Lecture 9 – Classification and Regression

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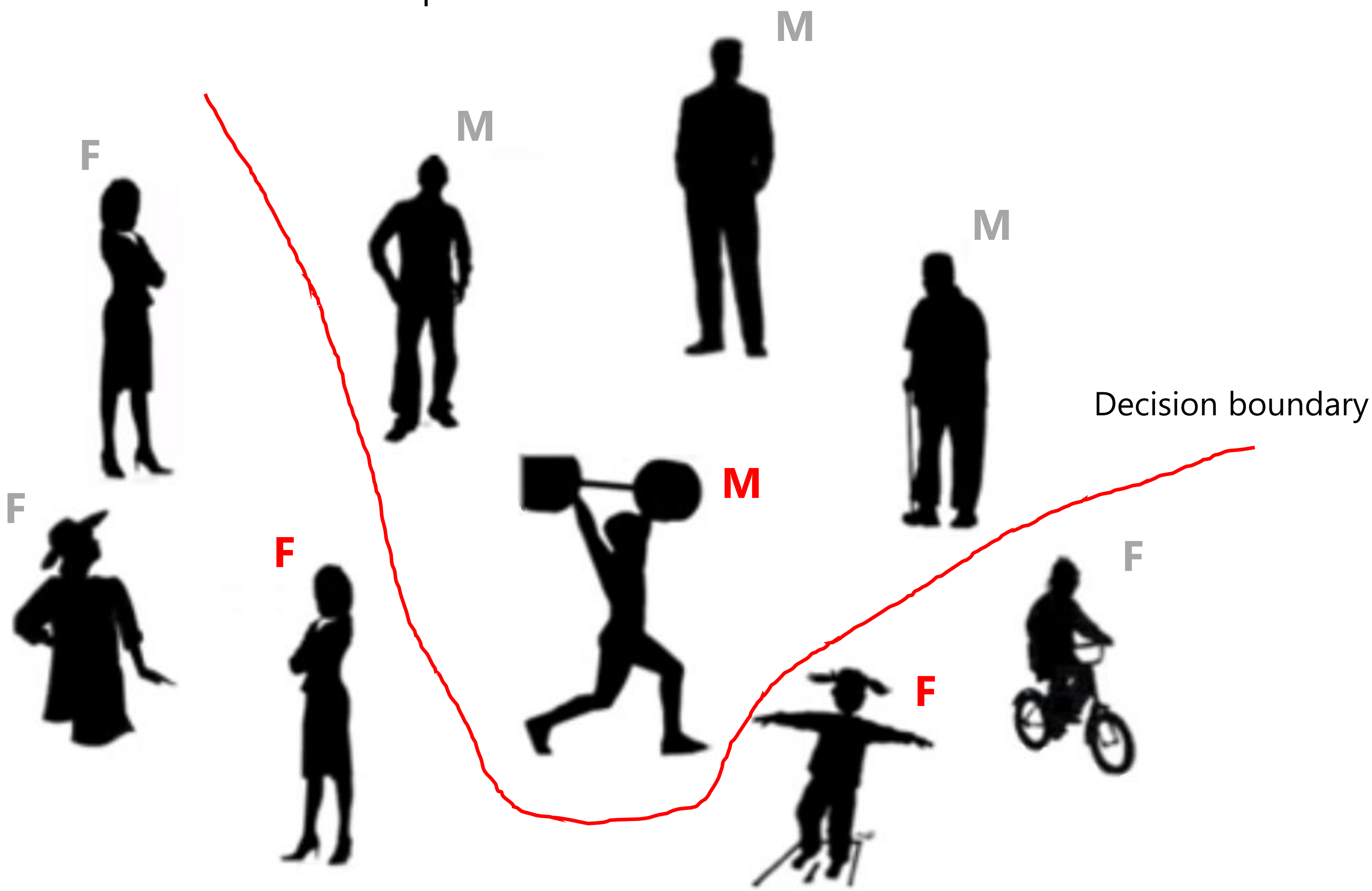
Objectives

- What is classification
- Training/validation/testing datasets
- K-nearest neighbours
- Support vector machines
- Classification performance evaluation

Classification

- Supervised
  - We have a database with samples and their labels



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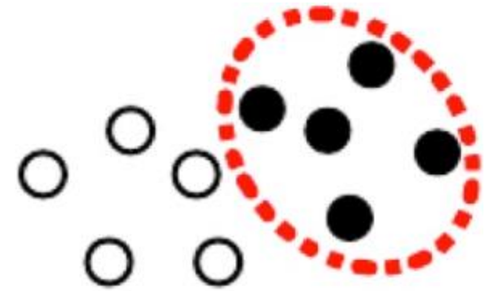
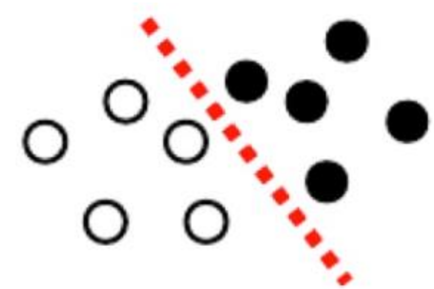
Generative vs Discriminative models

- Generative:
  - Computes probabilistic model for each class
  - Can use unlabeled data



- Discriminative:
  - Focus on separation of classes
  - Cannot use unlabeled data



Training/Validation/Testing datasets

- Training dataset:
  - Model can use both training features and labels for changing its parameters.
- Validation dataset:
  - Needed to estimate how suitable is the selected model for solving the target problem.
- Testing dataset:
  - Can only be used when the model is completely finalized. Cannot be used to update anything about the model

Training/Validation dataset example

- Dataset:

	Student 1	Student 2	Student 3	Student 4	Student 5
Name	Thomas	Victor	Diana	Tiffany	Andrew
Hours of preparation	12	25	10	21	1
Grade [0-10]	5	9	4	10	1

Training set

Validation set

- Two models trained on training set:
  - Grade depends on student's name:
    name starts with [A-M] – grade < 5
    name starts with [N-Z] – grade ≥ 5
  - Grade depends on the length of preparation:
    # hours < 12 – grade < 5
    # hours ≥ 12 – grade ≥ 5
  - How to know which one is more reasonable

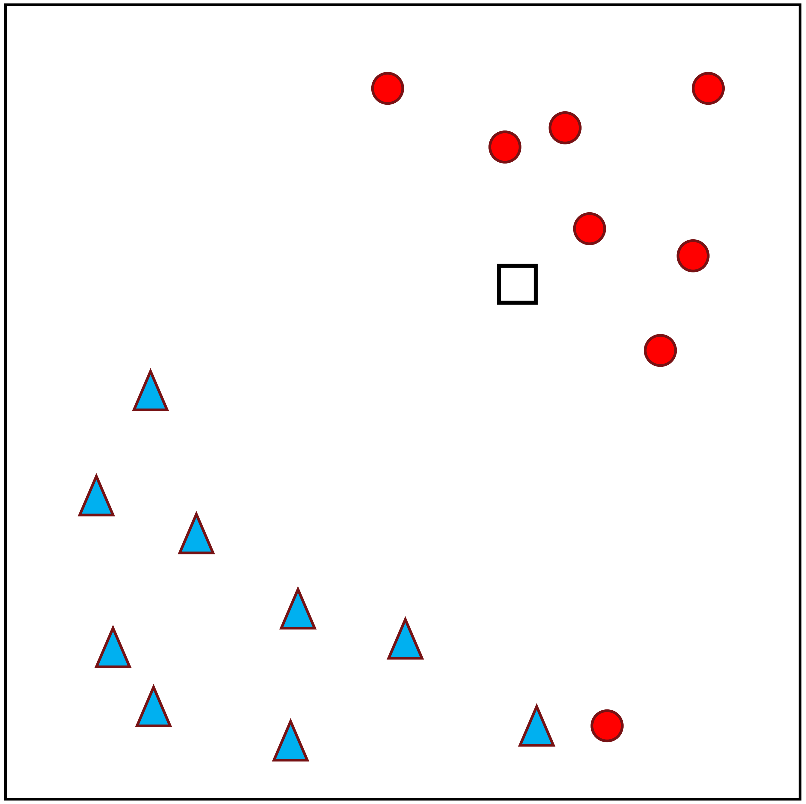
Accuracy on validation

50%

75%

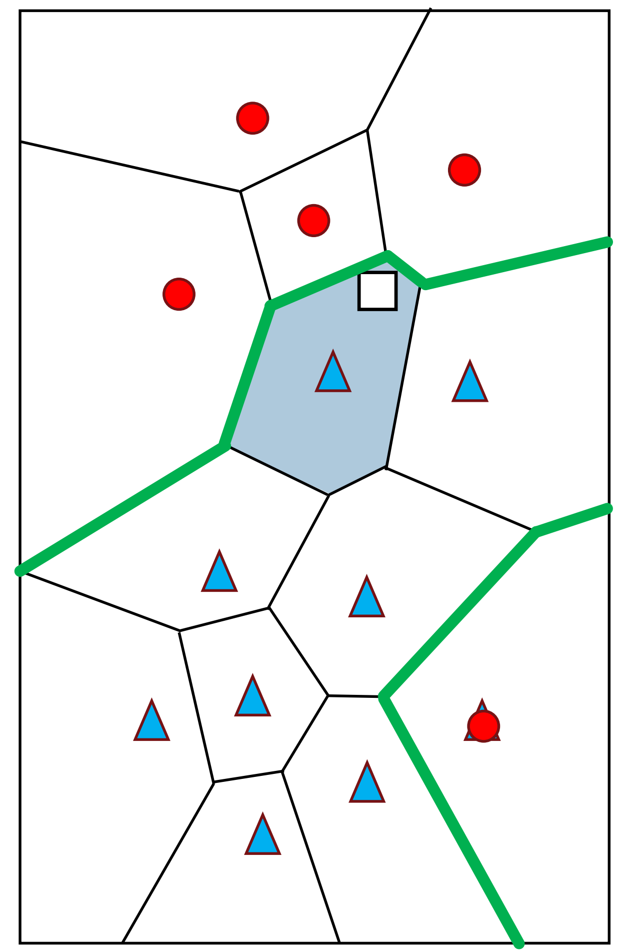
k-nearest neighbor classifier

- How would you classify the white box:
  - Red or blue class?
- How did you do it:
  - Fit gaussian?
  - Coded a neural network?
- Nearby elements are red



1-nearest neighbor classifier

- If we formalize this intuition:
  - Find the most similar training example x'
  - Use its label y' as the prediction
- Voronoi tessellation:
  - Separates space according to classes
  - Used to compute classification boundary
- Sensitive to outliers:
  - One point can change a very large regions
- Check more than 1 nearest neighbor



k-nearest neighbor (kNN) classifier

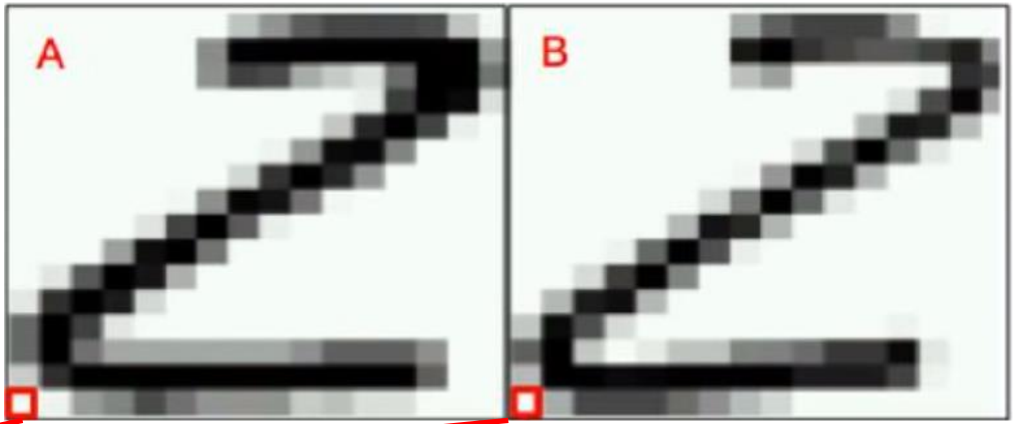
- Input:
  - Training examples $\{x_i, l_i\}$:
    - x_i - features of i-th examples
    - l_i - label of i-th examples

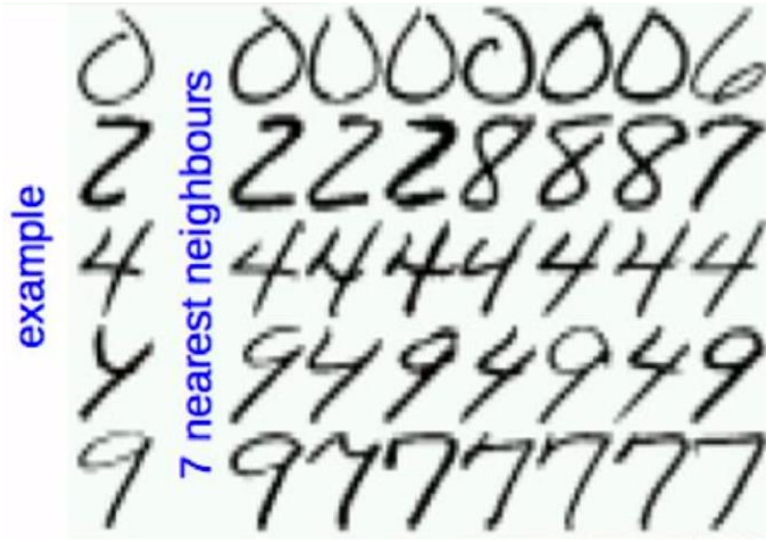
- Goal is to classify new example $\{z\}$

- Algorithm:
  - Compute distance $\mathrm{D}(z, x_i)$ to every training example x_i
  - Select k closest examples $x_{i1} \ldots x_{ik}$ and their labels $l_{i1} \ldots l_{ik}$
  - Output the most frequent class from $l_{i1} \ldots l_{ik}$

Example: digit classification 7NN

- Database of 16x16 grayscale scale bitmaps of digits with known labels
- Recognize digit on new 16x16 grayscale bitmap
- Distance metric:
  - $D(A,B) = \sqrt{\sum_i \sum_j \left(A_{i,j} - B_{i,j}\right)^2}$





Predictions

- **0**; as majority voting
- **2**; parity voting, but 2s have higher scores
- **4**; unanimously voting
- **9**; as majority voting
- **7**; as majority voting

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kNN regression

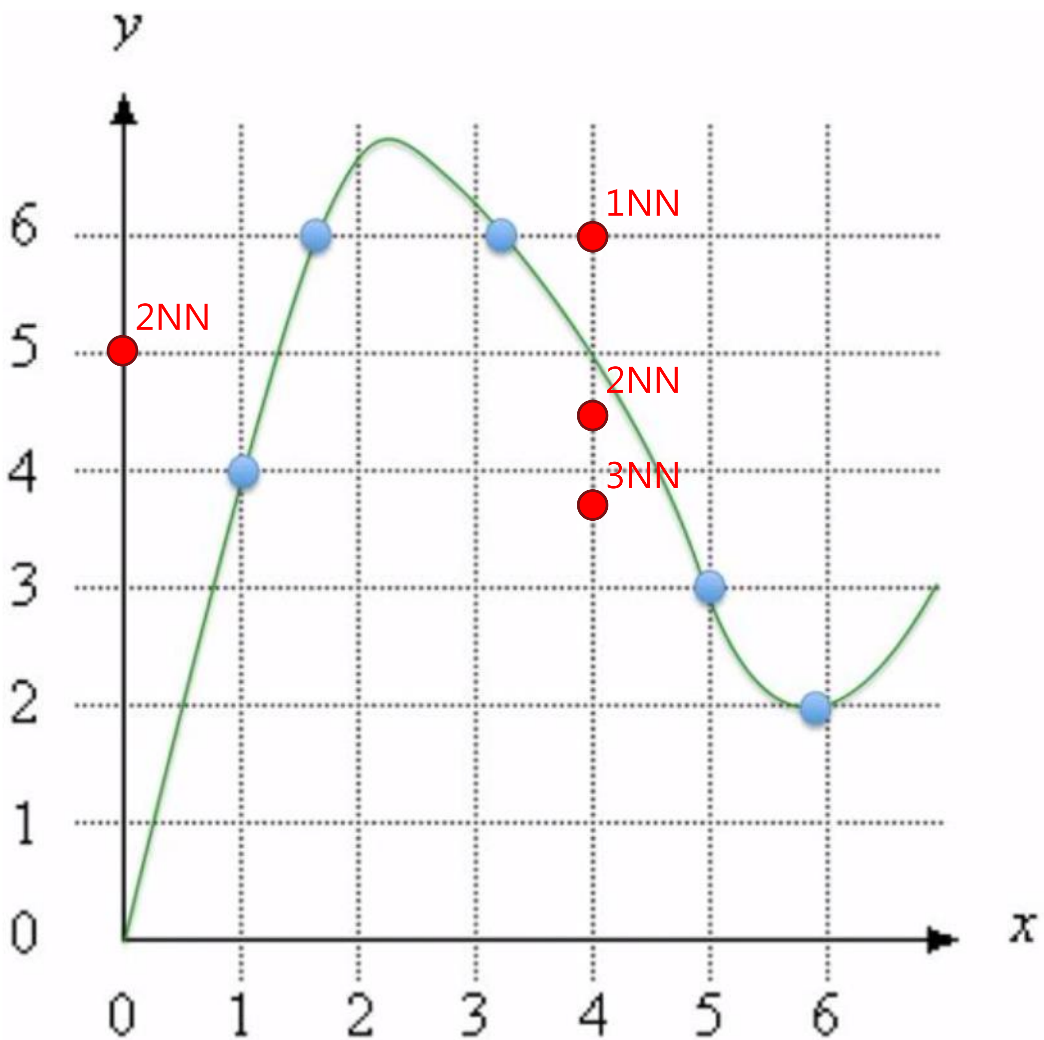
- Input:
  - Training examples $\{x_i, y_i\}$:
    - x_i - features of i-th examples
    - y_i - real value associated with examples (profit, exam result)

- Goal is to assign value to new example$\{z\}$

- Algorithm:
  - Compute distance $\mathrm{D}(z, x_i)$ to every training example x_i
  - Select k closest examples $x_{i1} \dots x_{ik}$and their values $y_{i1} \dots y_{ik}$
  - Output the mean of $y_{i1} \dots y_{ik}$

Example: kNN regression

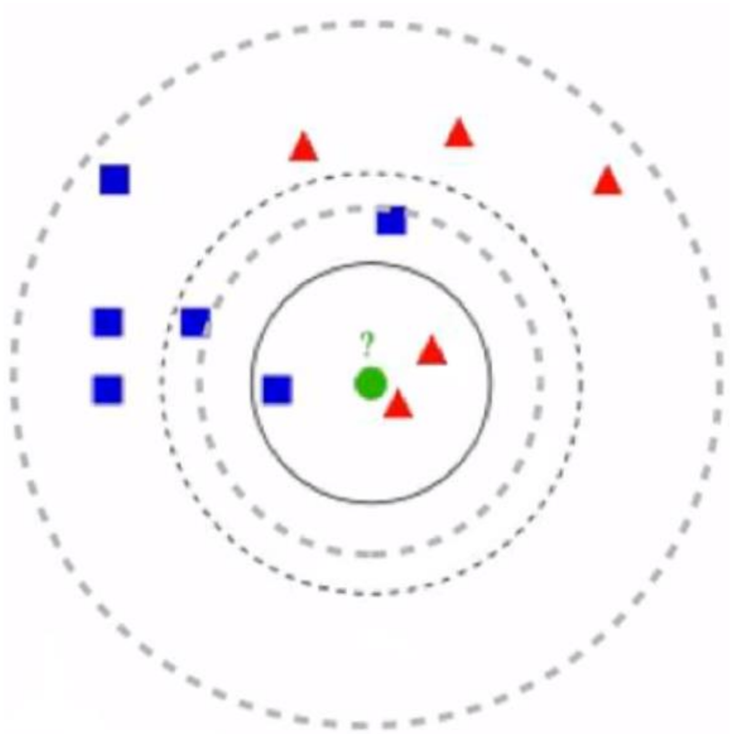
- Let's predict values for x=4:
  - 1NN regression
  - 2NN regression
  - 3NN regression
  - etc.



- Results may significantly depend on the k selection:
  - What if we choose k = database size
- Which k is good for predicting for x=0?
- Extrapolation is less accurate than interpolation

kNN: how to select k?

- What will be the prediction for green point for:
  - 1NN classification
  - 2NN classification
  - 5NN classification



- Let's say you have a database of 10000 points in space with known red/blue labels. How to choose good k?

- Validation set!

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kNN: Distance measure

- Euclidian distance:

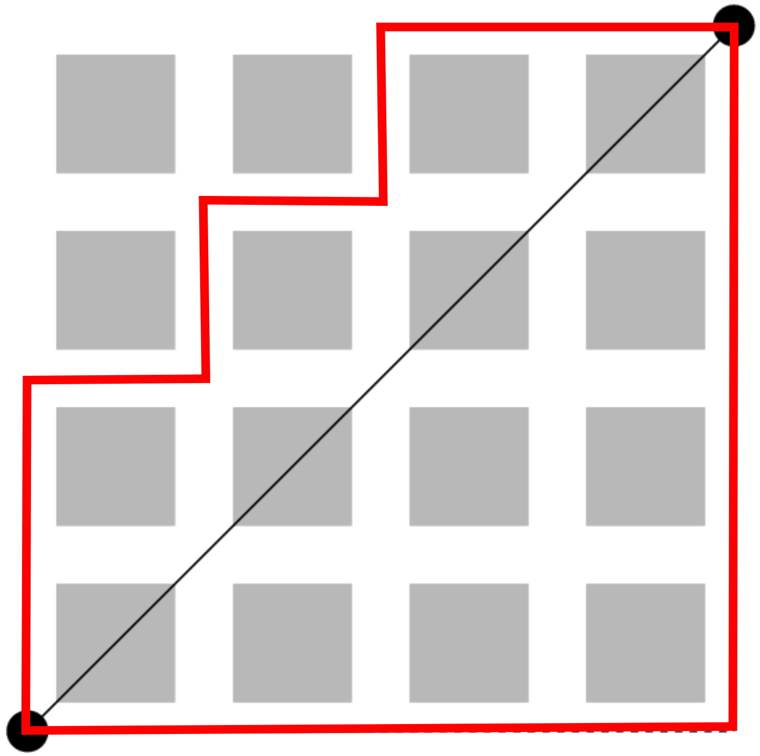
$$D(x, x') = \sqrt{\sum_d |x_d - x'_d|^2}$$

- Manhattan distance:

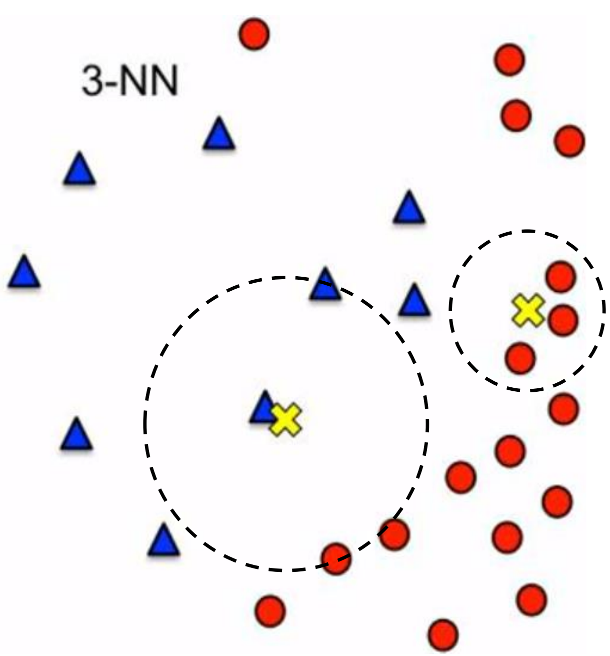
$$D(x, x') = \sum_d |x_d - x'_d|$$

- Logical distance (categorical attributes):

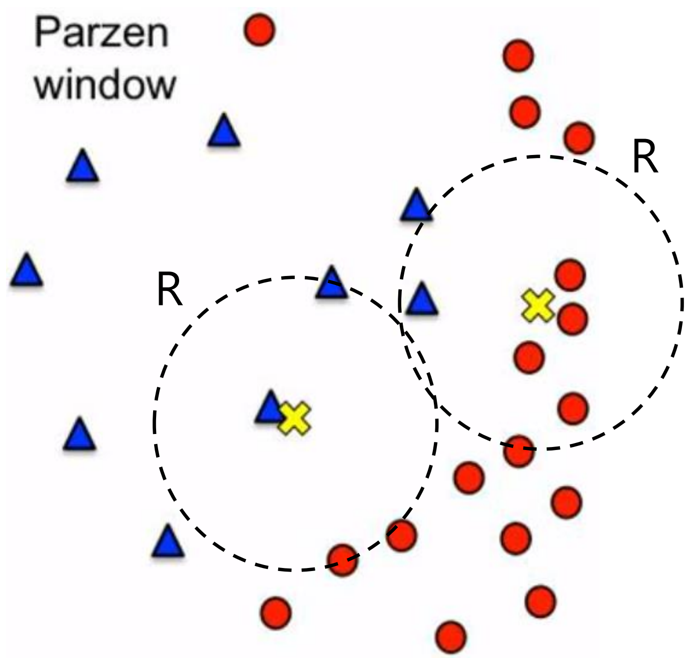
$$D(x, x') = \sum_d 1_{x_d \neq x'_d}$$



kNN and Parzen Windows



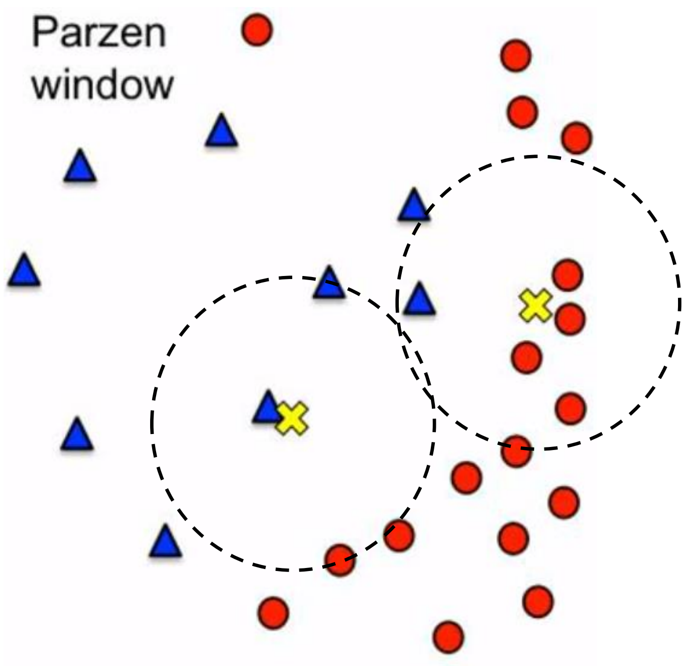
The size of the neighborhoods can be very different

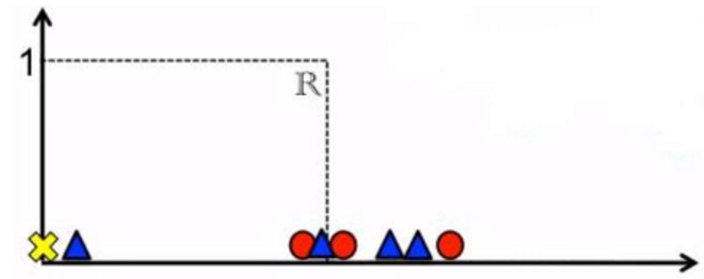


The size of the neighborhoods is the same

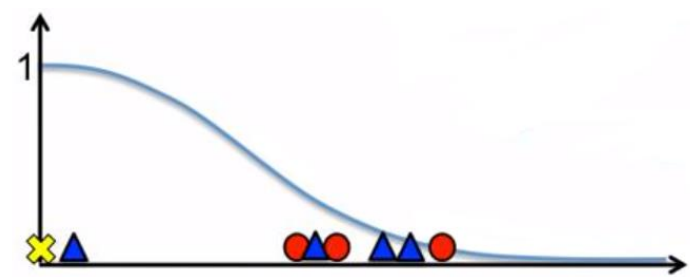
$$P(red|x) = \frac{\sum_i 1_{l_i=red} \cdot 1_{x_i \in R(x)}}{\sum_i 1_{x_i \in R(x)}}$$

kNN, Parzen Windows and Kernels





What is the problem with $1_{x_i \in R(x)}$?



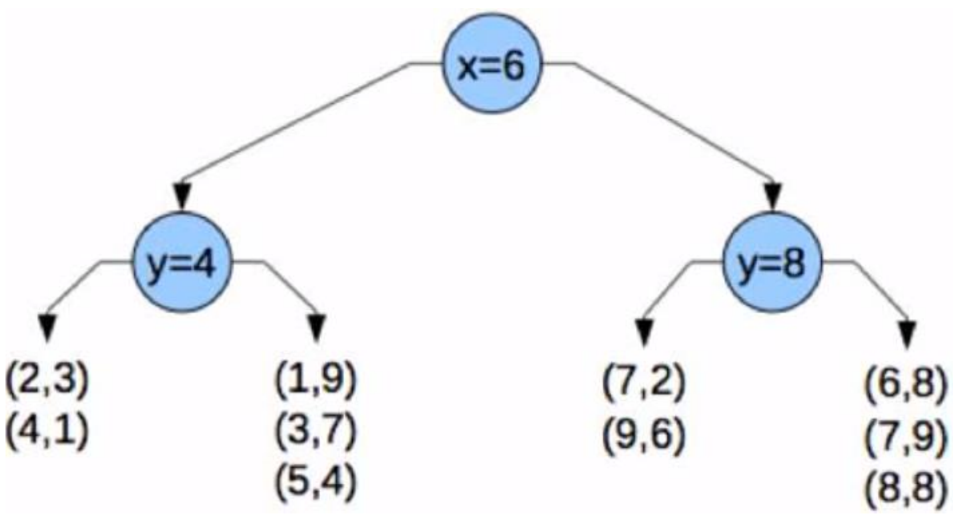
Kernel-based predictor

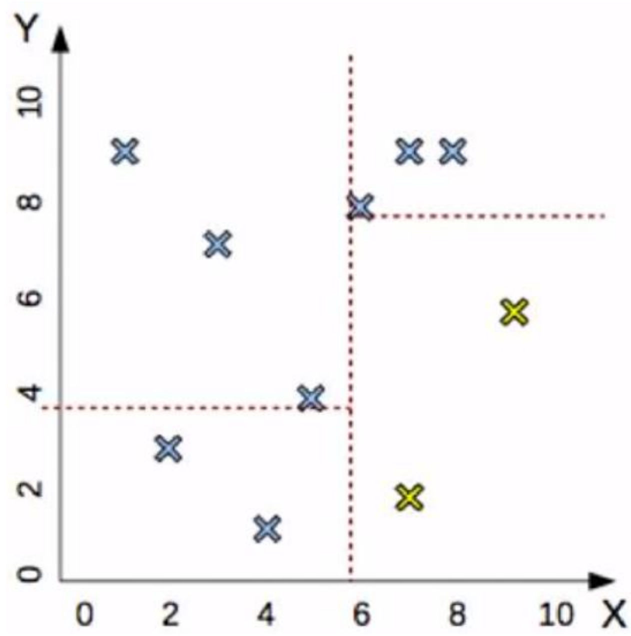
$$P(red|x) = \frac{\sum_i 1_{l_i=red} \cdot 1_{x_i \in R(x)}}{\sum_i 1_{x_i \in R(x)}}$$

$$P(red|x) = \frac{\sum_i 1_{l_i=red} \cdot K(x_i, x)}{\sum_i K(x_i, x)}$$

kNN problem: speed!

- There are 60000 examples digit recognition database:
  - It will be extremely slow to measure distance to all of them
- Many acceleration techniques. For example, KD search tree:
  - Training samples: {(1, 9), (2, 3), (4, 1), (3, 7), (5, 4), (6, 8), (7, 2), (8, 8), (7, 9), (9, 6)}
  - Pick random dimension, find median, split
  - For a test sample (7, 4), follow the tree and search the specific subregion





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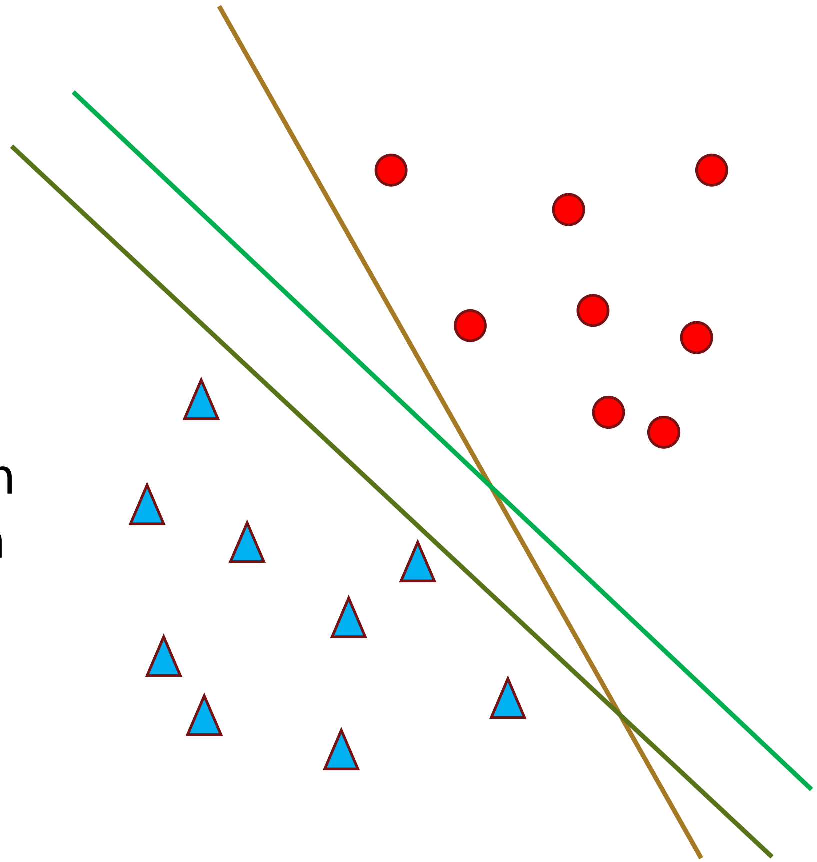
Support vector machines

- Let's say we want to best separate red and blue points
- Many solutions are possible, but are they equally good?
- Somehow this solution looks better than other solutions. How did you make such intuitive conclusion?



Support vector machines

- Let's say the points above the line have positive labels (+1), while points below – negative (-1)

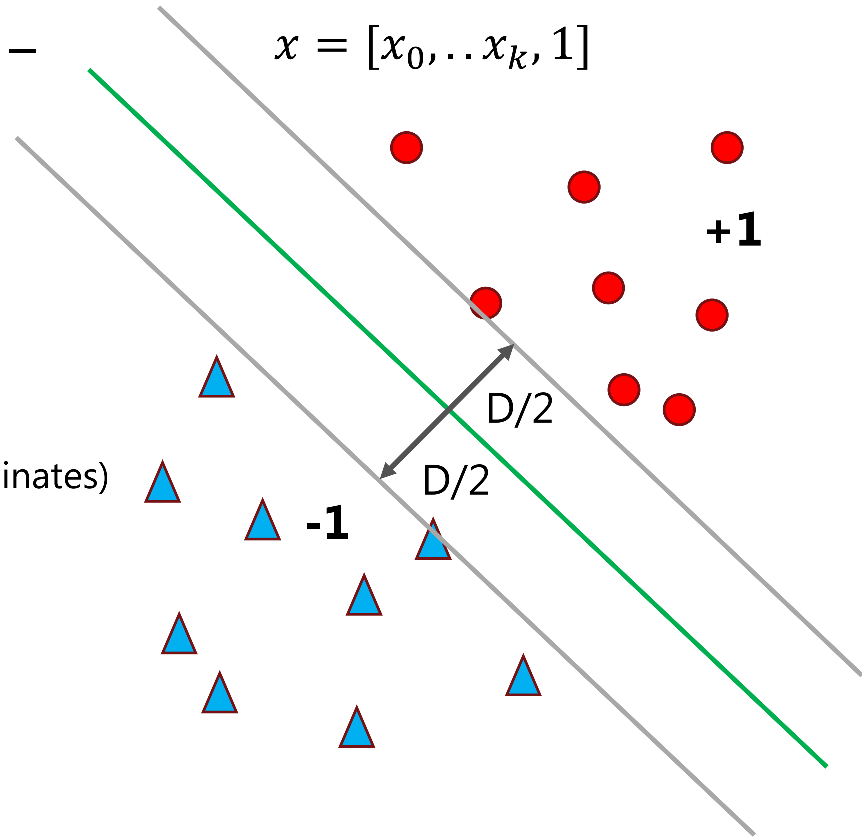
- A prediction line can be defined as:

$$y = w^T x$$

label

Features (point coordinates)

$$x = [x_0, .. x_k, 1]$$



Support vector machines

- The prediction is uncertain at the green borderline:

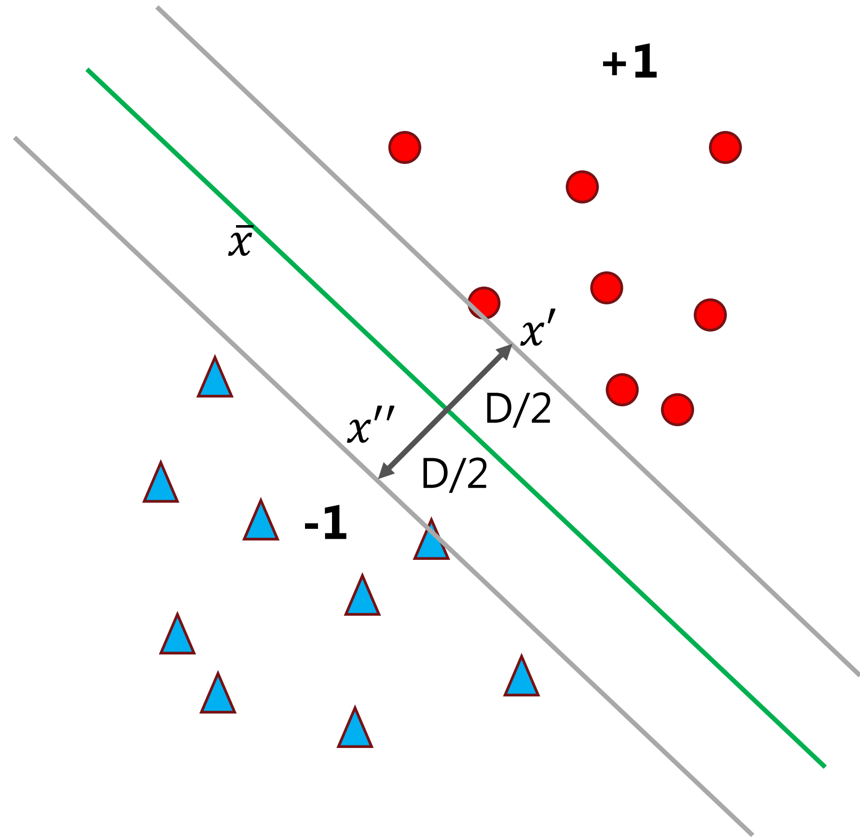
$$w^T \bar{x} = 0$$

- What is the equations for points above the upper gray line:

$$w^T x' \geq 1$$

- The equations for points below the lower gray line:

$$w^T x'' \leq -1$$



Support vector machines

- Hinge loss function:

$$h(x, y, w^T x\ ) = \begin{cases} 0 & \text{if } y \cdot w^T x\ \geq 1 \\ 1 - y \cdot w^T x & \text{else} \end{cases}$$

- L2 Regularization (*why do we need it?*):

$$l = \|w\|^2$$

- We want to optimize:

$$\min_w \left(\lambda \|w\|^2 + h(x, y, w^T x\ )\right)$$

Support vector machines

- Partial derivatives of $\min_{w}\left(\lambda\|w\|^2 + h(x, y, w^T x\ )\right)$:

$$\frac{\delta}{\delta w_k}\lambda\|w\|^2 = 2\lambda w_k \qquad \frac{\delta}{\delta w_k}h(\cdot) = \begin{cases} 0 & \text{if } y \cdot w^T x\ \geq 1 \\ -y_i x_{ik} & \text{else} \end{cases}$$

- Update of w:

for mis-classified samples:

$$w = w - \eta(-y_i x_{ik} + 2\lambda w_k)$$

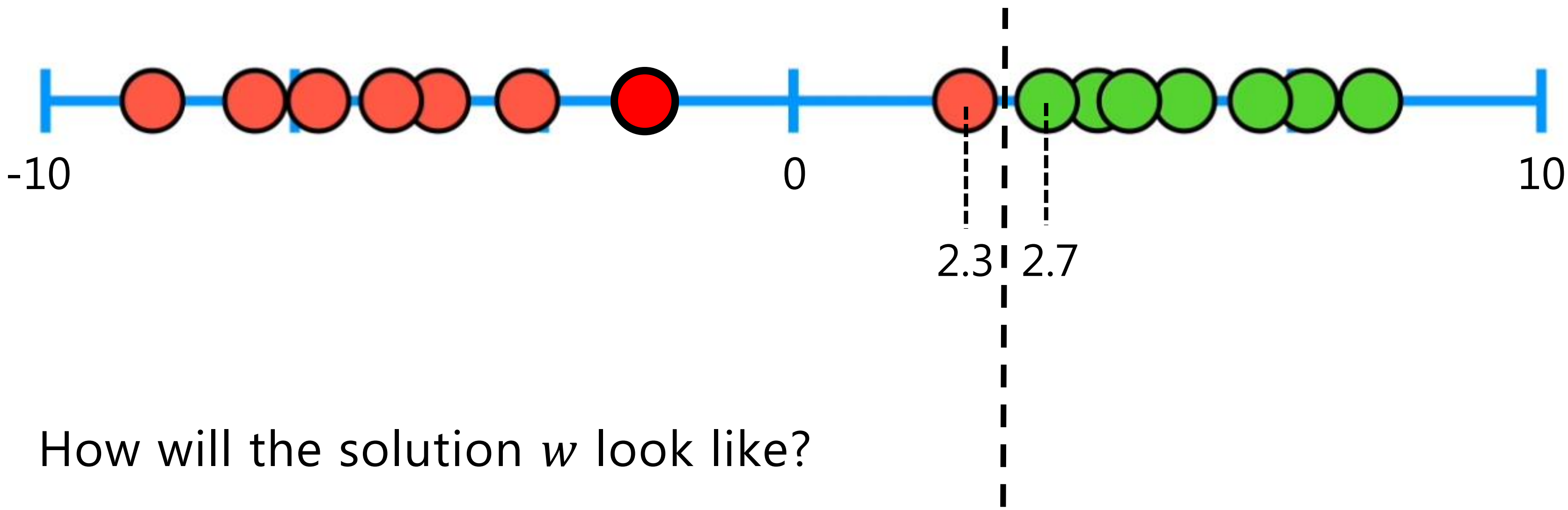
for correctly classified samples:

$$w = w - \eta(2\lambda w_k)$$

Support vector machines: regularization

- Separation with very low $\lambda = 1e - 10$:

$$\min_{w}\left(\lambda\|w\|^2 + h(x, y, w^T x)\right)$$



- How will the solution w look like?

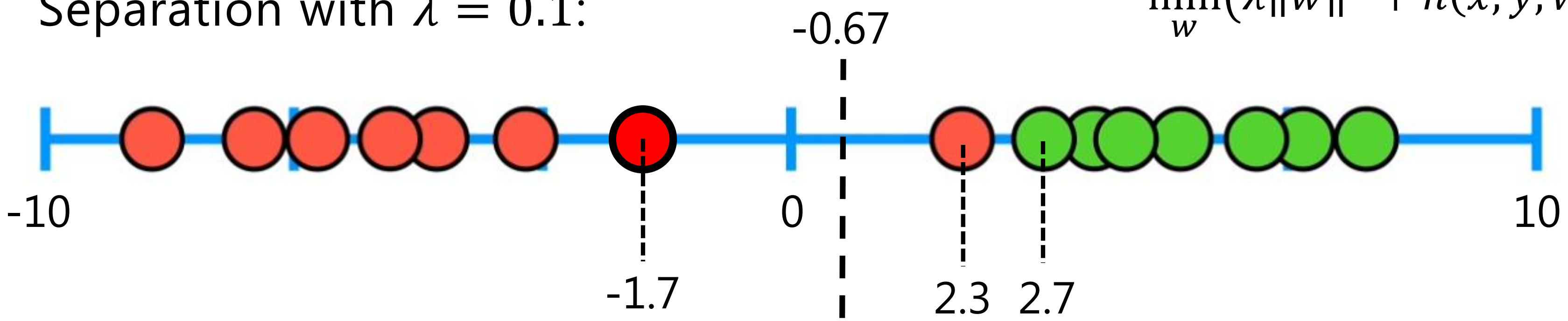
$$\boxed{w = 5x - 12.5}$$

- Could we get something like?
  - $w = 10x - 25$
- Is this a good solution?

Support vector machines: regularization

$$\min_{w}\left(\lambda\|w\|^2 + h(x, y, w^T x)\right)$$

- Separation with $\lambda = 0.1$:



- The solution w will look like:

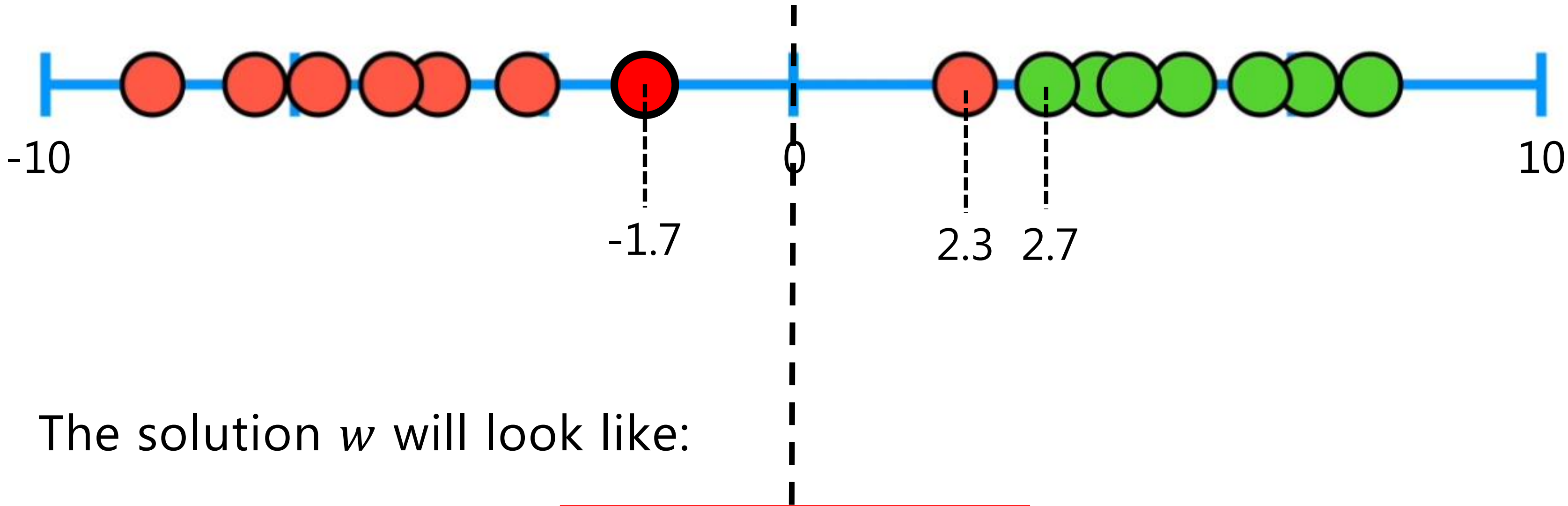
$$\boxed{w = 0.43x - 0.28}$$

- This separation does not classify samples perfectly, but seems to be more reliable

Support vector machines: regularization

- Separation with $\lambda = 10$:

$$\min_{w}\left(\lambda\|w\|^2 + h(x, y, w^T x\,)\right)$$



- The solution w will look like:

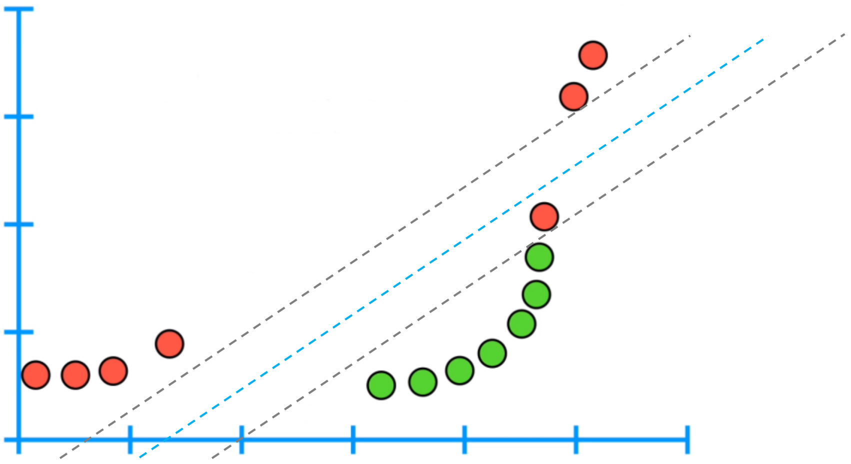
$$\boxed{w = 0.065x}$$

- The solution w comes closer to 0, with growth of λ:

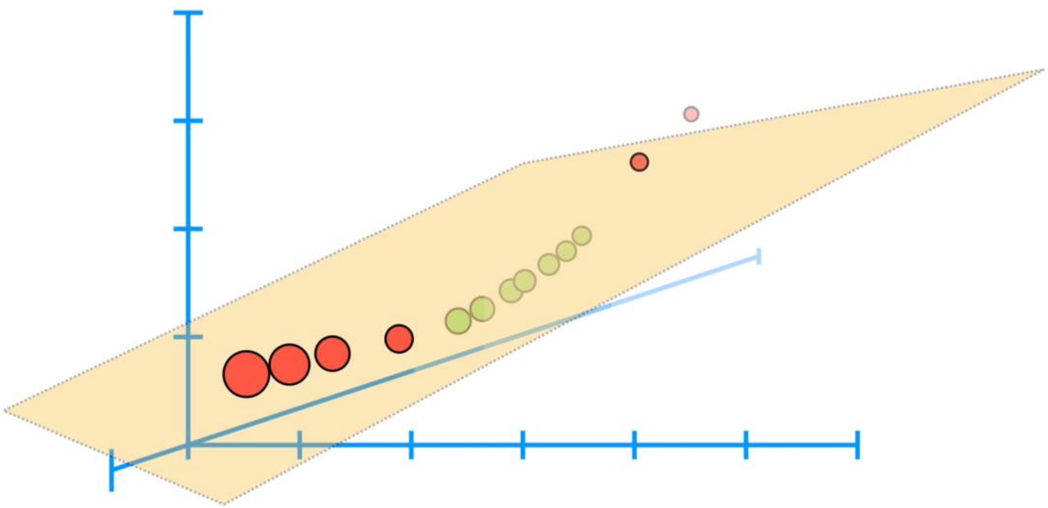
λ	w
1e-10	[5, -12.5]
0.1	[0.43, -0.28]
10	[0.065, 0]

Support vector machines: dimensionality

- 2D data:

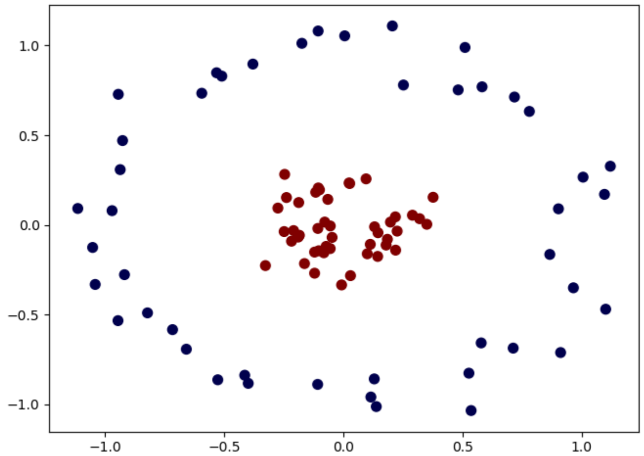


- 3D data:



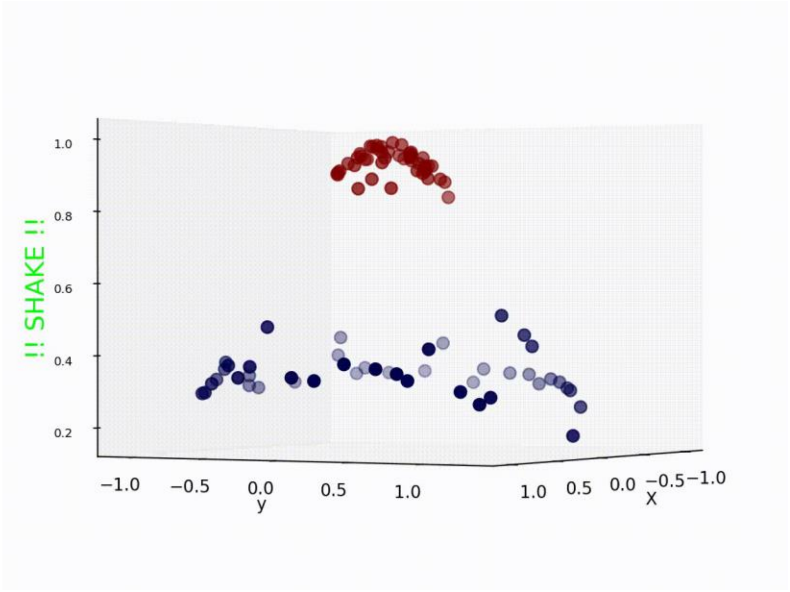
Support vector machines: kernel

- Can we classify these samples with support vectors:



- Let's transform data:

$$z = e^{-\|x\|^2}$$

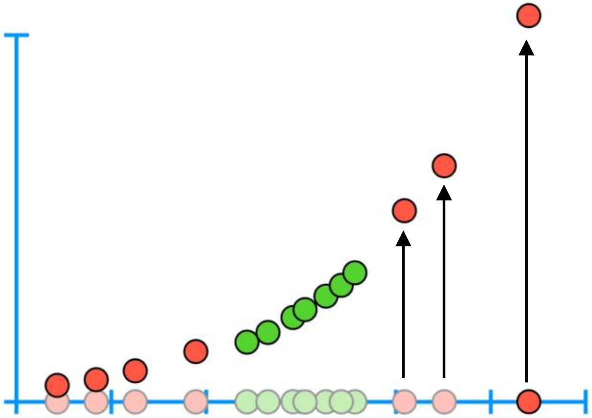


https://towardsdatascience.com/understanding-support-vector-machine-part-2-kernel-trick-mercers-theorem-e1e6848c6c4d

Support vector machines: kernels

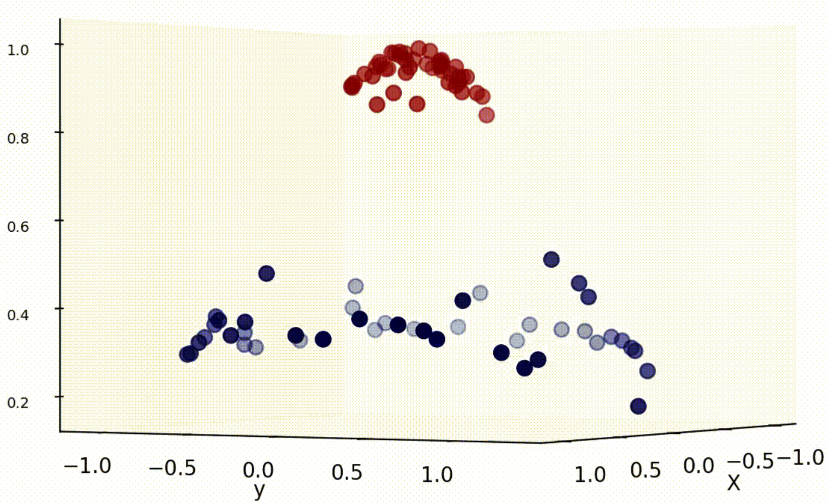
- Polynomial kernel:

$$K(x_i, x_j) = (x_i \cdot x_j + 1)^p$$



- Radial basis function kernel:

$$K(x_i, x_j) = e^{-\gamma (x_i - x_j)^2}$$



- Hinge loss:
$h(x, y, w^T x) = h(x, y, K(w, x))$

Classification performance evaluation: 2 classes

- Accuracy:

$$A = \frac{\sum_i \text{sign}(y_i f(x_i))}{|y|}$$

correctly classified testing examples

testing examples

- What are the problems of such metric:
  - Class imbalance problem:
    - 0.9 healthy subject, 0.1 diseased
    - Naïve classification will result in 0.9 accuracy

  - Let's say $f(x) \in [-1,1]$, $f(x) = 0.01$ will be as good as $f(x) = 0.99$ for $y = 1$

Performance evaluation: sensitivity/specificity

- Let's normalize all labels y and $f(x)$ to $[0, 1]$
- True positive (TP) - # of cases, where $y_i = 1$ and $f(x_i) \geq 0$
- True negative (TN) - # of cases, where $y_i = -1$ and $f(x_i) < 0$
- False positive (FP) - # of cases, where $y_i = -1$ and $f(x_i) \geq 0$
- False negative (FN) - # of cases, where $y_i = 1$ and $f(x_i) < 0$

- Sensitivity:

$$\frac{TP}{TP + FN}$$

- Specificity:

$$\frac{TN}{TN + FP}$$

Performance evaluation: ROC curve

- Example of testing mosquito killing spray:

Among survivals, how many survived receiving the current dose?

Among dead, how many died because of the current dose?

	A	B	C	D	E	F	G
3	ROC Table						
4							
5		Observed		Cumulative			
6	*Dosage*	*Lives*	*Dies*	*Lives*	*Dies*	*FPR*	*TPR*
7				0	0	1	1
8	less than 2.00	34	3	34	3	0.935484	0.989247
9	2.00 - 3.99	63	7	97	10	0.815939	0.964158
10	4.00 - 5.99	88	11	185	21	0.648956	0.924731
11	6.00 - 7.99	105	14	290	35	0.449715	0.874552
12	8.00 - 9.99	123	23	413	58	0.216319	0.792115
13	10.00 - 11.99	95	60	508	118	0.036053	0.577061
14	12.00 - 13.99	9	75	517	193	0.018975	0.308244
15	14.00 - 15.99	6	41	523	234	0.00759	0.16129
16	16.00 -17.99	4	30	527	264	0	0.053763
17	18.00 or more	0	15	527	279	0	0
18		527	279				

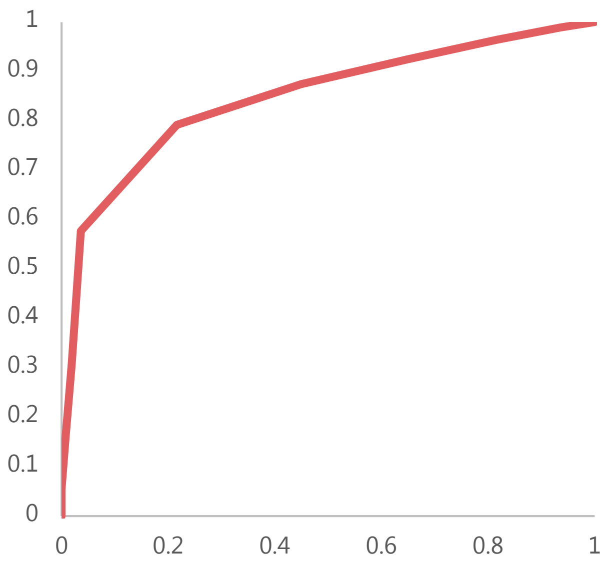
$$1 - \frac{35}{279}$$

$$1 - \frac{290}{527}$$

Performance evaluation: ROC curve

- Receiving operator curve:

FPR	TPR	AUC
1	1	0.064516
0.935484	0.989247	0.118259
0.815939	0.964158	0.160998
0.648956	0.924731	0.184244
0.449715	0.874552	0.204117
0.216319	0.792115	0.142791
0.036053	0.577061	0.009855
0.018975	0.308244	0.003509
0.00759	0.16129	0.001224
0	0.053763	0
0	0	0
		0.889515



- Closer AUC to 1 the better

Questions?