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**Algorithm 1** k-Nearest Neighbor [Tay et al., 2014] link:36

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**Input:** X: training data, Y:Class labels of X,  $x$ : unknown sample

**Output:** Class label of unknown sample Classify  $X, Y, x$   $i = 1$  to  $m$

- 1: Compute distance  $d(X_i, x)$
  - 2: Compute set  $I$  containing indices for the  $k$  smallest distances  $d(X_i, x)$
  - 3: Return majority label  $\{Y_i \text{ where } i \in I\}$
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**Algorithm 2** Adaboost [Schapire, 2014]

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**Input:**

Training data  $\{(x_i, y_i)_{i=1}^N$  where  $x_i \in \mathbb{R}^k$  and  $y_i \in \{-1, 1\}\}$   
Large number of classifiers denoted by  $f_m(x) \in \{-1, 1\}$   
0-1 loss function  $I$  defined as

$$I(f_m(x, y)) = \begin{cases} 0, & \text{if } f_m(x_i) = y_i \\ 1, & \text{if } f_m(x_i) \neq y_i \end{cases} \quad (1)$$

**Output:** The final classifier

$i = 1$  to  $N$   $i = 1$  to  $M$

- 1: Fit weak classifier  $m$  to minimize the objective function:
  - 2:  $\epsilon_m = \frac{\sum_{i=1}^N w_i^m I(f_m(x_i) \neq y_i)}{x^2 + 2x + 1}$
  - 3: where  $I(f_m(x_i) \neq y_i) = 1$  if  $f_m(x_i) \neq y_i$  and 0 otherwise
  - 4:  $\alpha_m = \ln \frac{1 - \epsilon_m}{\epsilon_m}$
  - all  $i$
  - 5:  $w_i^{m+1} = w_i^{(m)} e^{\alpha_m I(f_m(x_i) \neq y_i)}$
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**Algorithm 3** Adaboost [Hertzmamn et al., 2015]

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**Input:**

Training data  $\{(x_i, y_i)_{i=1}^N$  where  $x_i \in \mathbb{R}^k$  and  $y_i \in \{-1, 1\}\}$

**Output:** Weighted sum that represents the final output of the boosted classifier

- 1: Given Training data  $\{(x_i, y_i) \text{ where } y_i \in \{-1, 1\}\}$
- 2: initialize  $D_1$  = uniform distribution on training examples  $t = 1$  to  $T$
- 3: Train weak classifier  $h_t$  on  $D_t$
- 4: choose  $\alpha_t > 0$
- 5: compute new distribution  $D_{t+1}$ : all  $i$
- 6: multiply  $D_t(x)$  by

$$\begin{cases} e^{-\alpha_t}, & (< 1) \text{ if } y_i = h_t(x_i) \\ e^{\alpha_t}, & (> 1) \text{ if } y_i \neq h_t(x_i) \end{cases} \quad (3)$$

$$\quad (4)$$

7: renormalize

8: output final classifier  $H_{final(x)} = \text{sign}(\sum \alpha_t h_t(x))$

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**Algorithm 4** Random forest [Bernstein, 2016] Link:42

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**Input:** S: training set, F: Features and number of trees in forest  $B$

**Output:** Constructed tree RANDOMFORESTS,  $F$

- 1:  $H \leftarrow \emptyset$   $i = 1, \dots, B$
  - 2:  $S^{(i)} \leftarrow$  A bootstrap sample from  $S$
  - 3:  $h_i \leftarrow \text{RANDOMIZEDTREELEARN}(S^{(i)}, F)$
  - 4:  $H \leftarrow H \cup \{h_i\}$
  - 5: return  $H$
  - RANDOMIZEDTREELEARN,  $F$
  - 6: At each node:
  - 7:  $f \leftarrow$  a very small subset of  $F$
  - 8: Split on best feature in  $f$
  - 9: return The learned tree
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**Algorithm 5** Iterative Dichotomiser 3 [[., 2015a](#)] Link:40

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**Input:**  $D$  : Training Data,  $X$  : Set of Input Attributes

**Output:** A decision tree ID3 $D, X$

- 1: Let  $T$  be a new tree all instances in  $D$  have the same class  $c$
  - 2: Label( $T$ ) =  $c$ ; Return  $T$   $X = \emptyset$  or no attribute has positive information gain
  - 3: Label( $T$ ) = most common class in  $D$ ; Return  $T$
  - 4:  $X \leftarrow$  attribute with highest information gain
  - 5: Label( $T$ ) =  $X$  each value  $x$  of  $X$
  - 6:  $D_x \leftarrow$  instances in  $D$  with  $X = x$   $D_x$  is empty
  - 7: Let  $T_x$  be a new tree
  - 8: Label( $T_x$ ) = most common class in  $D$
  - 9:  $T_x = \text{ID3}(D_x, X - \{x\})$
  - 10: Add a branch from  $T$  to  $T_x$  labeled by  $x$
  - 11: return  $T$
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**Algorithm 6** Perceptron [[Brownlee, 2015d](#)] Link:65

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**Input:**  $ProblemSize, InputPatterns, iterations_{max}, learn_{rate}$

**Output:**  $Weights$

$i = 1$  to  $iterations_{max}$

- 1:  $Pattern_i \leftarrow \text{SelectInputPattern}(InputPatterns)$
  - 2:  $Activation_i \leftarrow \text{ActivateNetwork}(Pattern_i, Weights)$
  - 3:  $Output_i \leftarrow \text{TransferActivation}(Activation_i)$
  - 4:  $\text{UpdateWeights}(Pattern_i, Output_i, learn_{rate})$
  - 5: Return  $Weights$
- 

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**Algorithm 7** Back-propagation [[Brownlee, 2015a](#)] Link:17,42

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**Input:**  $ProblemSize, InputPatterns, iterations_{max}, learn_{rate}$

**Output:**  $Network$

- 1:  $Network \leftarrow \text{ConstructNetworkLayers}()$
  - 2:  $Network_{weights} \leftarrow \text{InitializeWeights}(Network, ProblemSize)$
  - $i = 1$  to  $iterations_{max}$
  - 3:  $Pattern_i \leftarrow \text{SelectInputPattern}(InputPatterns)$
  - 4:  $Output_i \leftarrow \text{ForwardPropagate}(Pattern_i, Network)$
  - 5:  $\text{BackwardPropagateError}(Pattern_i, Output_i, Network)$
  - 6:  $\text{UpdateWeights}(Pattern_i, Output_i, Network, learn_{rate})$
  - 7: Return  $Network$
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**Algorithm 8** Back-propagation2 [[Ng,](#) ]

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**Input:**

Training Set  $x^{(1)}, y^{(1)}, \dots, (x^{(m)}, y^{(m)})$

**Output:**

Gradient of the cost function

- 1:  $\Delta_{ij}^{(l)} = 0$  (for all  $l, i, j$ )  $i = 1$  to  $m$
  - 2: Set  $a^{(1)} = x^{(i)}$
  - 3: Perform forward propagation to compute  $a^{(l)}$  for  $l = 2, 3, \dots, L$
  - 4: Using  $y^{(i)}$ , compute  $\delta^{(L)} = a^{(L)} - y^{(i)}$
  - 5: Compute  $\delta^{(L-1)}, \delta^{(L-2)}, \dots, \delta^{(2)}$
  - 6:  $\Delta_{ij}^{(l)} := \Delta_{ij}^{(l)} + a_j^{(l)} \delta_i^{(l+1)}$
  - 7:  $D_{ij}^{(l)} := \frac{1}{m} \Delta_{ij} + \lambda \theta_{ij}^{(l)}$  if  $j \neq 0$
  - 8:  $D_{ij}^{(l)} := \frac{1}{m} \Delta_{ij}$  if  $j = 0$
  - 9:  $\frac{\partial}{\partial \theta_{ij}^{(l)}} J(\theta) = D_{ij}^{(l)}$
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**Algorithm 9** Learning Vector Quantization [Brownlee, 2015c]**Input:**  $ProblemSize, InputPatterns, iterations_{max}, CodebookVectors_{num}, learn_{rate}$ **Output:**  $CodebookVectors$ 

- 1:  $CodebookVectors \leftarrow InitializeCodebookVectors(CodebookVectors_{num}, ProblemSize)$   
 $i = 1$  to  $iterations_{max}$
  - 2:  $Pattern_i \leftarrow SelectInputPattern(InputPatterns)$
  - 3:  $Bmu_i \leftarrow SelectBestMatchingUnit(Pattern_i, CodebookVectors)$   $Bmu_i^{attribute} \in Bmu_i$   $Bmu_i^{class} \equiv Pattern_i^{class}$
  - 4:  $Bmu_i^{attribute} \leftarrow Bmu_i^{attribute} + learn_{rate} \times (Pattern_i^{attribute} - Bmu_i^{attribute})$
  - 5:  $Bmu_i^{attribute} \leftarrow Bmu_i^{attribute} - learn_{rate} \times (Pattern_i^{attribute} - Bmu_i^{attribute})$
  - 6: Return  $CodebookVectors$
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**Algorithm 10** Self Organizing Map [Brownlee, 2015b] Link:45**Input:**  $InputPatterns, iterations_{max}, learn_{rate}, Grid_{width}, Grid_{height}$ **Output:**  $CodebookVectors$ 

- 1:  $CodebookVectors \leftarrow InitializeCodebookVectors(Grid_{width}, Grid_{height}, InputPatterns)$   
 $i = 1$  to  $iterations_{max}$
  - 2:  $Learn_{rate}^i \leftarrow CalculateLearningRate(i, learn_{rate}^{init})$
  - 3:  $neighborhood_{size}^i \leftarrow CalculateNeighborhoodSize(i, neighborhood_{init}^{size})$
  - 4:  $Pattern_i \leftarrow SelectInputPattern(InputPatterns)$
  - 5:  $Bmu_i \leftarrow SelectBestMatchingUnit(Pattern_i, CodebookVectors)$
  - 6:  $Neighborhood \leftarrow Bmu_i$
  - 7:  $Neighborhood \leftarrow SelectNeighbors(Bmu_i, CodebookVectors, neighborhood_{size}^i)$   $Vector_i \in Neighborhood$   
 $Vector_i^{attribute} \in Vector_i$
  - 8:  $Vector_i^{attribute} \leftarrow Vector_i^{attribute} + learn_{rate} \times (Pattern_i^{attribute} - Vector_i^{attribute})$
  - 9: Return  $CodebookVectors$
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**Algorithm 11** Hierarchial Agglomerative Algorithm [Stein, 2016a]**Input:**

$\langle V, E, w \rangle$ . Weighted graph  
 $d_c$ . Distance measure for two clusters

**Output:**  $\langle V_T, E_T \rangle$ . Cluster hierarchy or dendrogram

- 1:  $C = \{\{v \mid v \in V\}\}$  {Initial Clustering}
  - 2:  $V_t = \{v_C \mid C \in C\}, E_T = \emptyset$  {Initial Dendrogram}  $|C| > 1$
  - 3:  $update\_distance\_matrix(C, G, d_c)$
  - 4:  $\{C, C'\} = \underset{\{C_i, C_j\} \in C: C_i \neq C_j}{argmin} d_c(C_i, C_j)$
  - 5:  $C = (C \setminus \{C, C'\}) \cup \{C \cup C'\}$  {Merging}
  - 6:  $V_T = V_T \cup \{v_{C, C'}\}, E_T = E_T \cup \{\{v_{C, C'}, v_C\}, \{v_{C, C'}, v_{C'}\}\}$  {Dendrogram}
  - 7: Return  $T$
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**Algorithm 12** Hierarchial Agglomerative Algorithm 2 [?]**Input:**

$\langle V, E, w \rangle$ . Weighted graph  
 $d_c$ . Distance measure for two clusters

**Output:**  $\langle V_T, E_T \rangle$ . Cluster hierarchy or dendrogram

- 1: **repeat**
  - 2:   Compute the proximity graph if necessary
  - 3:   **repeat**
  - 4:     Merge the closest two clusters.
  - 5:     Update the proximity matrix to reflect the proximity between the new cluster and the original clusters.
  - 6:   **until**
  - 7: Only singleton clusters remain
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**Algorithm 13** Hierarchial Divisive Algorithm [Stein, 2016b]

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**Input:**

$\langle V, E, w \rangle$ . Weighted graph  
 $d_c$ . Distance measure for two clusters

**Output:**  $\langle V_T, E_T \rangle$ . Cluster hierarchy or dendogram

- 1:  $C = \{V\}$  {Initial Clustering}
  - 2:  $V_t = \{v_C \mid C \in C\}, E_T = \emptyset$  {Initial Dendogram}  $\exists C_x : (C_x \in C \wedge |C| > 1)$
  - 3: *update\_distance\_matrix*( $C, G, d_c$ )
  - 4:  $\{C, C'\} = \underset{\{C_i, C_j\} : C_i \cup C_j = C_x \wedge C_i \cap C_j = \emptyset}{argmax} d_c(C_i, C_j)$
  - 5:  $C = (C \setminus \{C, C'\}) \cup \{C \cup C'\}$  {Merging}
  - 6:  $V_T = V_T \cup \{v_{C, C'}\}, E_T = E_T \cup \{\{v_{C, C'}, v_C\}, \{v_{C, C'}, v_{C'}\}\}$  {Dendogram}
  - 7: Return  $T$
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**Algorithm 14** Hierarchial Divisive Algorithm [Stein, 2016b]

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**Input:**

$\langle V, E, w \rangle$ . Weighted graph  
 $d_c$ . Distance measure for two clusters

**Output:**  $\langle V_T, E_T \rangle$ . Cluster hierarchy or dendogram

- 1: **repeat**
  - 2:   Create a new cluster by breaking the link corresponding to the largest distance (smallest similarity).
  - 3: **until** Only one cluster remains
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**Algorithm 15** C4.5 [Dai and Ji, 2014]

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**Input:**

$T$  : Training dataset  
 $S$  : Attributes

**Output:** decision tree *Tree* C4.5T  $T$  is *NULL*

- 1: return failure  
    $S$  is *NULL*
  - 2: return *Tree* as a single node with most frequent class label in  $T$   
    $|S| = 1$
  - 3: return *Tree* as a single node  $S$
  - 4: set  $Tree = \{\}$   
    $a \in S$
  - 5: set  $Info(a, T) = 0$  and  $SplitInfo(a, T) = 0$
  - 6: compute  $Entropy(a)$   $v \in values(a, T)$
  - 7: set  $T_{a,v}$  as the subset of  $T$  with attribute  $a = v$
  - 8:  $Info(a, T) + = \frac{|T_{a,v}|}{|T_a|} Entropy(a)$
  - 9:  $SplitInfo(a, T) + = -\frac{|T_{a,v}|}{|T_a|} \log \frac{|T_{a,v}|}{|T_a|}$
  - 10:  $Gain(a, T) = Entropy(a) - Info(a, T)$
  - 11:  $GainRatio(a, T) = \frac{Gain(a, T)}{SplitInfo(a, T)}$
  - 12: set  $a_{best} = argmax\{GainRatio(a, T)\}$
  - 13:  $a_{best}$  into *Tree*  $v \in values(a_{best}, T)$  call C4.5( $T_{a,v}$ )
  - 14: return *Tree*
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**Algorithm 16** Gradient Descent [[.](#), [2015b](#)]

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**Input:**

$f$   
starting value  $x_1$   
termination tolerances

**Output:**  $x_{maxIters}$ 

$i = 1$  to  $maxIters$

- 1: Compute the search direction  $d_t = -\delta f(x_t)$   $|d_T| < \epsilon_g$
  - 2: return "Converged to critical point", output  $x_t$
  - 3: Find  $\alpha_t$  so that  $f(x_t + \alpha_t d_t) < f(x_t)$   
 $|\alpha_t d_T| < \epsilon_x$
  - 4: return "Converged in x", output  $x_t$
  - 5: Find  $\alpha_t$  so that  $f(x_t + \alpha_t d_t) < f(x_t)$
  - 6: Let  $x_{t+1} = x_t + \alpha_t d_t$
  - 7: Return "Max number of iterations reached", output  $x_{maxIters}$
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**Algorithm 17** Naive Bayes [[.](#), [d](#)]

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**Input:**

$C$  : A fixed set of classes  
 $D$  : Documents

**Output:** Category(Class) of the Documents TrainMultinomialNBC,  $D$ 

- 1:  $V \leftarrow EXTRACTVOCABULARY(D)$
  - 2:  $N \leftarrow COUNTDOCS(D)$  each  $c \in C$
  - 3:  $N_c \leftarrow COUNTDOCSINCLASS(D, c)$
  - 4:  $prior|c| \leftarrow N_c/N$
  - 5:  $text_c \leftarrow CONCATENATETEXTTOFALLDOCSINCLASS(D, C)$  each  $t \in V$
  - 6:  $condprob|t||c| \leftarrow \frac{T_{ct}+1}{\sum_{t'}(T_{ct'}+1)}$
  - 7: return  $V, prior, condprob$   
ApplyMultinomialNBC,  $D, prior, condprob, d$
  - 8:  $W \leftarrow EXTRACTTOKENSFROMDOC(V, d)$   
each  $c \in C$
  - 9:  $score|c| \leftarrow \log prior|c|$  each  $t \in W$
  - 10:  $score|c| + = \log condprob|t||c|$
  - 11: return  $arg \max_{c \in C} score|c|$
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**Algorithm 18** Lasso Regression

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**Input:**

$ipy$  : Inner product vector,  $ipy_i = \langle y, X_{.i} \rangle$   
 $ipx$  : Inner product matrix,  $ipx_{ij} = \langle X_{.i}, X_{.j} \rangle$   
 $\lambda$  : Penalty parameter  
 $N$  : Number of samples

**Output:**  $beta$  : Regression parameter vector FastLassoipy,  $ipx, \lambda, N$ 

- 1: **stop\_thr** {Threshold for stopping iteration}
  - 2:  $p \leftarrow length(ipy)$
  - 3:  $beta \leftarrow 0$  with length  $p$
  - 4:  $gc \leftarrow 0$  with length  $p$   $diffBeta_{max} \geq stop\_thr$
  - 5:  $diffBeta_{max} \leftarrow 0$   
 $j = 1 \leftarrow p$
  - 6:  $z \leftarrow (ipy[j] - gc[j])/N + beta[j]$
  - 7: **beta\_tmp**  $\leftarrow \max(0, z - \lambda) - \max(0, -z - \lambda)$
  - 8:  $diffBeta \leftarrow beta\_tmp - beta[j]$
  - 9:  $diffabs \leftarrow abs(diffBeta)$   $diffabs > 0$
  - 10:  $beta[j] \leftarrow beta\_tmp$
  - 11:  $gc \leftarrow gc + ipx[j] \times diffBeta$
  - 12:  $diffBeta_{max} = \max(diffBeta_{max}, diffabs)$
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**Algorithm 19** Bagging [., a]

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**Input:**

B: the number of bags or base hypotheses  
L: Base Learning Algorithm

**Output:** New Training Sets Bagging  $examples, B, L$   $i = 1$  to  $B$ 

- 1:  $examples_i \leftarrow$  a bootstrap sample of  $examples$
  - 2: Compute set  $I$  containing indices for the  $k$  smallest distances  $d(X_i, x)$
  - 3:  $h_i \leftarrow$  apply  $L$  to  $examples_i$
  - 4: Return  $h_1, h_2, \dots, h_B$
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**Algorithm 20** Deep Q-Learning with Experience Replay [Mnih et al., 2013]

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**Input:**

D: data set  
Q: Action-Value Function

**Output:** New Training Sets

$i = 1$  to  $M$

- 1: Initialise sequence  $s_1 = \{x_1\}$  and preprocessed sequenced  $\phi = \phi(s_1)$   $i = 1$  to  $T$
- 2: With probability  $\epsilon$  select a random action  $a_t$  otherwise select  $a_t = \max_a Q * (\phi(s_t).a : \theta)$
- 3: Execute action  $a_t$  in emulator and observe reward  $r$  and image  $x_{t+1}$
- 4: Set  $s_{t+1} = s_t, a_t, x_{t+1}$  and preprocess  $\phi_{t+1} = \phi(s_{t+1})$
- 5: Store transition  $(\phi_t, a_t, r_t, \phi_{t+1})$  in  $D$
- 6: Set  $y_j =$

$$\begin{cases} r_j, & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta), & \text{for terminal } \phi_{j+1} \end{cases} \quad (5)$$

$$(6)$$

- 7: Perform a gradient descent step on  $(y_j - Q(\phi_j, a_j; \theta))^2$  according to the following equation
- 8:

$$\Delta_{\theta} L_i(\theta_i) = \mathbb{E}_{s, a \sim \rho(\cdot); s' \sim \epsilon} [(r + \gamma \max_{a'} Q(s', a'; \theta_{i-1}) - Q(s, a; \theta_i)) \Delta_{\theta_i} Q(s, a; \theta_i)]$$

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**Algorithm 21** PageRank [., e]

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**Input:**

G: inlink file  
iteration: Number of iteration

**Output:** PageRank PageRankG, iteration

- 1:  $d \leftarrow 0.85$  {damping factor: 0.85}
  - 2:  $oh \leftarrow G$  {get outlink hash from G}
  - 3:  $ih \leftarrow G$  {get inlink hash from G}
  - 4:  $N \leftarrow G$  {get number of pages from G} all  $p$  in the graph
  - 5:  $opg[p] \leftarrow \frac{1}{N}$  iteration  $> 0$
  - 6:  $dp \leftarrow 0$  all  $p$  that has no out-links
  - 7:  $dp \leftarrow dp + d * \frac{opg[p]}{N}$  all  $p$  in the graph
  - 8:  $npg[p] \leftarrow dp + \frac{[1-d]}{N}$  all  $ip$  in  $ih[p]$
  - 9:  $npg[p] \leftarrow dp + \frac{d * opg[ip]}{oh[ip]}$
  - 10:  $opg \leftarrow npg$
  - 11: iteration  $\leftarrow$  iteration  $- 1$
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**Algorithm 22** DBSCAN link:42 [Ram et al., 2010]

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**Input:**

$D$ : Data

$\epsilon$ : Threshold distance

$MinPts$  : Minimum number of points required to form a cluster

**Output:** Clustered Data DBSCAN( $D, \epsilon, minPts$ )

- 1:  $C = 0$  each point  $P$  in dataset  $D$  is visited
  - 2: continue next point
  - 3: mark  $P$  as visited
  - 4:  $NeighborPts = regionQuery(P, \epsilon)$   $sizeof(NeighborPts) < MinPts$
  - 5: mark  $P$  as NOISE
  - 6:  $C =$  next cluster
  - 7:  $expandCluster(P, NeighborPts, C, \epsilon, MinPts)$   
     $expandCluster(P, NeighborPts, C, \epsilon, MinPts)$
  - 8: add  $P$  to Cluster  $C$  each point  $P'$  in  $NeighborPts$   $P'$  is not visited
  - 9: mark  $P'$  as visited
  - 10:  $NeighborPts' = regionQuery(P', \epsilon)$   $sizeof(NeighborPts') \geq MinPts$
  - 11:  $NeighborPts = NeighborPts$  joined with  $NeighborPts'$   $P'$  is not yet member of any cluster
  - 12: add  $P'$  to cluster  $C$   
     $regionQuery(P, \epsilon)$
  - 13: return all points within  $P's \in neighborhood$
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**Algorithm 23** Logistic Regression [., c]

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**Input:**

Training data of the form  $\{(x_1, 1), (x_2, 0), ..\}$

$x$ : unknown sample

**Output:** The output is a probability that the given input point belongs to a certain class

1:  $0 \leftarrow \beta$

2: Compute  $y$  by setting its elements to

$$y = \begin{cases} 1, & \text{if } g_i = 1 \\ 0, & \text{if } g_i = 2 \end{cases} \quad (7)$$

$$(8)$$

$i = 1, 2, ..N$

3: Compute  $p$  by setting its elements to

$$p(x_i, \beta) = \frac{e^{\beta^T x_i}}{1 + e^{\beta^T x_i}}$$

$i = 1, 2, ..N$

4: Compute the diagonal matrix  $W$ . The  $i$ th diagonal element is  $p(x_i, \beta)(1 - p(x_i, \beta))$

5:  $z \leftarrow X\beta + W^{-1}(y - p)$

6:  $\beta \leftarrow (X^T W X)^{-1} X^T W z$

7: If the stopping criteria, stop; otherwise go back to step 3

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**Algorithm 24** Gaussian Process [., b]

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**Input:**

$$X = \begin{bmatrix} x_1^T \\ \dots \\ x_n^T \end{bmatrix} \in \mathbb{R}^{n \times D}, \text{ m training inputs}$$

$$y = \begin{bmatrix} y_1^T \\ \dots \\ y_n^T \end{bmatrix} \in \mathbb{R}^n$$

$$k(.,.) : \mathbb{R}^{D \times D}$$

$x_*$  test input

$\sigma^2$  noise level on the observations

$$[y(x) = f(x) + \epsilon, \epsilon \sim N(0, \sigma^2)]$$

**Output:**

$$f_*$$

$$\text{cov}(f_*)$$

1:  $K \in \mathbb{R}^{n \times n}$  Gram matrix.  $K_{ij} = k(x_i, x_j)$

$$k(x_*) = k_* = k(X, x_*) = \begin{bmatrix} k(x_1, x_*) \\ \dots \\ k(x_n, x_*) \end{bmatrix} \in \mathbb{R}$$

2:  $\alpha = (K + \sigma_2 \mathbb{I}_n)^{-1} y$

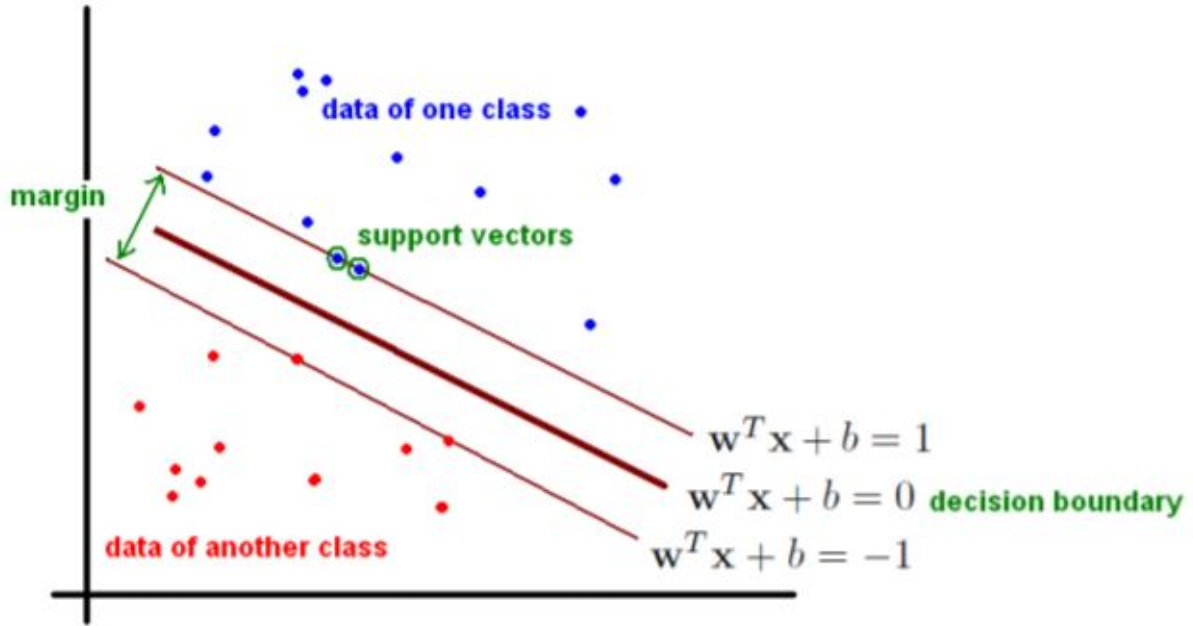
3:  $f_* = k_*^T \alpha \in \mathbb{R}$

4:  $\text{cov}(f_*) = k(x_*, x_*) - k_*^T [K + \sigma_2 \mathbb{I}_n]^{-1} k_*$

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**Input:**

Set of  $N$  input-output pairs  $\{x, y\}^{N_1}$   $x$ : input vectors of the same dimension and  $y$ : set of output target labels  $y_i = \{0, 1\}$



## 1 Simple case : linearly-separable data, binary classification

Goal: we want to find the hyperplane (i.e. decision boundary) linearly separating our classes. Our boundary will have the equation:  $\mathbf{w}^T \mathbf{x} + \mathbf{b} = 0$

Anything above the decision boundary should have label 1 i.e.,  $\mathbf{w}^T \mathbf{x}_i + b > 0$  will have corresponding  $y_i = 1$

Similarly, anything below the decision boundary should have label -1 i.e.  $\mathbf{w}^T \mathbf{x}_i + b < 0$  will have corresponding  $y_i = -1$

The reason for this labeling scheme is that it lets us condense for the decision function to

$$f(x) = \text{sign}(\mathbf{w}^T \mathbf{x} + b)$$

since  $f(x) = +1$  for all  $x$  above the boundary, and  $f(x) = -1$  for all  $x$  below the boundary.

Thus, we can figure out if an instance has been classified properly by checking that  $y(\mathbf{w}^T \mathbf{x} + b) \geq 1$  (which will be the case as long as either both  $y, \mathbf{w}^T \mathbf{x} + b > 0$  or else  $y, \mathbf{w}^T \mathbf{x} + b < 0$ )

You'll notice that we will now have some space between our decision boundary and the nearest data points of either class. Thus, let's rescale the data such that anything on or above the boundary  $\mathbf{w}^T \mathbf{x} + b = 1$  is of one class (with label 1), and anything on or below the boundary  $\mathbf{w}^T \mathbf{x} + b = -1$  is of another class (with label -1)

What is the distance between these newly added boundaries?

First note that the two lines are parallel, and thus share their parameters  $w, b$ . Pick an arbitrary point  $x_1$  to lie on line  $\mathbf{w}^T \mathbf{x} + b = -1$ . Then the closest point on line  $\mathbf{w}^T \mathbf{x} + b = 1$  is the point  $\mathbf{x}_2 = \mathbf{x}_1 + \lambda \mathbf{w}$  (since the closest point will always lie on the perpendicular; recall that the vector  $\mathbf{w}$  is perpendicular to both lines). Using this formulation,  $\lambda \mathbf{w}$  will be the line segment connecting  $\mathbf{x}_1$  and  $\mathbf{x}_2$ , and thus,  $\lambda \|\mathbf{w}\|$ , the distance between  $\mathbf{x}_1$  and  $\mathbf{x}_2$  is the shortest distance between the two lines/boundaries.

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**Algorithm 25** Support Vector Machines (continued)

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Solving for  $\lambda : \mathbf{w}^T \mathbf{x}_2 + b = 1$  where  $\mathbf{x}_2 = \mathbf{x}_1 + \lambda \mathbf{w}$   
 $\mathbf{w}^T (\mathbf{x}_1 + \lambda \mathbf{w}) + b = 1 \Rightarrow \mathbf{w}^T \mathbf{x}_1 + \lambda \mathbf{w}^T \mathbf{w} + b = 1$   
 $\mathbf{w}^T \mathbf{x}_1 + b + \lambda \mathbf{w}^T \mathbf{w} = 1$  where  $\mathbf{w}^T \mathbf{x}_1 + b = -1$   
 $-1 + \lambda \mathbf{w}^T \mathbf{w} = 1$   
 $\lambda \mathbf{w}^T \mathbf{w} = 2$   
 $\lambda = \frac{2}{\mathbf{w}^T \mathbf{w}} = \frac{2}{\|\mathbf{w}\|^2}$   
 And, so the distance  $\lambda \|w\|$  is  $\frac{2}{\|\mathbf{w}\|^2} \|w\| = \frac{2}{\|\mathbf{w}\|} = \frac{2}{\sqrt{\mathbf{w}^T \mathbf{w}}}$

It's intuitive that we would want to maximize the distance between the two boundaries demarcating the classes (Why? We want to be as sure that we are not making classification mistakes and thus we want our data points from the two classes to lie as far away from each other as possible). This distance is called the margin, so we want to obtain the maximal margin.

Thus, we want to maximize  $\frac{2}{\sqrt{\mathbf{w}^T \mathbf{w}}}$ , which is equivalent to minimizing  $\frac{\sqrt{\mathbf{w}^T \mathbf{w}}}{2}$  which is in turn equivalent to minimizing  $\frac{\mathbf{w}^T \mathbf{w}}{2}$  (since square root is a monotonic function)

This quadratic programming problem is expressed as :

$$\min_{w,b} \frac{\mathbf{w}^T \mathbf{w}}{2}$$

subject to :  $y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 (\forall \text{ data points } \mathbf{x}_i)$

## 2 Soft-margin extension

Consider the case that your data isn't linearly separable. For instance, maybe you aren't guaranteed that all your data points are correctly labelled, so you want to allow some data points of one class to appear on the other side of the boundary.

We can introduce *slack variables*  $\epsilon_i \geq 0$ . Our quadratic programming problem becomes:

$$\min_{\mathbf{w}, b, \epsilon} \frac{\mathbf{w}^T \mathbf{w}}{2} + C \sum_i \epsilon_i$$

subject to :  $y_i(\mathbf{w}^T \mathbf{x}_i + b) \geq 1 - \epsilon_i$

## 3 Nonlinear decision boundary

Mapping your data vectors,  $x_i$ , into a higher-dimension (even infinite) feature space may make them linearly separable in that space (whereas they may not be linearly separable in the original space). The formation of the quadratic programming problem is as above, but with all  $\mathbf{x}_i$  replaced with  $\phi(\mathbf{x}_i)$ , where  $\phi$  provides the higher-dimensional mapping. So we have the standard SVM formulation:

$$\min_{\mathbf{w}, b, \epsilon} \frac{\mathbf{w}^T \mathbf{w}}{2}$$

subject to :  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1 - \epsilon_i$  and  $\epsilon_i \geq 0 (\forall \text{ data points } \mathbf{x}_i)$

## 4 Reformulating as a Lagrangian

We can introduce Lagrange multipliers to represent the condition:  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)$  must be as close to 1 as possible. This condition is captured by:  $\max_{\alpha_i \geq 0} \alpha_i [1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)]$ . This ensures that when  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) \geq 1$ , the expression above is maximal when  $\alpha_i = 0$  (since  $[1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)]$  ends up being negative). Otherwise,  $y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b) < 1$ , so  $[1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)]$  is a positive value, and the expression is maximal when  $\alpha_i \rightarrow \infty$ . This has the effect of penalizing any misclassified data points, while assigning 0 penalty to properly classified instances.

We thus have the following formulation:

$$\min_{w,b} \left[ \frac{\mathbf{w}^T \mathbf{w}}{2} + \sum_i \max_{\alpha_i \geq 0} \alpha_i [1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)] \right]$$

To allow for slack (soft-margin), preventing the  $\alpha$  variables from going to  $\infty$ , we can impose constraints on the Lagrange multipliers to lie within:  $0 \leq \alpha_i \leq C$ . We can define the dual problem by interchanging the max and min as follows (i.e minimize after fixing alpha):

$$\max_{\alpha} \left[ \min_{w,b} J(\mathbf{w}, b; \alpha) \right] \text{ where } J(\mathbf{w}, b; \alpha) = \frac{\mathbf{w}^T \mathbf{w}}{2} + \sum_i \alpha_i [1 - y_i(\mathbf{w}^T \phi(\mathbf{x}_i) + b)]$$


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**Algorithm 25** Support Vector Machines (continued)

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Since, we're solving an optimization problem, we set  $\frac{\partial J}{\partial \mathbf{w}} = 0$  and discover that the optimal setting of  $\mathbf{w}$  is  $\sum_i \alpha_i y_i \phi(\mathbf{x}_i)$ , while setting  $\frac{\partial J}{\partial b} = 0$  yields the constraint  $\sum_i \alpha_i y_i = 0$

Thus, after substituting and simplifying, we get:

$$\begin{aligned} \min_{w,b} J(\mathbf{w}, b, \alpha) &= \sum_i \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j) \text{ And thus our dual is:} \\ \max_{\alpha \geq 0} & [\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)] \\ \text{Subject to: } & \sum_i \alpha_i y_i = 0 \text{ and } 0 \leq \alpha_i \leq C \end{aligned}$$

## 5 Kernel trick

Because we're working in a higher-dimension space (and potentially even an infinite-dimensional space), calculating  $\phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$  may be intractable. However, it turns out there are special *kernel* functions that operate on the lower dimension vectors  $\mathbf{x}_i$  and  $\mathbf{x}_j$  to produce a value equivalent to the dot-product of the higher dimensional vectors. For instance, consider the function  $\phi: \mathbb{R}^3 \mapsto \mathbb{R}^{10}$ , where  $\phi(x) = (1, \sqrt{2}x^{(1)}, \sqrt{2}x^{(2)}, \sqrt{2}x^{(3)}, [\mathbf{x}^{(1)}]^2, [\mathbf{x}^{(2)}]^2, [\mathbf{x}^{(3)}]^2, \sqrt{2}x^{(1)(2)}, \sqrt{2}x^{(1)(3)}, \sqrt{2}x^{(2)(3)})$ . Instead, we have the kernel trick, which tells us that  $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^2 = \phi(\mathbf{x}_i)^T \phi(\mathbf{x}_j)$  for the given  $\phi$ . Thus, we can simplify our calculations. Re-writing the dual in terms of the kernel yields:  $\max_{\alpha \geq 0} [\sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)]$

## 6 Decision function

To classify a novel instance  $\mathbf{x}$  once you've learned the optimal  $\alpha_i$  parameters, all you have to do is calculate  $f(\mathbf{x}) = \text{sign}(\mathbf{w}^T \mathbf{x} + b) = \sum_i \alpha_i y_i \phi(\mathbf{x}_i)$  (and using the kernel trick). Note that  $\alpha_i$  is only non-zero for instances  $\phi(\mathbf{x}_i)$  on or near the boundary—those are called the *support vector* since they alone specify the decision boundary. We can toss out the other data points once training is complete. Thus, we only sum over the  $x_i$  which constitute the support vectors.

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