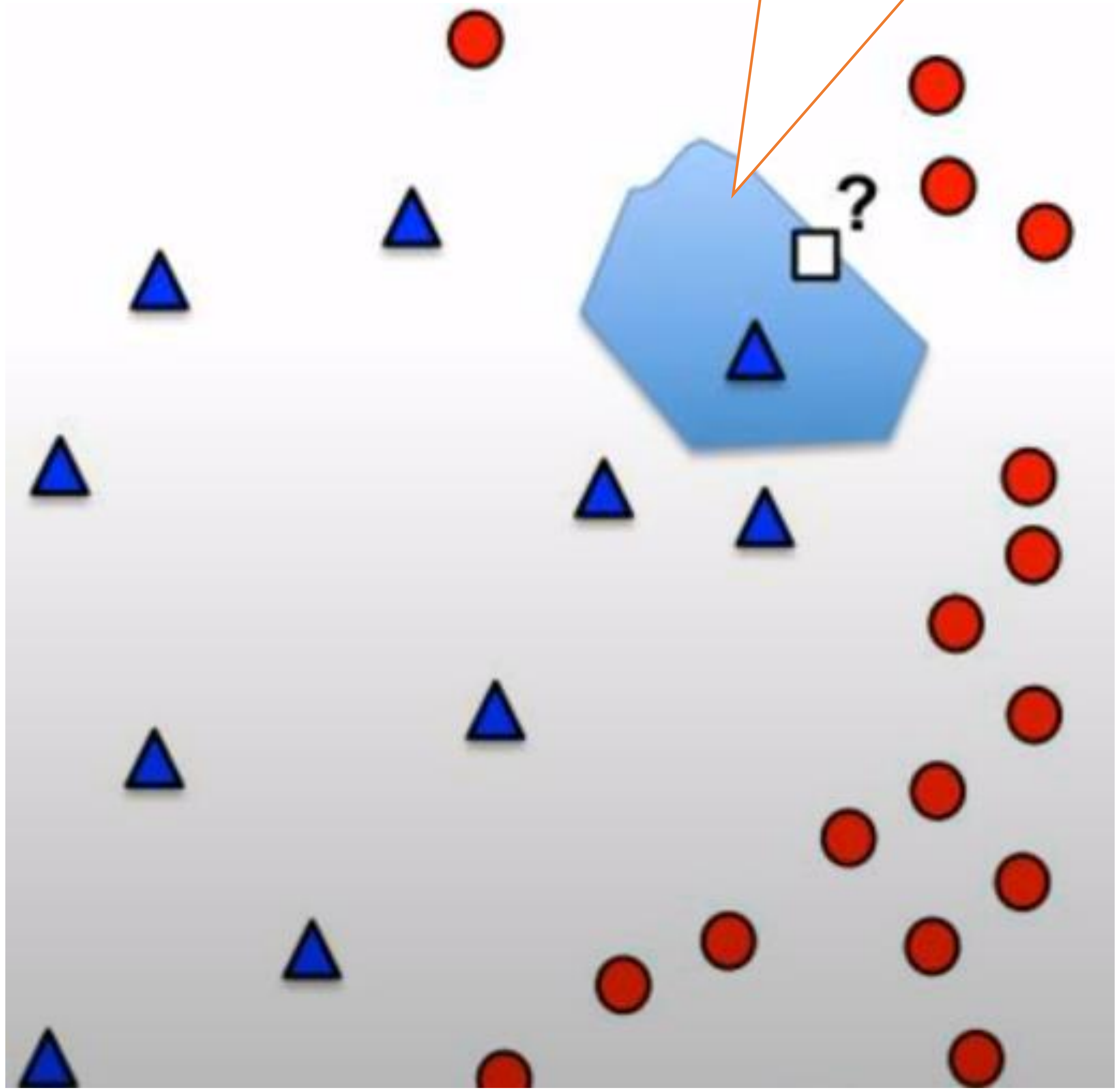

6
4
2
Age
10
1
2
3
4
5
Number of Surgeries
Nearest
Neighbors!

Mitigating overfitting in kNN

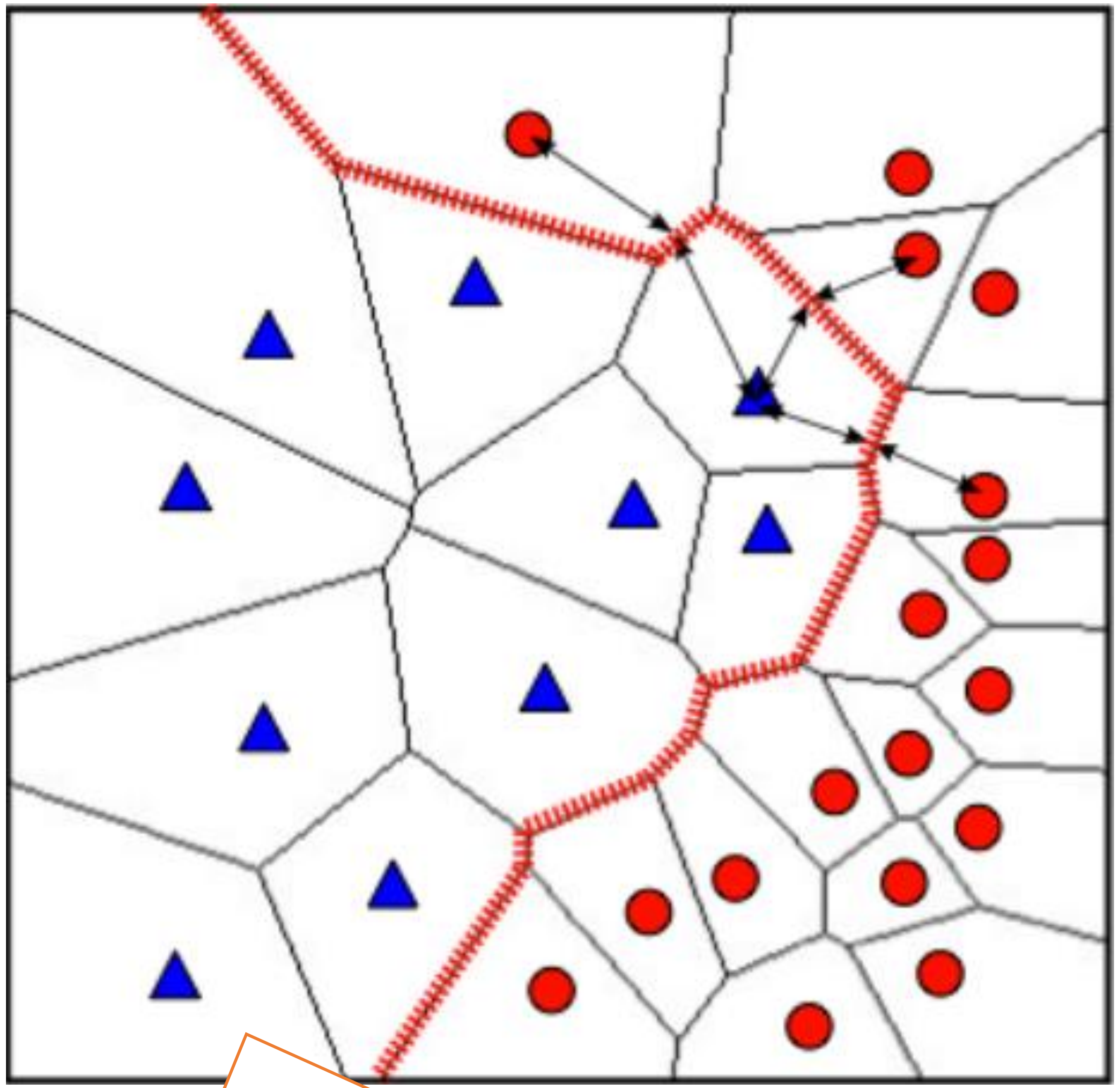
Decision Boundary in kNN

Voronoi cell: contains points closer to blue example than any other

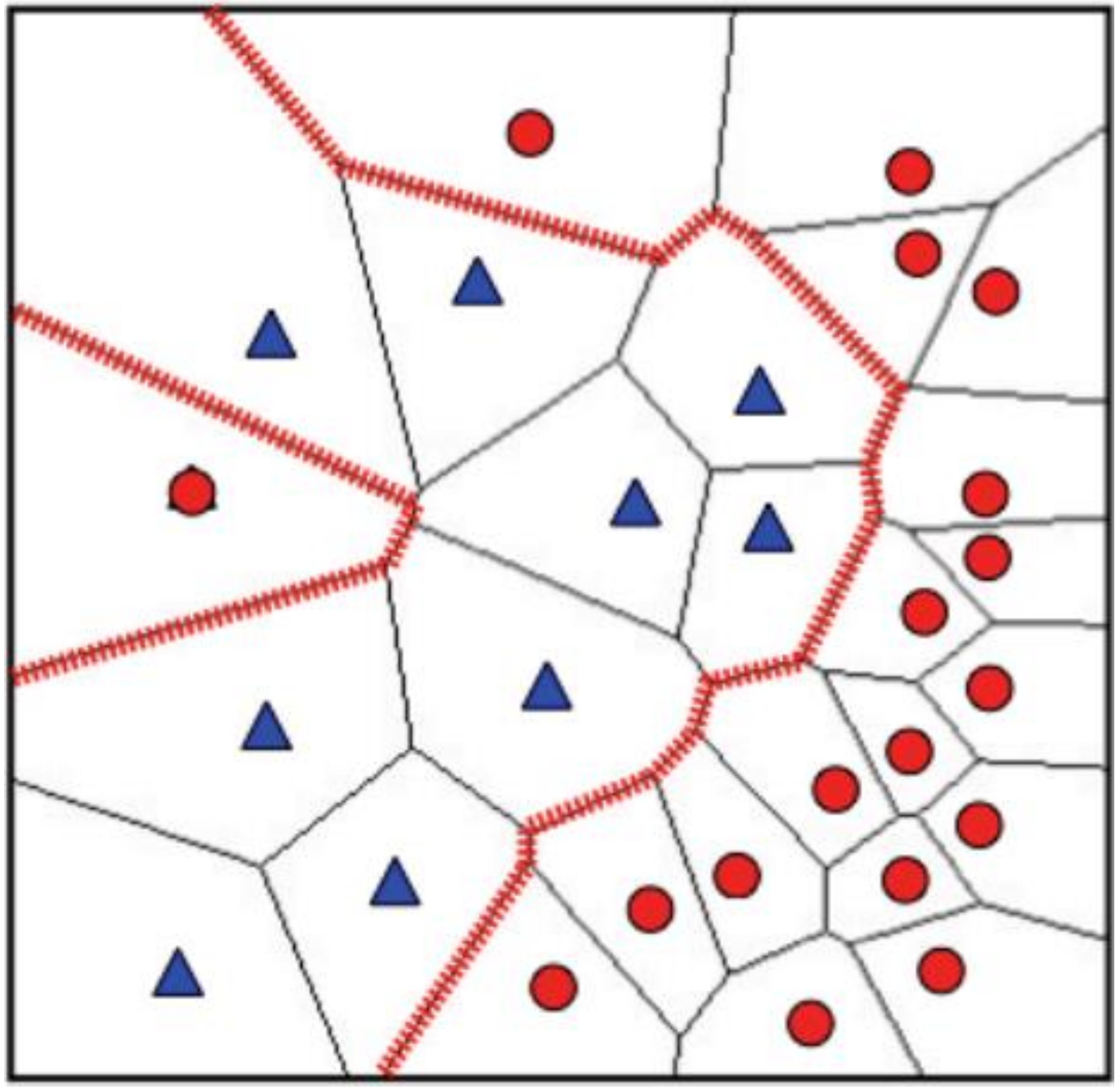




Decision Boundary in kNN (contd.)



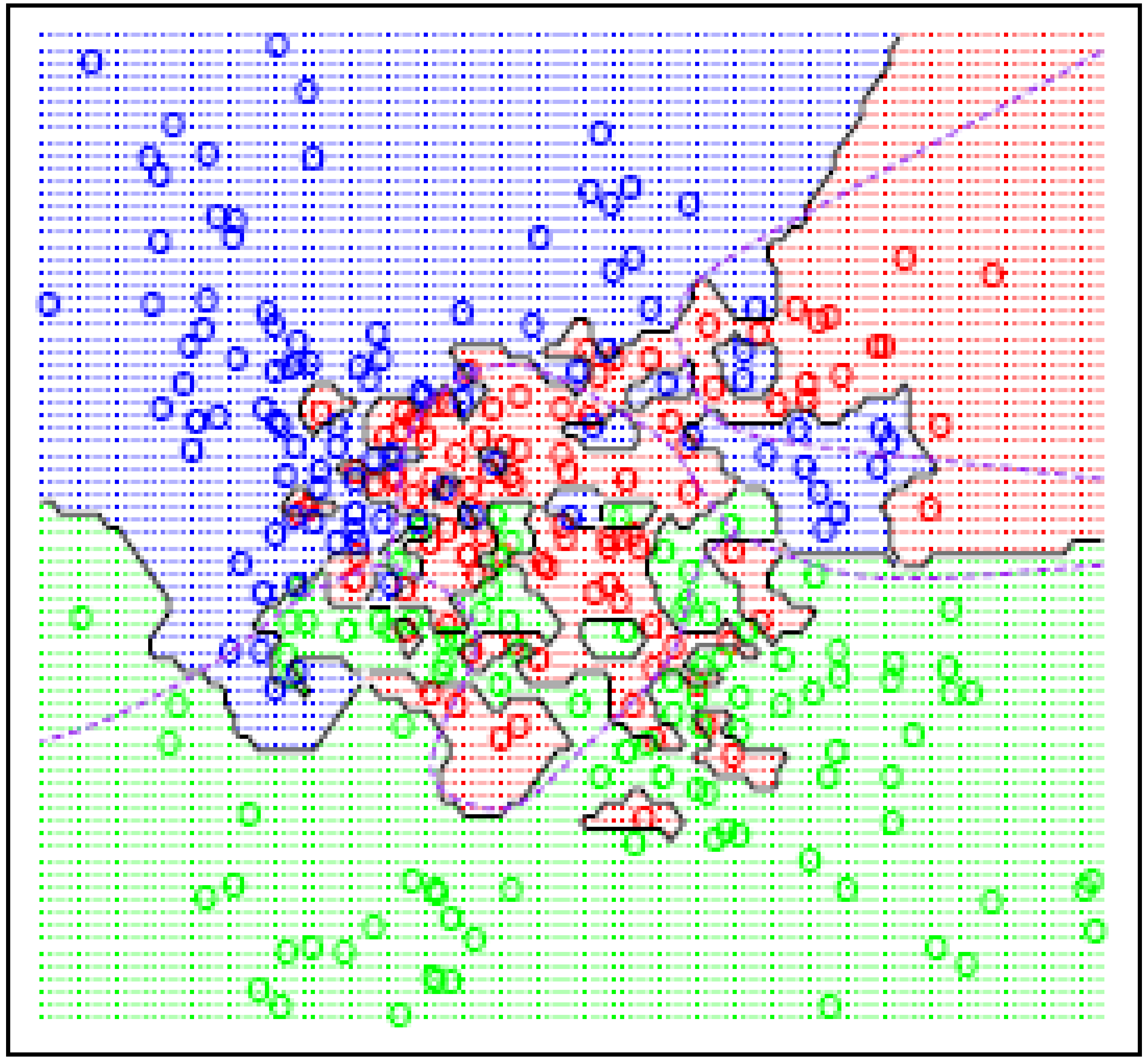
- Pretty impressive non-linear boundary
- Flexible implies risk for overfitting



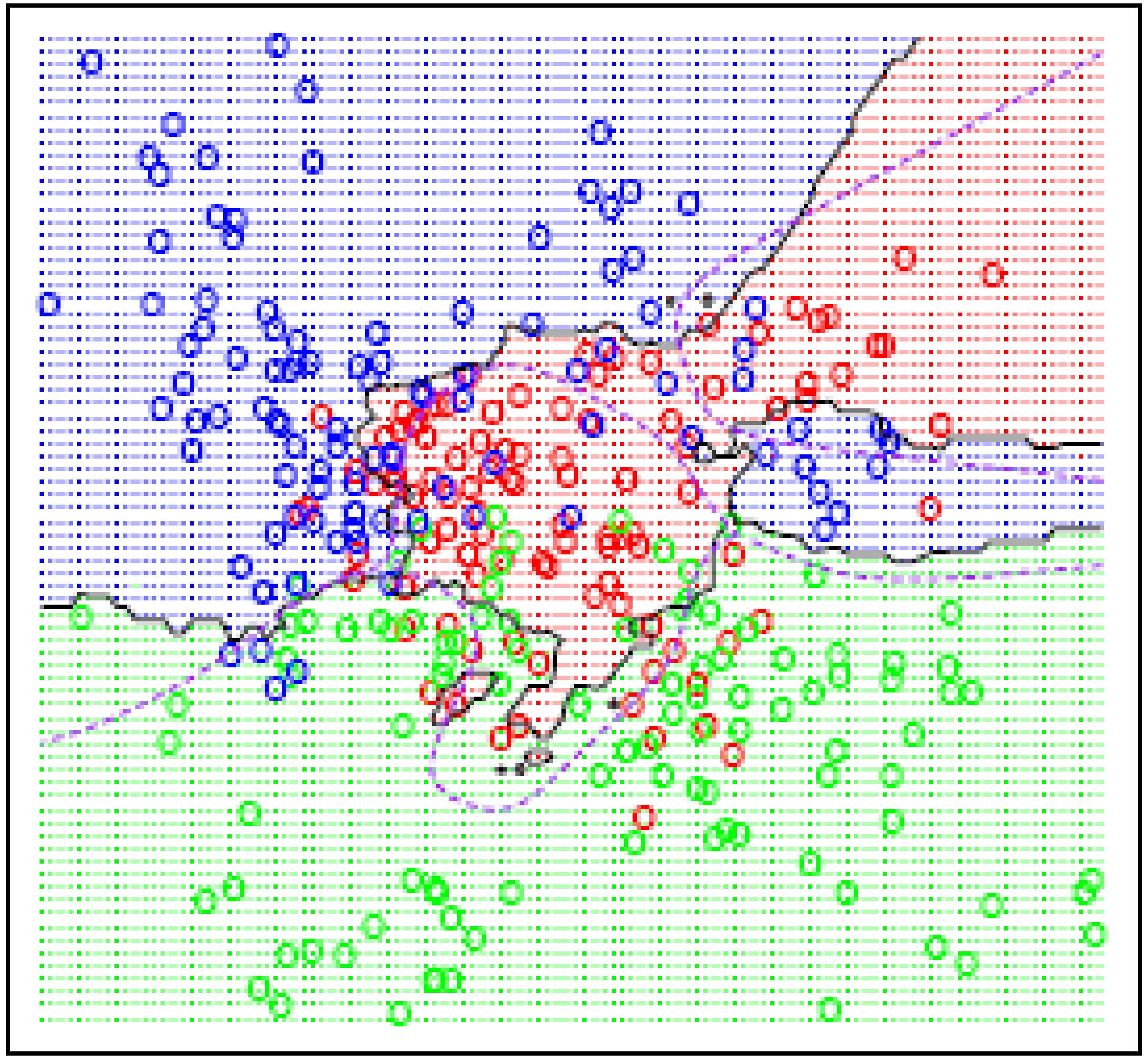
Voronoi Tessellation: Partitioned non overlapping space dominated by one type of training class

Decision Boundary in kNN (contd.)

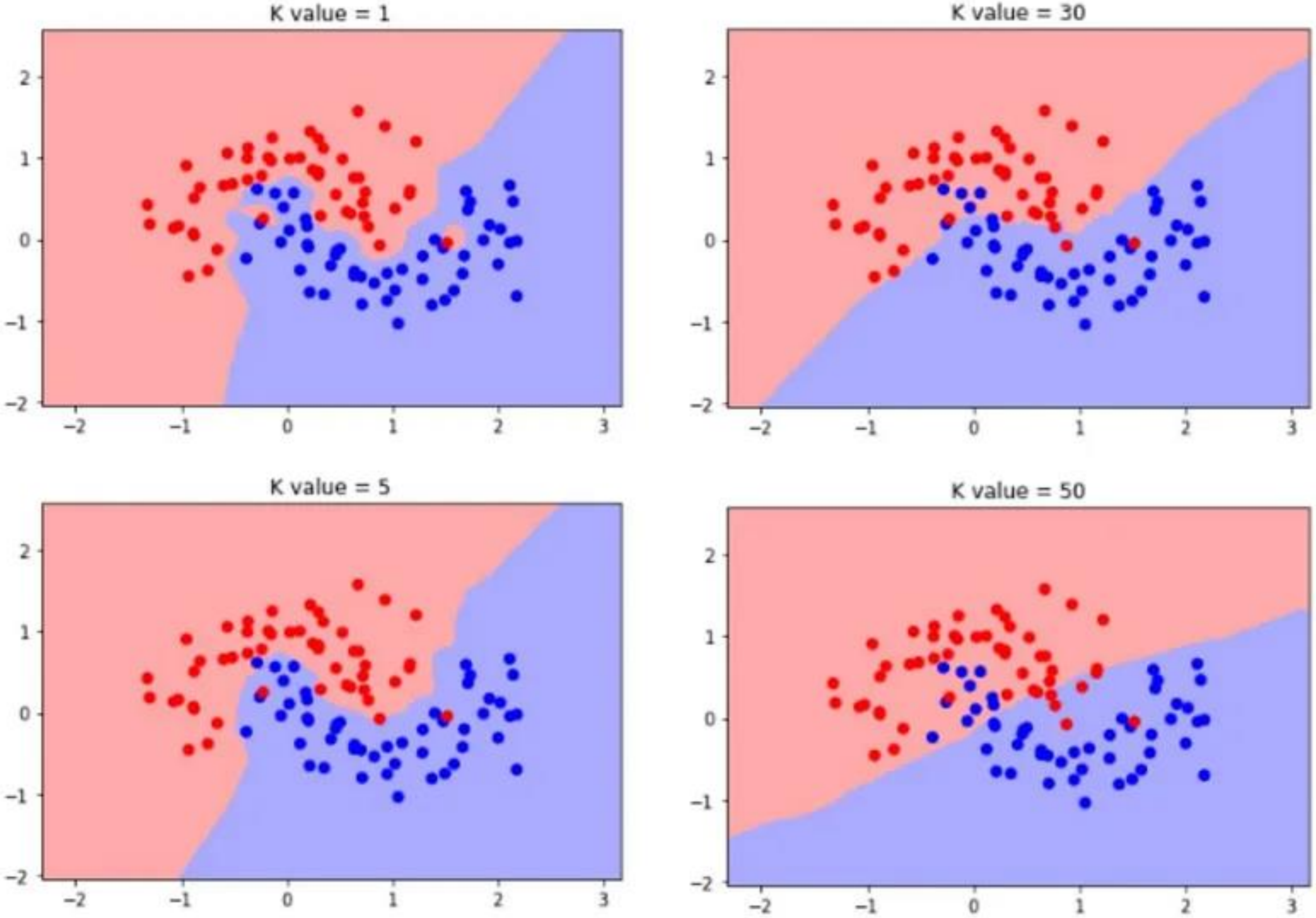
k=1



k=15

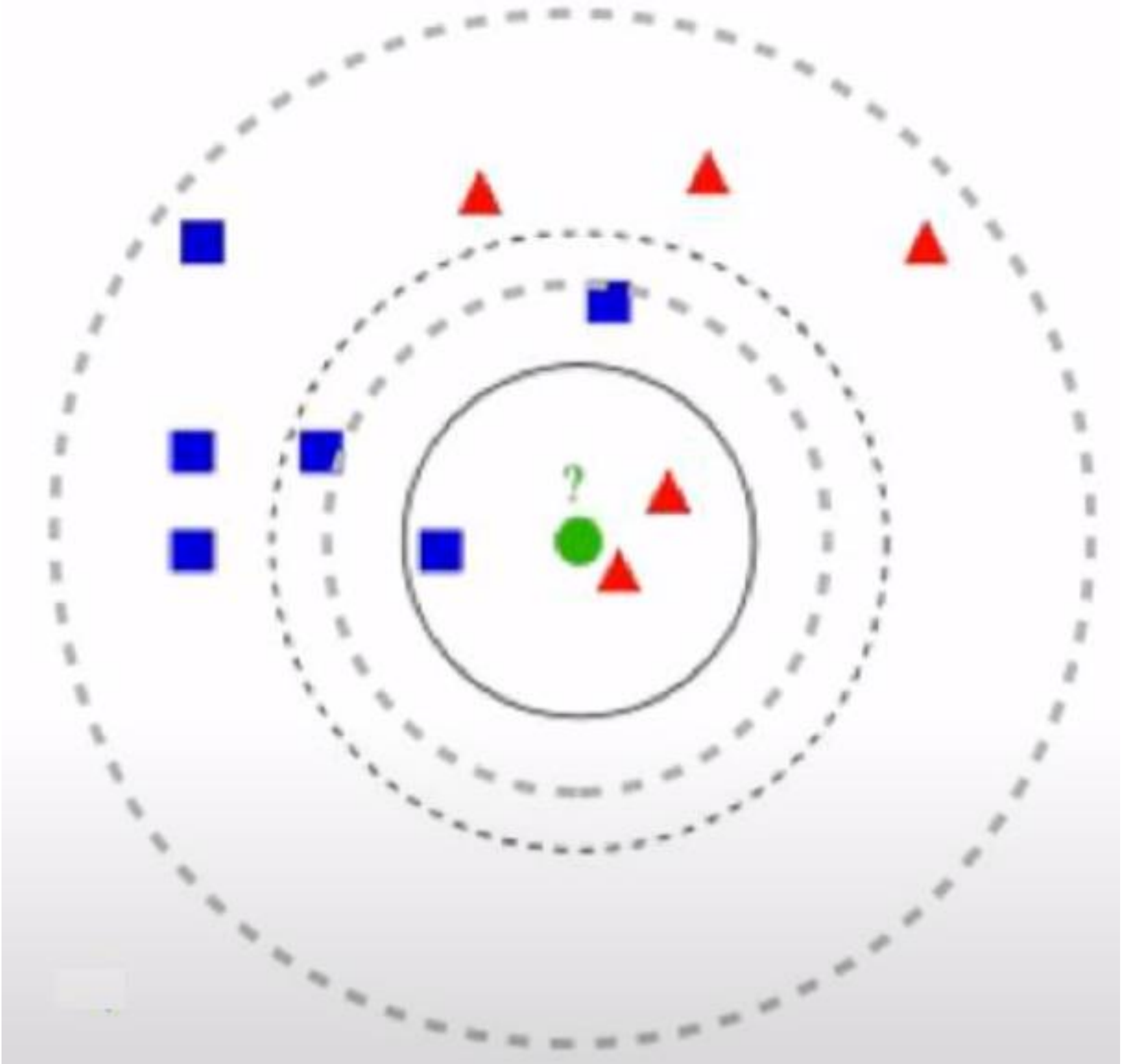


Decision Boundary in kNN (contd.)



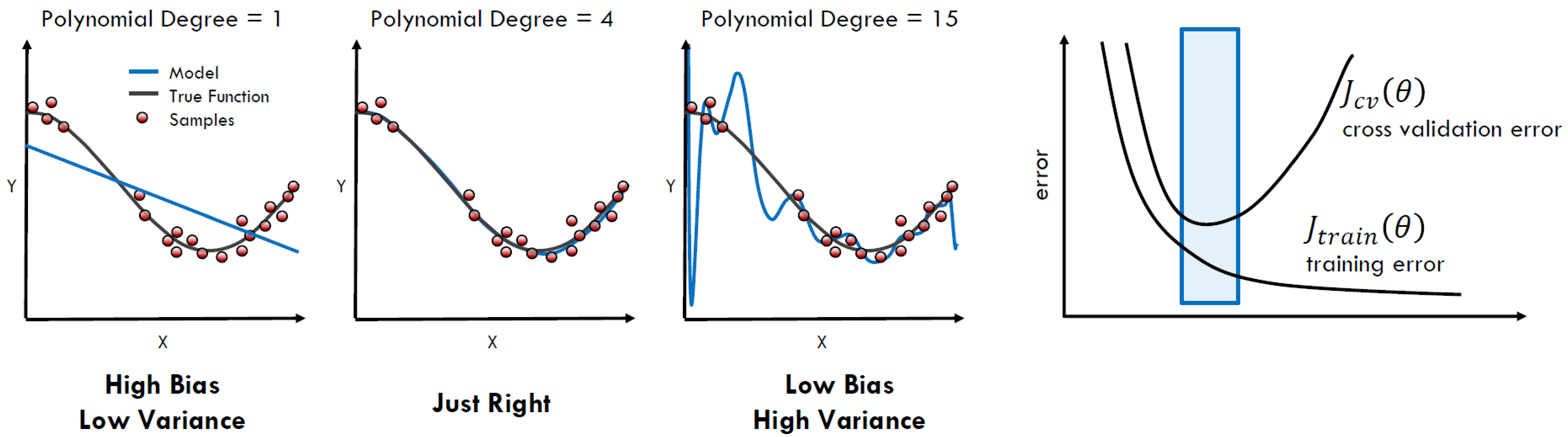
Impact of k

- Value of k has strong effect on kNN performance
- Small k -> unstable decision boundary
- Small change in training set leads to large change in classification



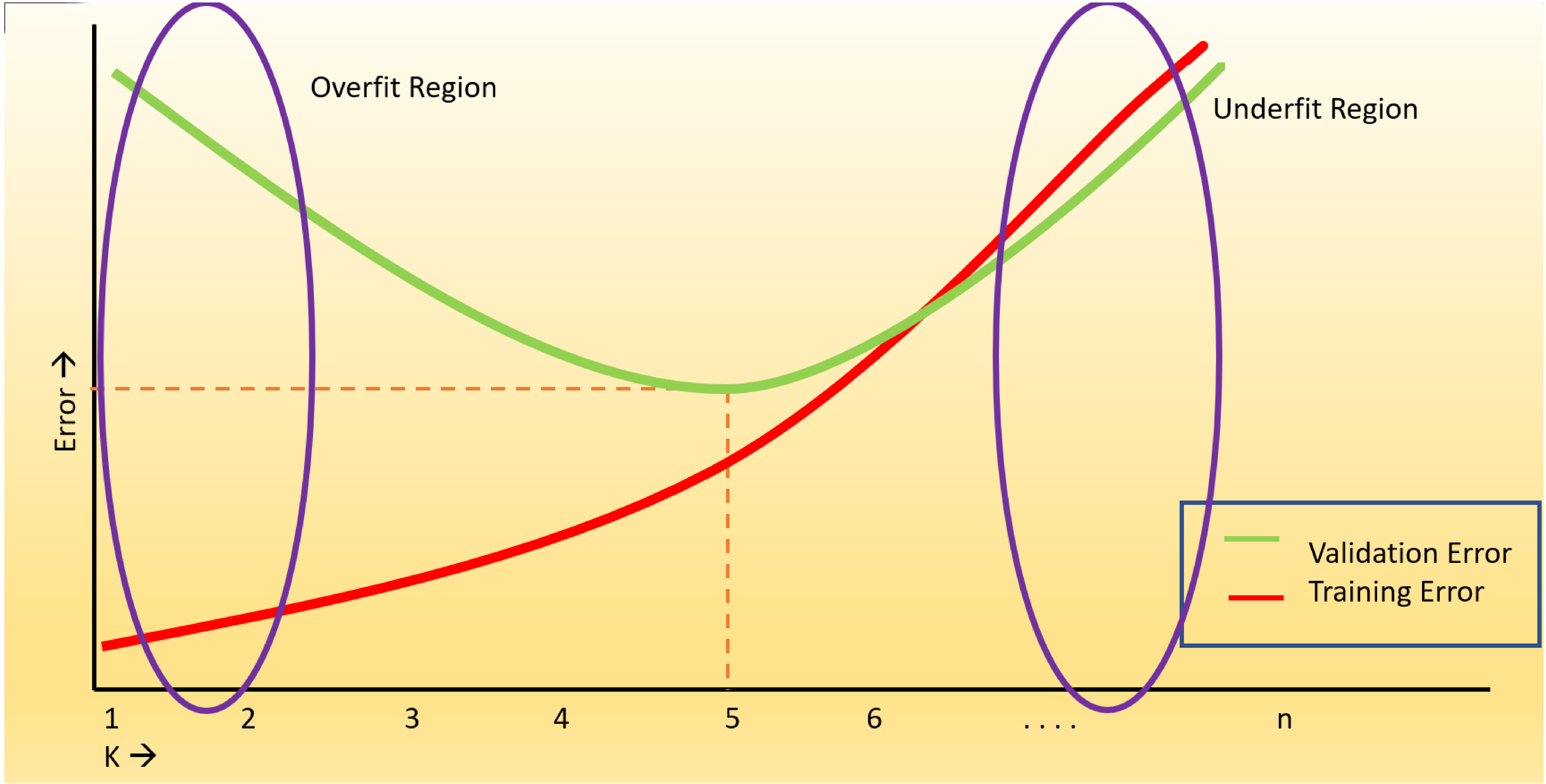
- Extreme case of large k: k=N
  - Every test point classified as the most probable class = P(y_maxclass) = Prior

Decision Boundary in kNN (contd.)

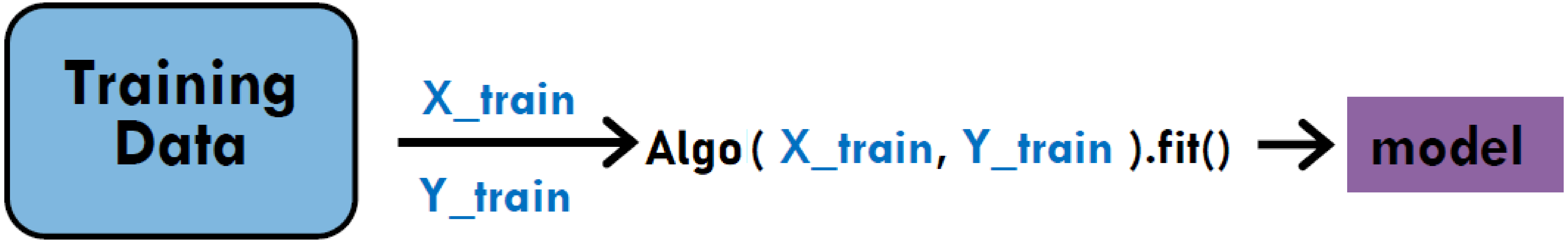


- In other ML algorithms, higher value (such as degree of polynomial in regression) leads to overfitting
- Reverse in kNN
- Overfitting for low k. Underfitting for high k

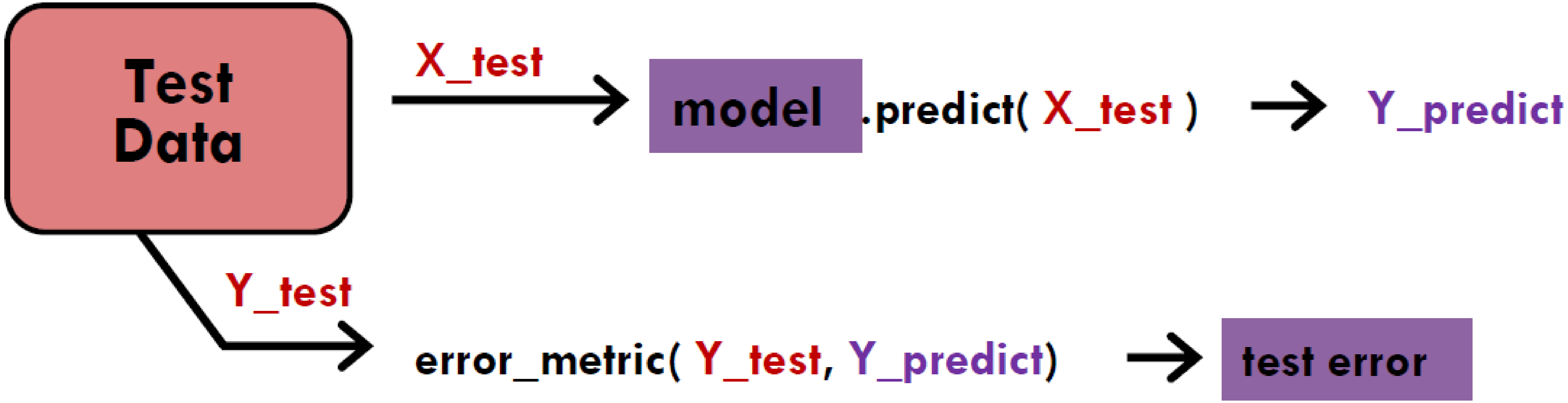
kNN Overfitting v/s Underfitting



Typical train-test steps



- Nearest Centroid training: extract centroids & classes
  - Throw away training data after that



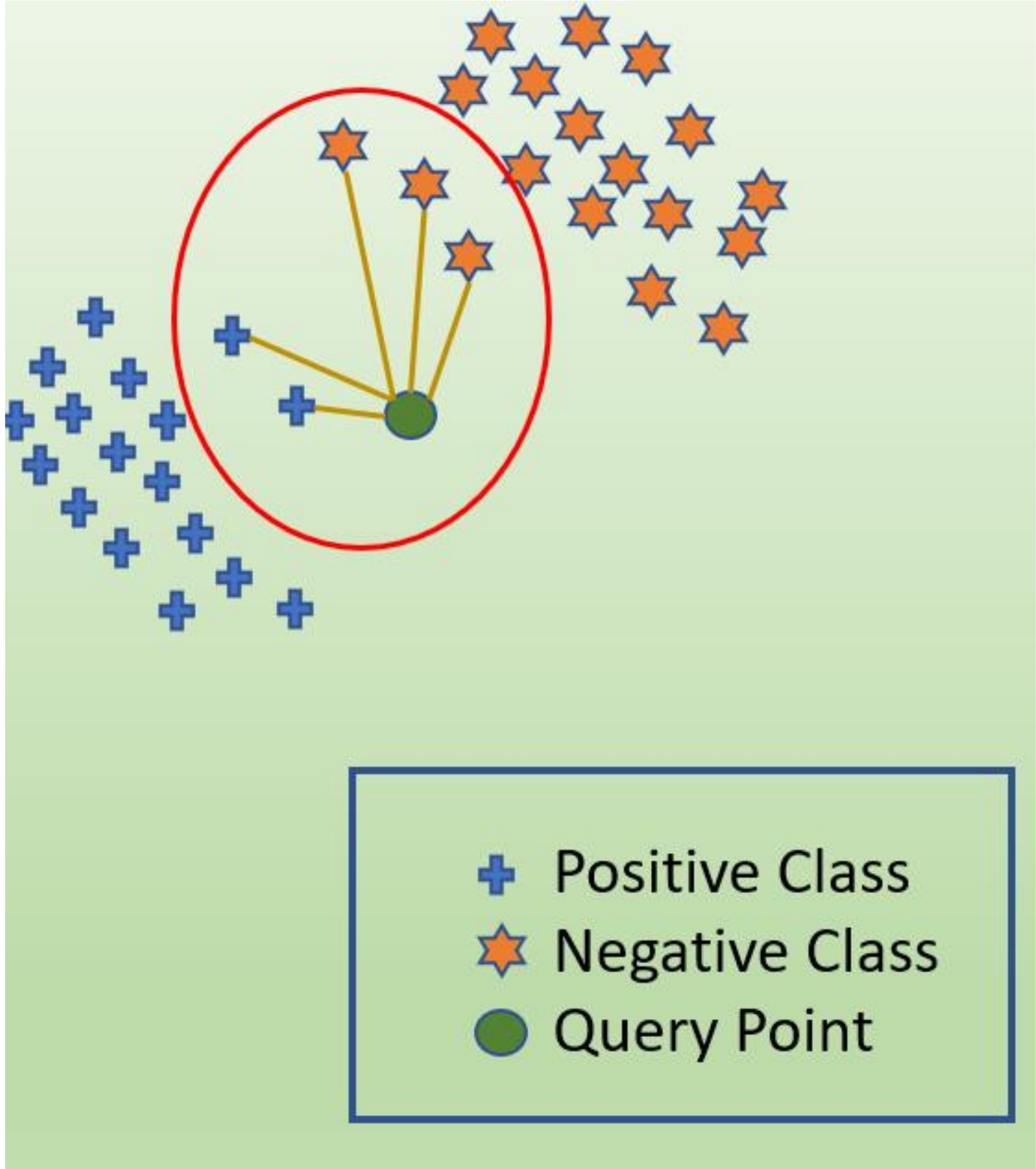
kNN train-test steps

- Train:
  - kNN training phase does nothing
  - Just holds onto the provided hyper params & data
- Test:
  - Multiple test points are provided
  - Runs pairwise distance between all train & test points (m x n distance computations)
  - Reports score
  - Computationally expensive at prediction time

Nearest Centroid v/s kNN comparison

Nearest Centroid	kNN
Eager	Lazy
Batch	Instance
Parametric	Non parametric
Discriminative	Discriminative

Weighted kNN



$$weight = \frac{1}{distance}$$

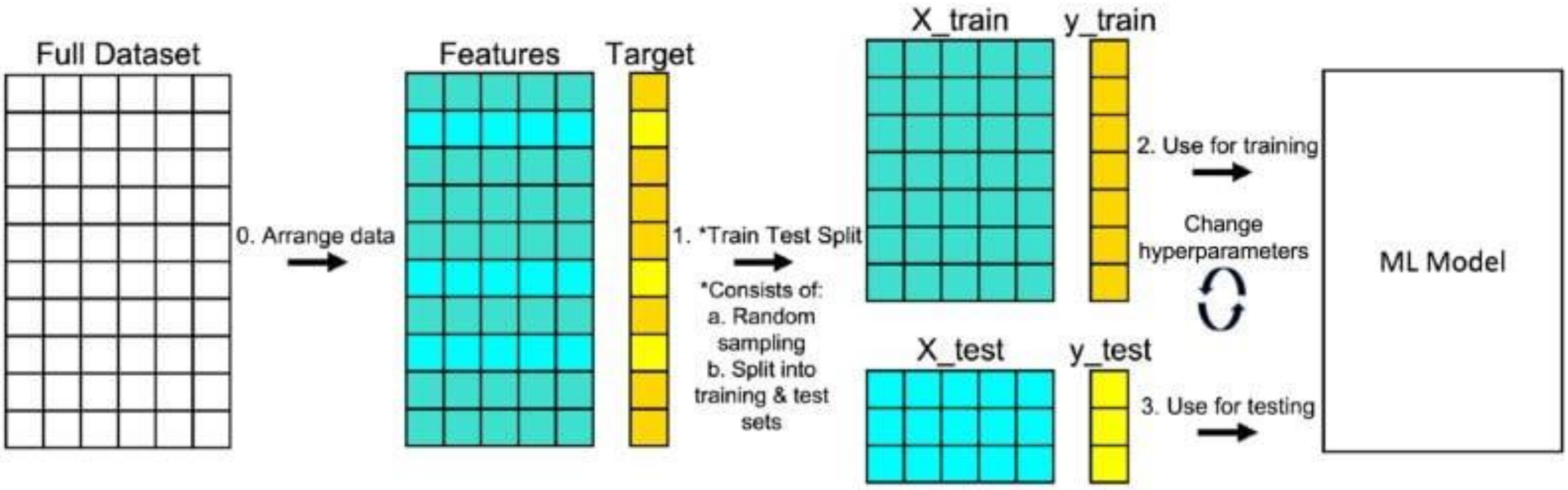
Neighbour	True Label	Distance	Weight	Sum of Weights
X_1	Positive	0.1	10	13.3
X_2	Positive	0.3	3.3	
X_3	Negative	1	1	1.8
X_4	Negative	2	0.5	
X_5	Negative	3	0.3	

Hyperparameter tuning with Cross validation

How to select a kNN model?

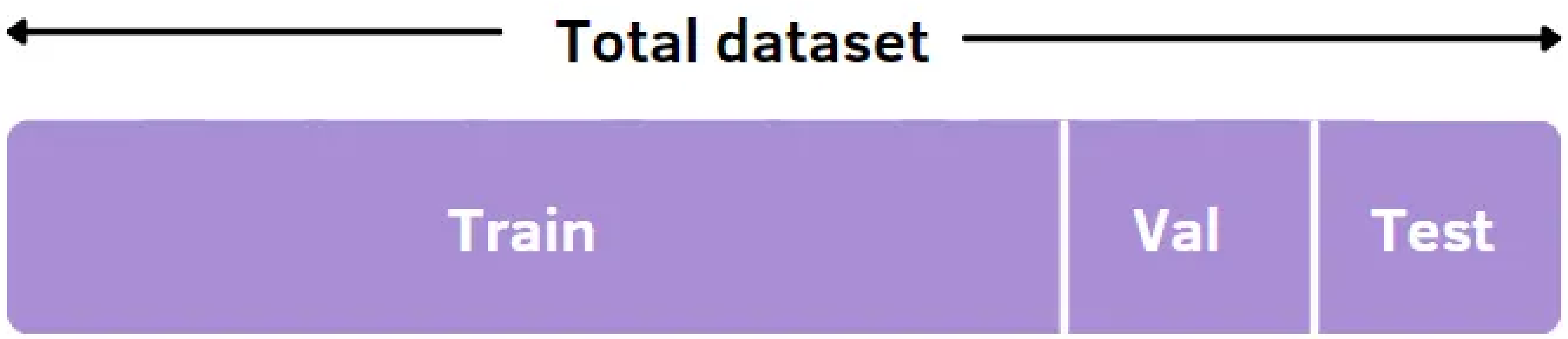
- Basic kNN - Two hyperparameters to choose
  - k – The number of nearest neighbors
  - Distance measure (Euclidean, Manhattan)
- Many more hyperparameters exist
  - How about weighted kNN?
- Parameters & hyperparams – What's the difference
- Hyperparameter tuning

Option 1: Use train-test split



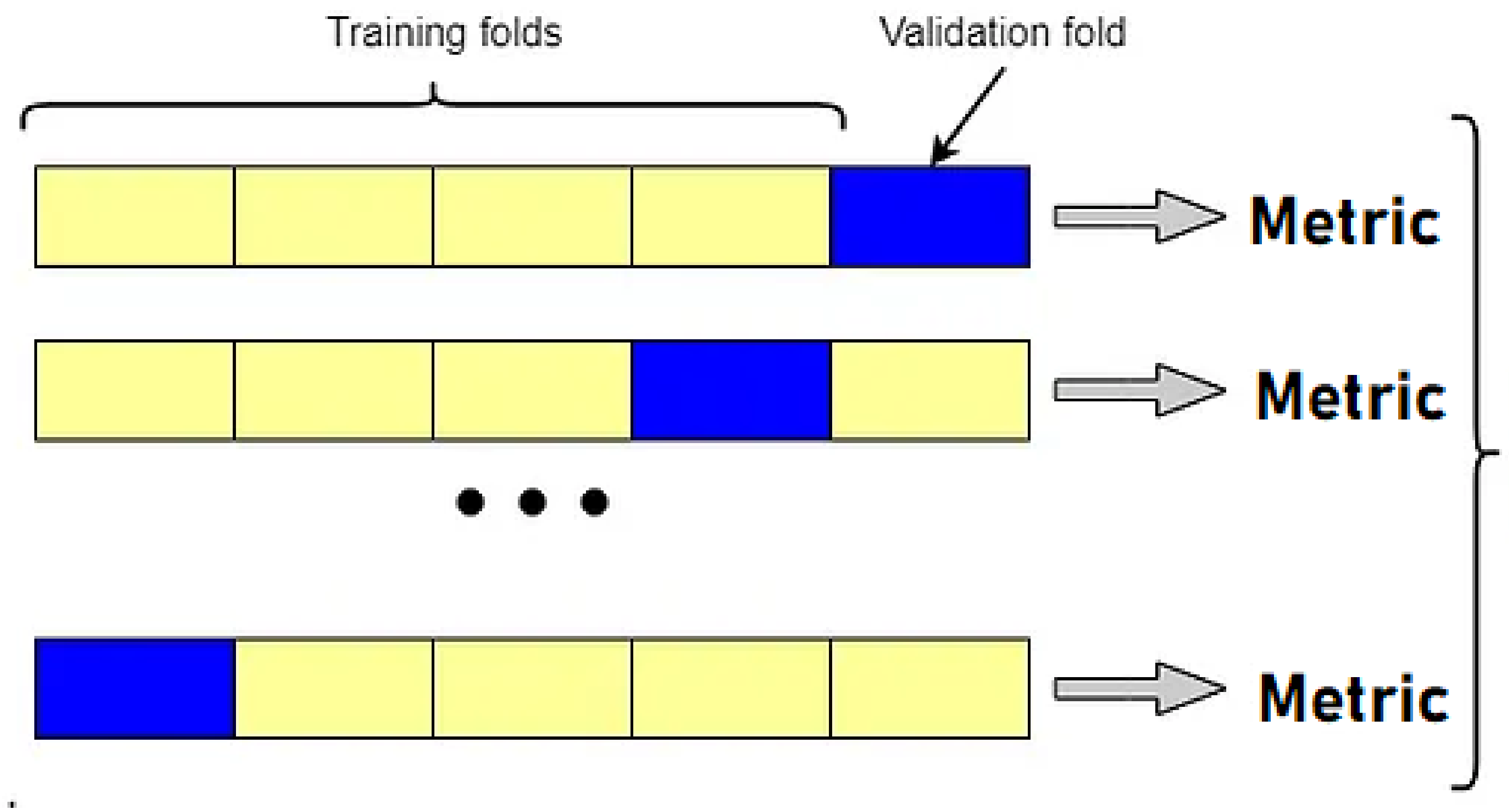
- Issue:
  - We will never know if a model is good without running on test split

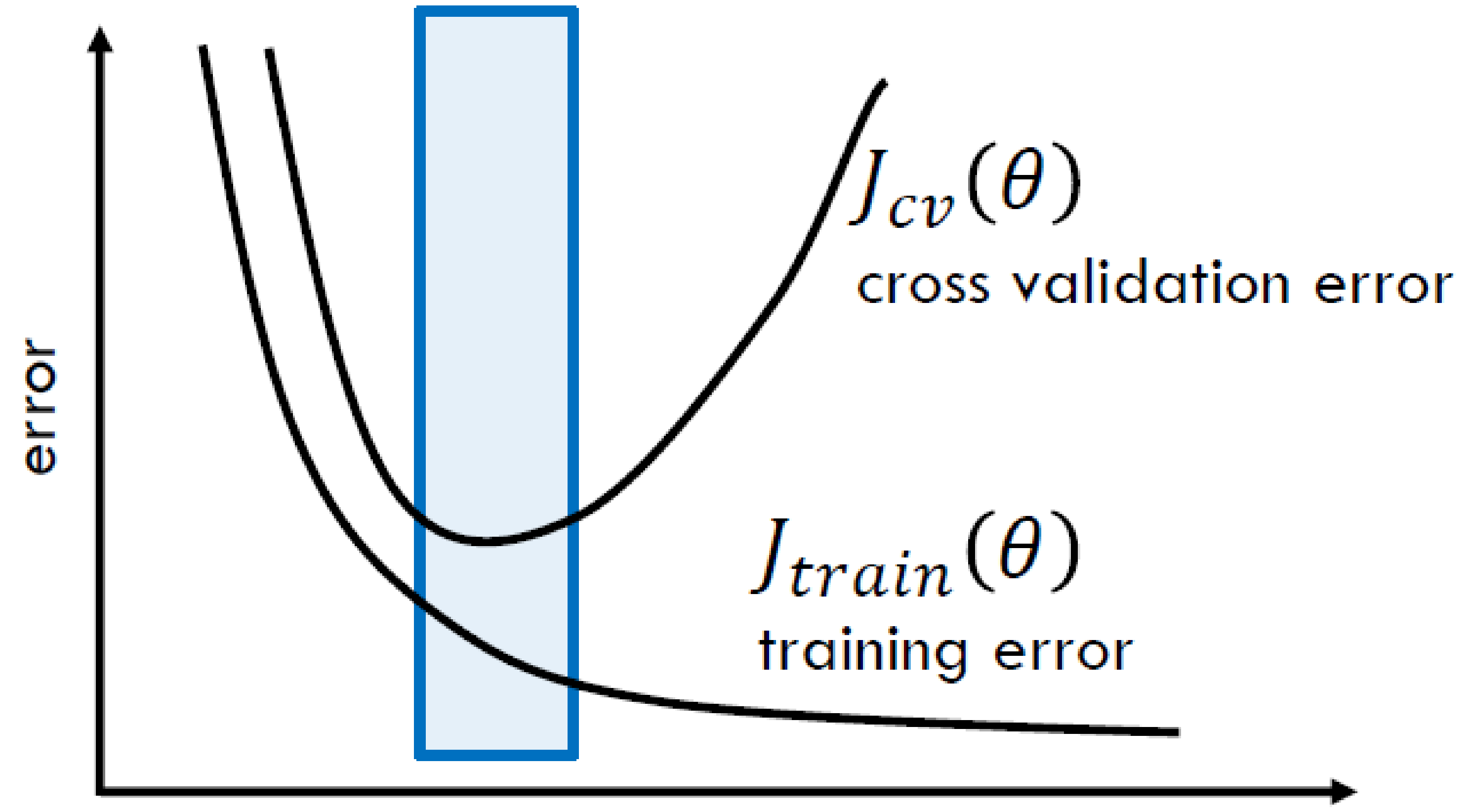
Option 2: train-validation-test split



- Classical, old fashioned approach: 60:20:20 split
- Acceptable when there is lot of data
- Issue:
  - Model does not generalize when less data
  - Results in overfitting

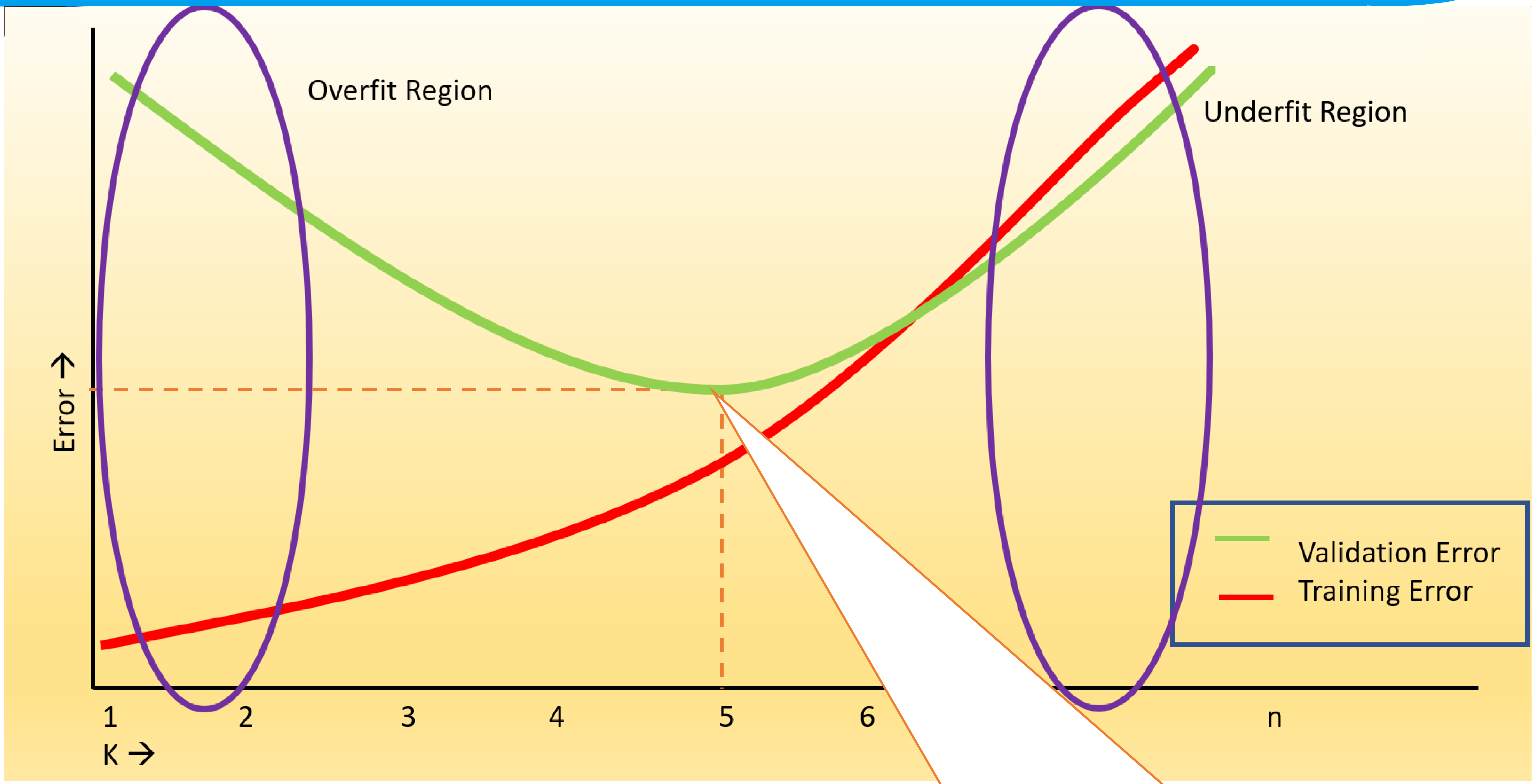
K-Fold CV (contd.)





- For each of k=1,3,5,7,10 in kNN:
  - Run 5-Fold CV
  - Get mean train and val error. Plot
- In general, k with lowest val error is best k

kNN K-Fold CV

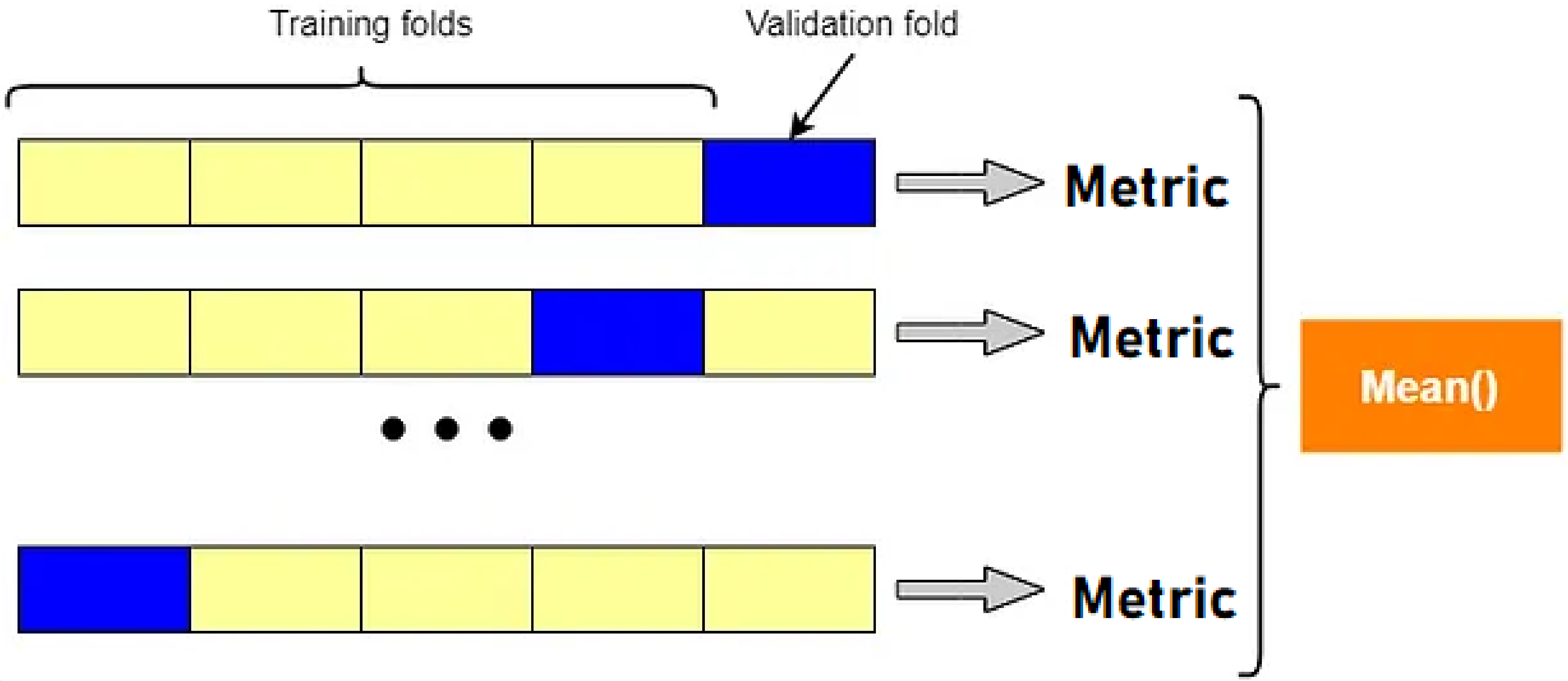


Classifier metric may measure accuracy & higher the better.
We look for best score in CV

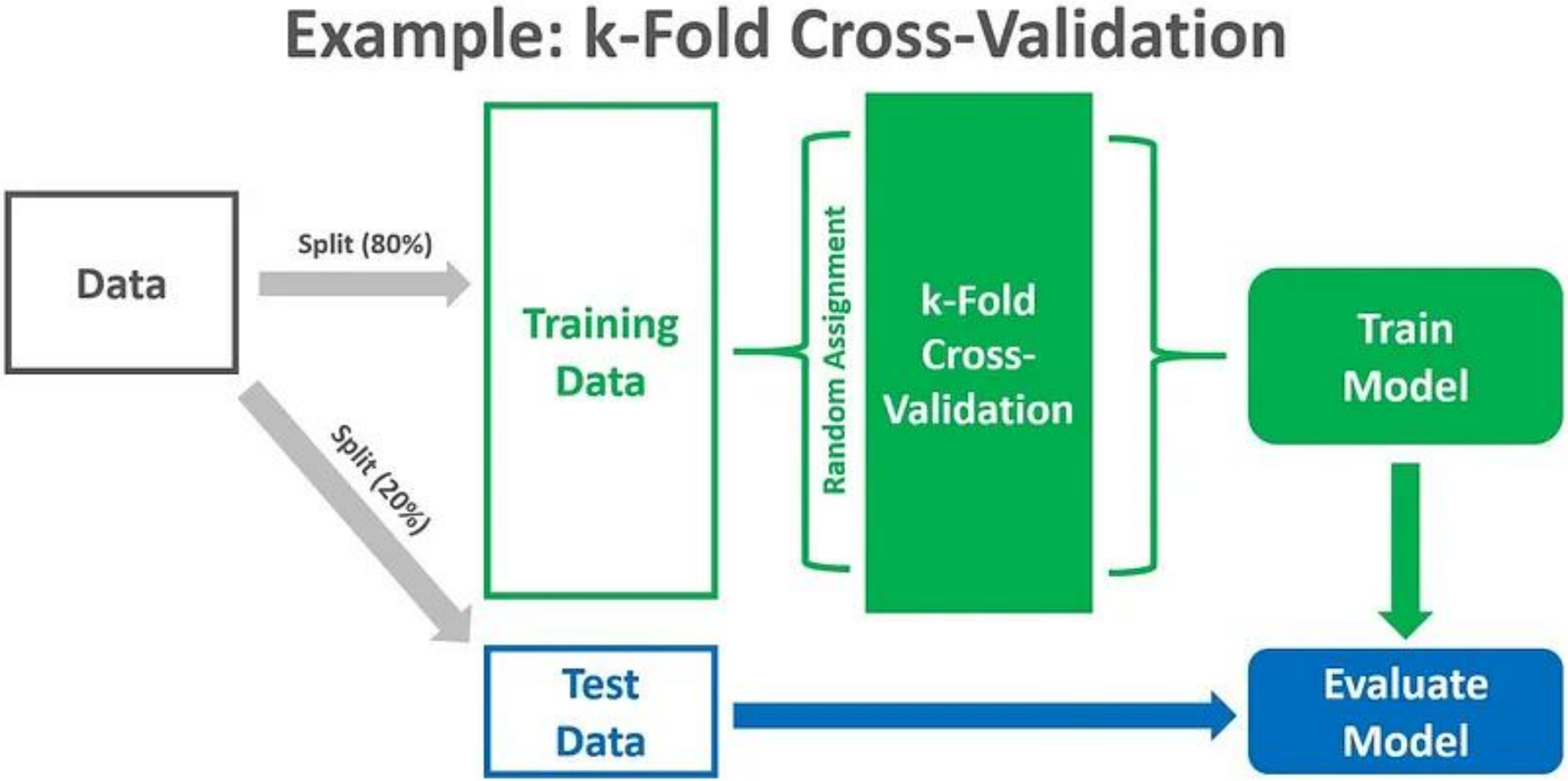
Option 3: K-Fold Cross Validation (CV)

Choose k = 1 for kNN (1 neighbor)

Repeat with k = 3, 5, 7 for kNN



- Mean errors for different k = [10.5 , 12 , 12 , 8.5 , 18]
- K-Fold CV is used to select best k for kNN
- Note: K in K-Fold CV got nothing to do with k in kNN
- Choose K = 5 (or 10) in K-Fold CV. This is constant

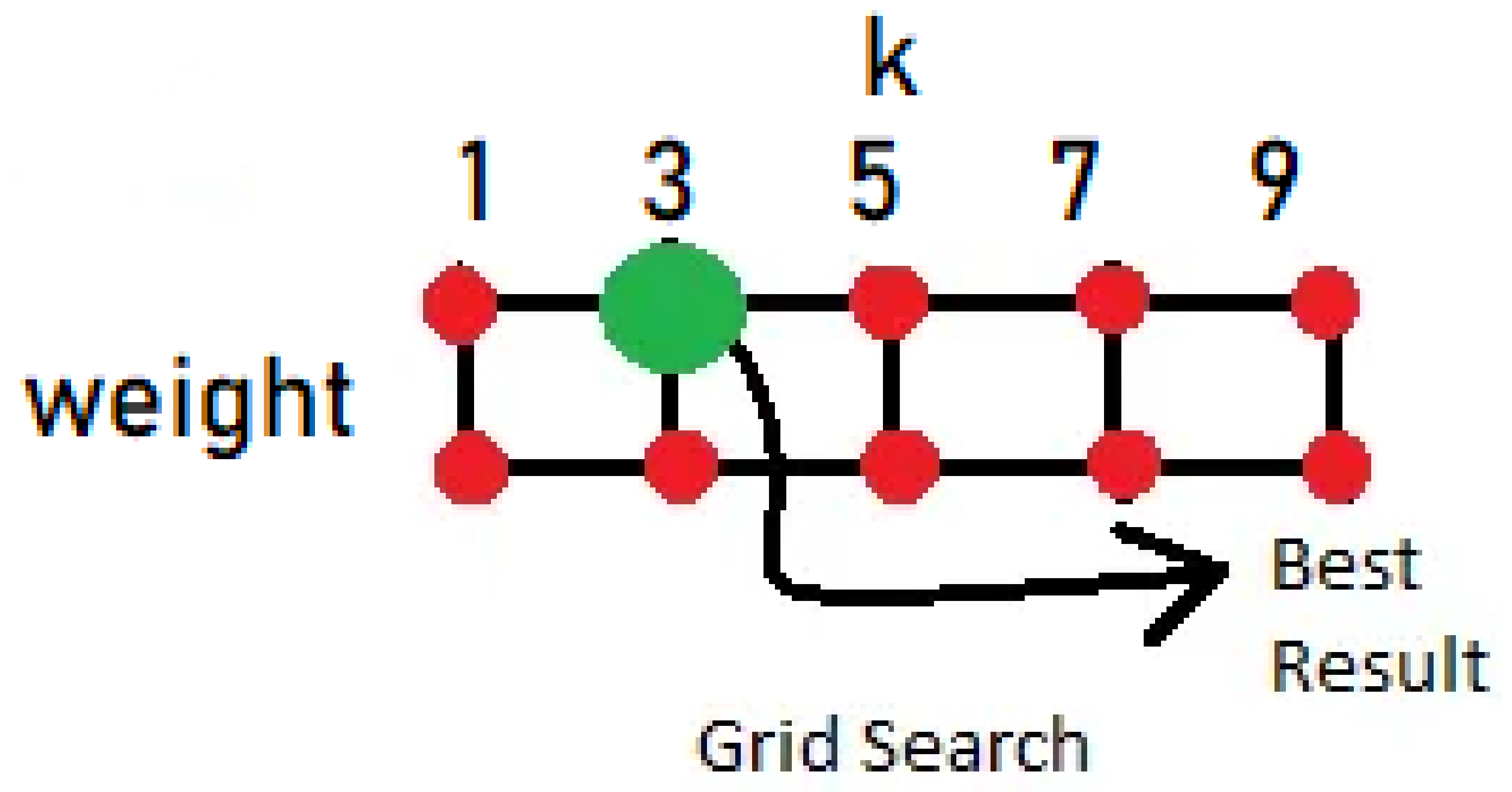


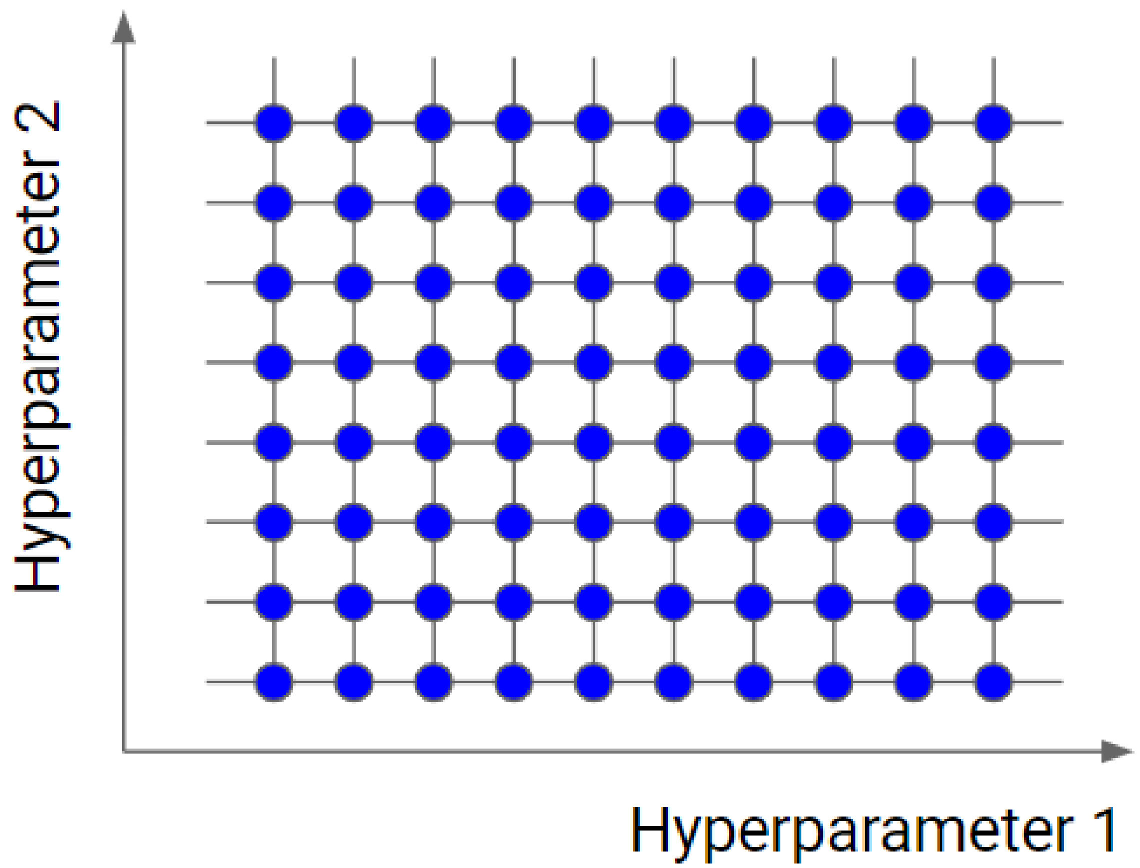
- Can we use K-Fold CV for Nearest Centroid?

Hyperparameter tuning with Grid Search and Bayesian Optimization

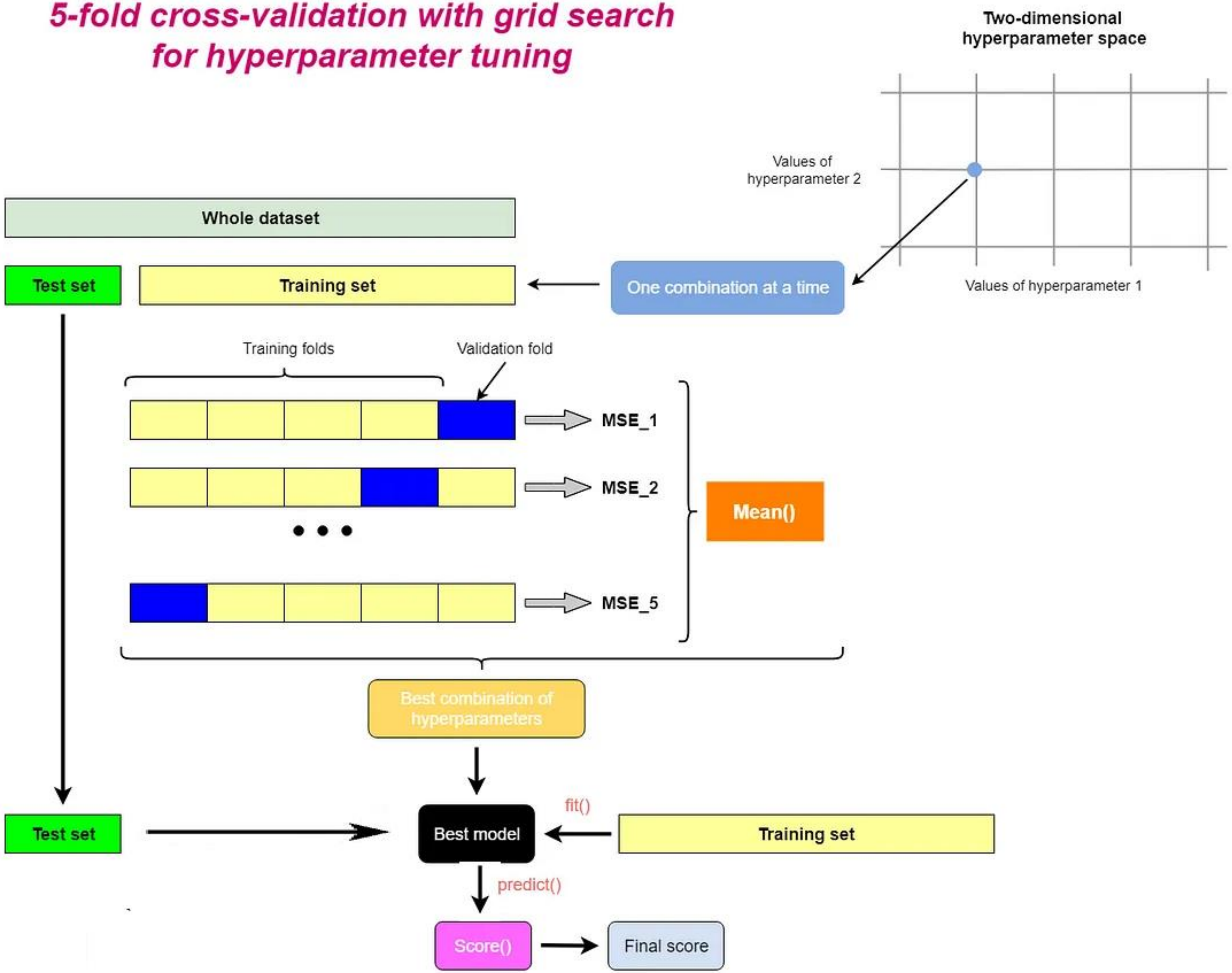
Multiple hyperparameter tuning

- kNN – k and weight
  - k={1,3,5,7,9}
  - weight={“uniform”, “distance”}
- K-Fold CV to be executed 5 x 2 = 10 times
- GridSearchCV

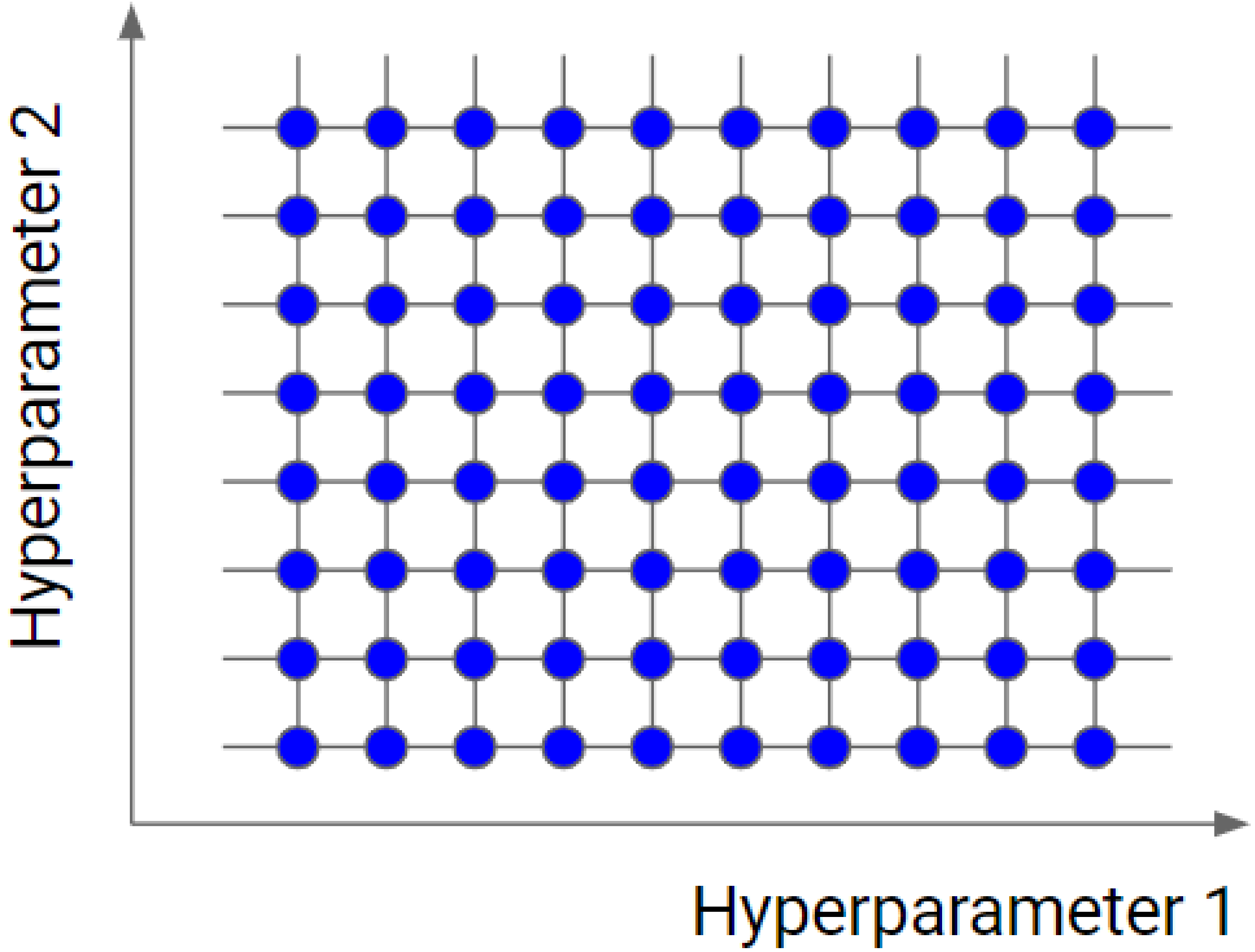


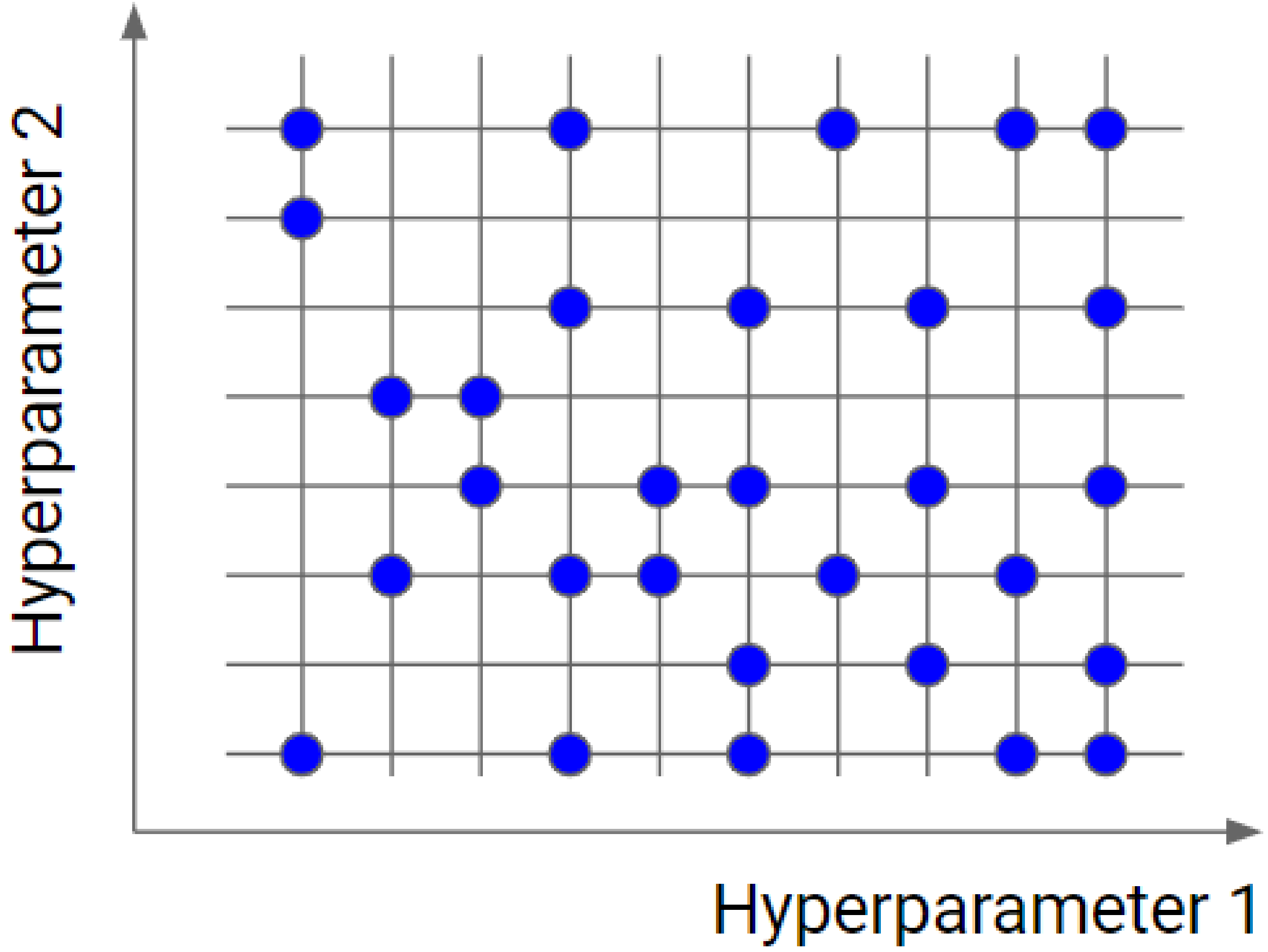


5-fold cross-validation with grid search for hyperparameter tuning



GridSearchCV & RandomSearchCV





Which option when? Dos and don’ts

- Regular machine learning
  - 1 hyperparam - K-Fold CV
  - Multiple hyperparams - GridSearchCV, RandomCV
- What about deep learning?
  - Lot’s of data, lengthy training process
  - Training neural network K-times CV is not feasible
- KerasTuner, Hyperopt, Optuna for both regular & deep learning

Why not Grid search

- Too many eval - Objective function eval is expensive
- Grid search is completely uninformed about past eval

- 3 spaces to be aware of:
- Feature space
- Parameter space
- Hyperparameter space

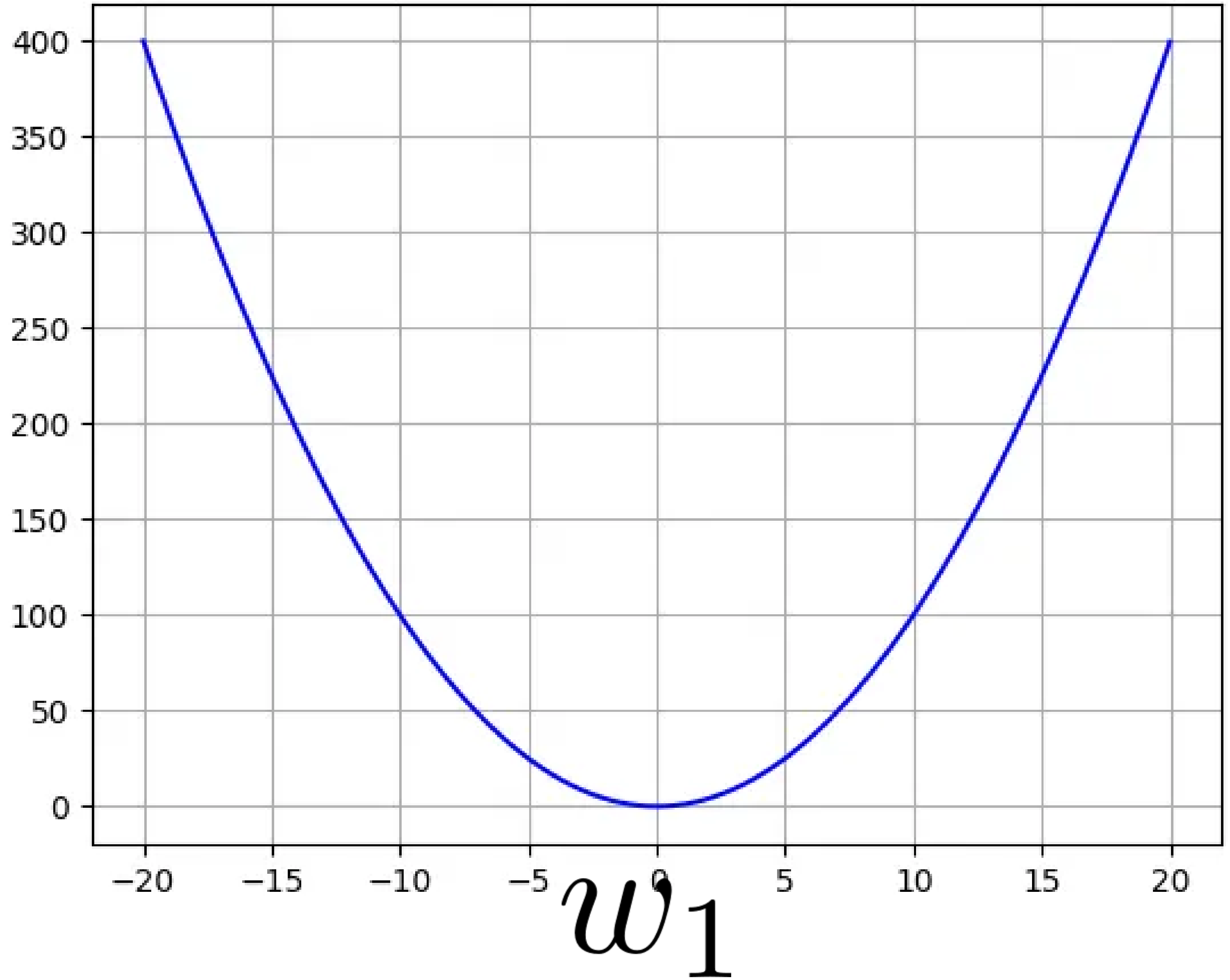
Understanding parameter space

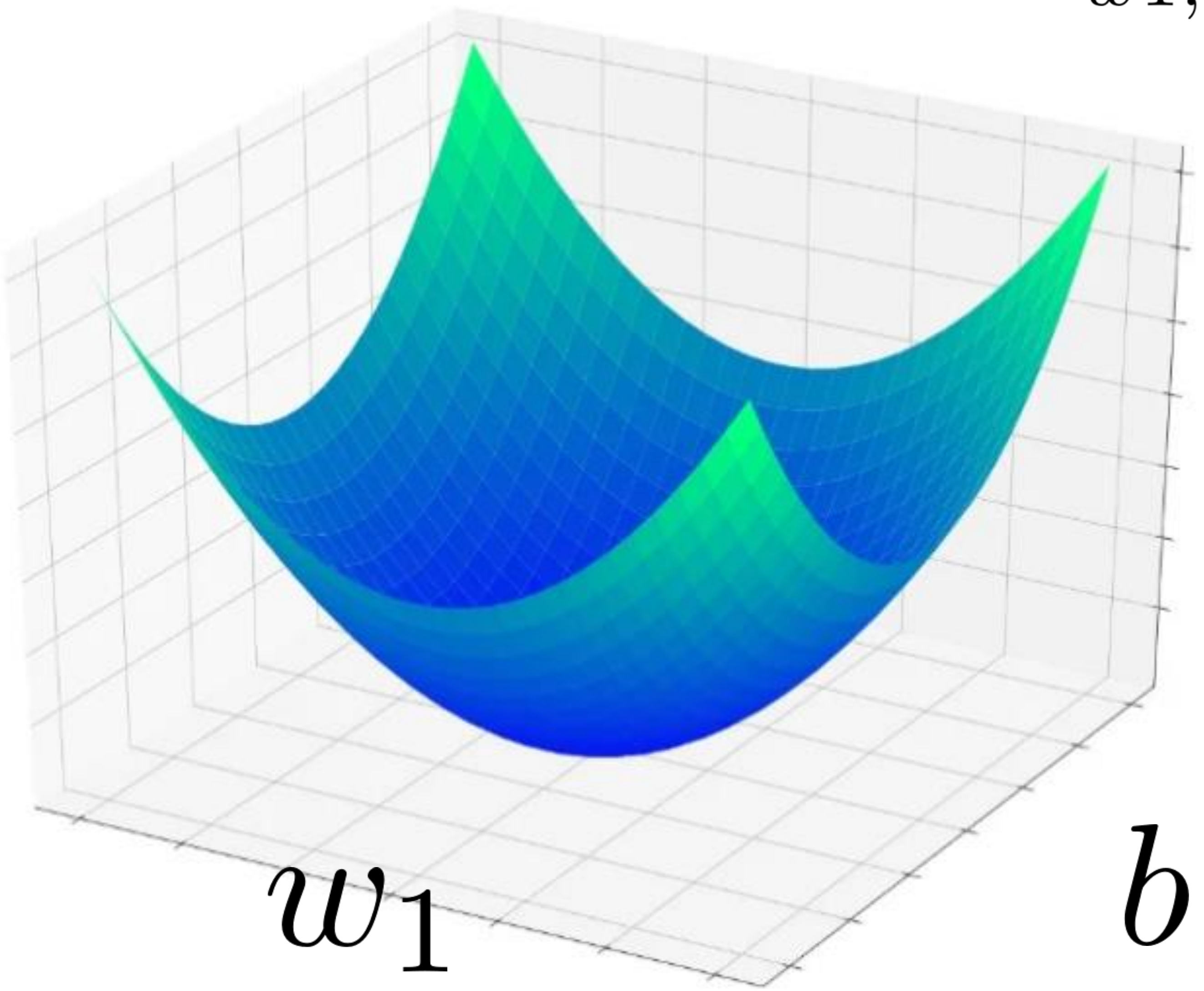
- Objective function is evaluated in parameter space

$$\hat{y}_i = x_i^T w + b \quad w \in \mathbb{R}^d$$

$$\text{MSE} = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2$$

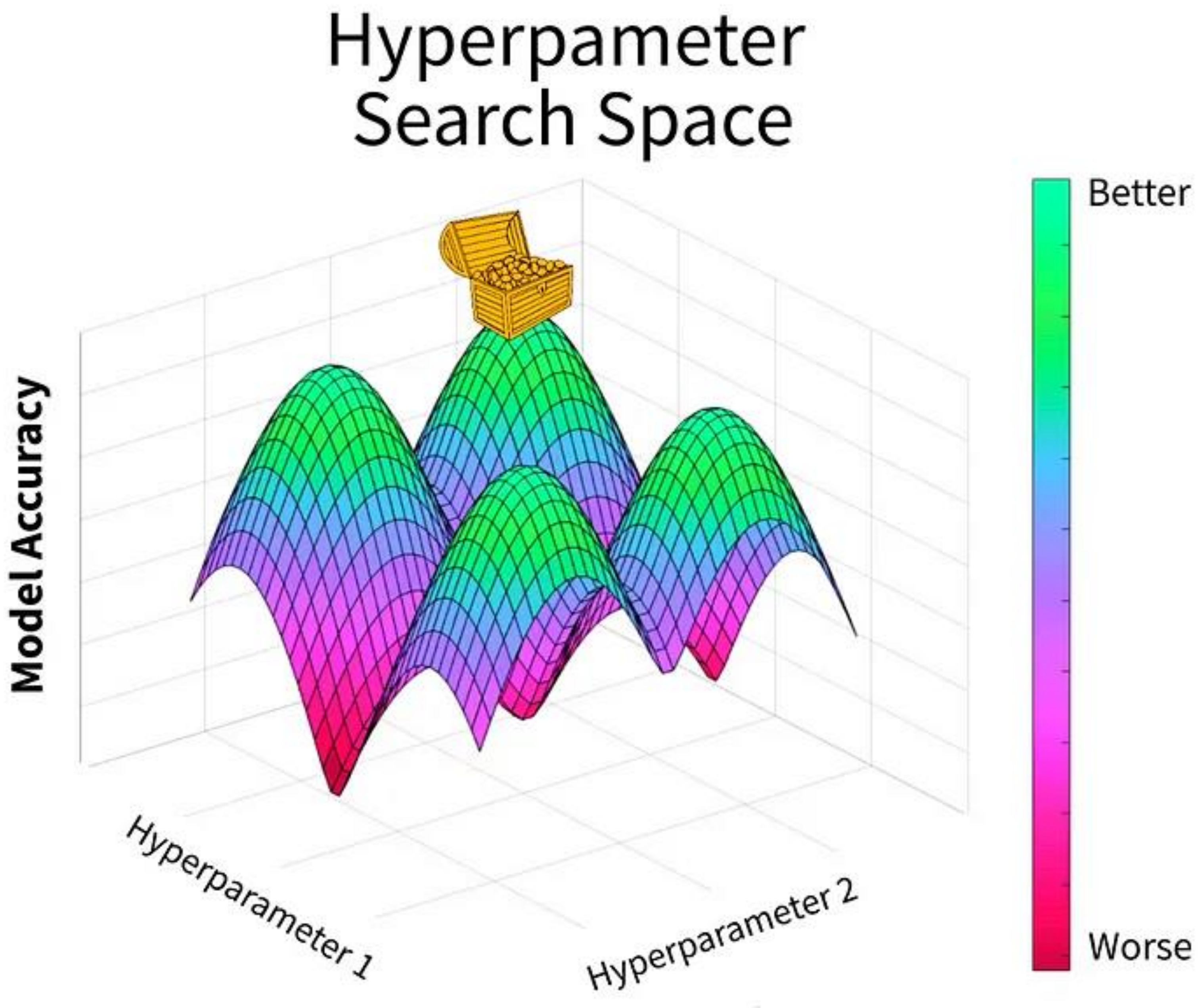
$$Objective = \arg\min_{w1,b} MSE$$





Why not Grid search

- Too many eval - Objective function eval is expensive
- Grid search is completely uninformed about past eval



- GridSearch happens in hyperparameter space

- There's also a hypothesis space. Don't worry about it

Hyperparameter tuning with Bayesian Optimization

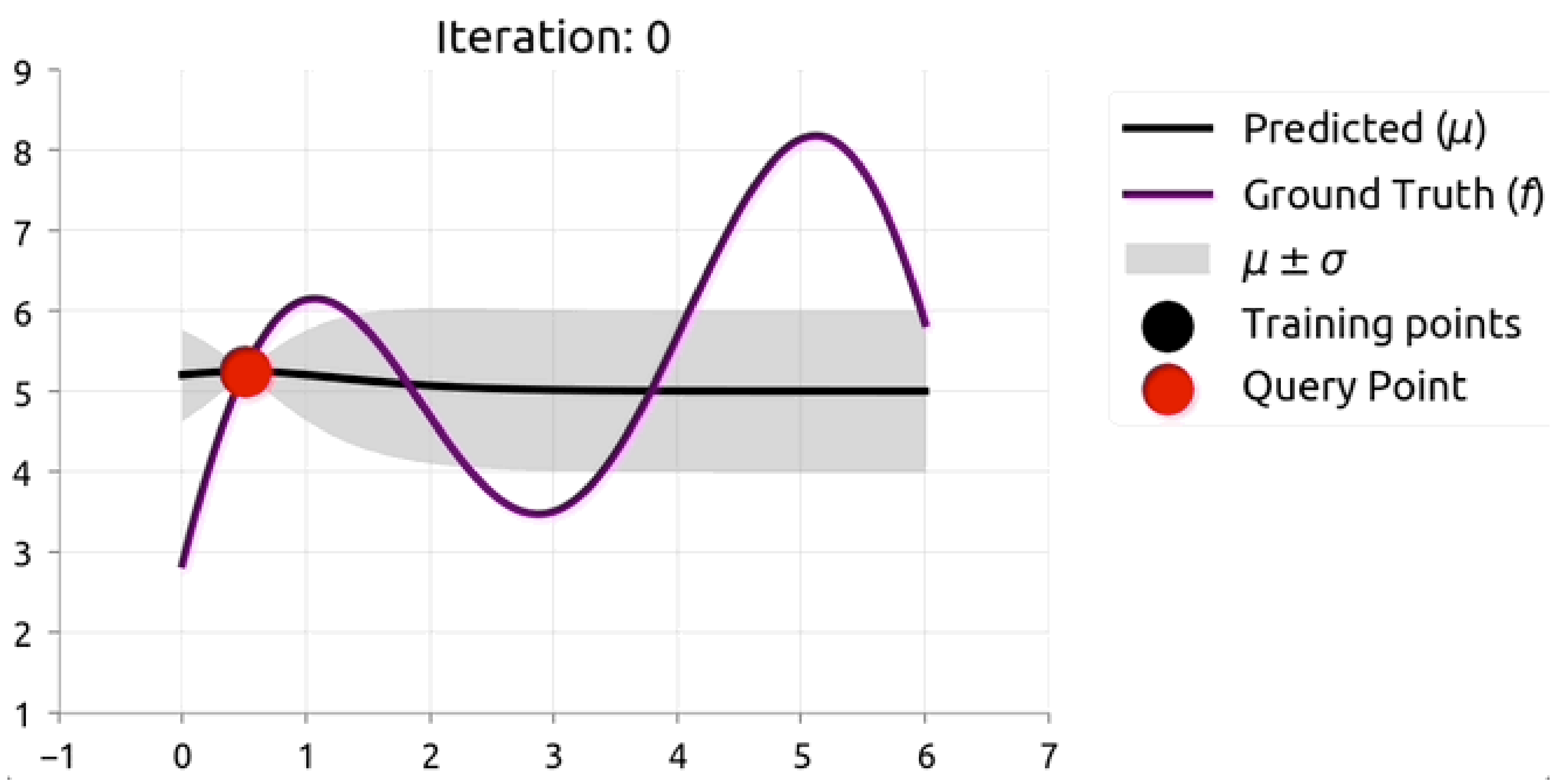
Surrogate function

Posterior

Likelihood

Prior

$$P(score|hyperparam) = \frac{P(hyperparam|score)P(score)}{P(hyperparam)}$$



- Prior, Likelihood & Posterior
- Posterior evaluated with surrogate function
- Cheap to evaluate

- Surrogate function modeled as a Gaussian Process (GP)
- GP gives a distribution of functions
- Very good at interpolating, not good at extrapolating

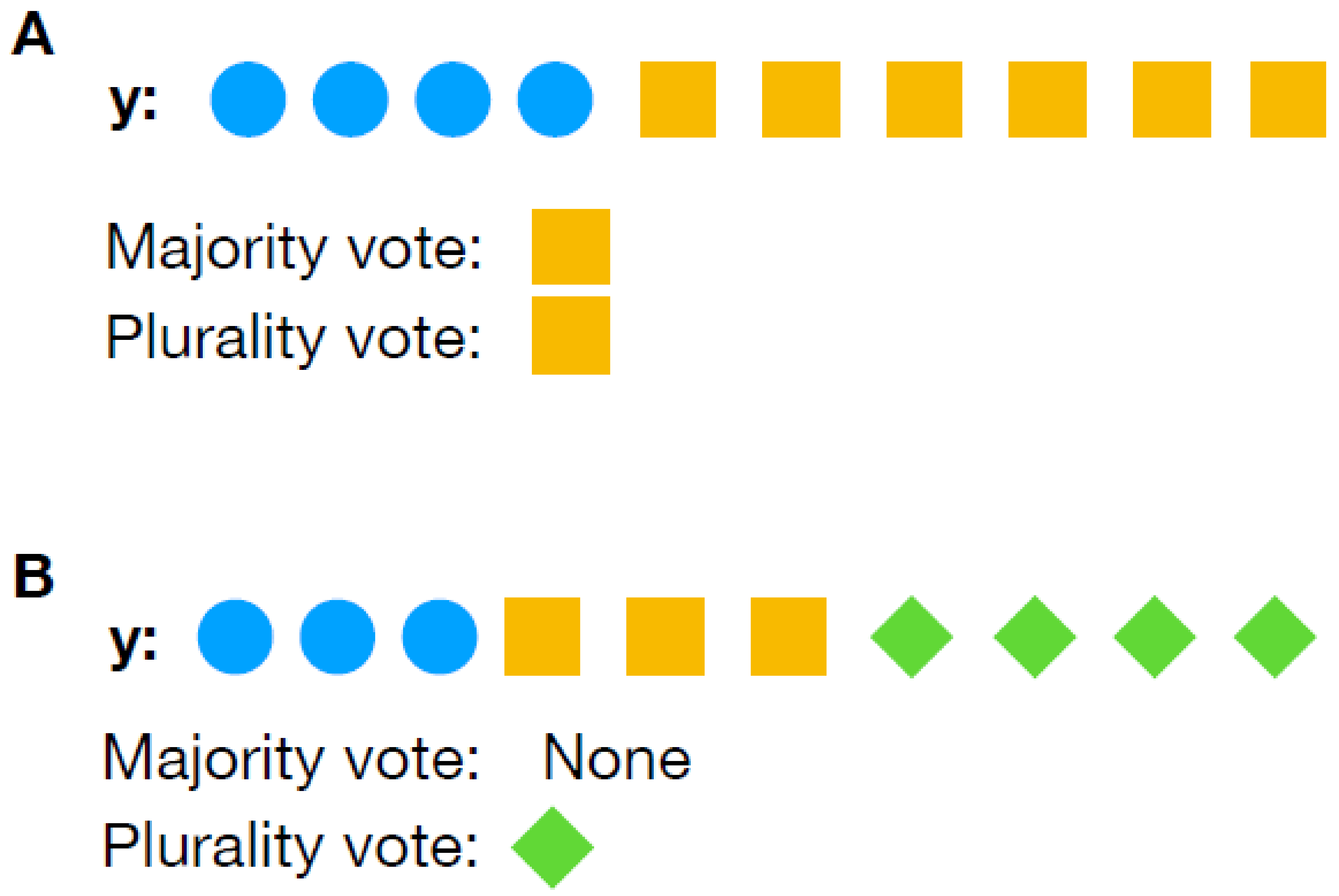
Types of Cross Validation

- Hold out (Train-test split)
- K-Fold Cross Validation
- Stratified K-Fold
- Repeated K-Fold
- Nested k-Fold
- Leave One Out (LOOCV)
- Let’s look at others in lab

Multiclass kNN & kNN Regression

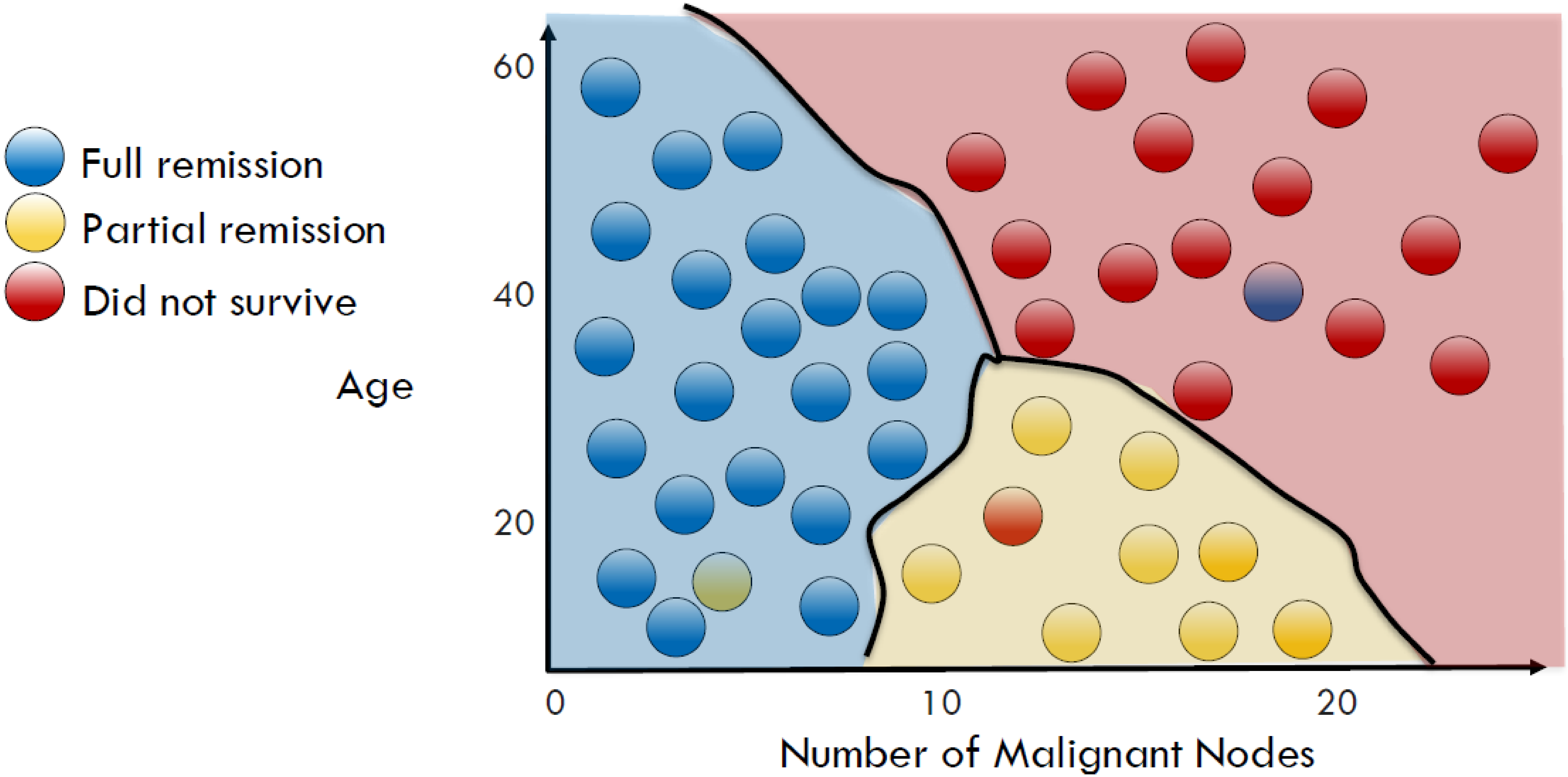
Multi class kNN

- Majority v/s plurality
- For 3 class
    - Majority = 50%+
    - Plurality = 33.33%+



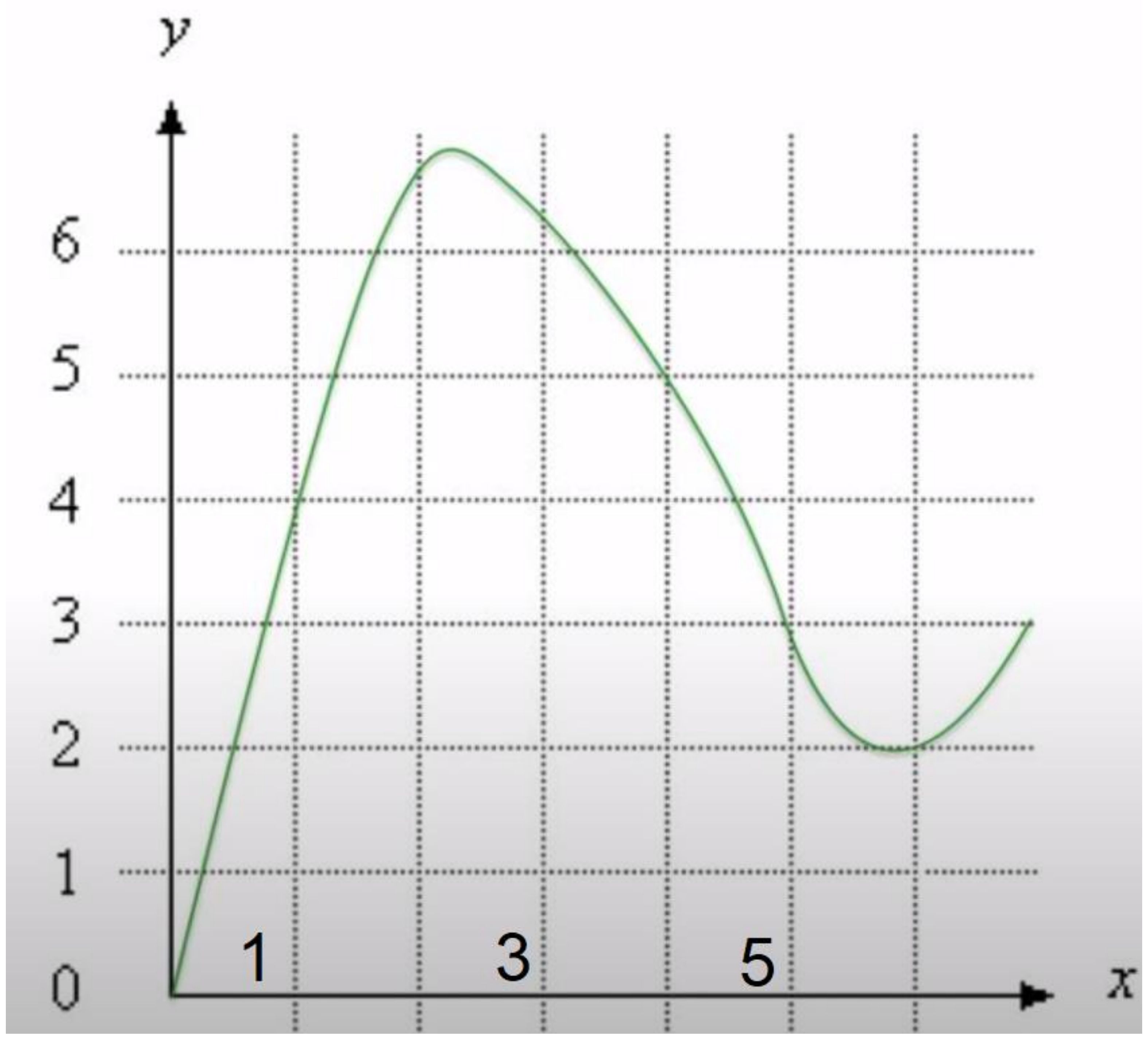
Multi class kNN decision boundary

K = 5

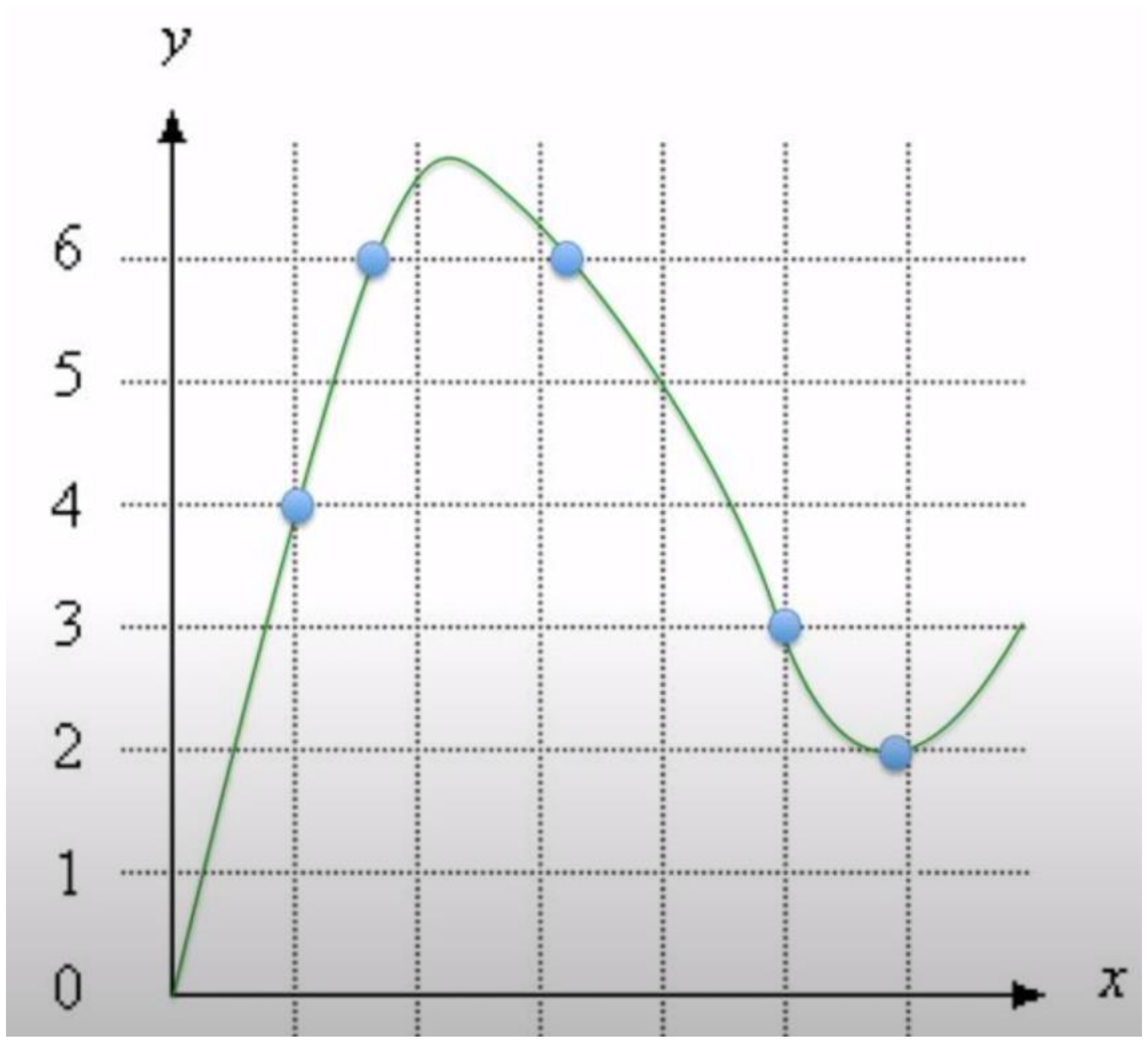


kNN Regression

Real function

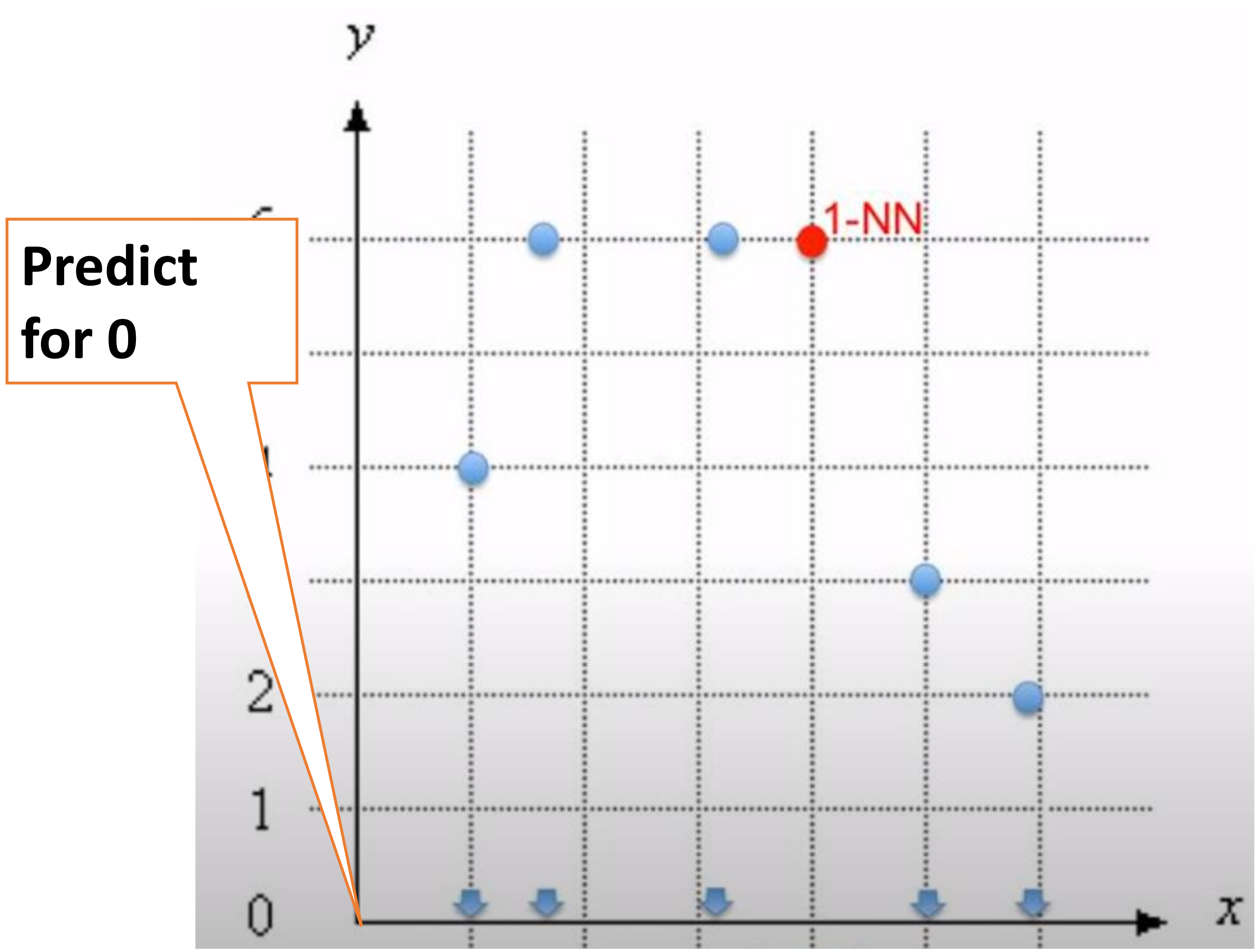


Actual data

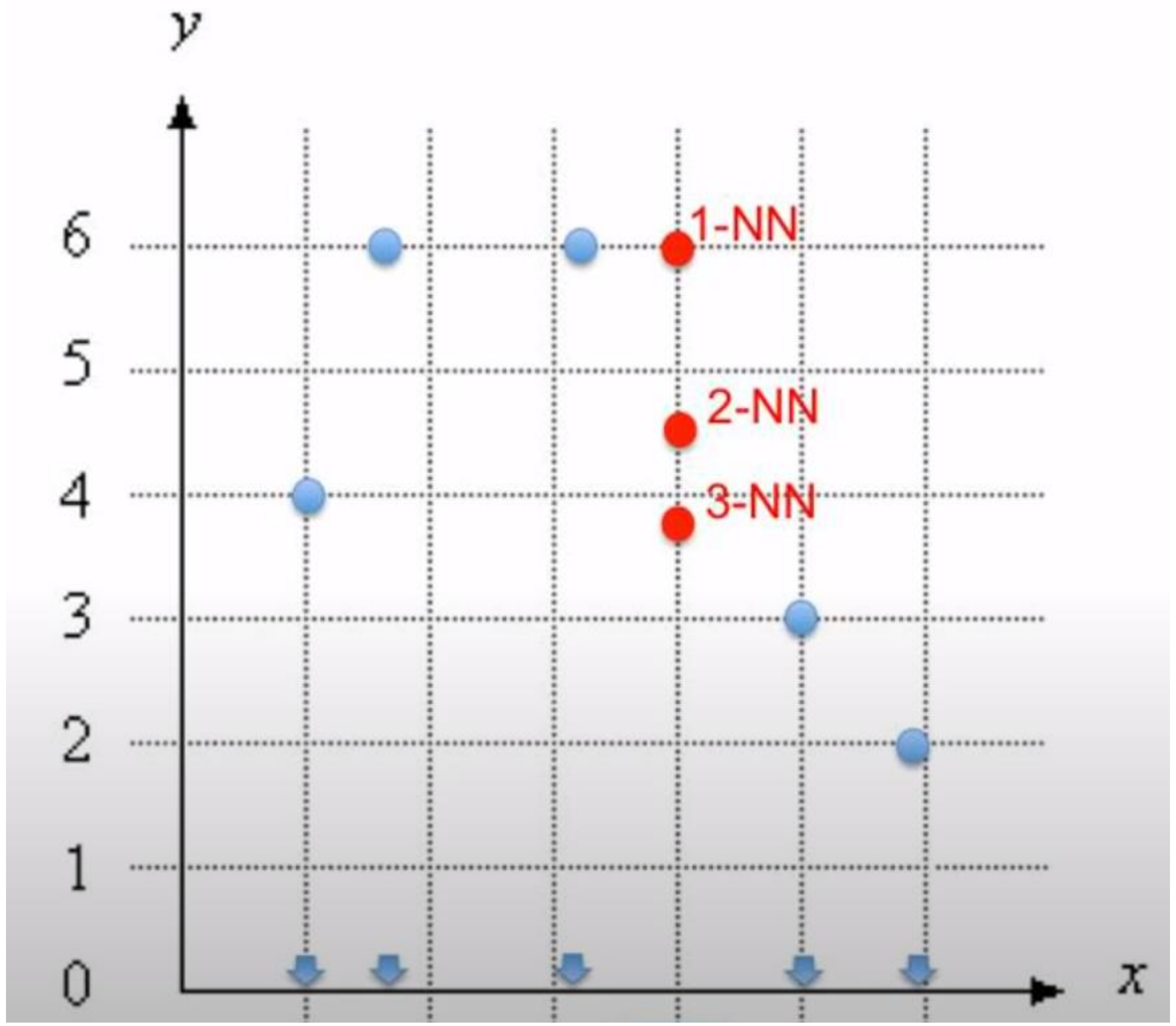


kNN Regression(contd.)

1-NN Regression

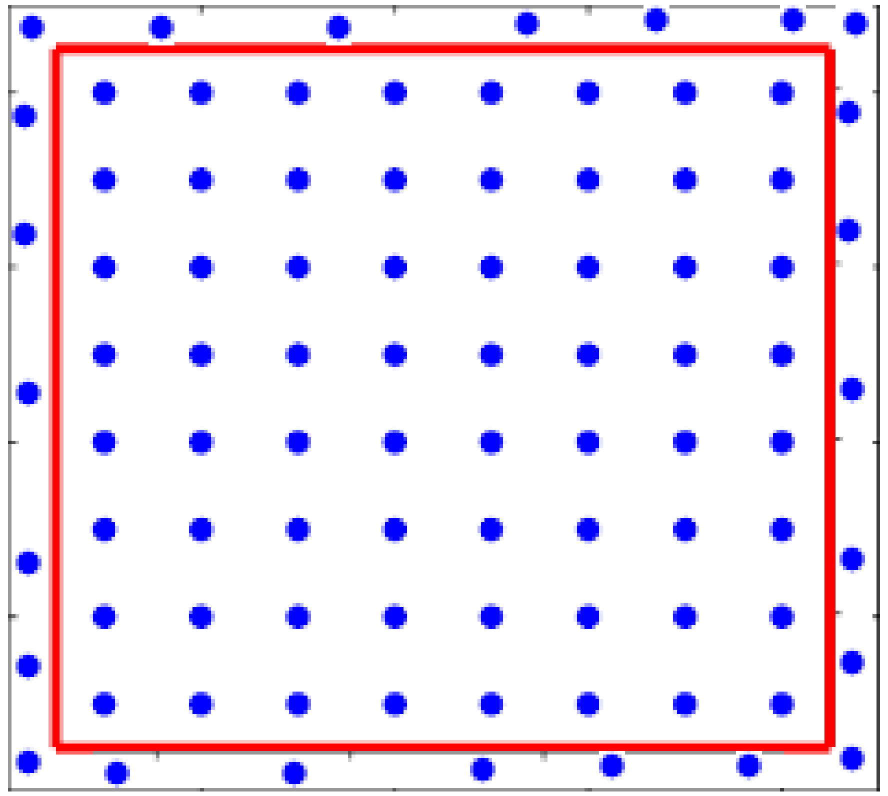


2-NN, 3-NN Regression



- kNN Regression good at interpolation bad for extrapolation

Curse of Dimensionality



- P(point < 0.01 units from border) =
  - 1 - P(point inside 0.99)
- P(point inside 0.99) = 0.99 * 0.99
- 1- 0.9801 = 0.0199

- P(point < 0.01 units from border) =

$$= 1 - (0.99)^3 = 1 - 0.9703 = 0.029$$

- For 1000 dimensions, P(point in 0.01 border) =

$$= 1 - (0.99)^{1000} = 1 - 0.00004317 = 0.99995683$$


QUESTIONS

Literature Survey