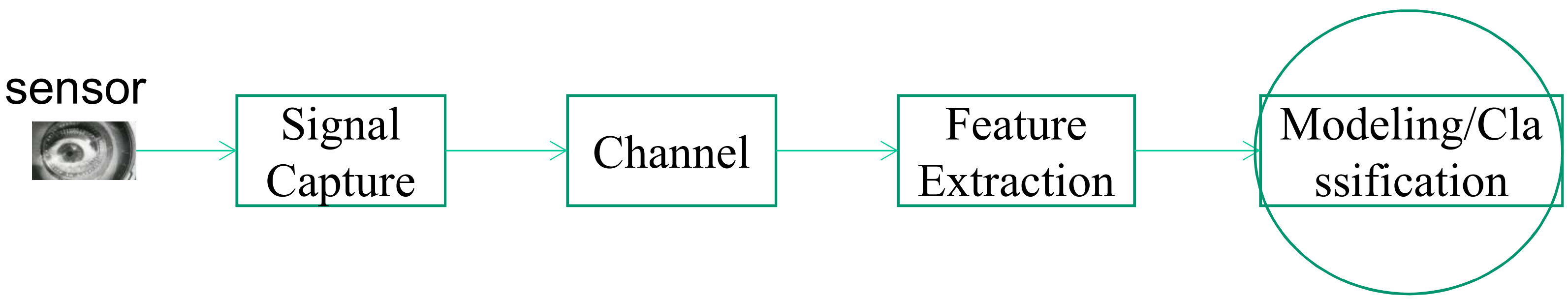
# Linear Classifiers
## (With slides from Najim Dehak)

# Recap

- Classification and KNN..

# MLSP

- Application of Machine Learning techniques to the analysis of signals




- Modeling
  - Classification: Model-Based vs instances-Based

# Machine Learning

- **Supervised:** We are given input samples (X) and output samples (y) of a function $y = f(X)$. We would like to "learn" f, and evaluate it on new data. Types:
  - **Classification:** y is discrete (class labels).
  - **Regression:** y is continuous, e.g. linear regression.

- **Unsupervised:** Given only samples X of the data, we compute a function f such that $y = f(X)$ is "simpler".
  - **Clustering:** y is discrete
  - Y is continuous: **Matrix factorization, Kalman filtering, unsupervised neural networks**.

# Machine Learning

- **Supervised:**
  - Is this image a cat, dog, car, house?
  - How would this user score that restaurant?
  - Is this email spam?
  - Is this blob a supernova?
- **Unsupervised**
  - Cluster some hand-written digit data into 10 classes.
  - What are the top 20 topics in Twitter right now?
  - Find and cluster distinct accents of people at Berkeley. (?)

# Multi-class Image Classification

# k-Nearest Neighbor classification

Given a query item:
Find k closest matches
in a labeled dataset ↓

# k-Nearest Neighbor classification

Given a query item:
Find k closest matches

Return the most
Frequent label

# k-Nearest Neighbor classification

k = 3 votes for “cat”

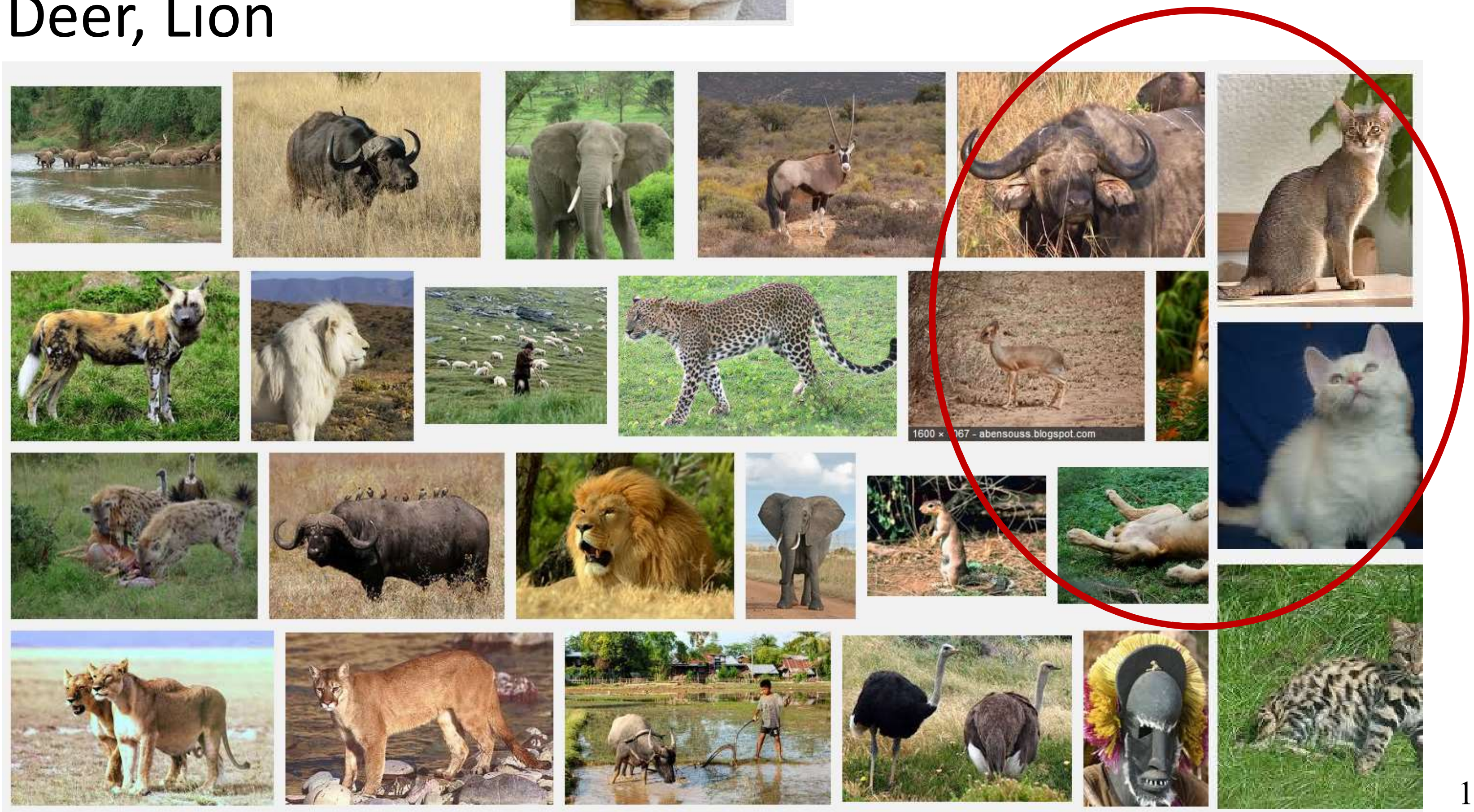
# k-Nearest Neighbors

2 votes for cat,

1 each for Buffalo,

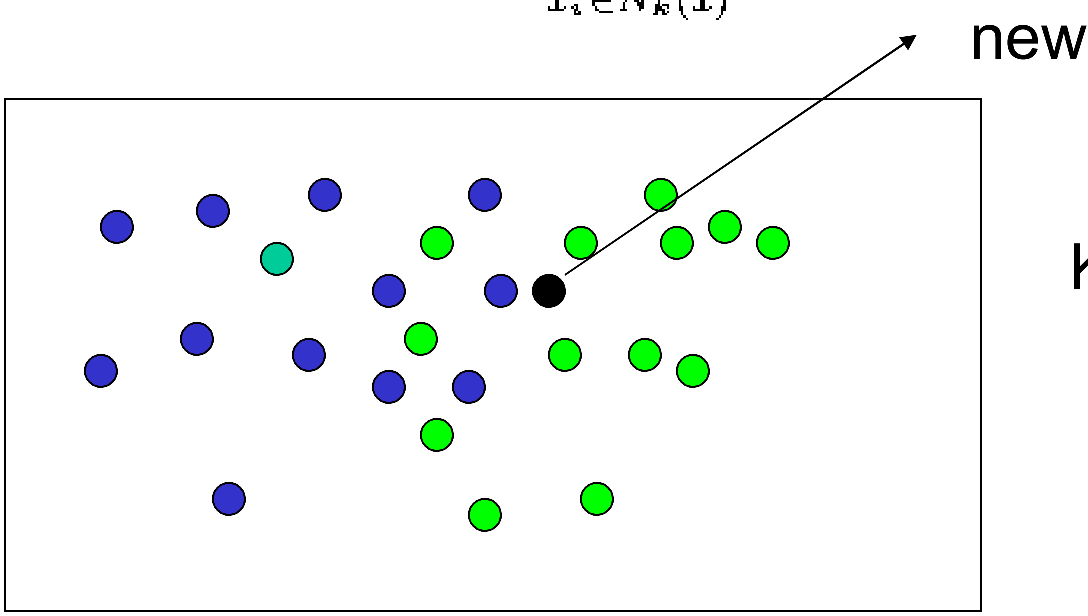
Deer, Lion

Cat wins…



# Nearest neighbor method

- Majority vote within the k nearest neighbors $\hat{Y}(x) = \frac{1}{k} \sum_{x_i \in N_k(x)} y_i$

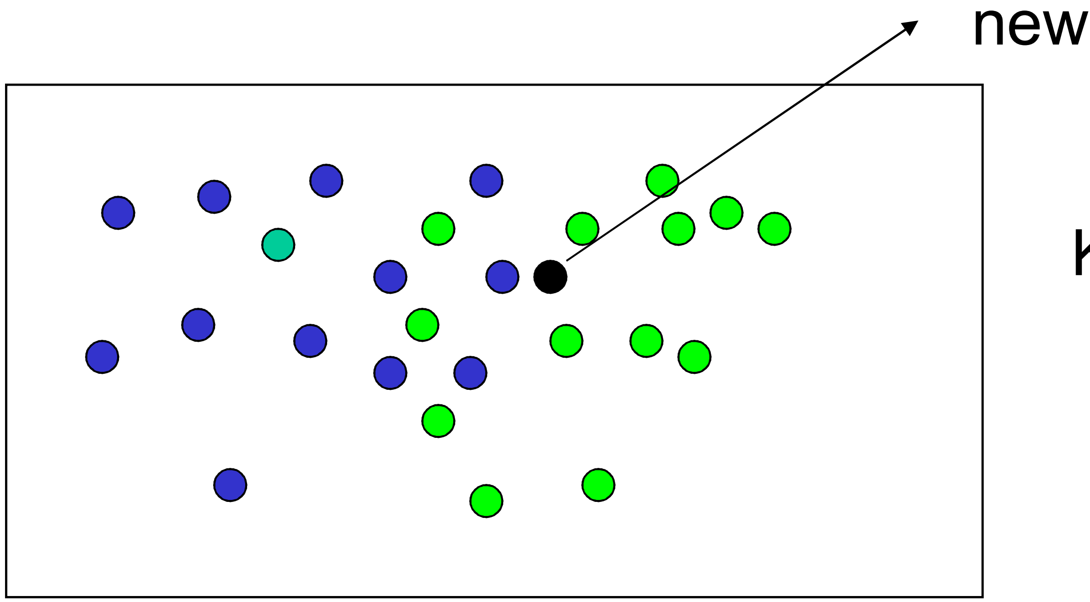



K= 1: blue
K= 3: green

# Nearest neighbor method

- Weighted majority vote

$$\hat{Y}(x) = \frac{1}{k}\sum_{i \in N_k(x)} w(x, x_i) y_i$$



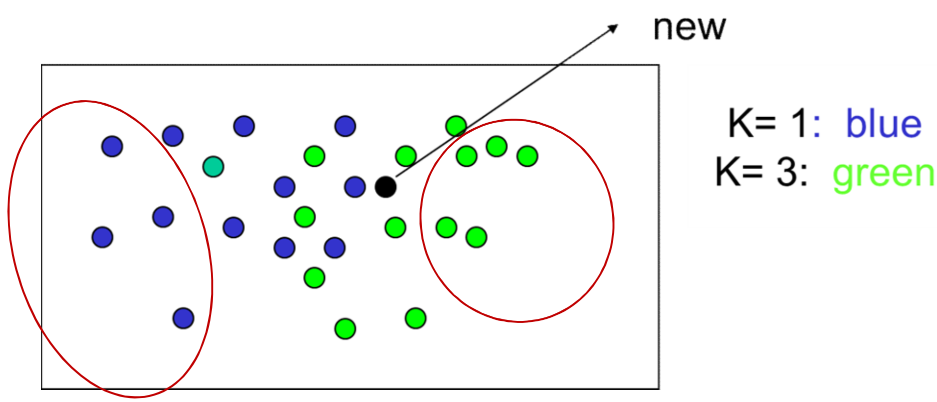

K= 1: blue
K= 3: green

# Nearest neighbor method

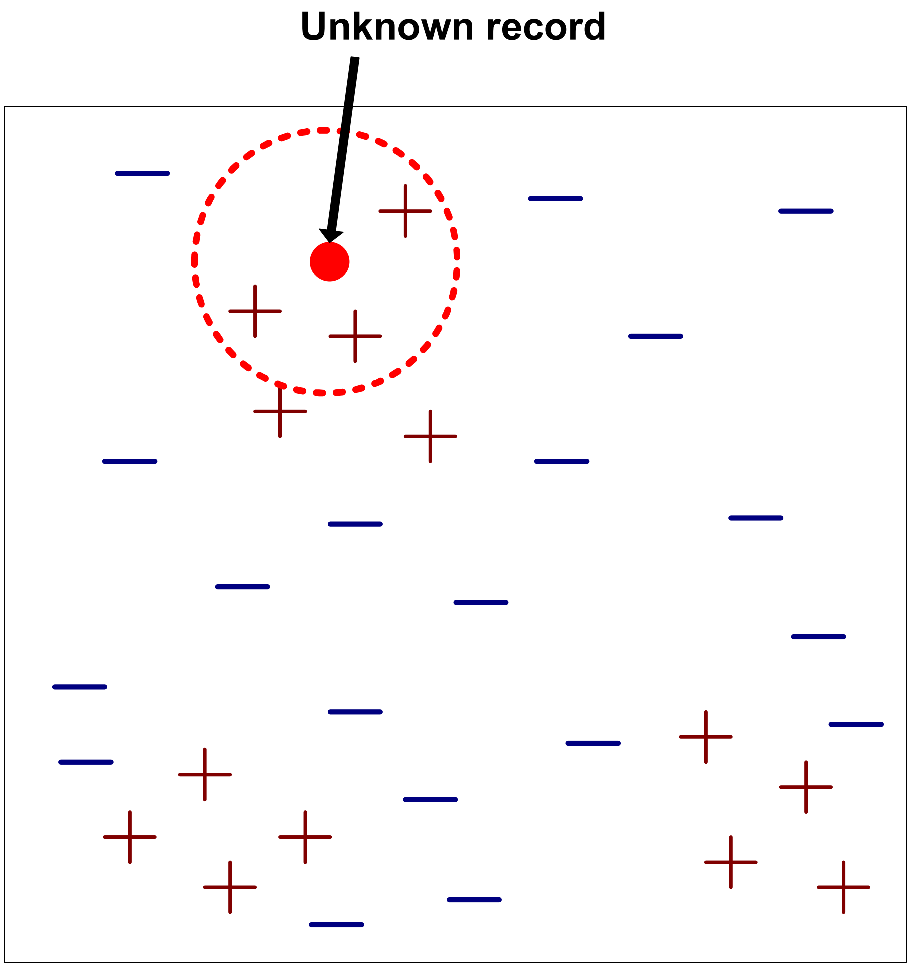
- Weighted majority vote within the k nearest neighbors
- Not *all* Ys are equally important
  - Outliers and training instances far away from the "confusing" regions don't really inform
  - Redundant training instances (very close to others) don't really add anything new

$$\hat{Y}(x) = \frac{1}{\sum_{i \in N_k(x)} \alpha_i} \sum_{i \in N_k(x)} w(x, x_i) \alpha_i y_i$$

- $\alpha_i$s may be binary (useful vs. useless)



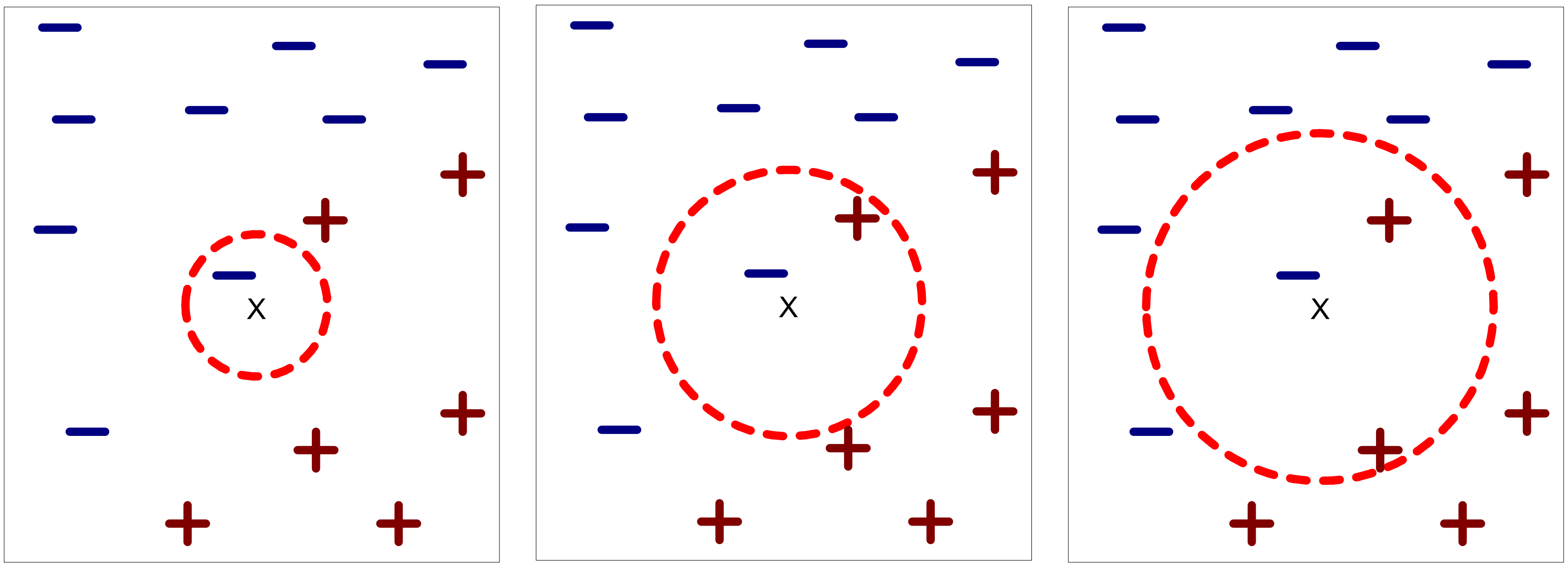
# Nearest-Neighbor Classifiers




- Requires three things
  - The set of stored records
  - Distance Metric to compute distance between records
  - The value of *k*, number of nearest neighbors to retrieve

- To classify new record:
  - Compute distance to other training records
  - Identify *k* nearest neighbors
  - Vote among nearest neighbors

# Definition of Nearest Neighbor

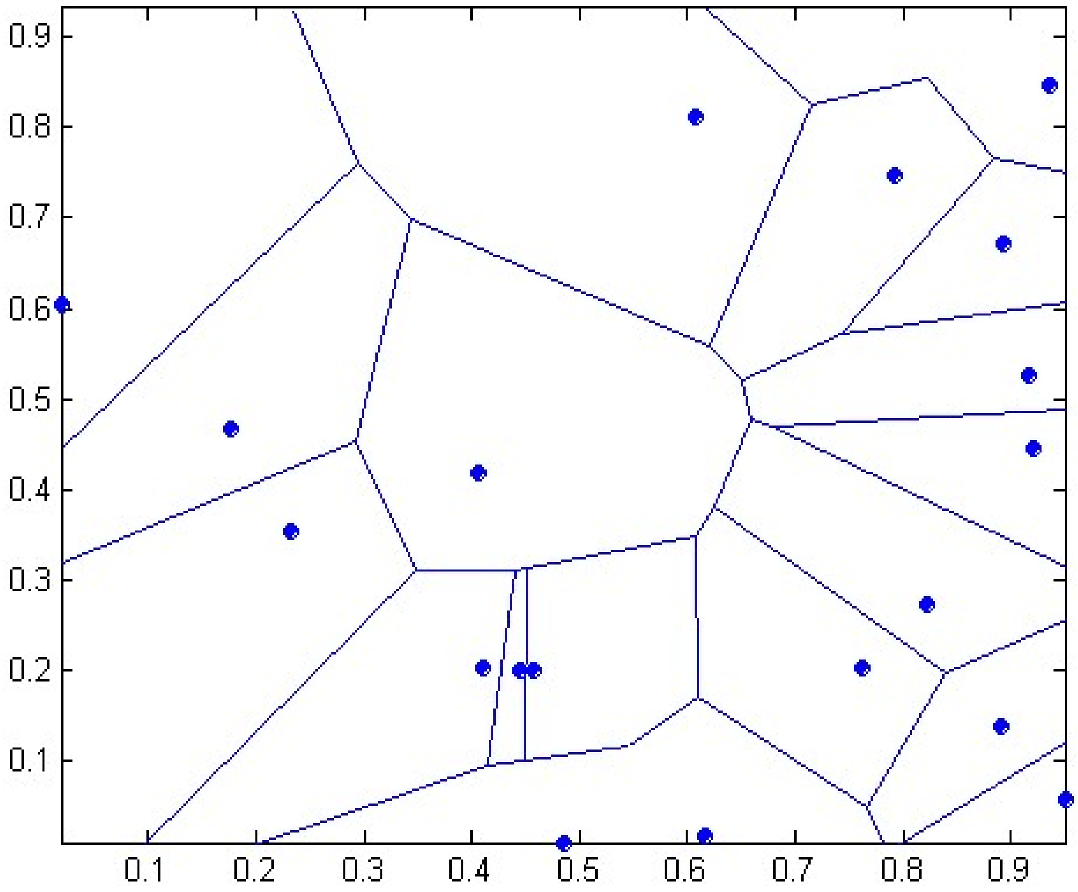



(a) 1-nearest neighbor (b) 2-nearest neighbor (c) 3-nearest neighbor

K-nearest neighbors of a record x are data points that have the k smallest distance to x

# 1 nearest-neighbor

Voronoi Diagram



# k-NN issues

## The Data is the Model

- No training needed.
- Accuracy generally improves with more data.
- Matching is simple and fast (and single pass).
- Usually need data in memory, but can be run off disk.

## Minimal Configuration:

- Only parameter is k (number of neighbors)
- Two other choices are important:
  - Weighting of neighbors (e.g. inverse distance)
  - Similarity metric

# K-NN metrics

- **Euclidean Distance:** Simplest, fast to compute
$$d(x, y) = \|x - y\|$$
- **Cosine Distance:** Good for documents, images, etc.
$$d(x, y) = 1 - \frac{x \cdot y}{\|x\|\|y\|}$$
- **Jaccard Distance:** For set data:
$$d(X, Y) = 1 - \frac{|X \cap Y|}{|X \cup Y|}$$
- **Hamming Distance:** For string data:
$$d(x, y) = \sum_{i=1}^{n} (x_i \neq y_i)$$

# K-NN metrics

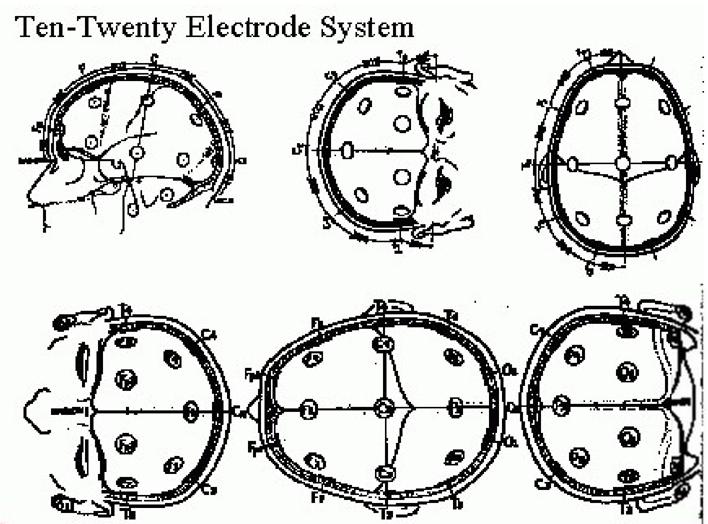
- **Manhattan Distance:** Coordinate-wise distance

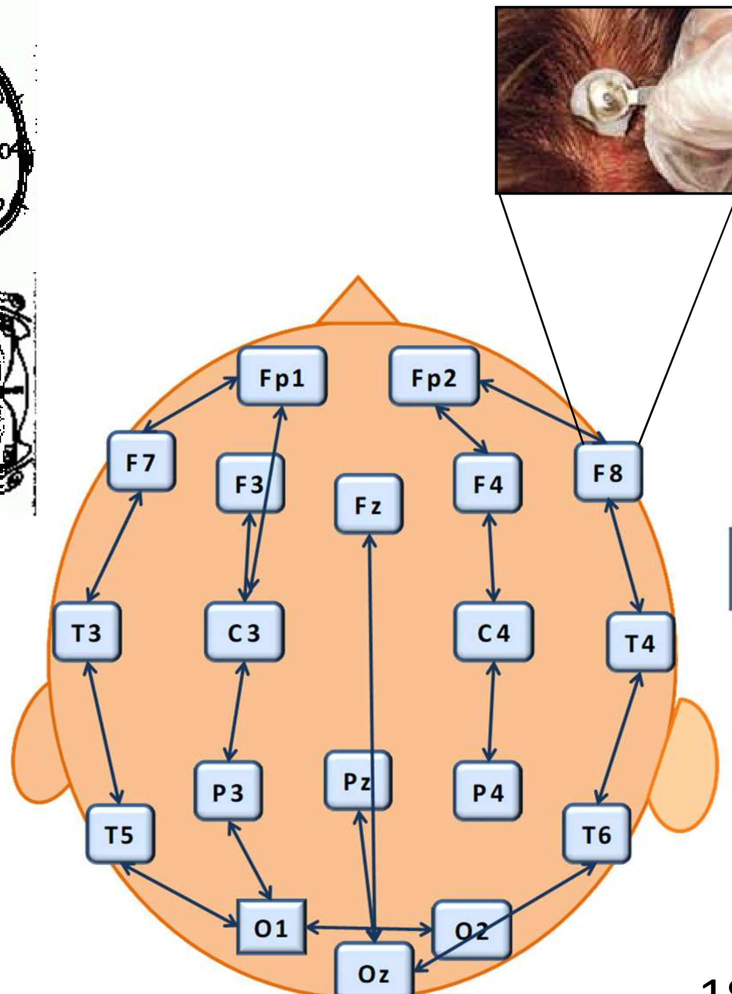
$$d(x, y) = \sum_{i=1}^{n} |x_i - y_i|$$

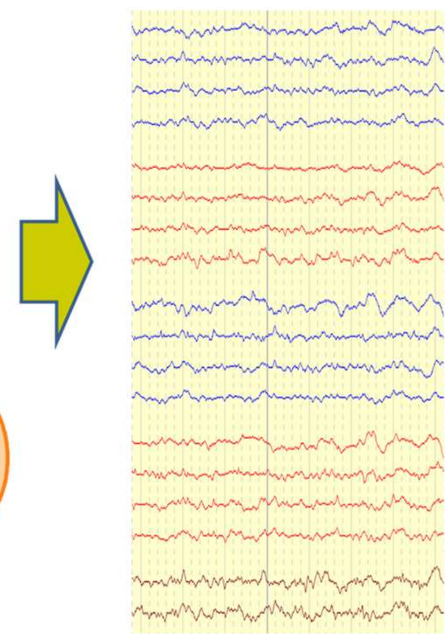
- **Edit Distance:** for strings, especially genetic data.

- **Mahalanobis Distance:** Normalized by the sample covariance matrix – unaffected by coordinate transformations.

# Scalp EEG Acquisition

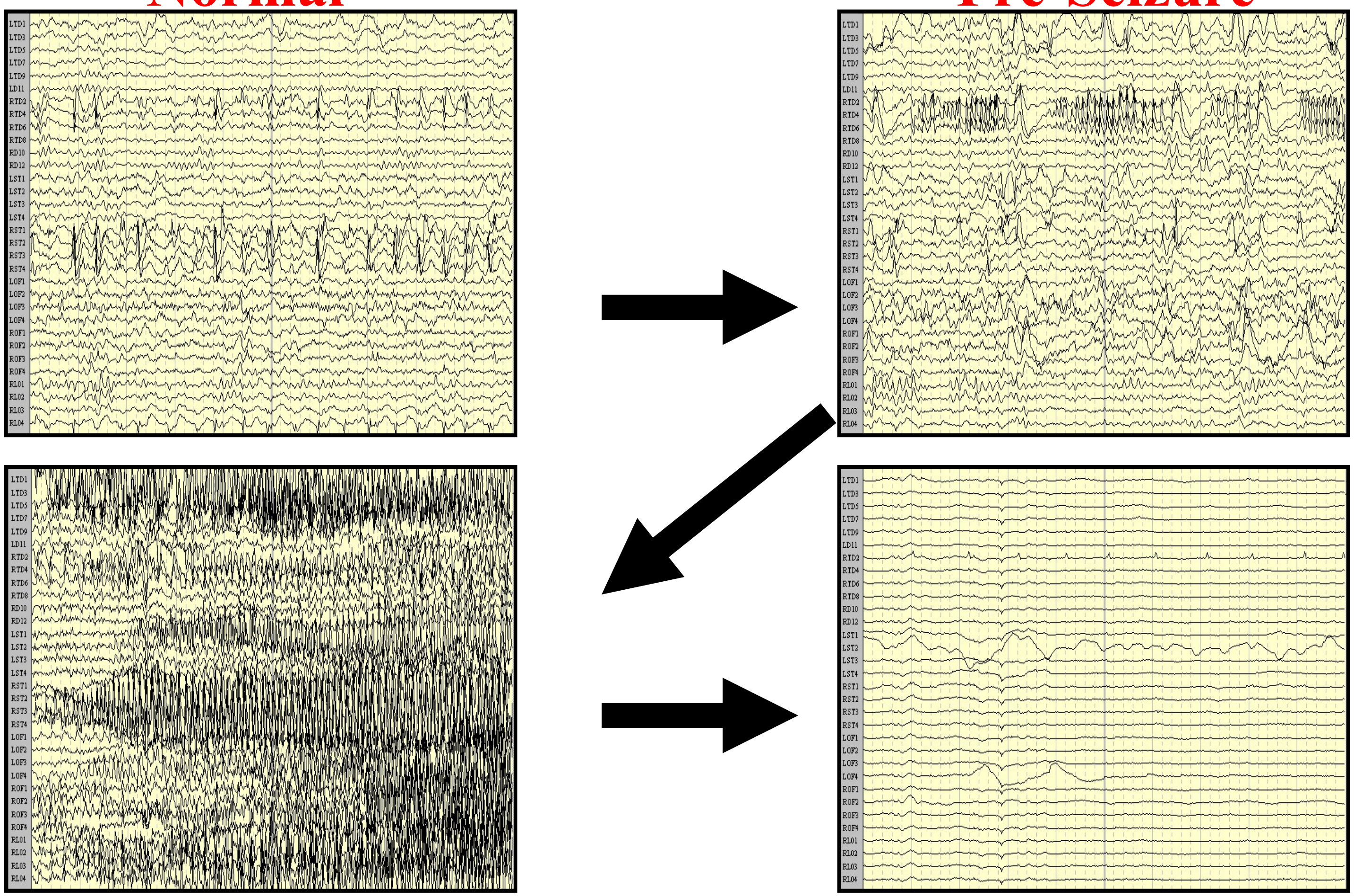


18 Bipolar Channels

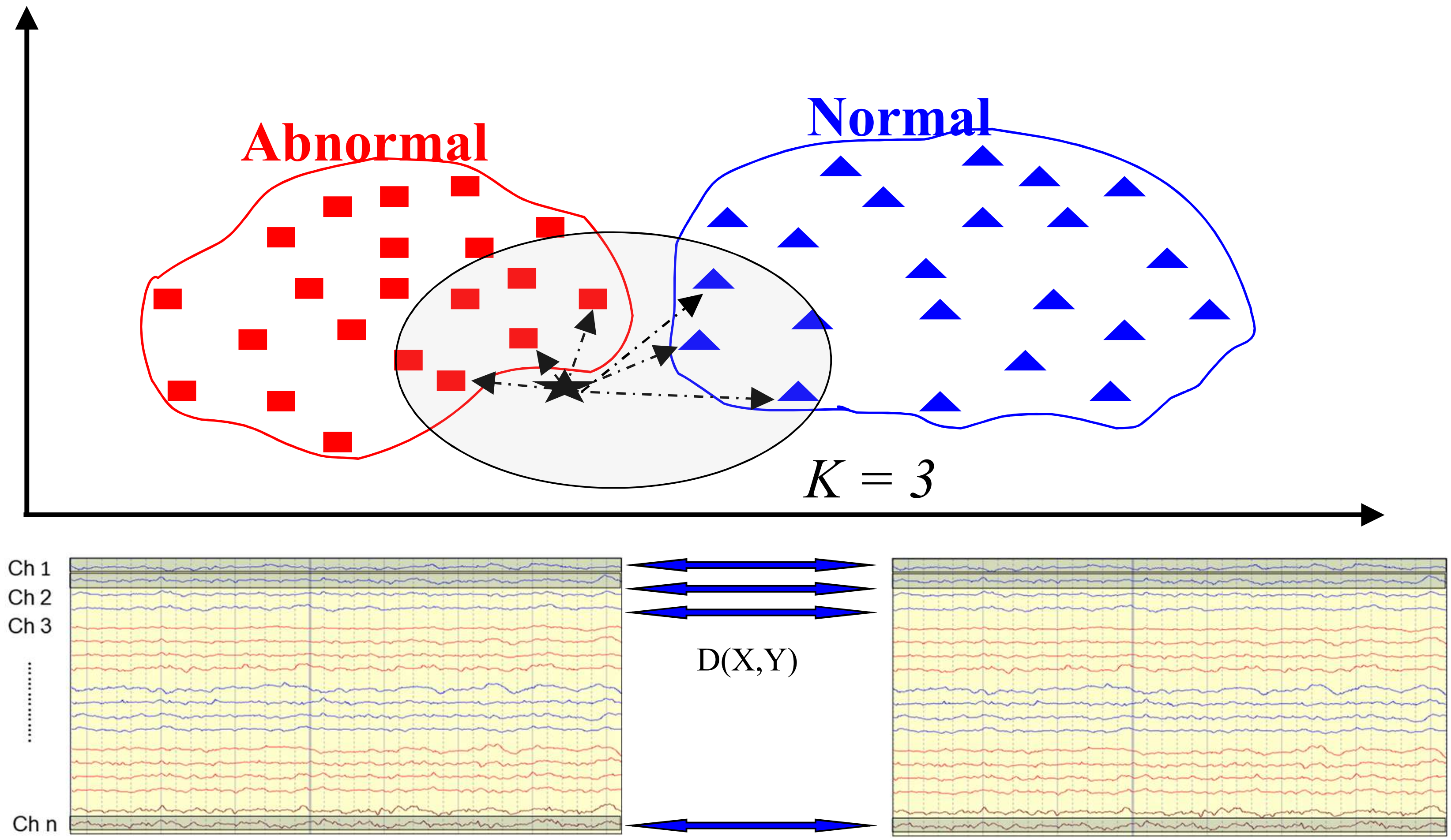
# 10-second EEGs: Seizure Evolution





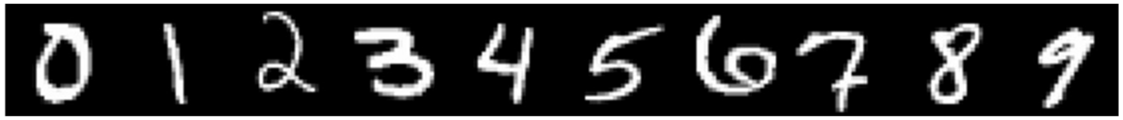

Chaovalitwongse et al., *Annals of Operations Research* (2006)

# K-Nearest Neighbor for seizure detection




**Time series distances:** *(1) Euclidean, (2) Dynamic Time Warping*

# Example: Digit Recognition



- Yann LeCunn – MNIST Digit Recognition
  - Handwritten digits
  - 28x28 pixel images: $d = 784$
  - 60,000 training samples
  - 10,000 test samples

| | Test Error Rate (%) |
|---|---|
| Linear classifier (1-layer NN) | 12.0 |
| K-nearest-neighbors, Euclidean | 5.0 |
| K-nearest-neighbors, Euclidean, deskewed | 2.4 |
| K-NN, Tangent Distance, 16x16 | 1.1 |
| K-NN, shape context matching | 0.67 |

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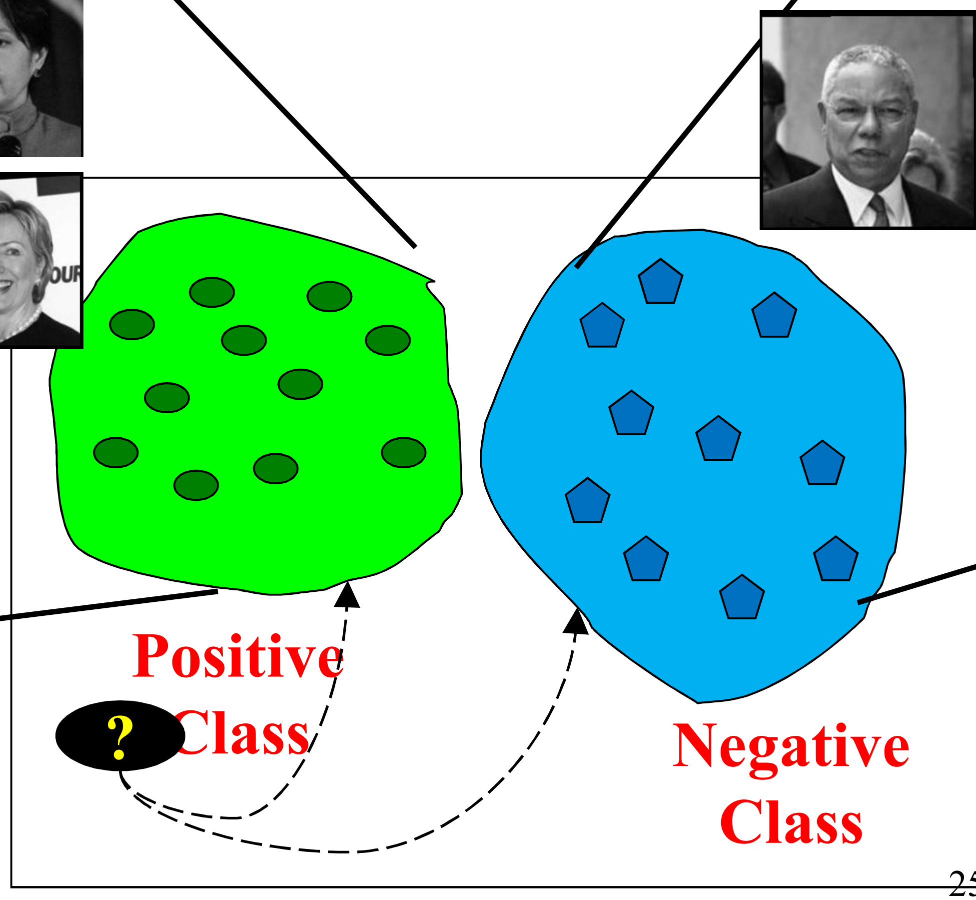
# More generally: Supervised classification

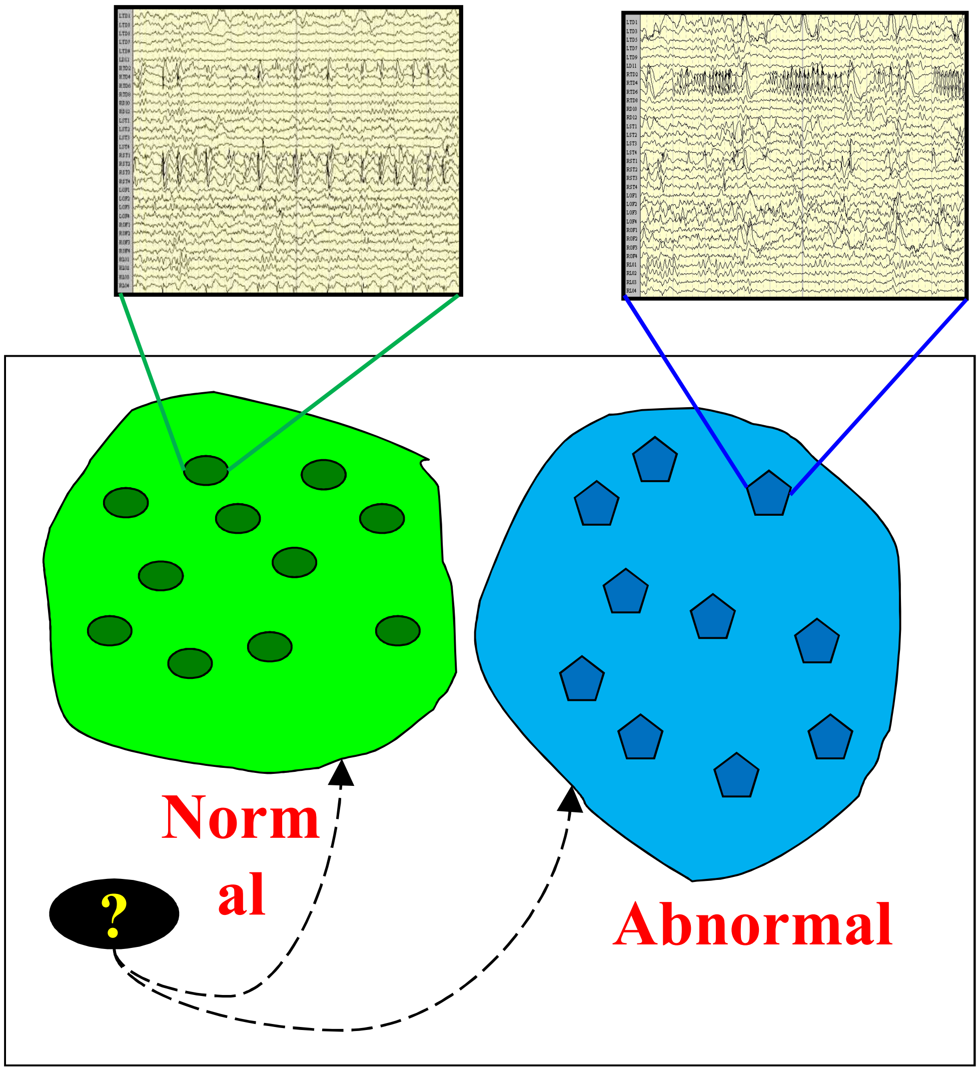
- A minor shift of gears..
- Given a set of labelled training instances, learn to classify a new test instance..
  - (K)NN was only one method

# Binary classification
# Gender identification

**<u>Supervised learning</u>:** A class (category) label for each pattern in the training set is provided.



# Multidimensional Time Series Classification in Medical Data




- Positive *versus* Negative
- Responsive *versus* Unresponsive

- ***Multidimensional Time Series Classification***
- ***Multisensor medical signals (e.g., EEG, ECG, EMG)***

# Classification and *discriminant* functions

- Define a "discriminant function" $g_i(\mathbf{x})$ for each class $\omega_i$ such that:

- the classifier assigns a feature vector $x$ to class $\omega_i$ if

$$g_i(\mathbf{x}) > g_j(\mathbf{x}) \qquad \text{for all } \; j \neq i$$

- For two-category case, $g(\mathbf{x}) \equiv g_1(\mathbf{x}) - g_2(\mathbf{x})$

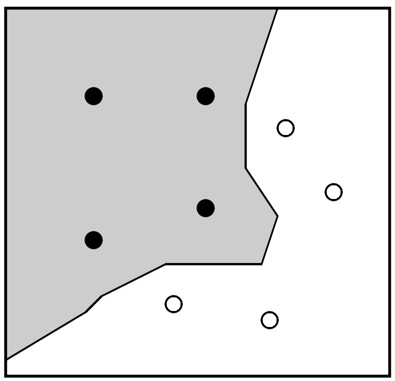
$$\text{Decide } \omega_1 \text{ if } g(\mathbf{x}) > 0; \text{ otherwise decide } \omega_2$$

- An example
  - Minimum-Error-Rate Classifier

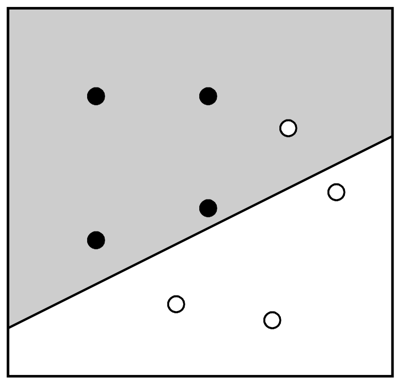
$$g(\mathbf{x}) \equiv p(\omega_1 \mid \mathbf{x}) - p(\omega_2 \mid \mathbf{x})$$

# Discriminant Function

- It can be arbitrary functions of *x*, such as:

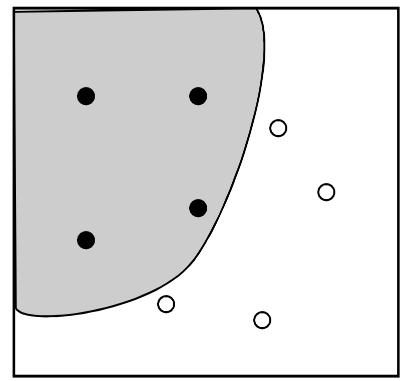


Nearest Neighbor



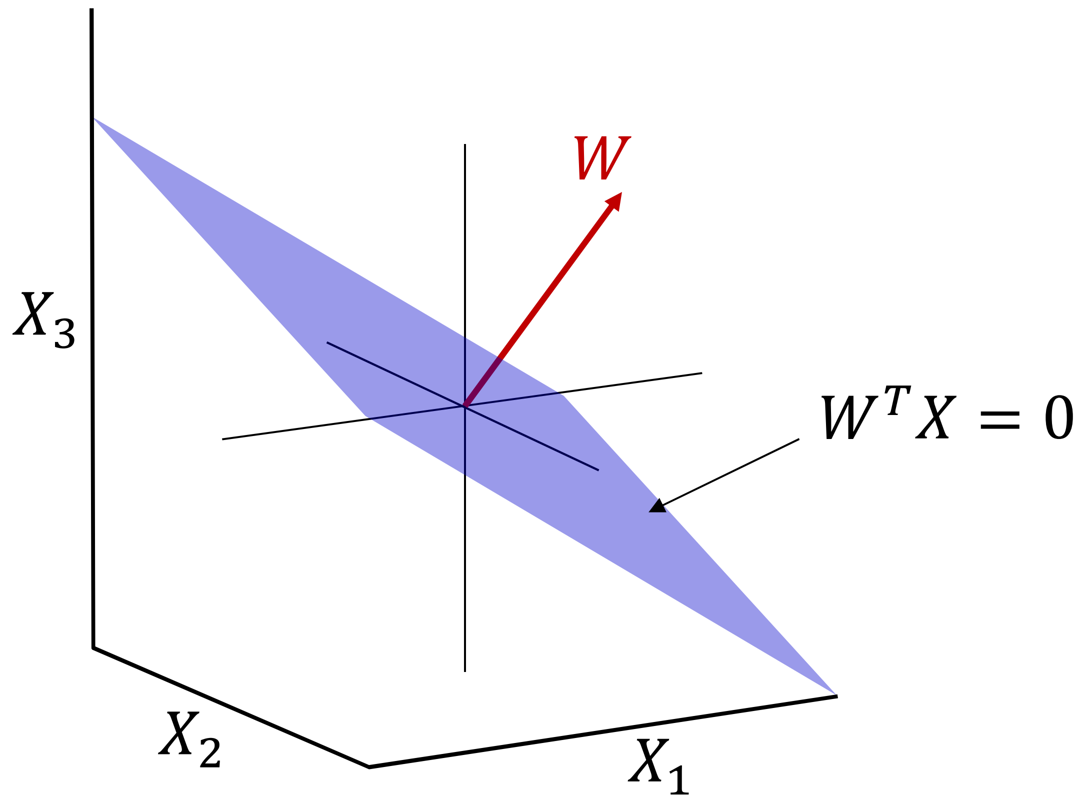
Linear Functions

$$g(\mathbf{x}) = \mathbf{w}^T \mathbf{x} + b$$



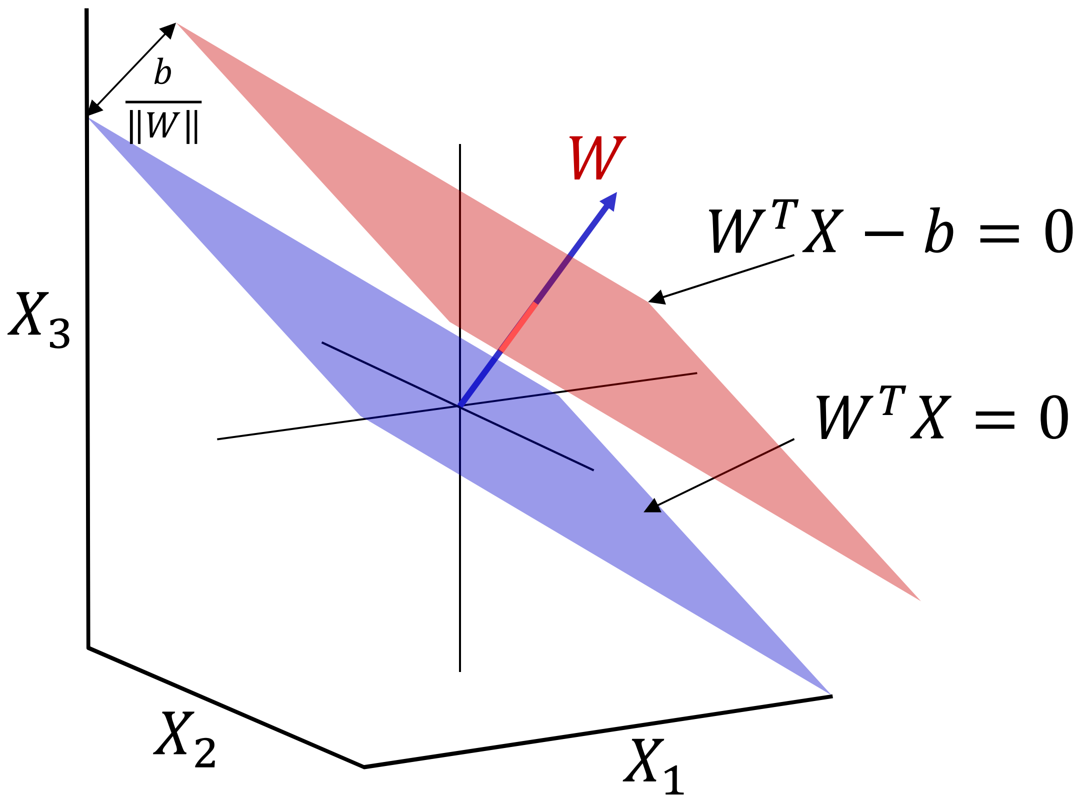
Nonlinear Functions

# The equation for a hyperplane



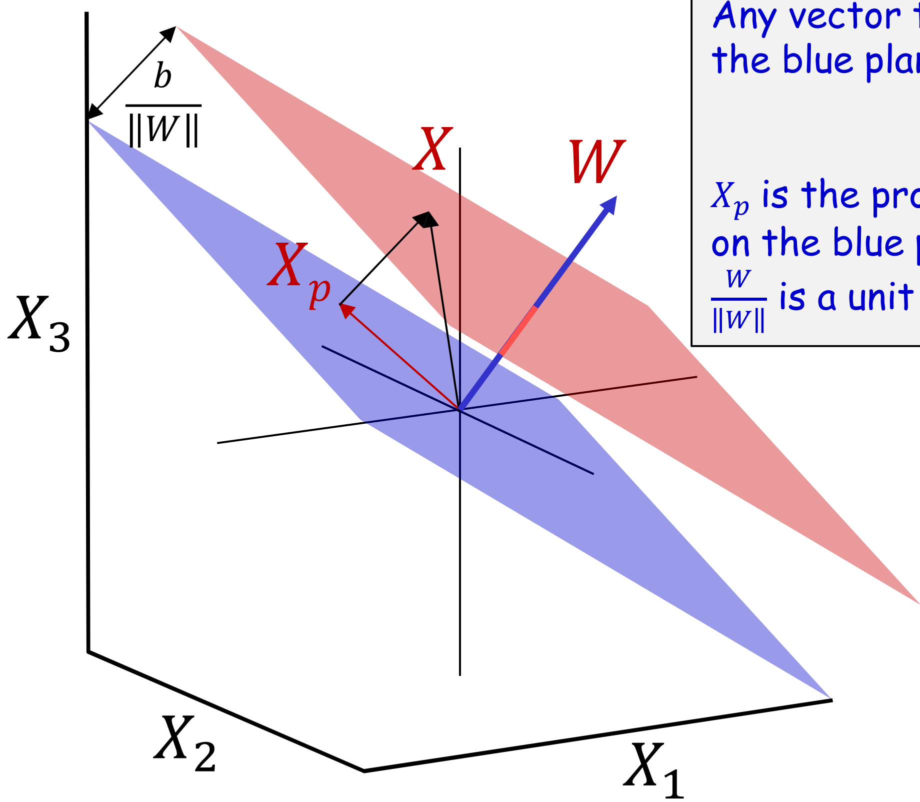

- $W^T X = 0$ is the equation representing the set of all vectors that are orthogonal to $W$

# The equation for a hyperplane




- $W^T X - b = 0$ is the equation representing plane that is orthogonal to $W$ and a distance $\frac{b}{\|W\|}$ from origin
  - The set of all vectors that are a distance $\frac{b}{\|W\|}$ from the blue plane

# The equation for a hyperplane




Any vector that is a distance $d$ from the blue plane can be written as

$$X = X_p + d\frac{W}{\|W\|}$$

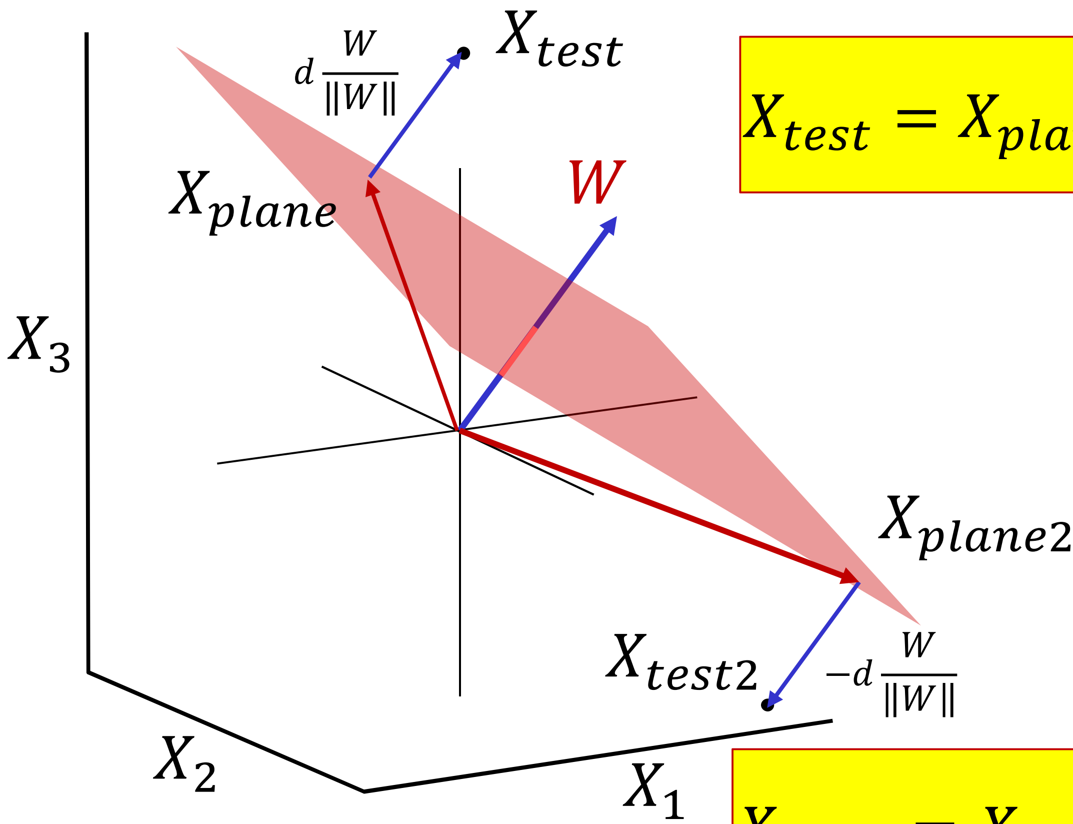
$X_p$ is the projection of the vector on the blue plane

$\frac{W}{\|W\|}$ is a unit vector in the direction of $W$

Trivial proof:

- On the red plane any $X = X_p + \left(\frac{b}{\|W\|}\right)\frac{W}{\|W\|}$
- $W^T X = W^T X_p + b\frac{W^T W}{\|W\|^2} = b$

# Distance from a hyperplane

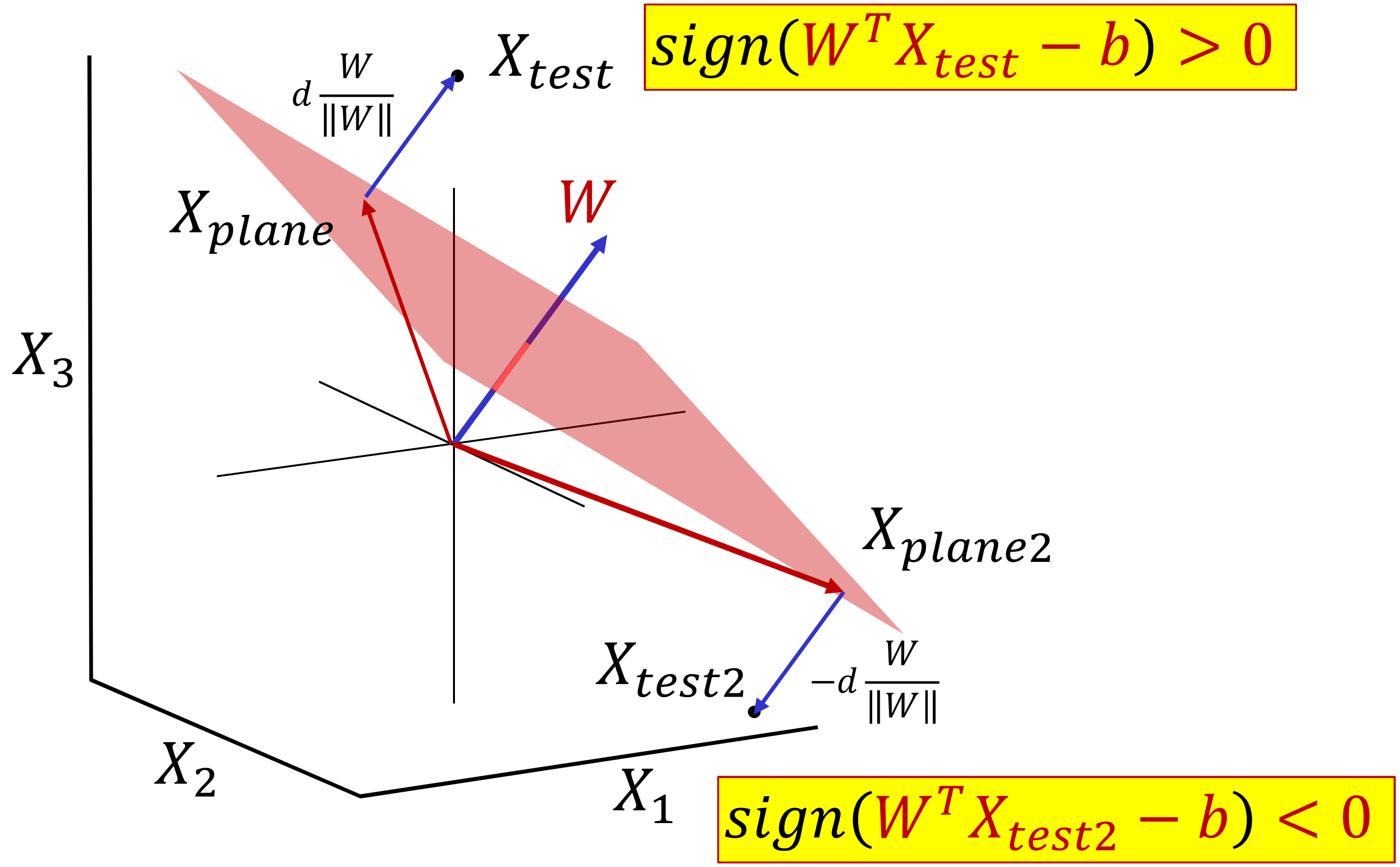



$$X_{test} = X_{plane} + d\frac{W}{\|W\|}$$

$$X_{test2} = X_{plane2} - d\frac{W}{\|W\|}$$

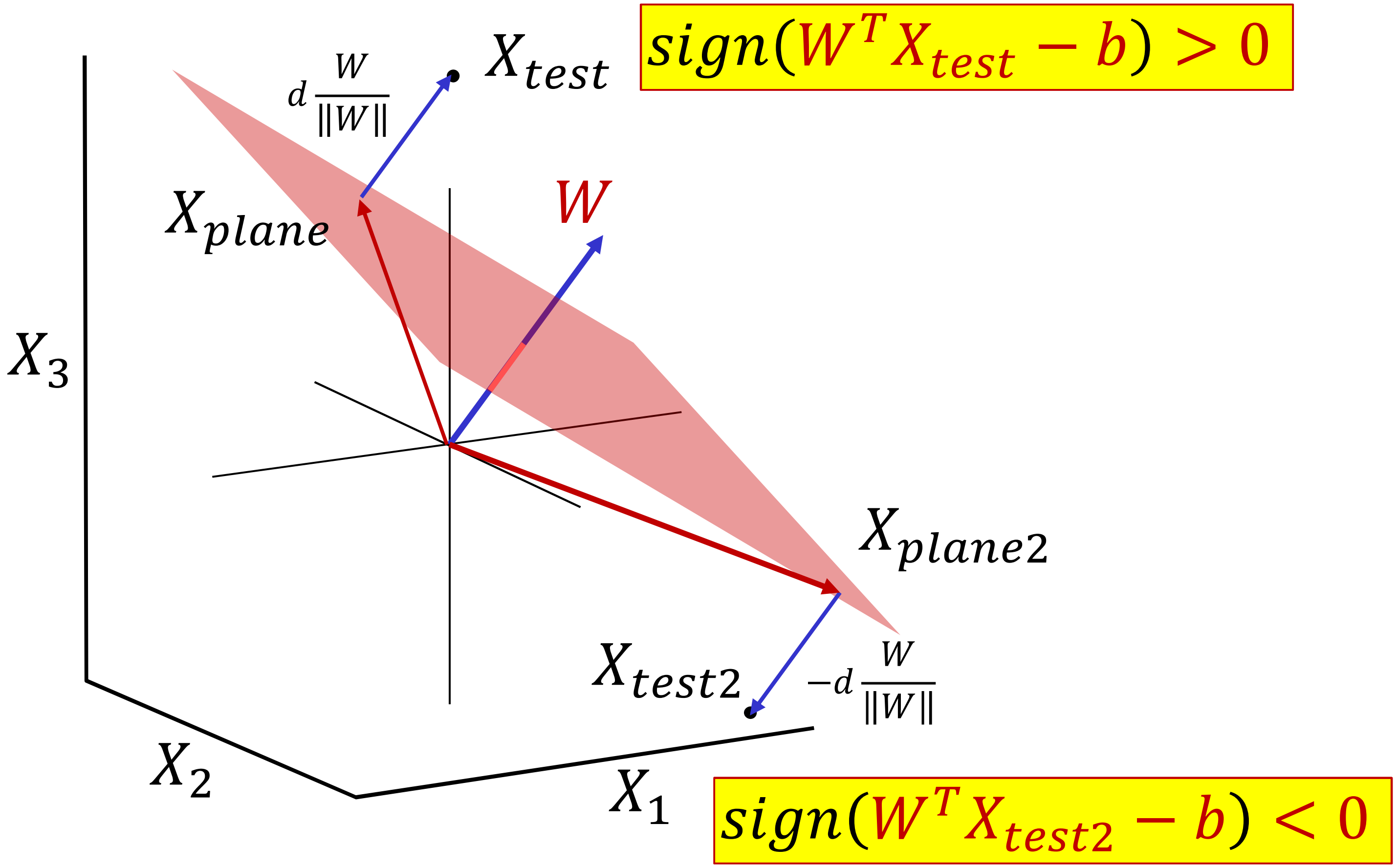
- The distance of any $X_{test}$ from the plane $W^T X - b = 0$ is $d = \frac{W^T X_{test} - b}{\|W\|}$
- This can be positive (in the direction of $W$) or negative (opposite to $W$)

# Sign of distance from hyperplane



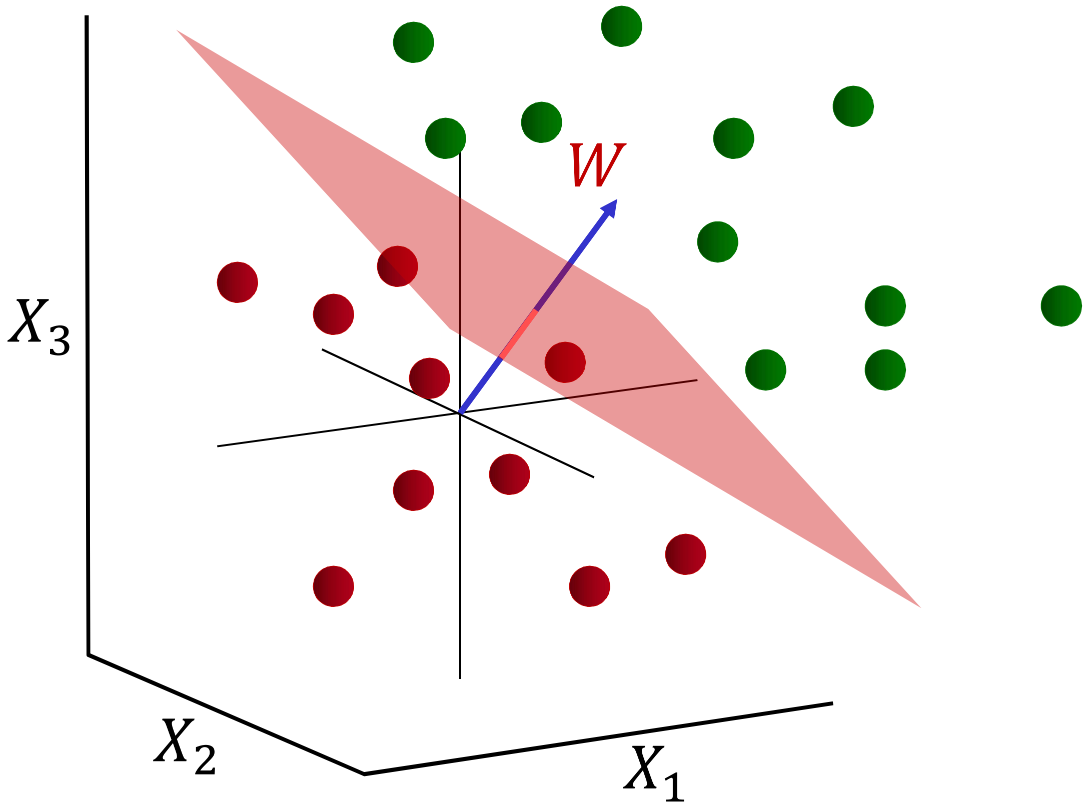

- The sign of $W^T X - b$ signifies which side of the plane the point $X$ is on

# Linear Classifier



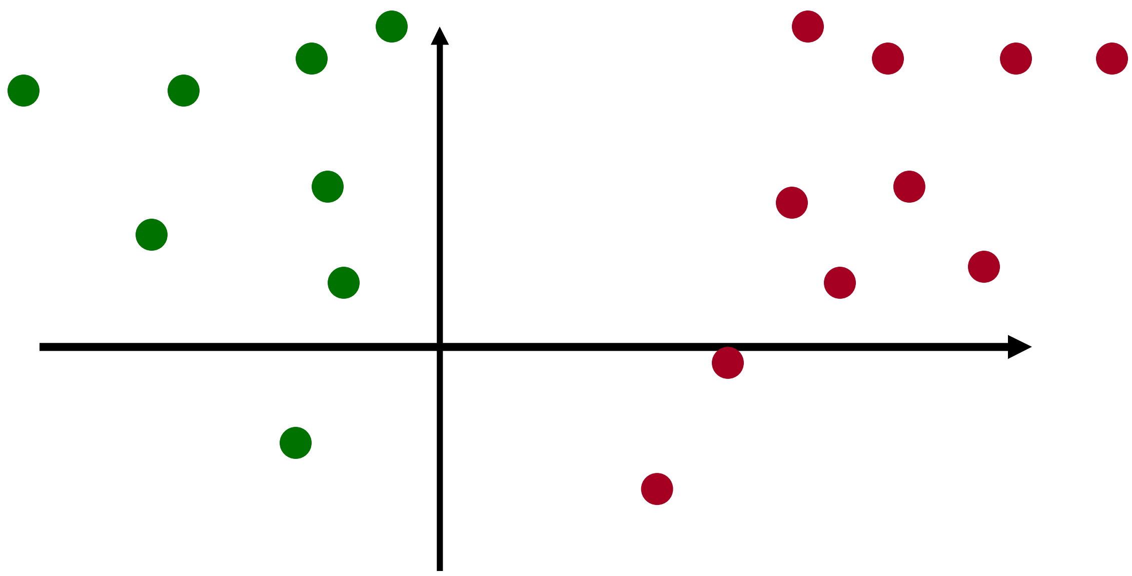

- The plane $W^T X - b$ is a linear classifier
  - The class is given by $sign(W^T X_{test} - b)$

# Linearly separable data



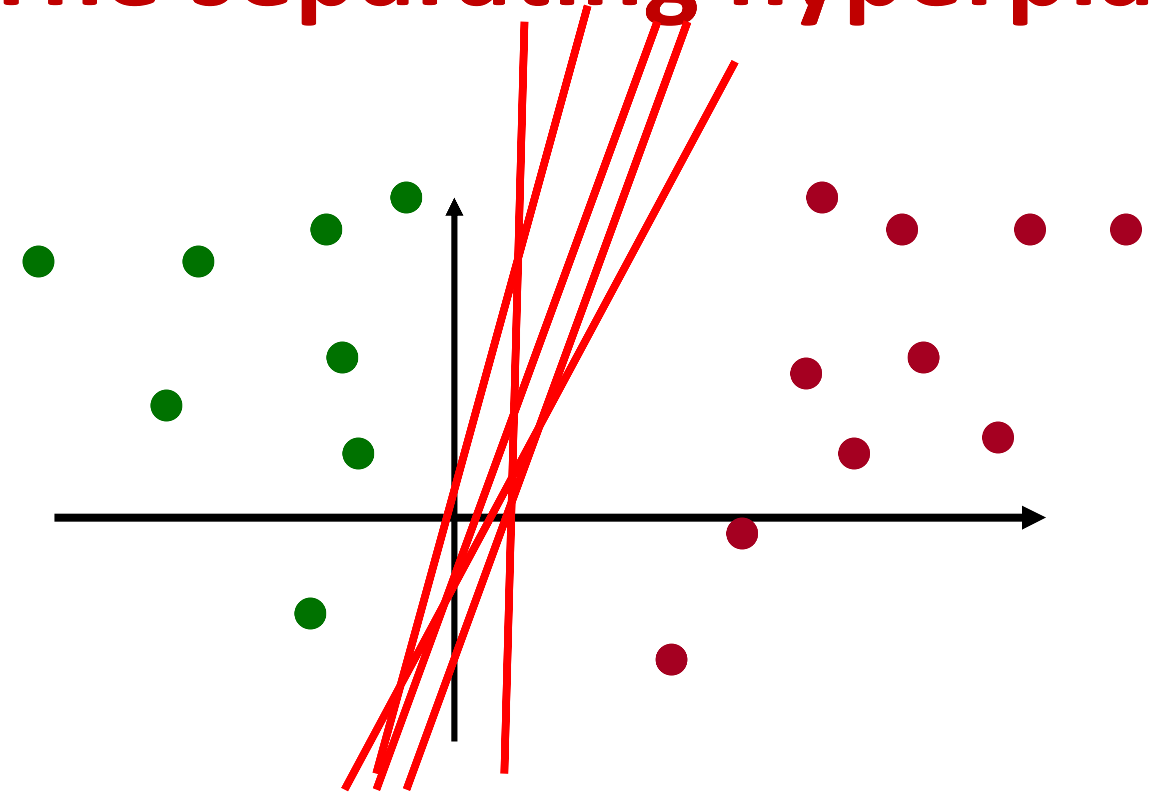

- Data where the two classes are separated by a hyperplane
  - And classification can be performed by $sign(W^T X_{test} - b)$ for any separating hyperplane

# 2D illustration, linearly separable data



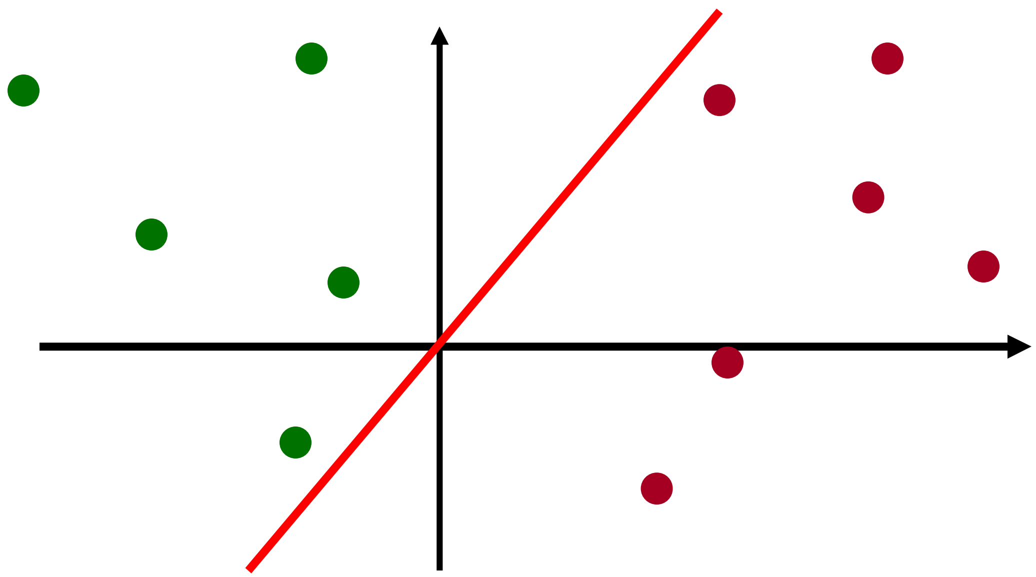
- Classes are linearly separable
- Dots represent “training” instances
- **Training problem**: Given these training instances find a separating hyperplane

# The separating hyperplane



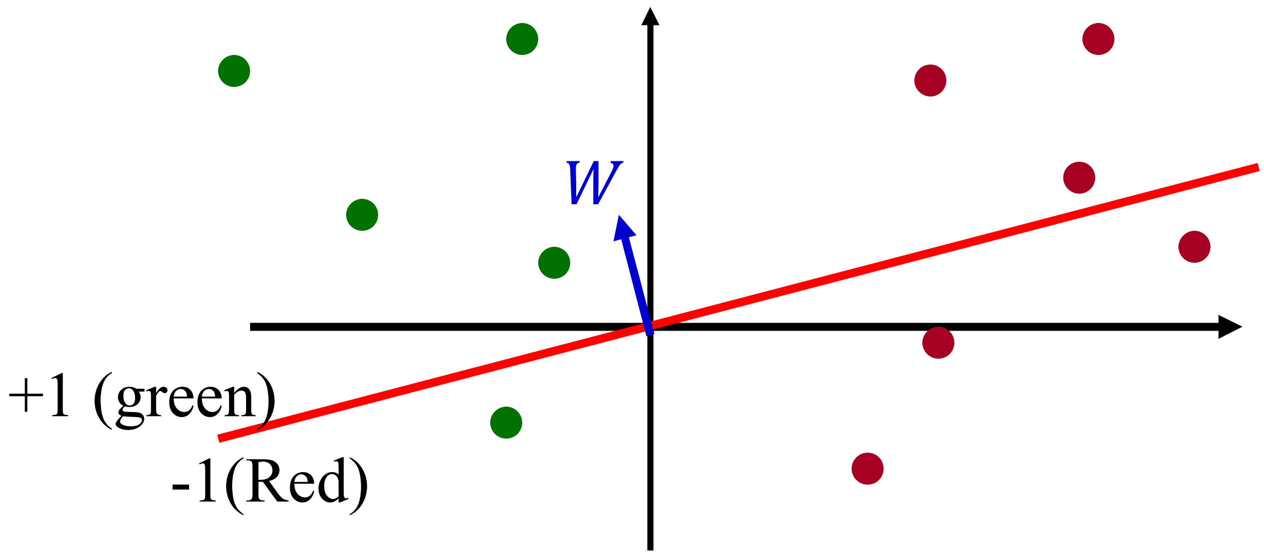
- Problem: Given these training instances find a separating hyperplane
- **Many ways of finding this hyperplane**
  - Any number of solution algorithms are possible

# A Simplifying Assumption



- **Simplifying assumption:** The separating hyperplane always goes through origin
  - Easily enforced by appending a constant 1 to every vector

# A Simple Method: The Perceptron Algorithm




- **Initialize:** Randomly initialize the hyperplane
  - I.e. randomly initialize the normal vector $W$
  - Classification rule $sign(W^T X)$
  - The random initial plane will make mistakes

# Perceptron Algorithm

- Given $N$ training instances $(X_1, Y_1), (X_2, Y_2), \ldots, (X_N, Y_N)$
  - $Y_i = +1$ or $-1$

- Initialize $W$
- Cycle through the training instances:
- While more classification errors
  - For $i = 1 \,..\, N_{train}$

$$O(X_i) = sign(W^T X_i)$$

    - If $O(X_i) \neq Y_i$

$$W = W + Y_i X_i$$

# Perceptron Algorithm: Summary

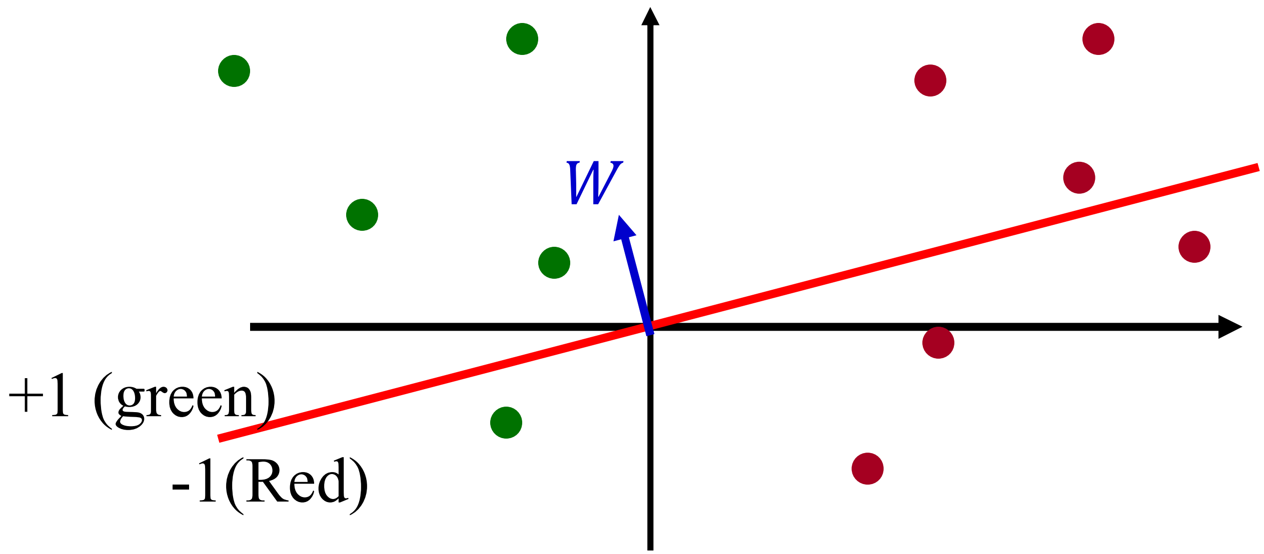
- Cycle through the training instances
- Only update $W$ on misclassified instances
- If instance misclassified:
  - If instance is positive class

$$W = W + X_i$$

  - If instance is negative class

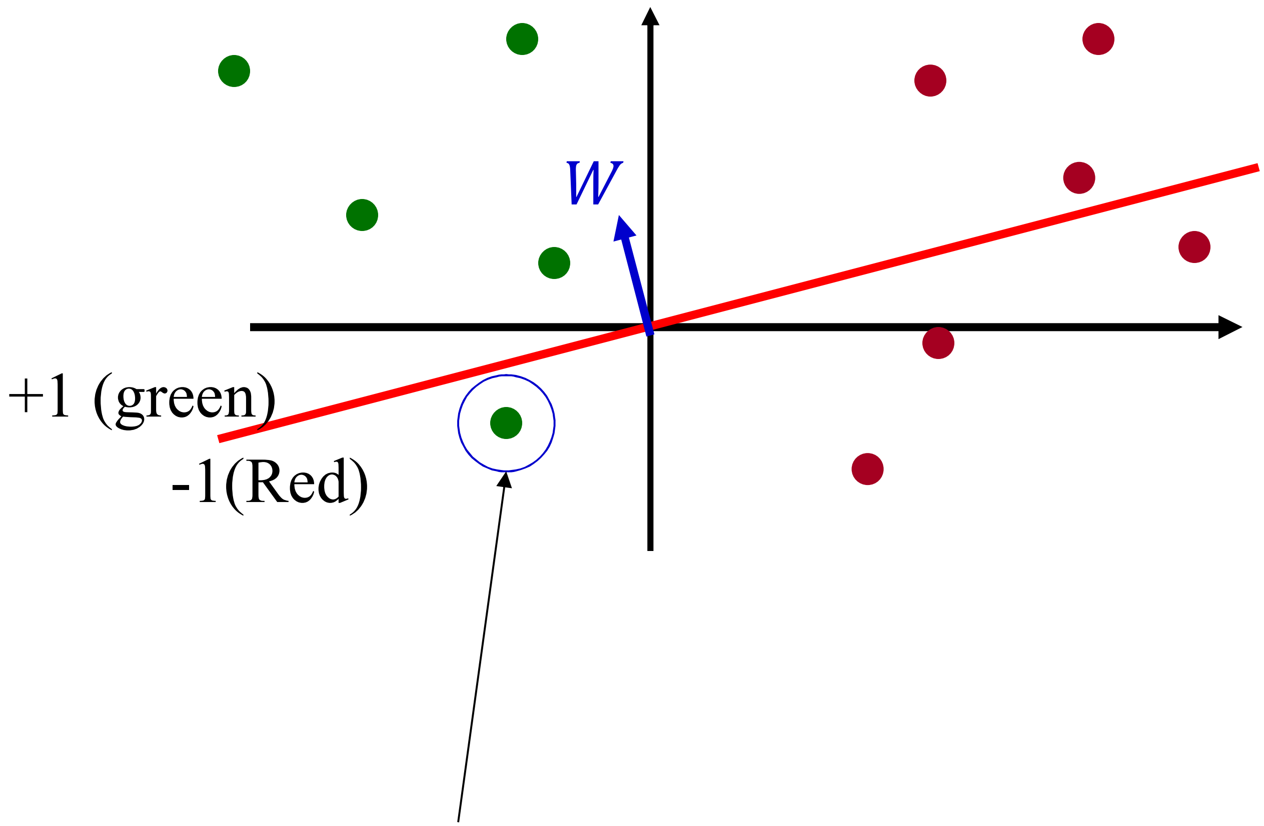
$$W = W - X_i$$

# Perceptron Algorithm



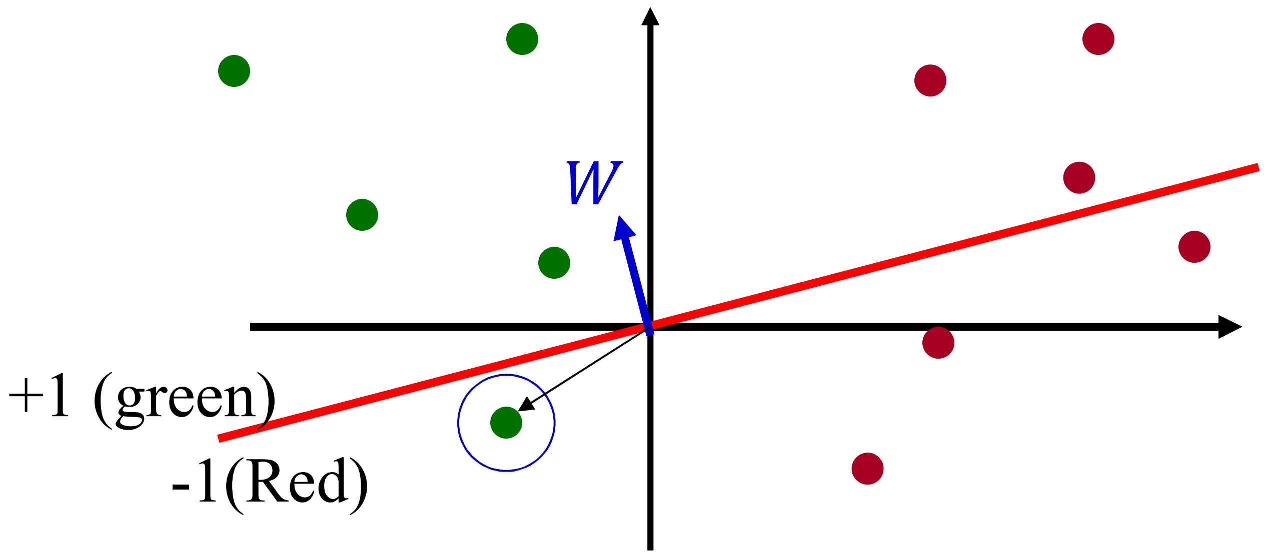

Initialization

# Perceptron Algorithm

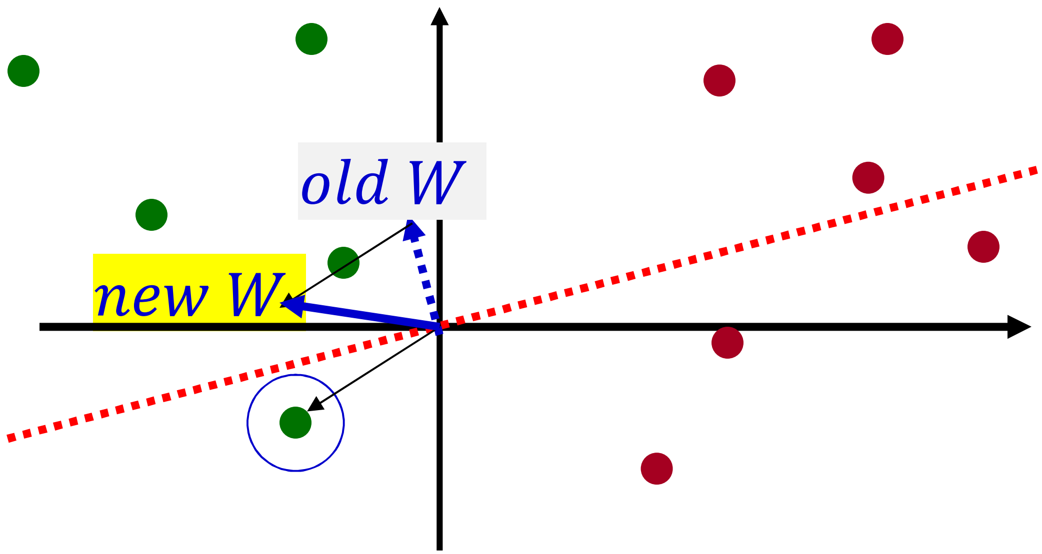



Misclassified positive instance

# Perceptron Algorithm

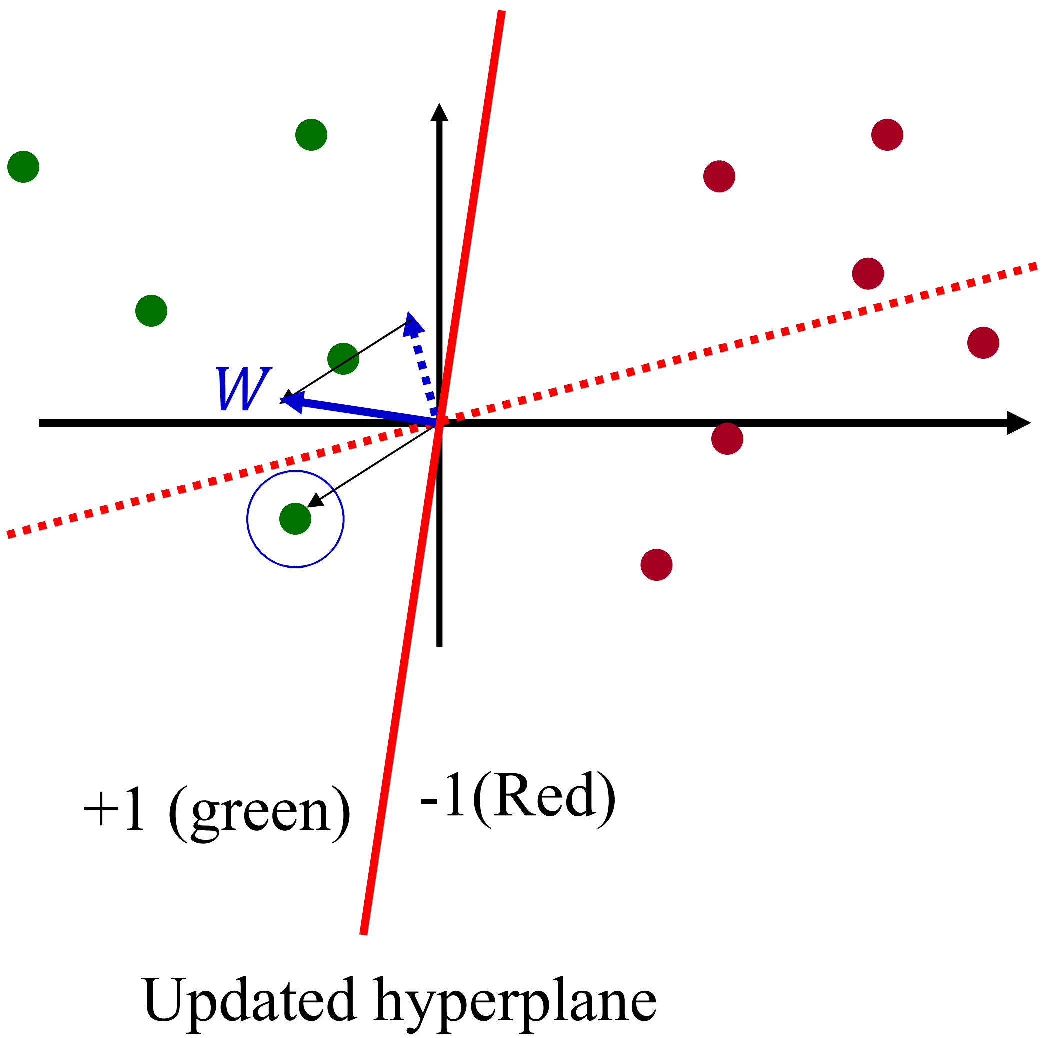


# Perceptron Algorithm




Updated weight vector

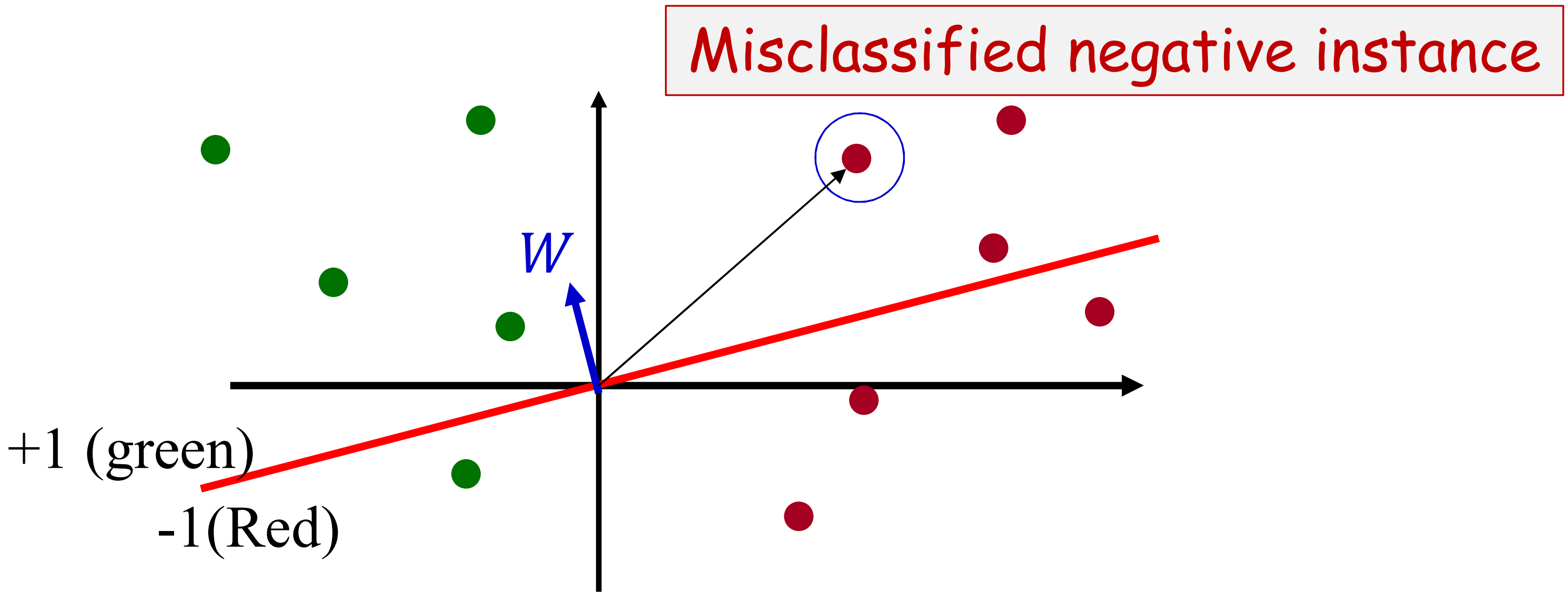
# Perceptron Algorithm



# Convergence of Perceptron Algorithm

- Guaranteed to converge
  - After no more than $\frac{R^2}{\gamma^2}$ misclassifications
  - $R$ is length of longest training point
  - $\gamma$ is the *best case* closest distance of a training point from the classifier
    - I.e the *largest* distance to the *closest* training instance to *any* appropriate classifier

# Problems with perceptron algorithm




- Final solution depends on order of processing of inputs
  - Can get different solutions for the same initial vector by changing the order in which instances are considered

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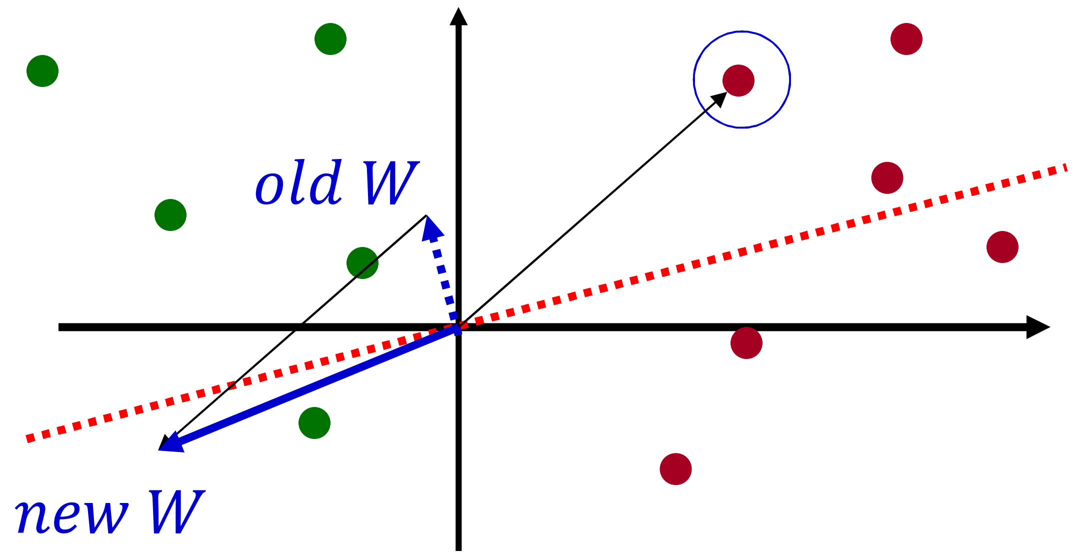


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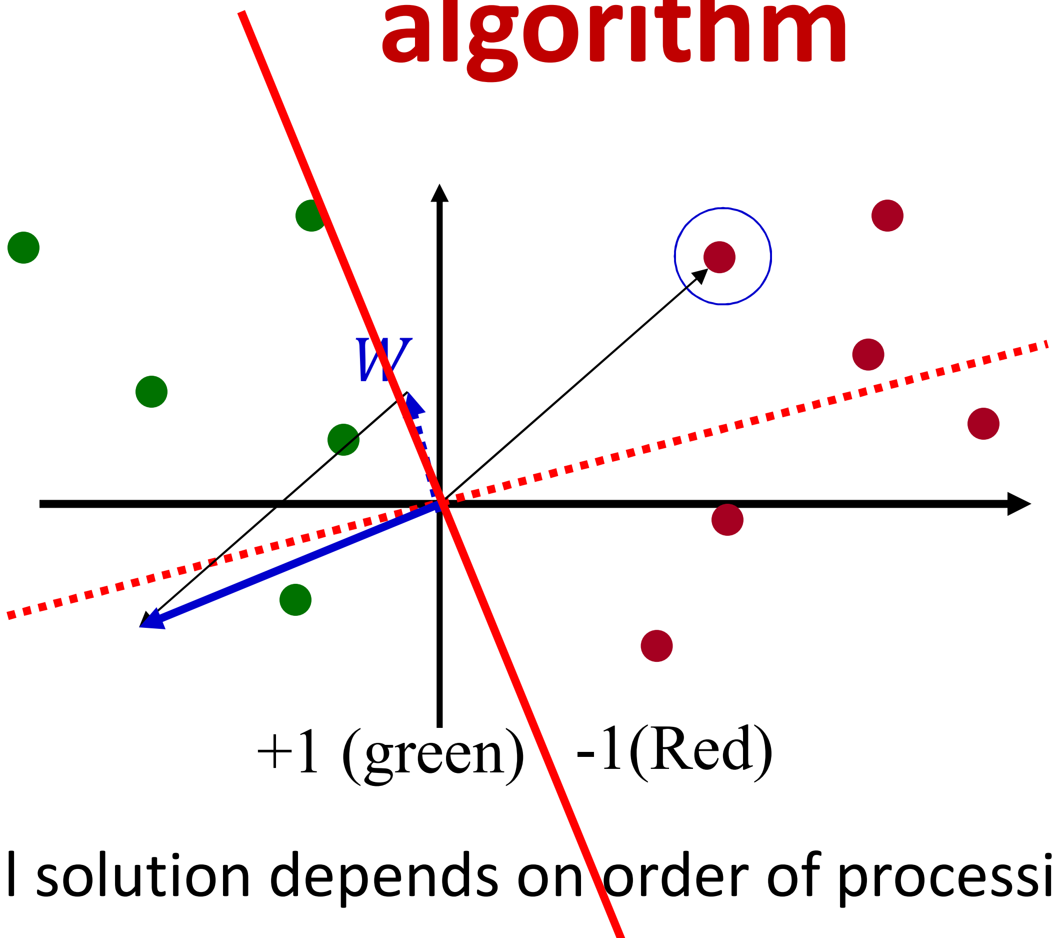


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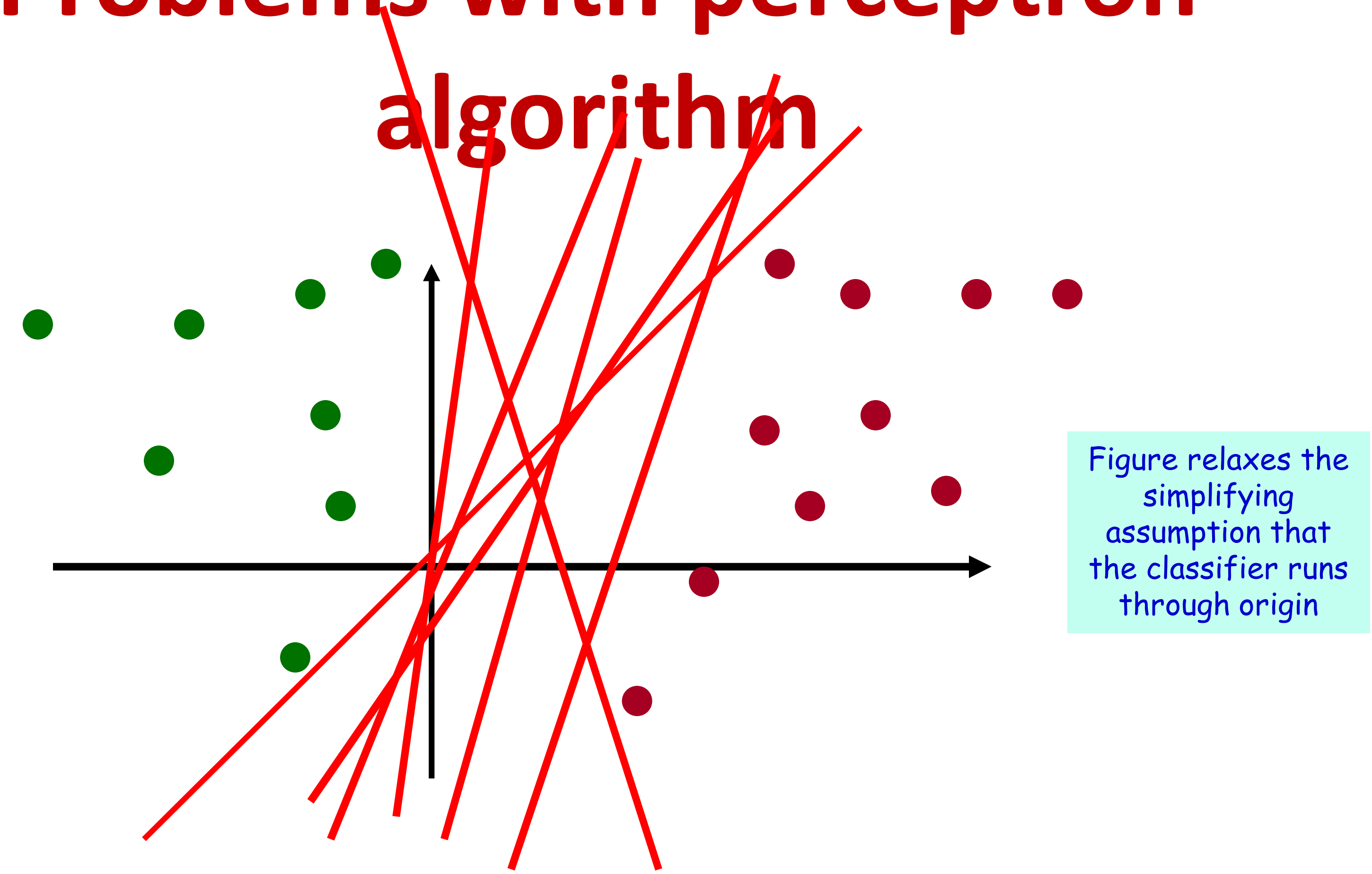


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  - $R$ is length of longest training point
  - $\gamma$ is the *best case* closest distance of a training point from the classifier
    - I.e the *largest* distance to the *closest* training instance to *any* appropriate classifier
- **Although the number of iterations is bounded by the distance of a "best-case" classifier, no guarantee that we will actually find this best-case classifier**
  - Algorithm stops updating after perfect training classification

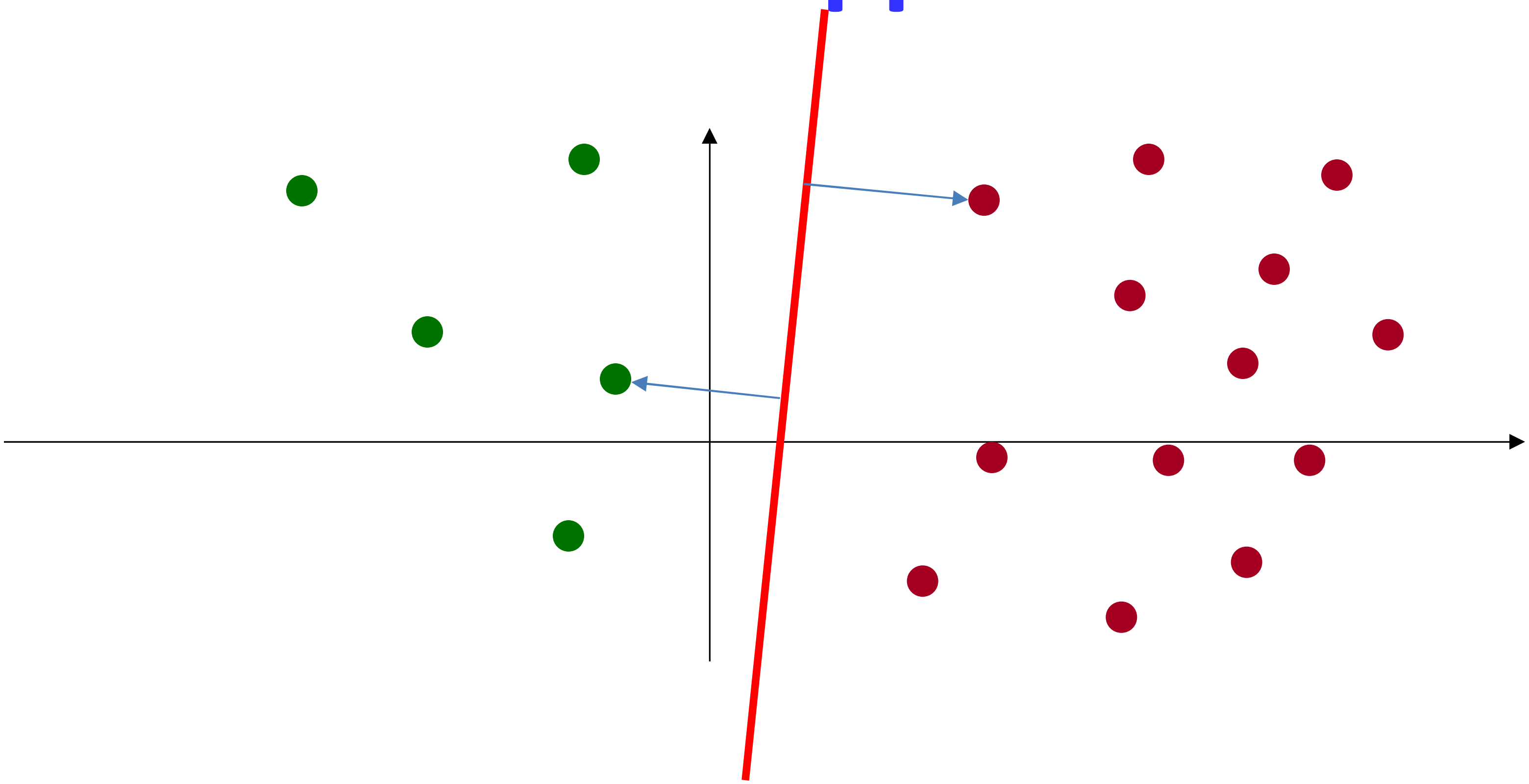
# Modification of perceptron to find margin

- Instead of updating only on misclassified instances, update on any vector within $0.5\gamma$ of boundary
- Guaranteed to converge
- Problem – you specify $\gamma$.
  - Overall optimality not guaranteed
  - But still, a pretty good algorithm

# Enter: Support Vector Machines

- Find a classifier that is maximally distant from the *closest* instances from either class

# A Better Approach

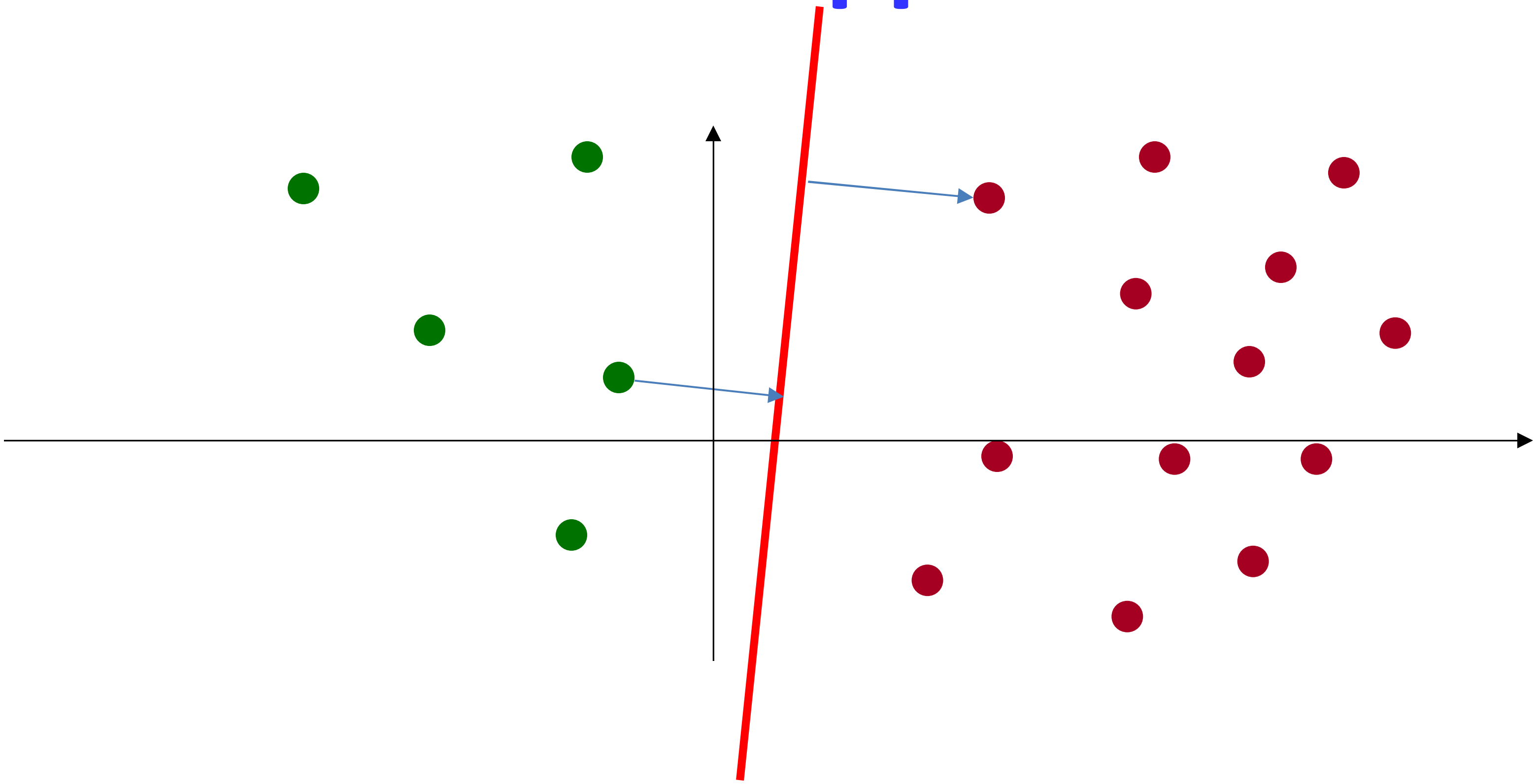


- Any linear classifier has some *closest* instances
- These instances will be at some distance from the boundary
- Changing the classifier will change both, the closest instance, and their distance from the boundary

# Returning to the *Perceptron* algorithm

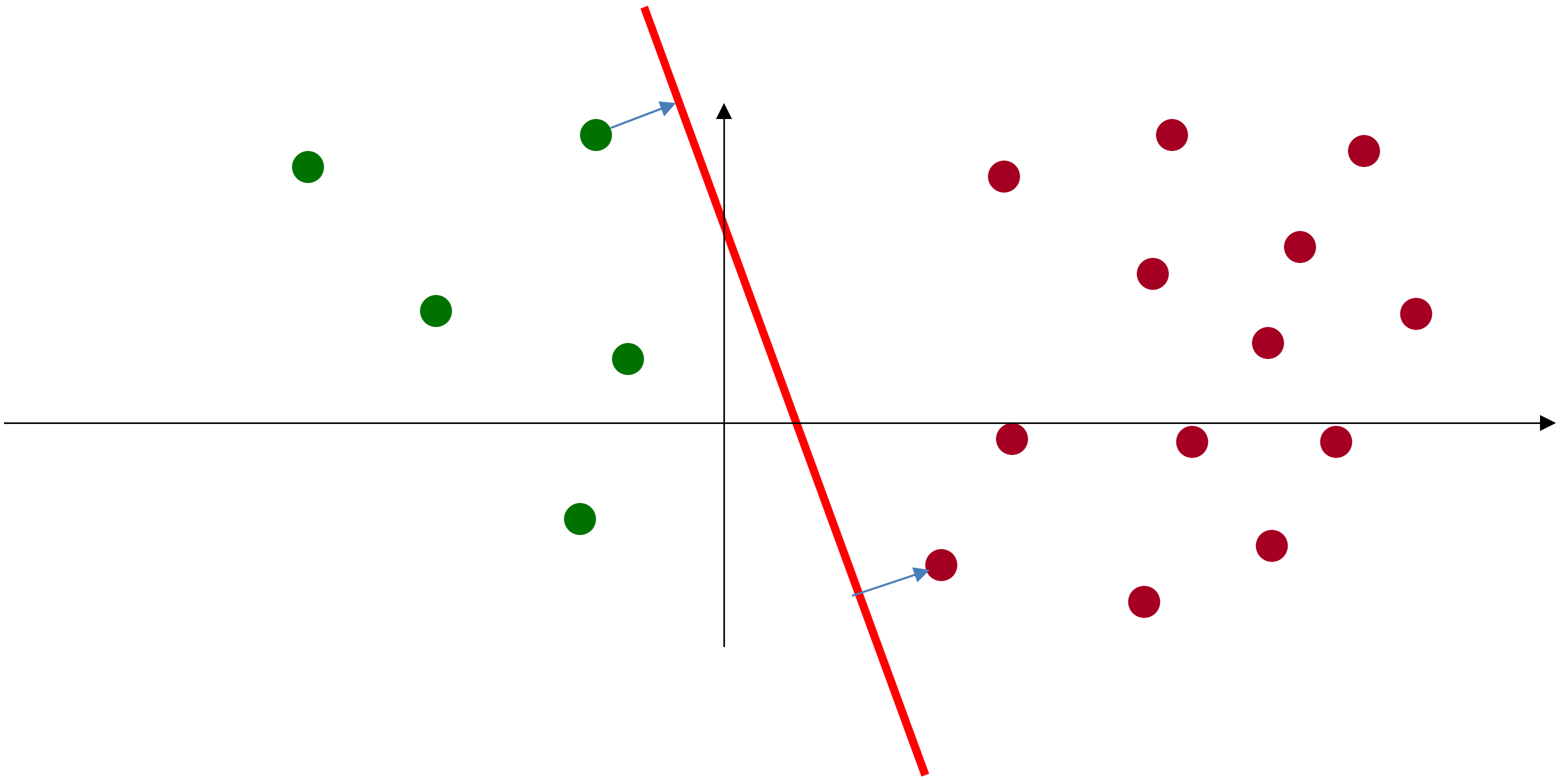
- Guaranteed to converge
  - After no more than $\frac{R^2}{\gamma^2}$ misclassifications
  - $R$ is length of longest training point
  - $\gamma$ is the *best case* closest distance of a training point from the classifier
    - I.e the *largest* distance to the *closest* training instance to *any* appropriate classifier
- No guarantee that we will actually find this best-case classifier
  - Algorithm stops updating after perfect training classification
- **Can we actually *make* it find this best case classifier**

# A Better Approach



- Search through all classifiers such that the distance to the closest points is maximized
  - Very conservative
  - Focuses on *worst-case* scenario
  - Maximizes the chance that the classifier will work well on new unseen data

# A Better Approach



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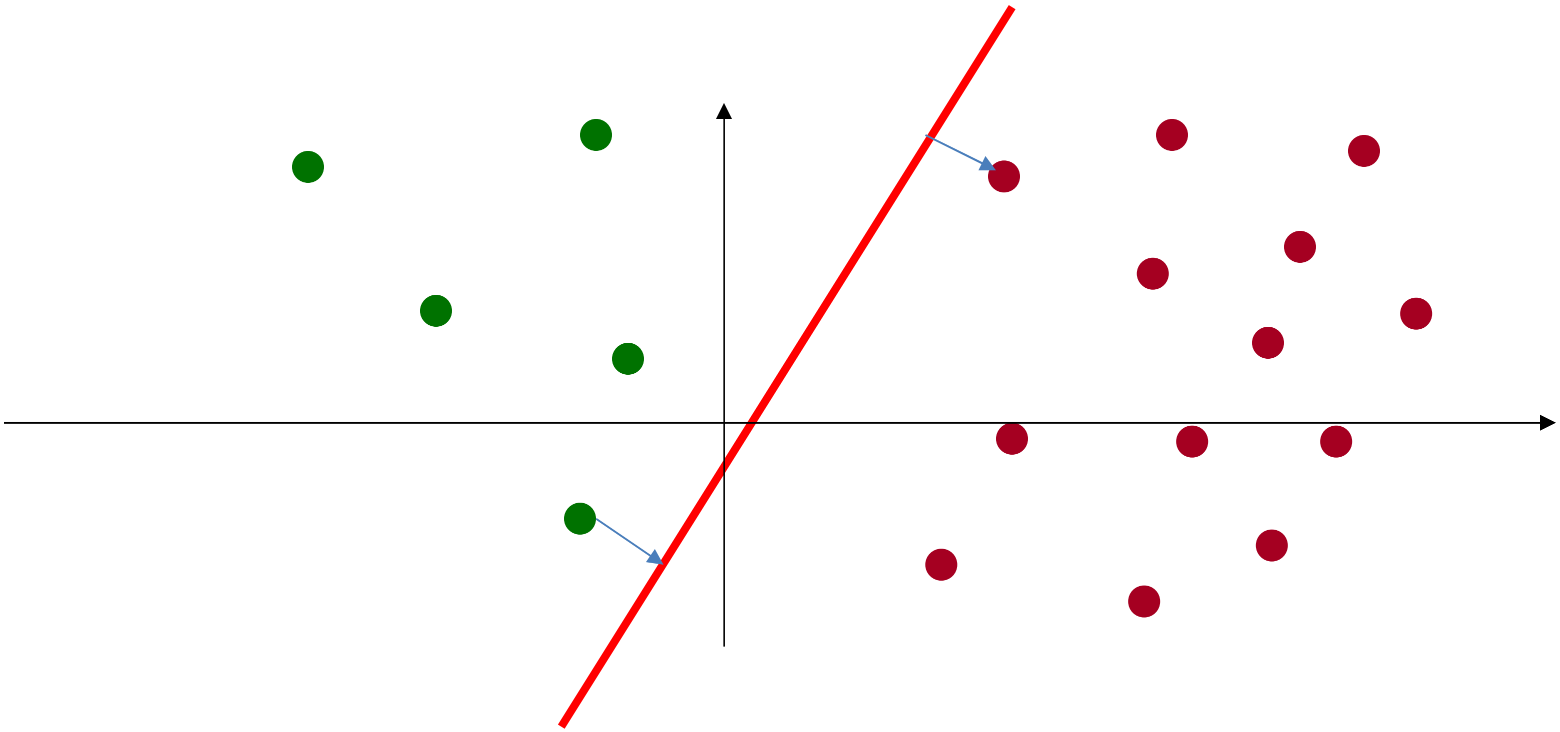
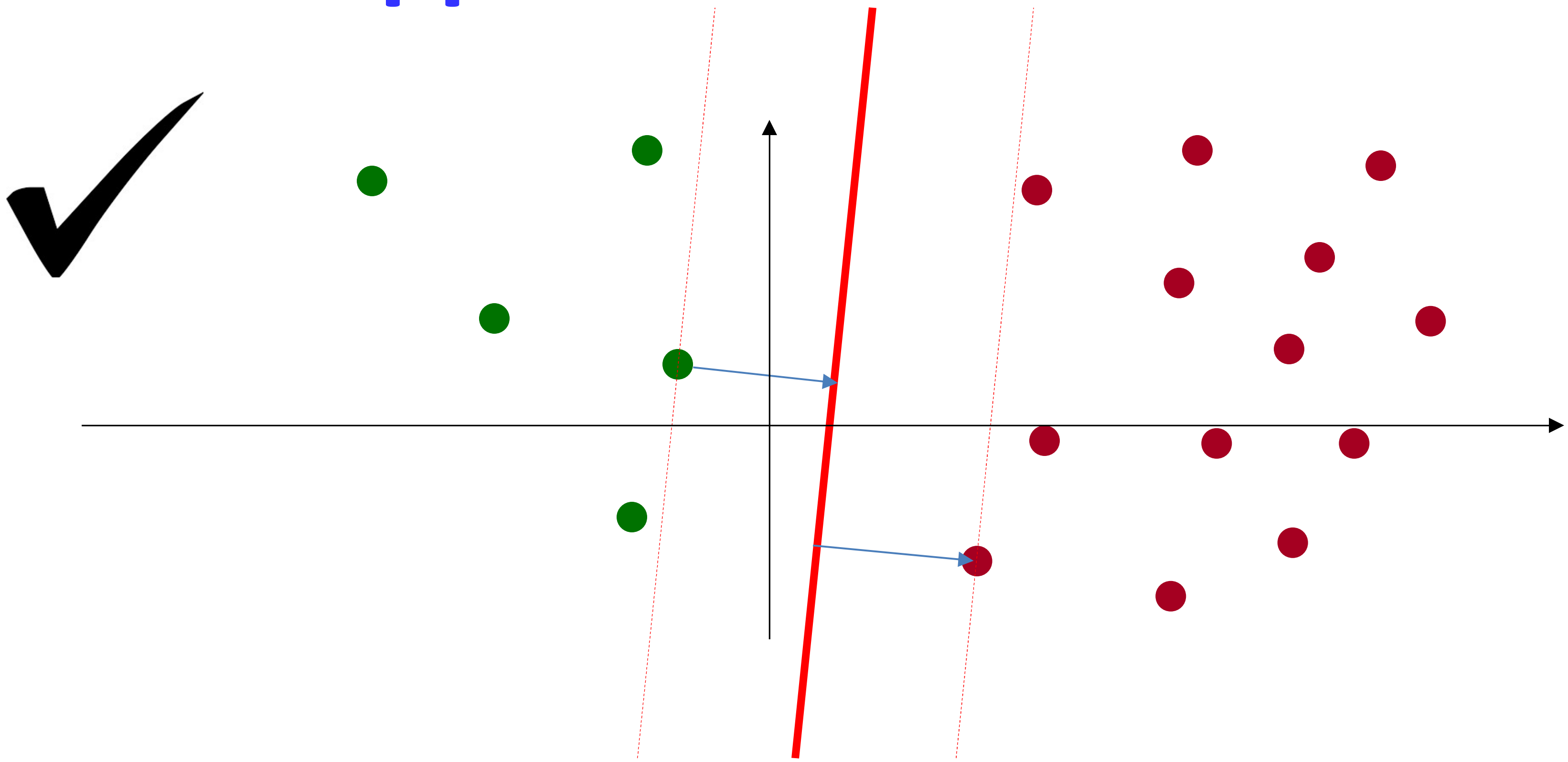
  - Very conservative
  - Focuses on *worst-case* scenario
  - Maximizes the chance that the classifier will work well on new unseen data

# A Better Approach



- Search through all classifiers such that the distance to the closest points is maximized
  - Very conservative
  - Focuses on *worst-case* scenario
  - Maximizes the chance that the classifier will work well on new unseen data

# Support Vector Machine



- Search through all classifiers such that the distance to the closest points is maximized
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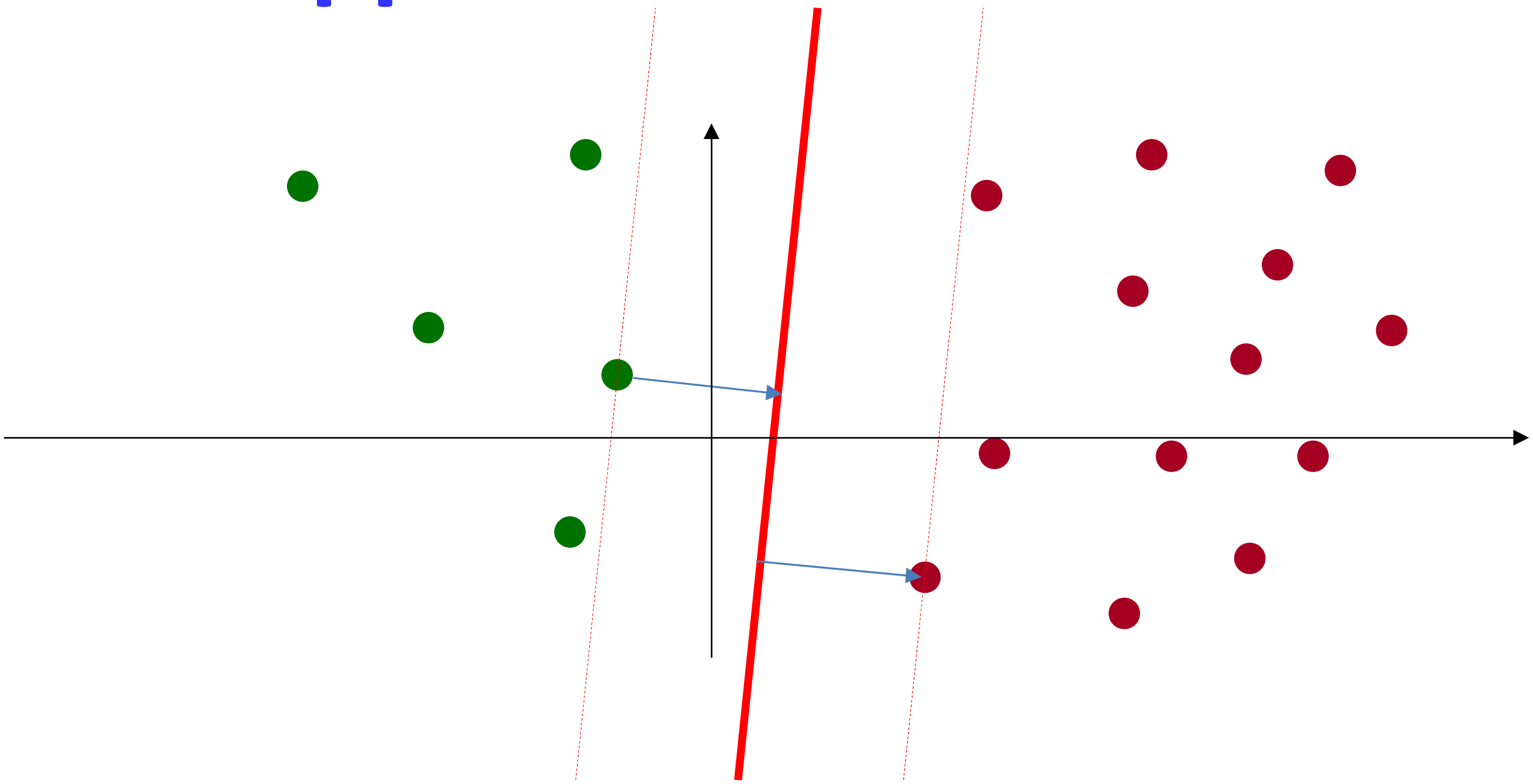
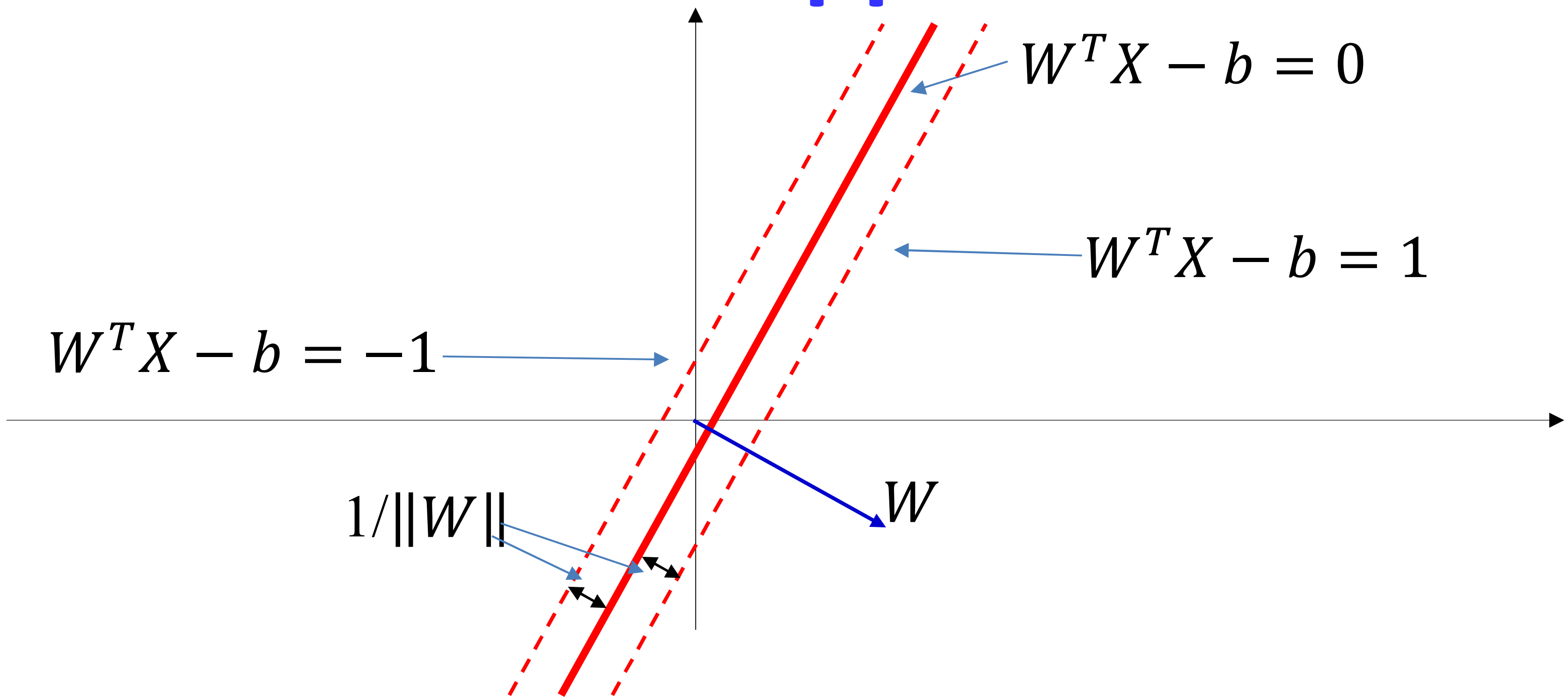
# Support Vector Machine



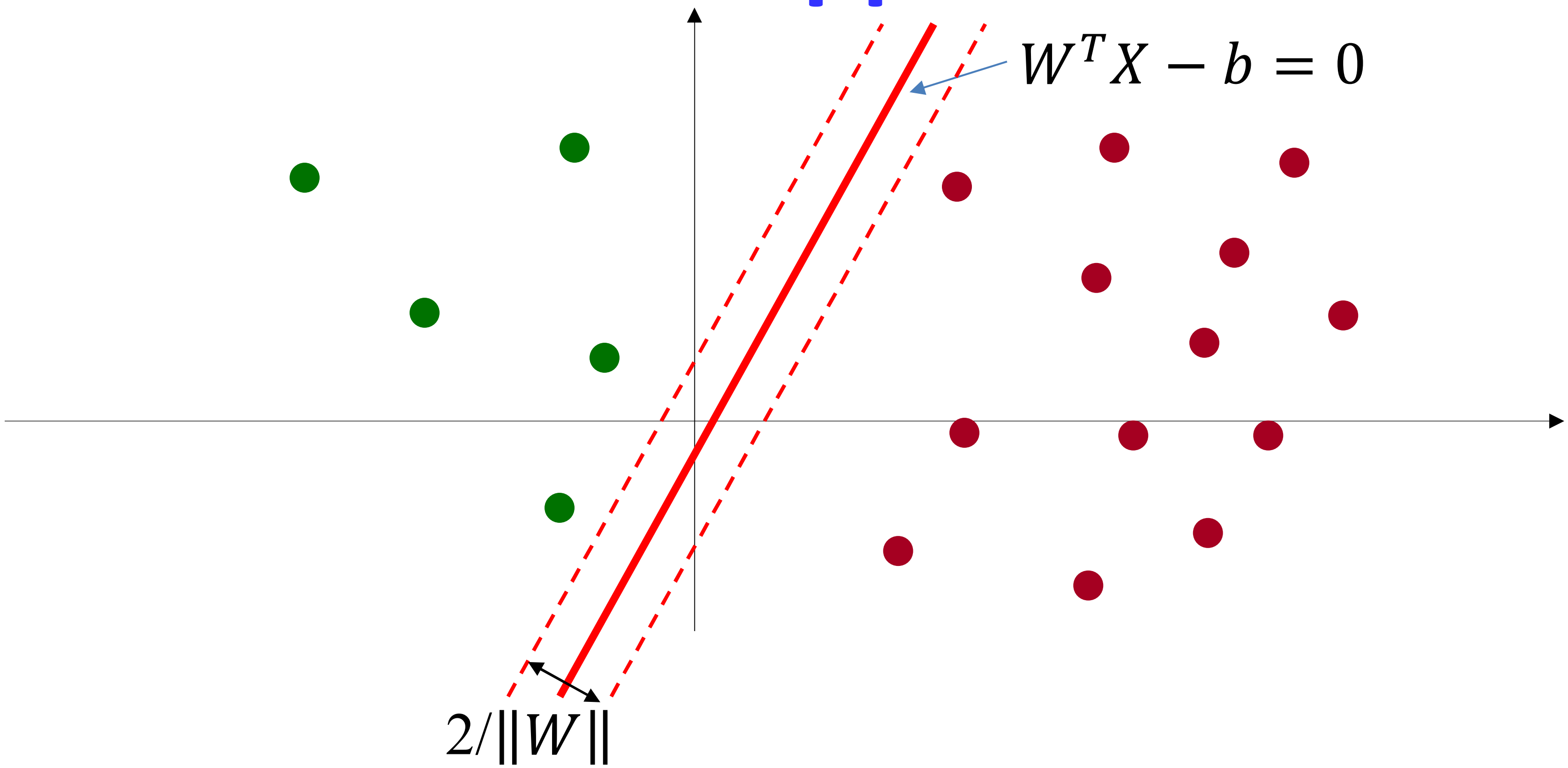
- Find the classifier such that the distance to the *closest* points is maximized
- I.e. solve *two* problems: find the closest points, and the classifier, such that the distance is maximum
  - Position the classifier in the *middle* so that the distance to the closest green = distance to the closest red
- Is this a combinatorial optimization problem??

# Solution Approach



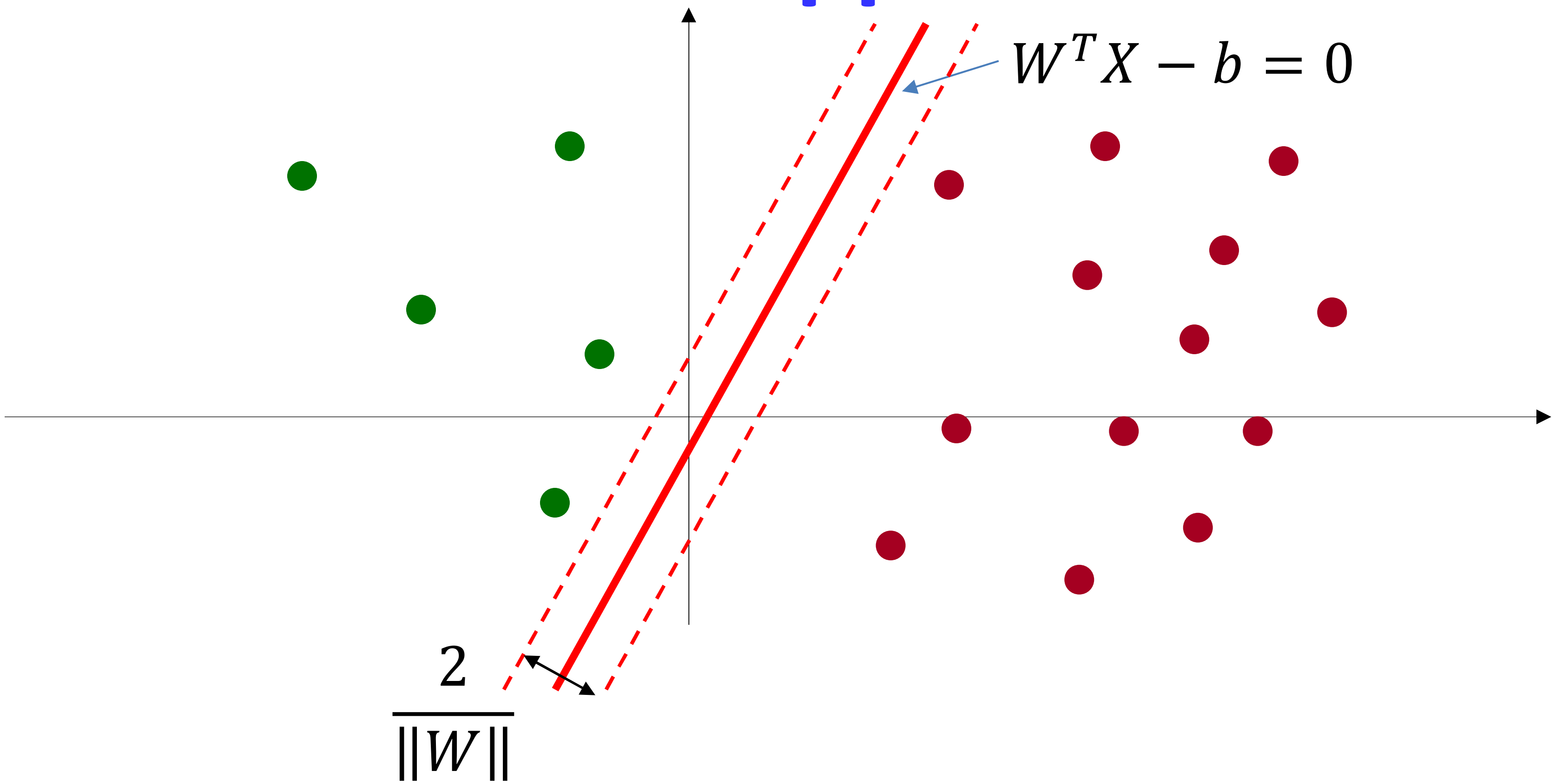

- For any hyperplane (linear classifier) $W^TX - b = 0$
- Choose two hyperplanes $W^TX - b = 1$ and $W^TX - b = -1$
  - The distance of these hyperplanes from the classifier is $1/||W||$
  - The total distance between the hyperplanes is $2/||W||$

# Solution Approach



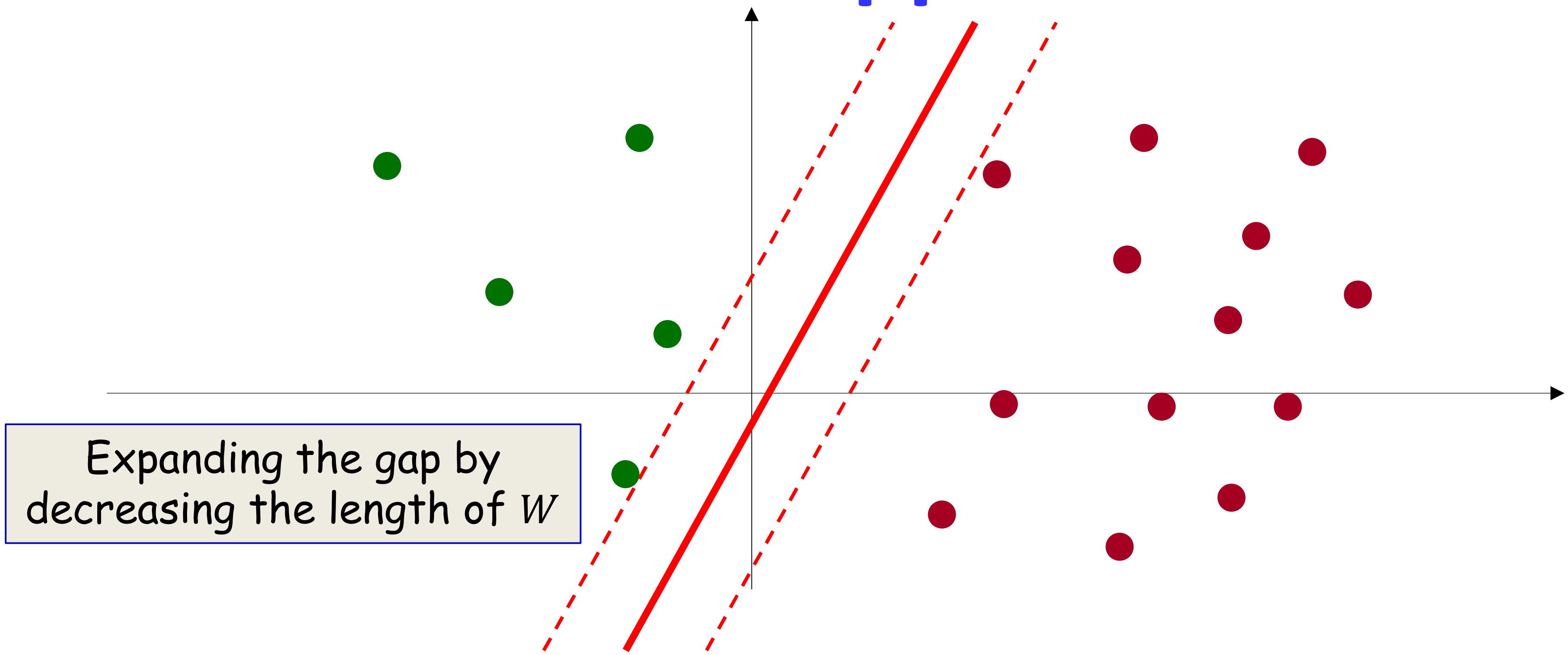

- Constraint: Perfect classification with a margin
- Choose the hyperplanes such that
  - All positive points are on the positive side of the positive hyperplane
  - All negative points are on the negative side of the negative hyperplane

# Solution Approach




- The distance between the hyperplanes is $\frac{2}{\|W\|}$
- Find the $W$ (and $b$) such that this is maximized, while maintaining the constraint that all training points are on the "outside" of the appropriate hyperplane

# Solution Approach

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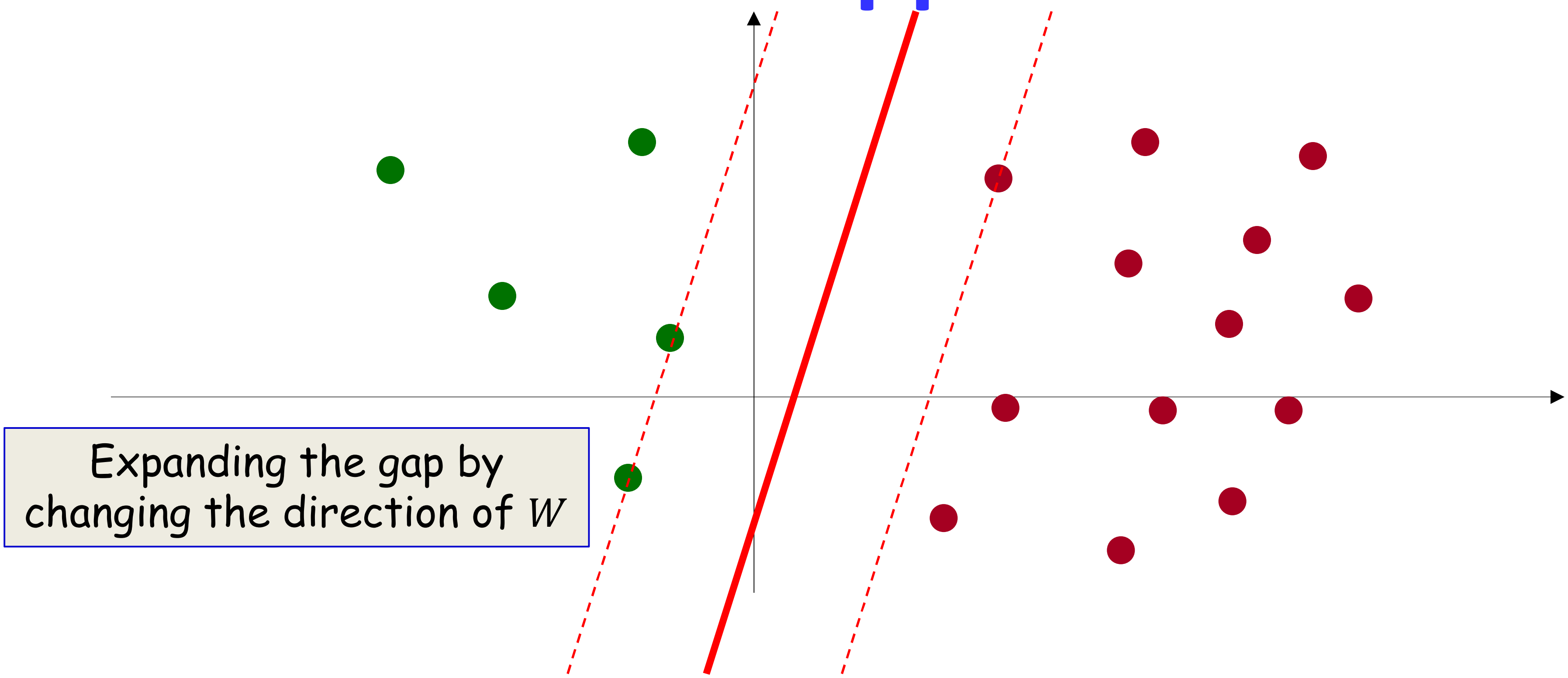
# Solution Approach




- The distance between the hyperplanes is $\frac{2}{\|W\|}$
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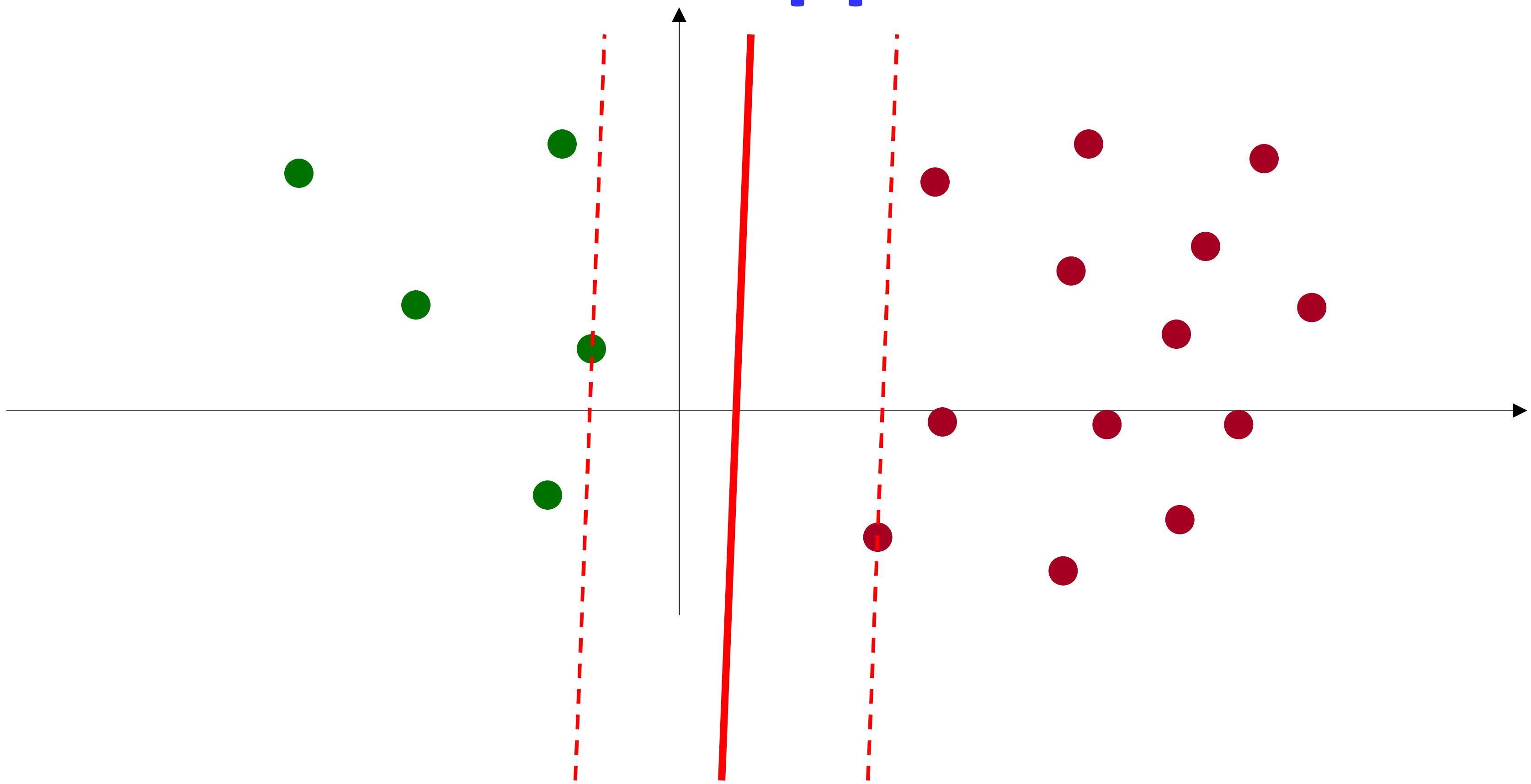
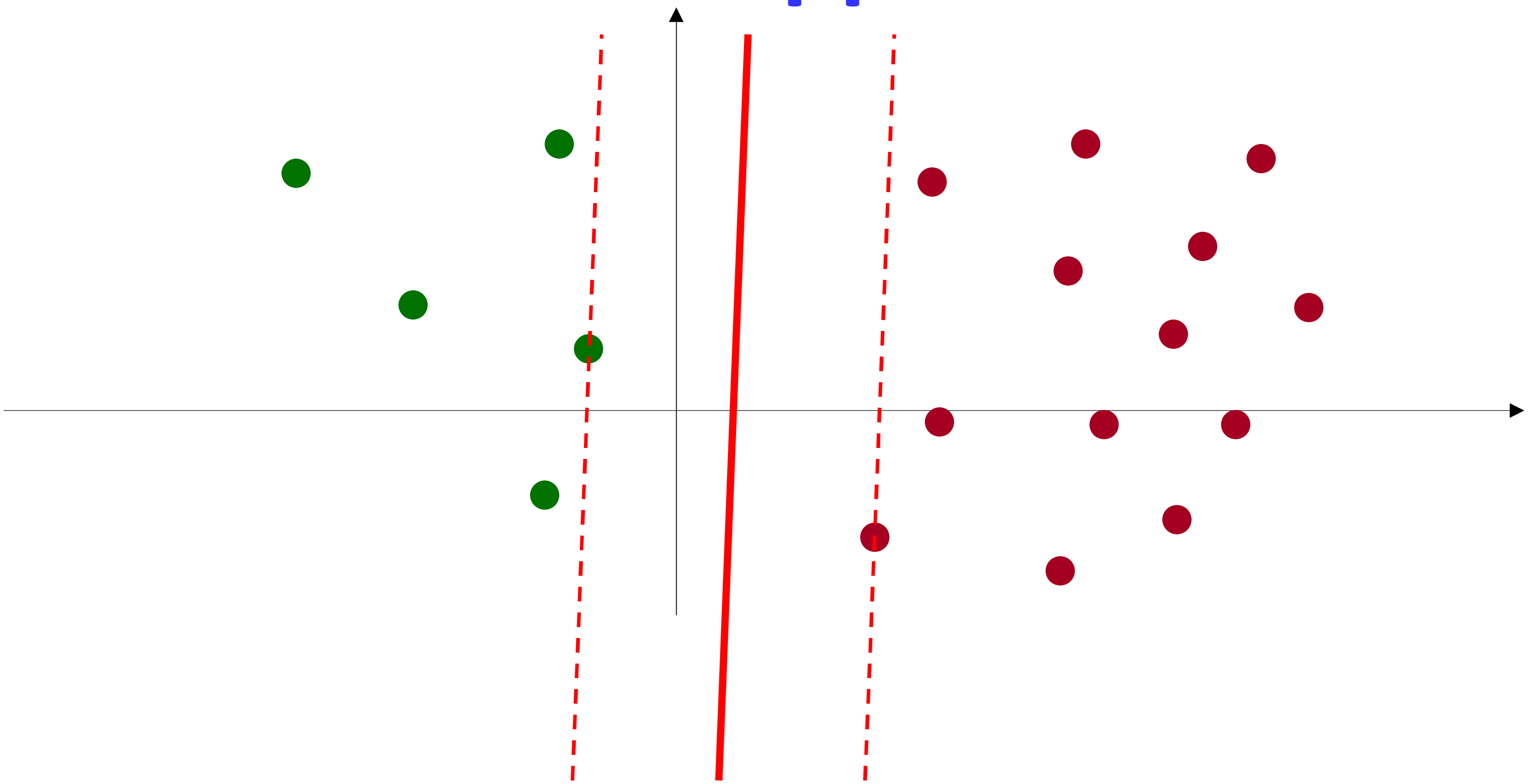
# Solution Approach



- The distance between the hyperplanes is $\frac{2}{\|W\|}$
- Find the $W$ (and $b$) such that this is maximized, while maintaining the constraint that all training points are on the "outside" of the appropriate hyperplane

# Solution Approach



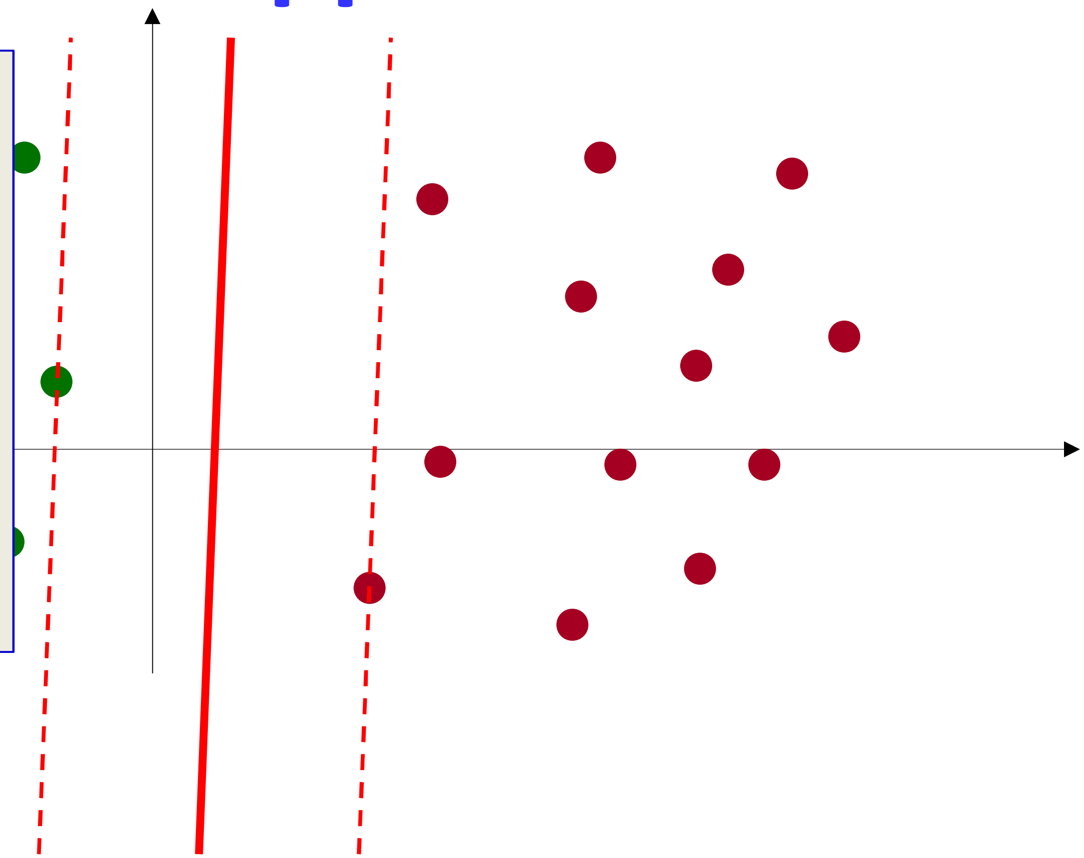
- The distance between the hyperplanes is $\frac{2}{||W||}$
- Maximize this distance. I.e. ..
- **Minimize $||W||$ such that**
  - all training points are on the "outside" of the appropriate hyperplane

# Solution Approach

Decreasing the length of $W$ will expand the gap between the boundary planes

Rotating it will *also* increase this length

Must find a formalism that explores both options simultaneously



- The distance between the hyperplanes is $\frac{2}{\|W\|}$
- Maximize this distance. I.e. ..
- **Minimize $\|W\|^2$ such that**
  - all training points are on the “outside” of the appropriate hyperplane

# Lets formalize this

- Constraint: Ensuring that all training instances are on the proper side of their respective hyperplanes
- For positive training instances $X_i$:

$$W^T X_i - b \geq 1$$

- For negative instances

$$W^T X_i - b \leq -1$$

- Generically stated, for all instances we want

$$Y_i(W^T X_i - b) \geq 1$$

# Solution Formalism

- Minimize $||W||$ such that
- For all training instances

$$Y_i(W^T X_i - b) \geq 1$$

- Formally

$$\hat{W} = \underset{W,b}{\operatorname{argmin}} \, ||W||^2$$
$$s.t. \; \forall \, i \quad Y_i(W^T X_i - b) \geq 1$$

# Solving the optimization

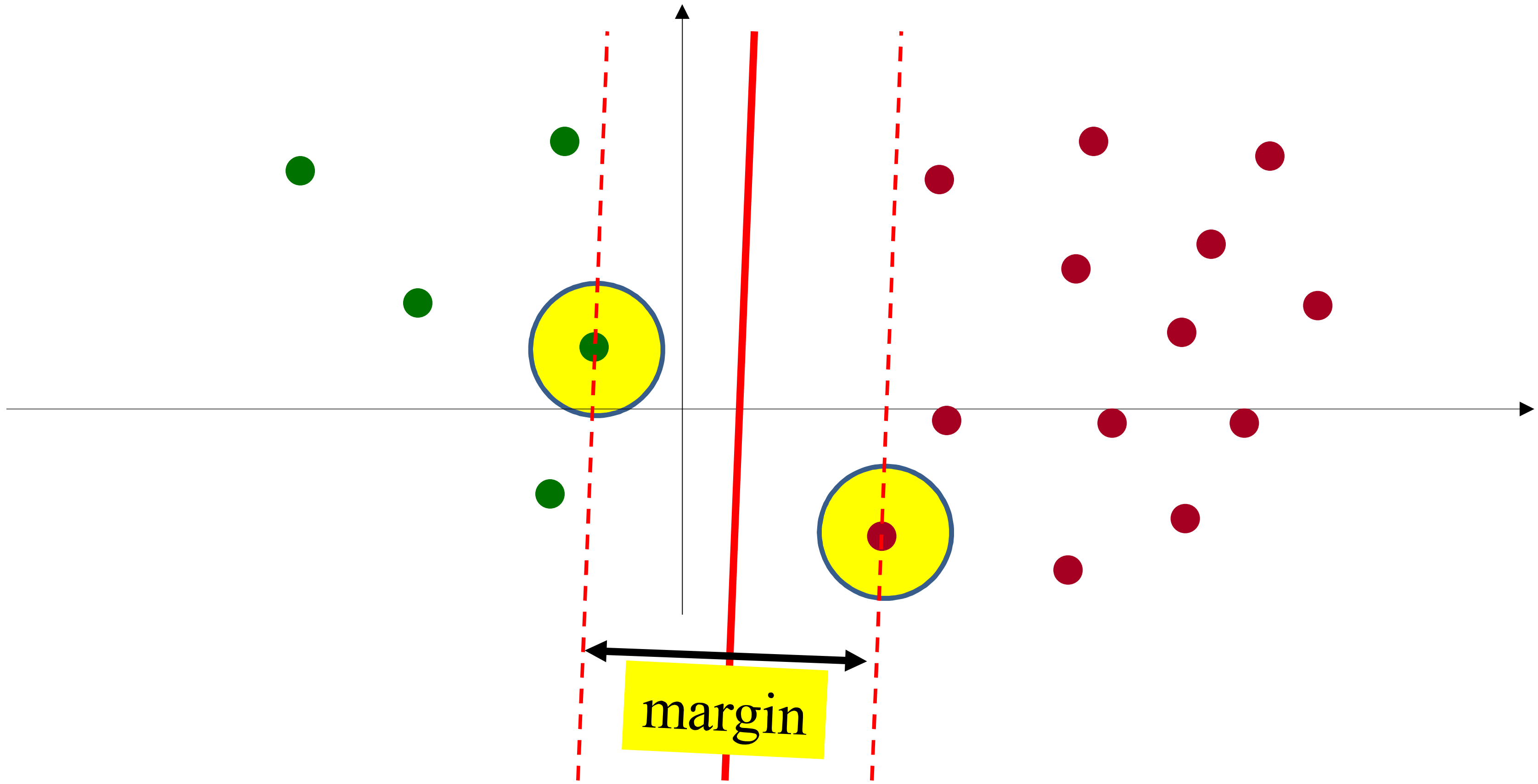
- This is a quadratic programming problem!

$$\widehat{W} = \underset{W,b}{\operatorname{argmin}} \|W\|^2$$

$$s.t.\ \forall\, i \quad Y_i(W^T X_i - b) \geq 1$$

- A variety of techniques can be applied
  - Interior point methods, active set methods, gradient descent, conjugate gradient
  - The objective function is convex, QP *will* find the (near) optimal solution
- Most useful solution is based on *Lagrangian duals*
  - Later..

# The solution

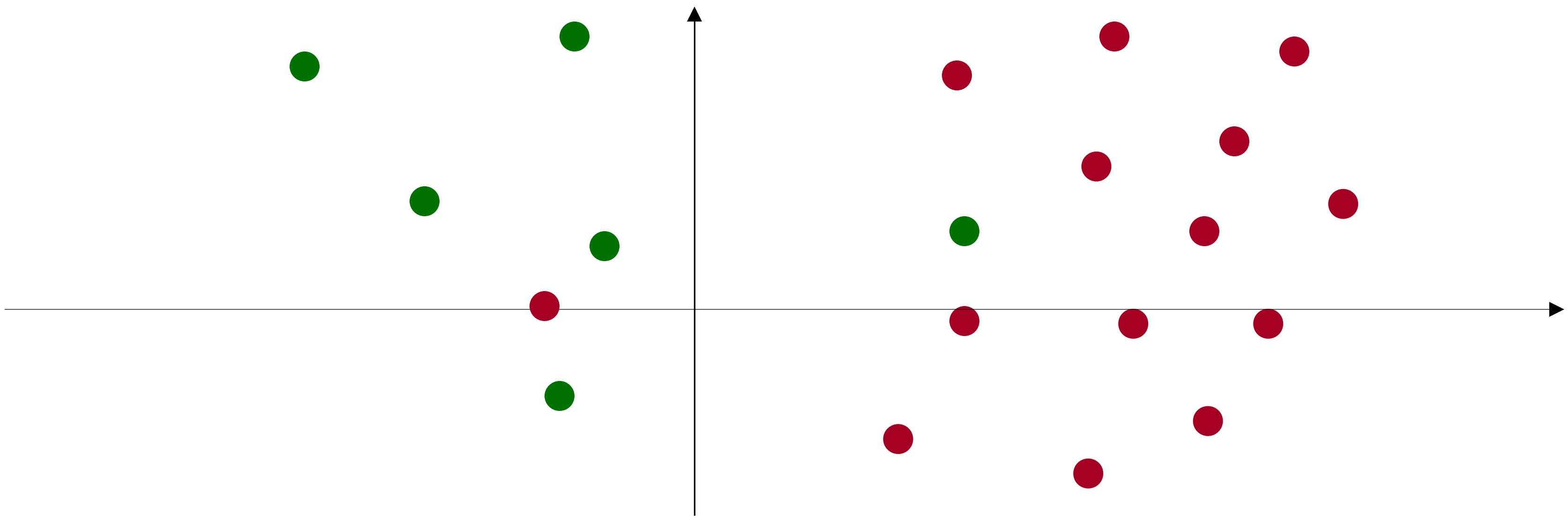



- Maximizes the *margin*
- This is a *max-margin* classifier
- The boundary samples are called support vectors
  - All the information about the classifier is in these support vectors

# Challenges

- What if the classes are not linearly *separable*
- What if the classes are not *linearly* separable?
- What if the classes are not *linearly separable*?

# What if they are not separable?



- What if the data are not separable?

# Original Problem

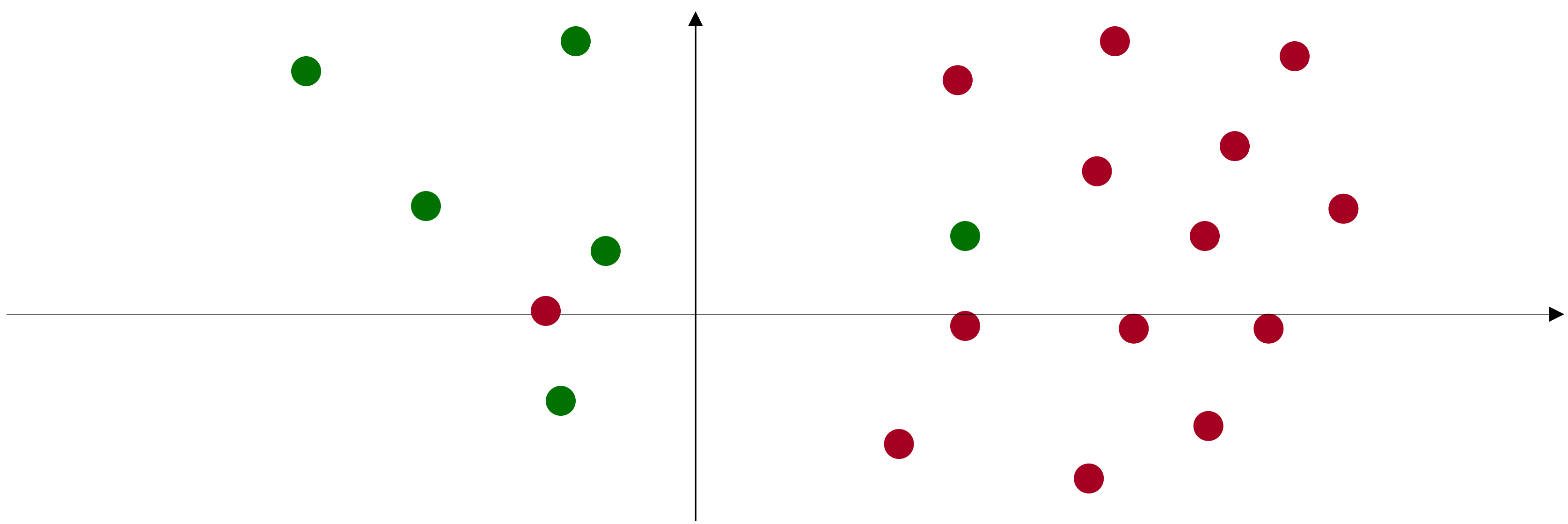
- This is a quadratic programming problem!

$$\hat{W} = \underset{W}{\operatorname{argmin}} \|W\|^2$$

$$s.t. \ \forall i \quad Y_i(W^T X_i - b) \geq 1$$

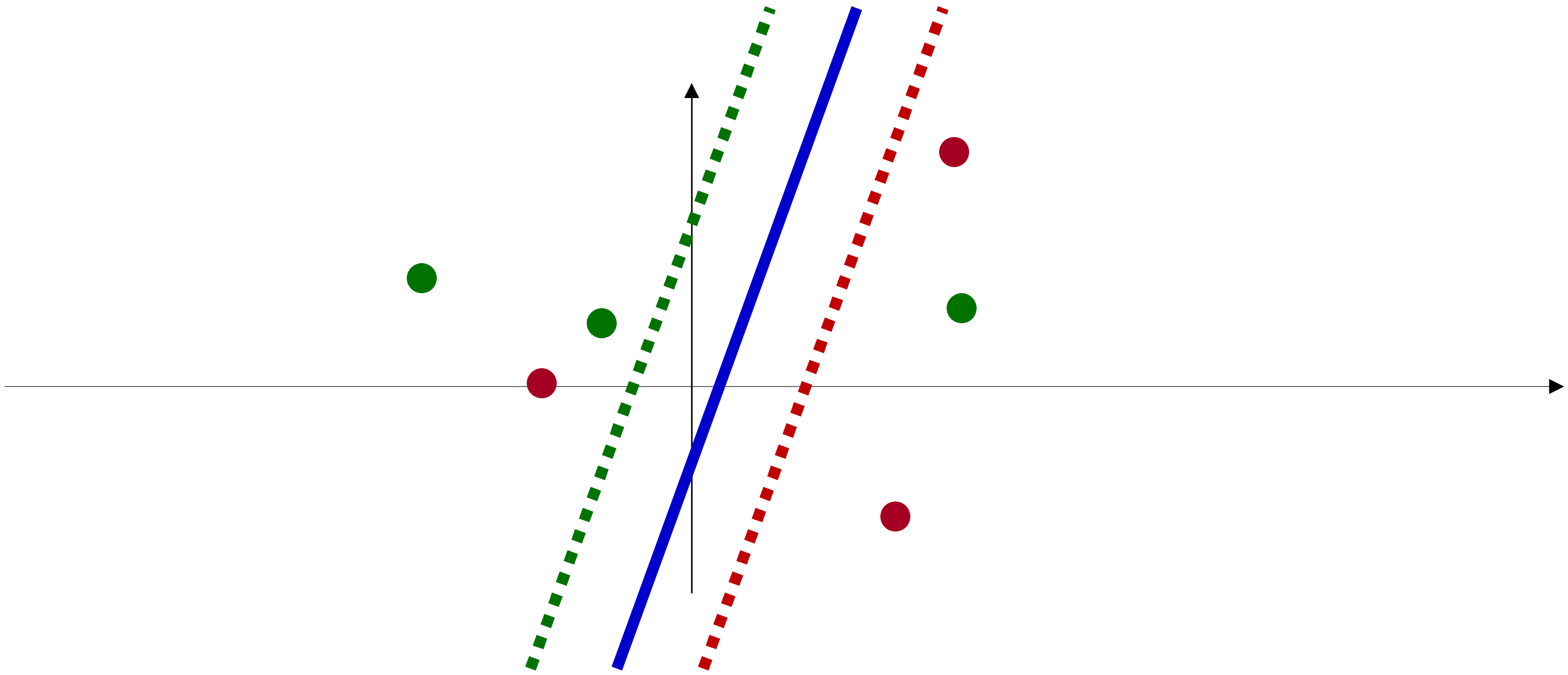
- Maximize the distance between the planes
- Subject to the constraint that all training data instances are on the "correct" side of the plane
- When data are not linearly separable, this constraint can never be satisfied

# Introducing the *slack* variable



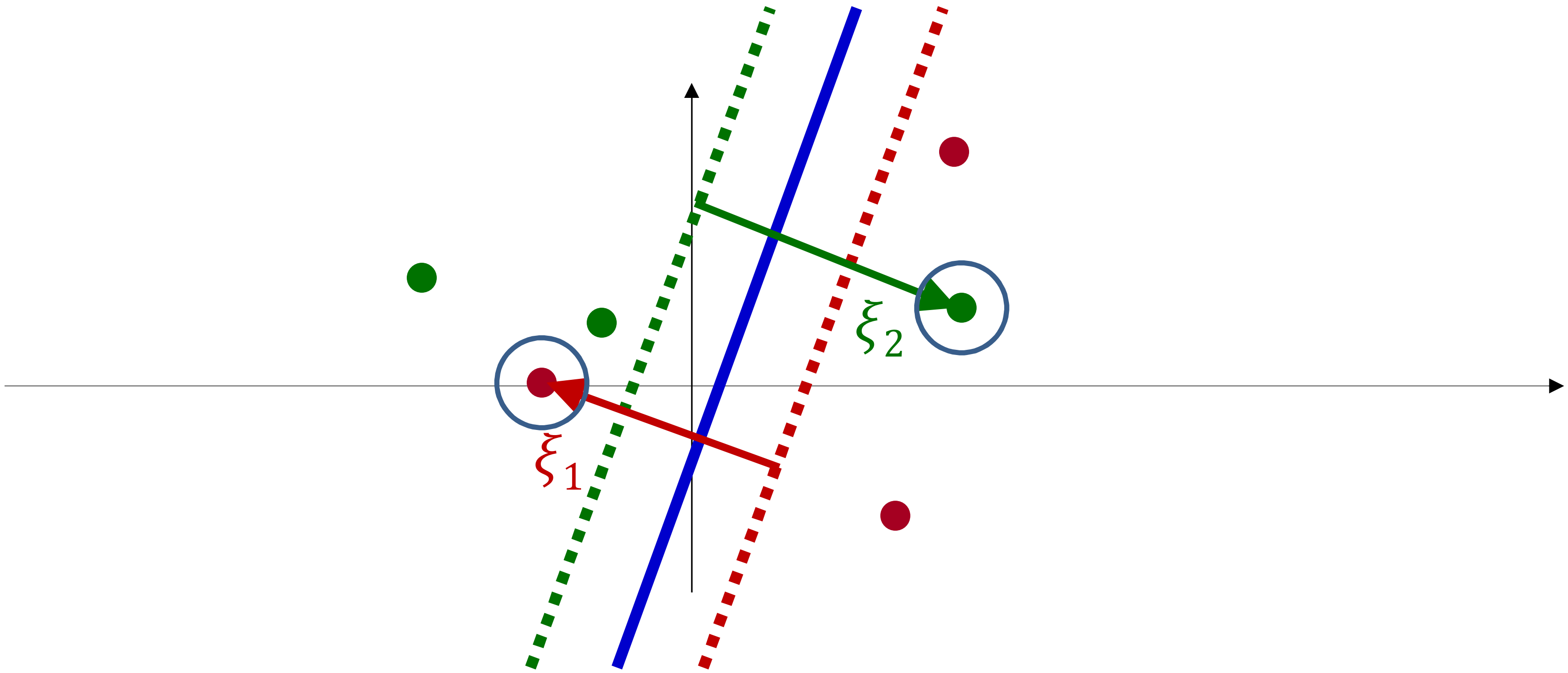
- What if the data are not separable?

# Introducing the *slack* variable



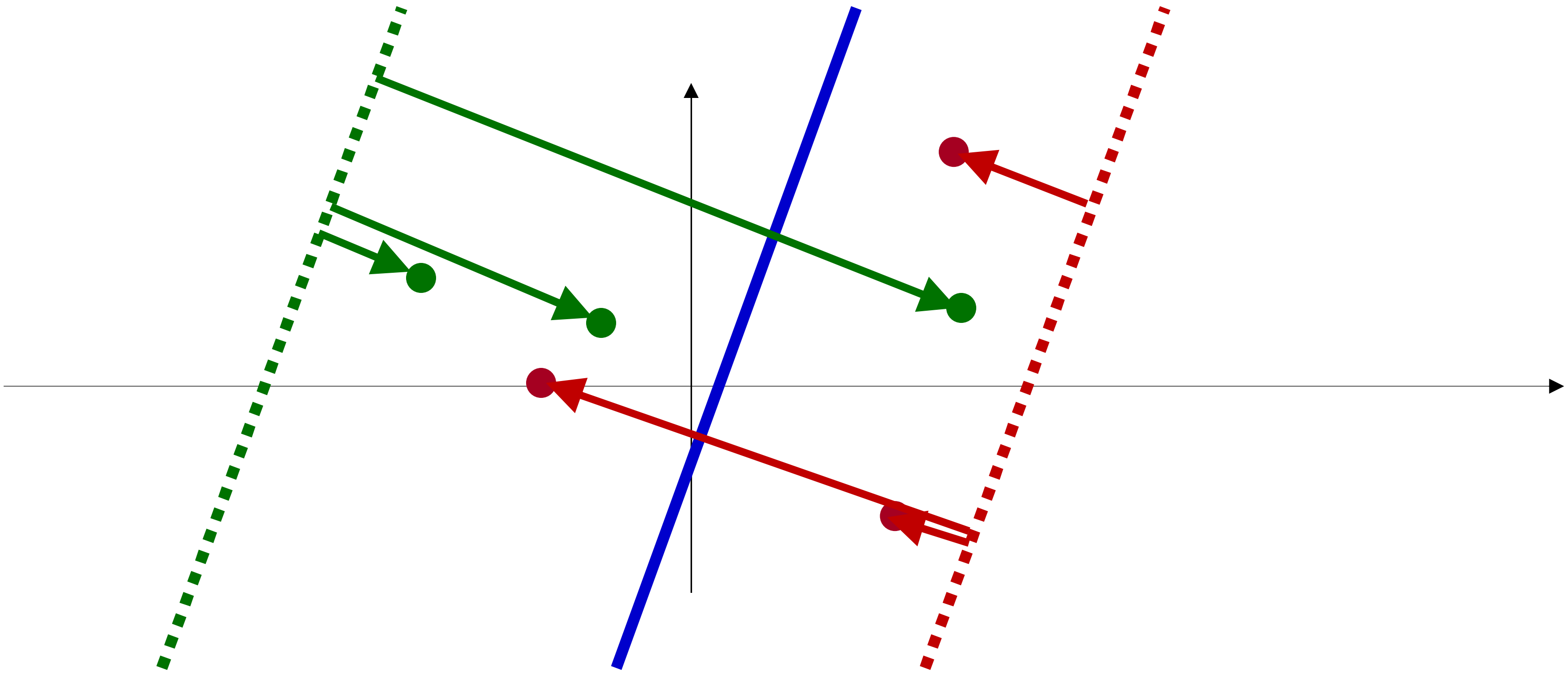
- For every training instance, introduce a *slack* variable $\xi$
- The slack variable is the maximum distance you have to *shift* the boundary plane to move the point to the "correct" side

# Introducing the *slack* variable



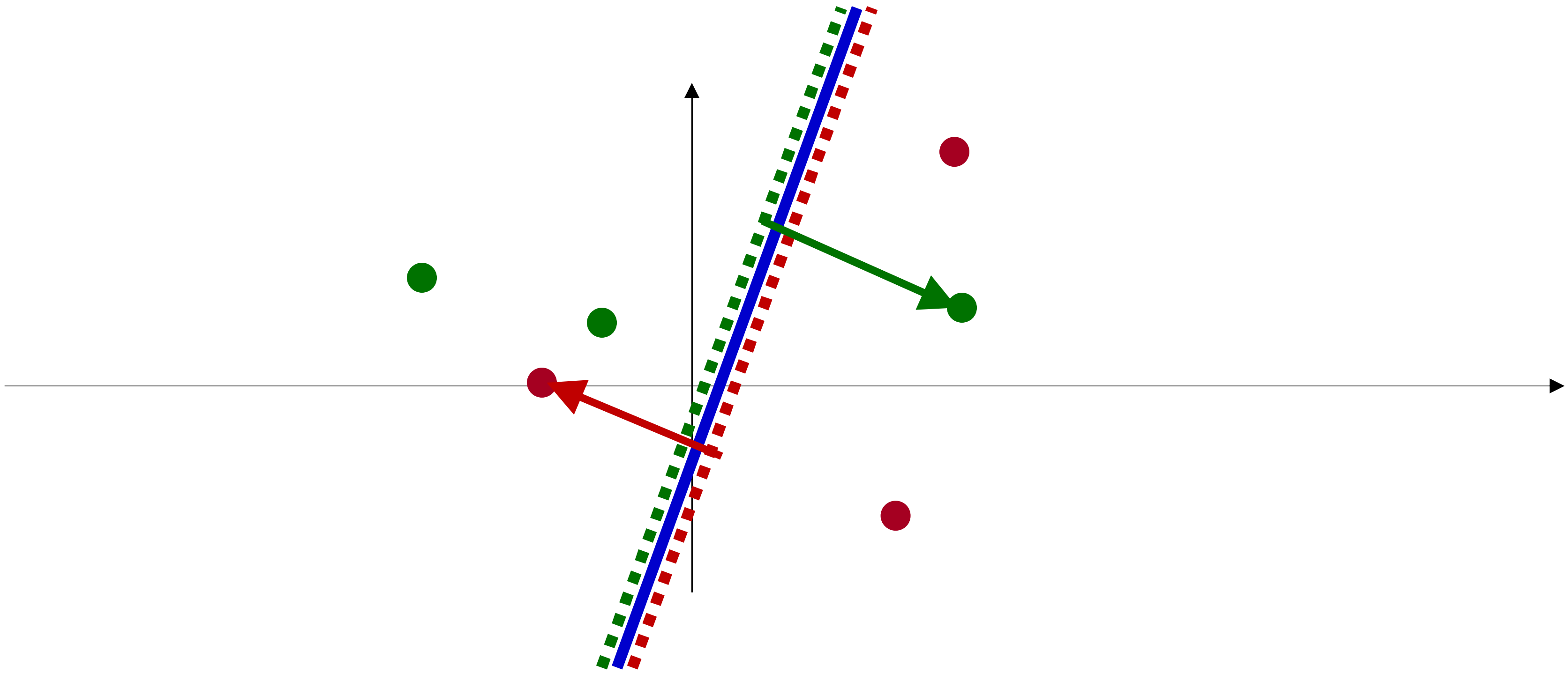

- For every training instance, introduce a *slack* variable $\xi$
- The slack variable is the *reverse* distance from the *margin* plane of the training instance
  - This will be non-zero only for some instances
  - **Ideally this should be minimum**

# Introducing the *slack* variable



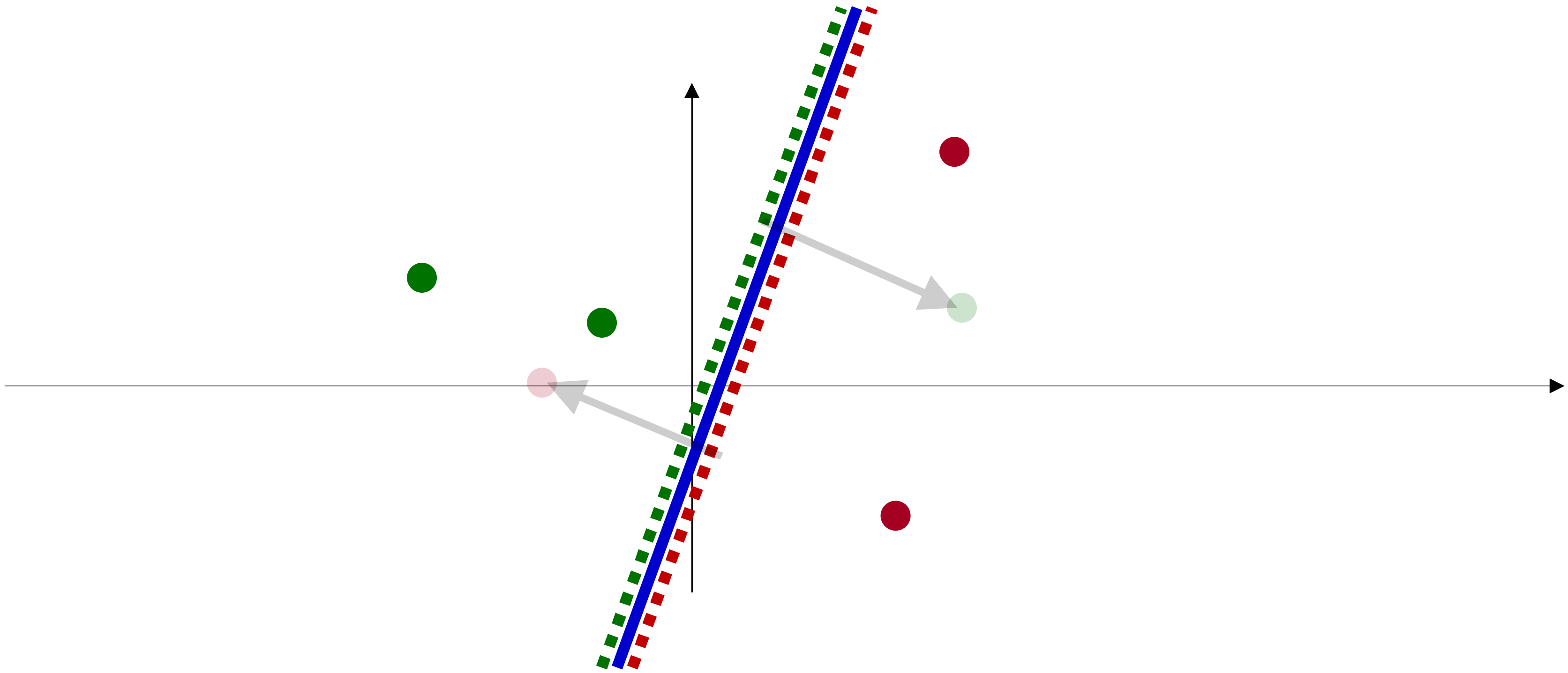
- The total length of slack variables varies with the boundary
- If you push the boundaries too far you will have a greater length of slack variable
  - Which contradicts our desire that they should be minimum

# Introducing the *slack* variable



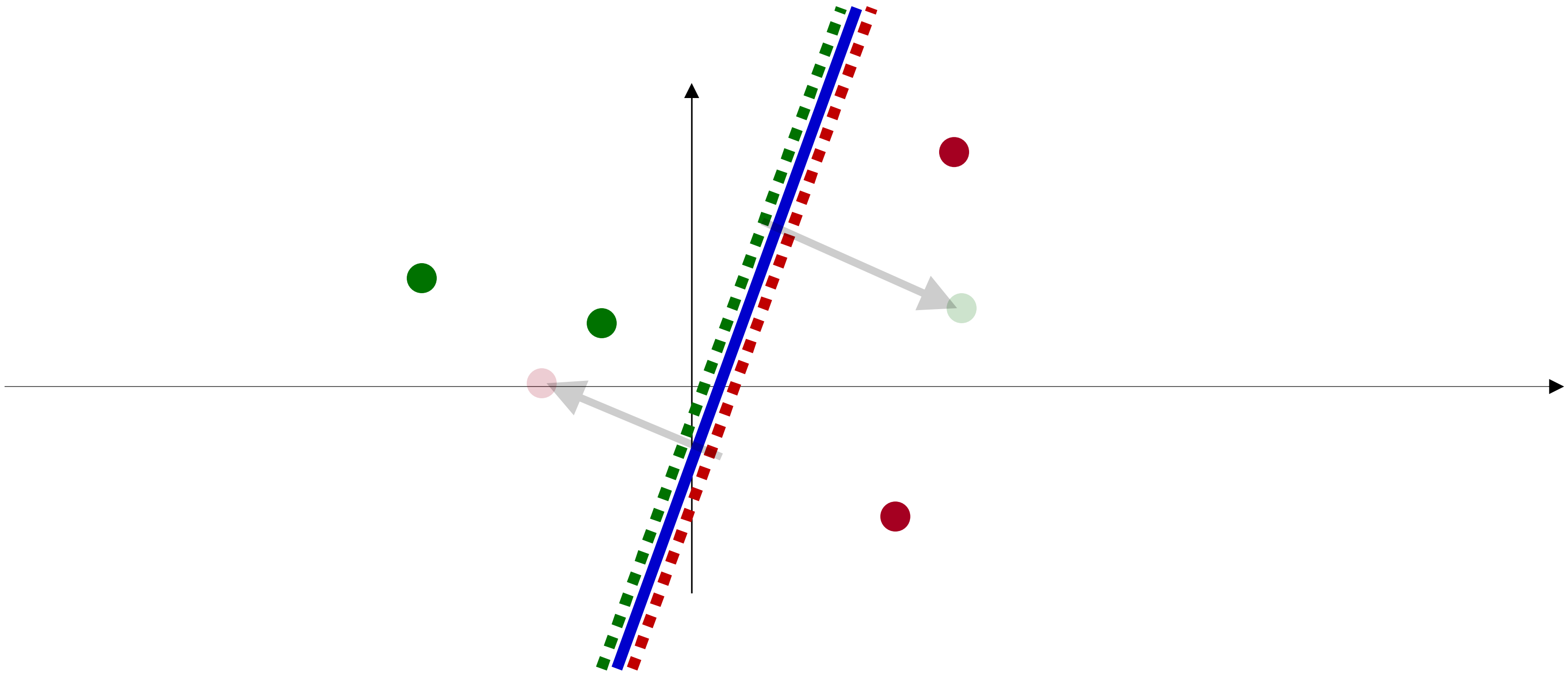
- If they are very close, only the *inseparable points* will have non-zero slack variable
  - The minimum slack value is when the margin planes coincide with the linear classifier

# Introducing the *slack* variable



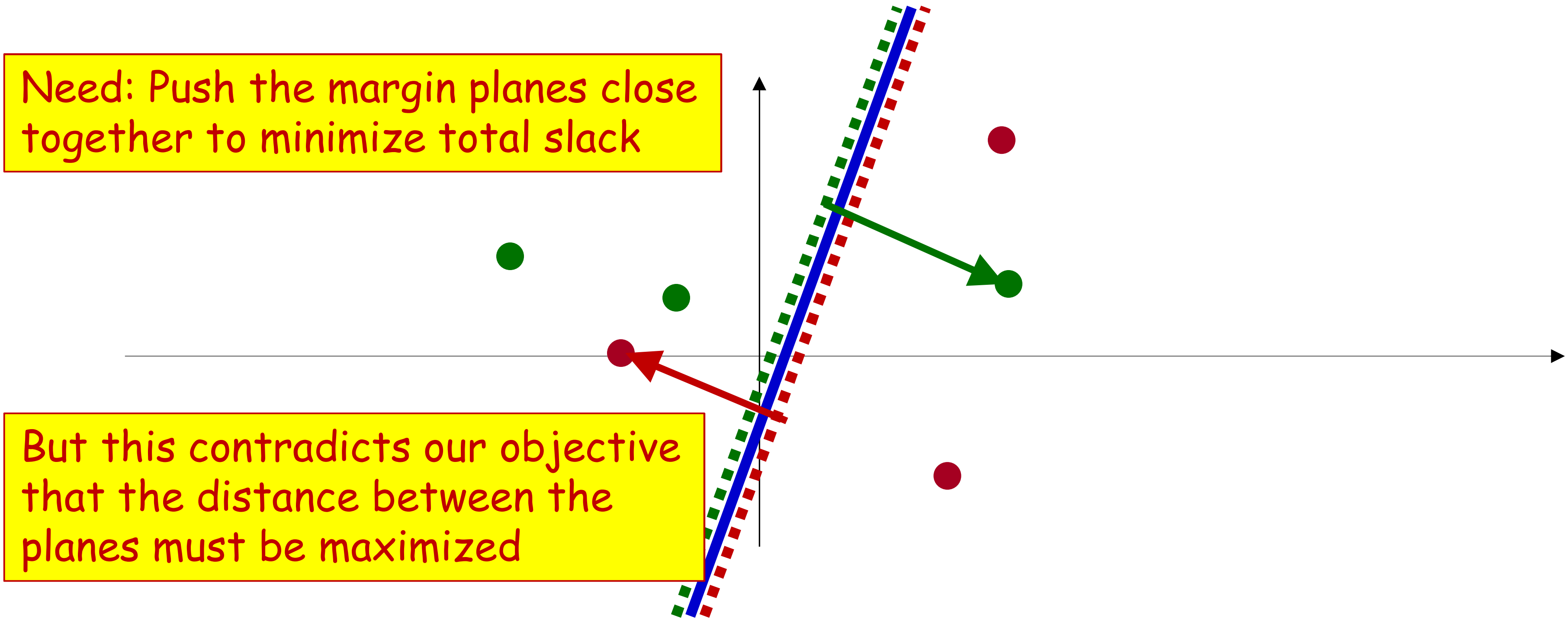
- If they are very close, only the *inseparable points* will have non-zero slack variable
  - The minimum slack value is when the margin planes coincide with the linear classifier
- For linearly separable classes, if the boundary planes are close enough, the total slack length will be 0

# Introducing the *slack* variable



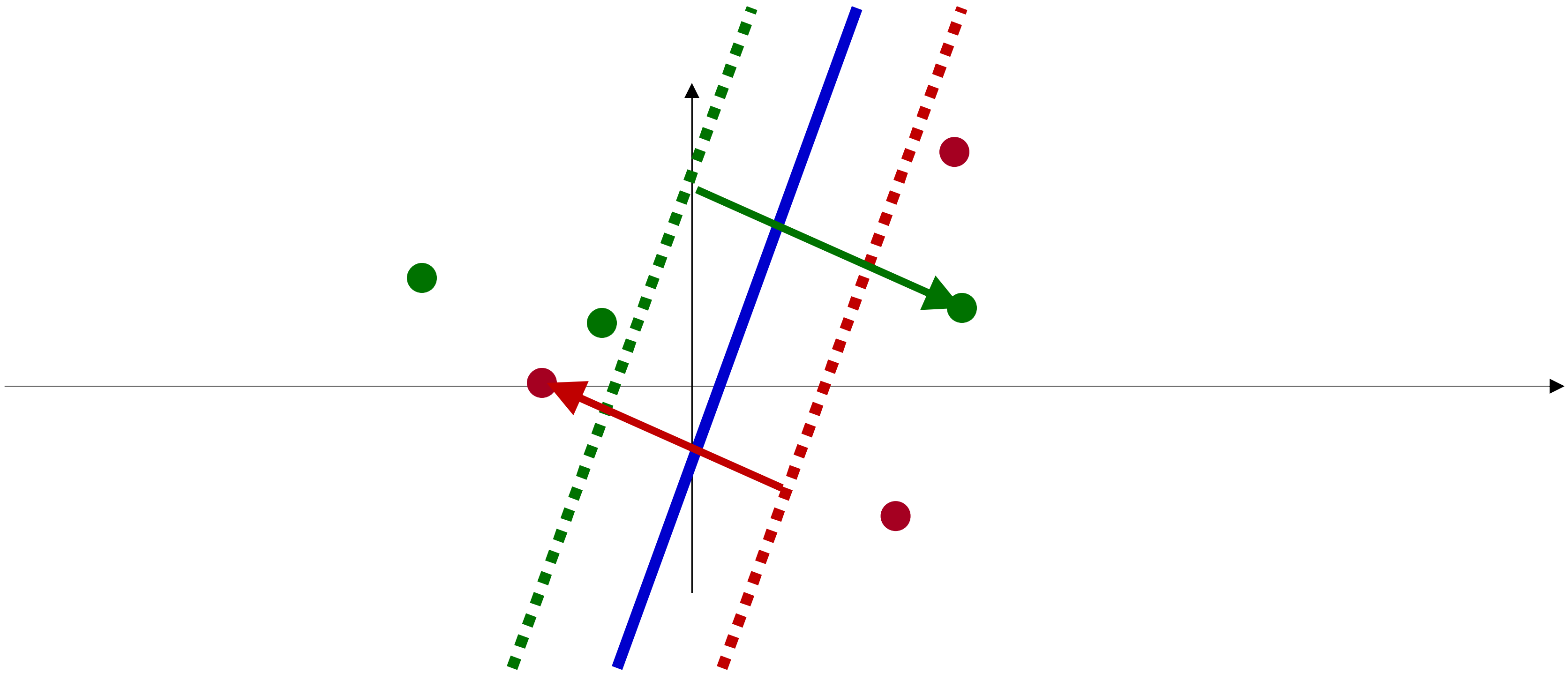
- Problem: If they are too close, the planes violate our desire to *maximize* the margin

# Introducing the *slack* variable



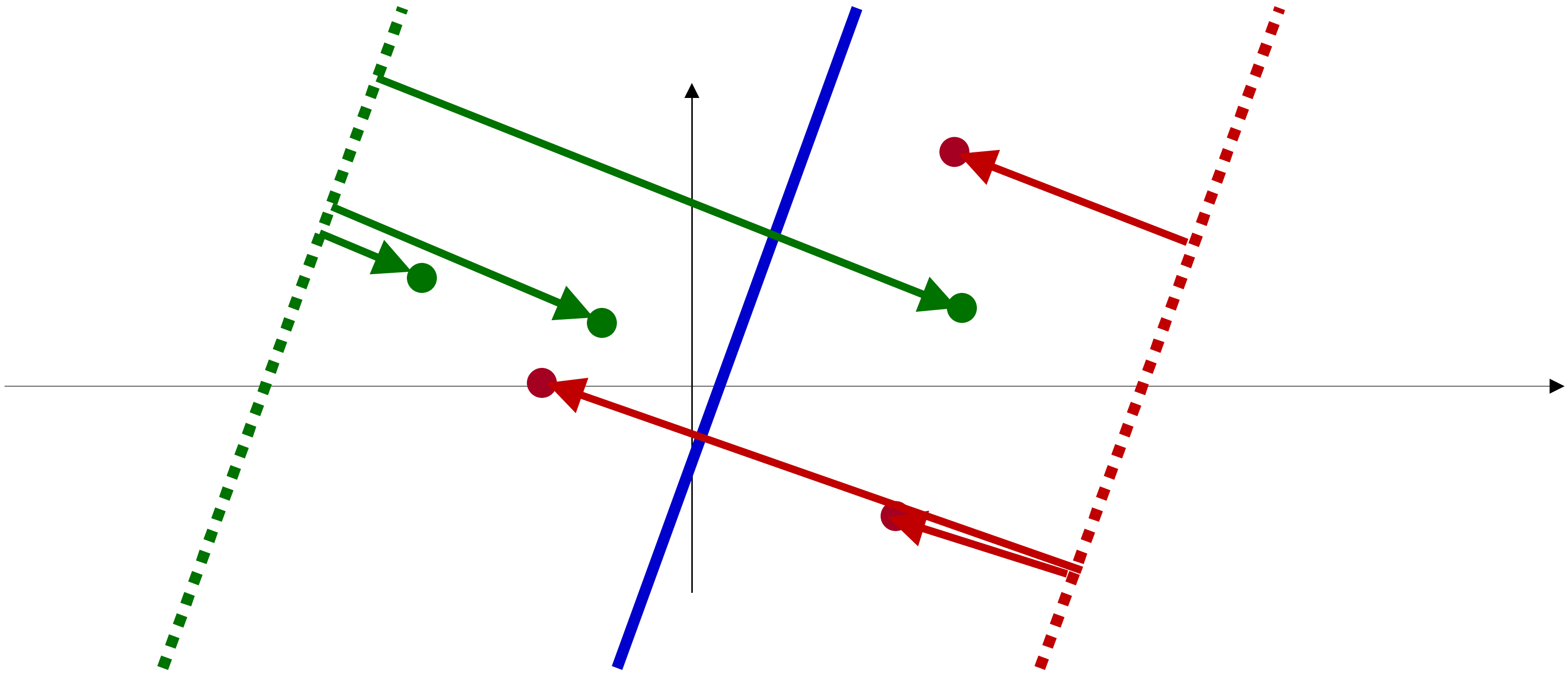

- Contradicting requirements..

# New Objective



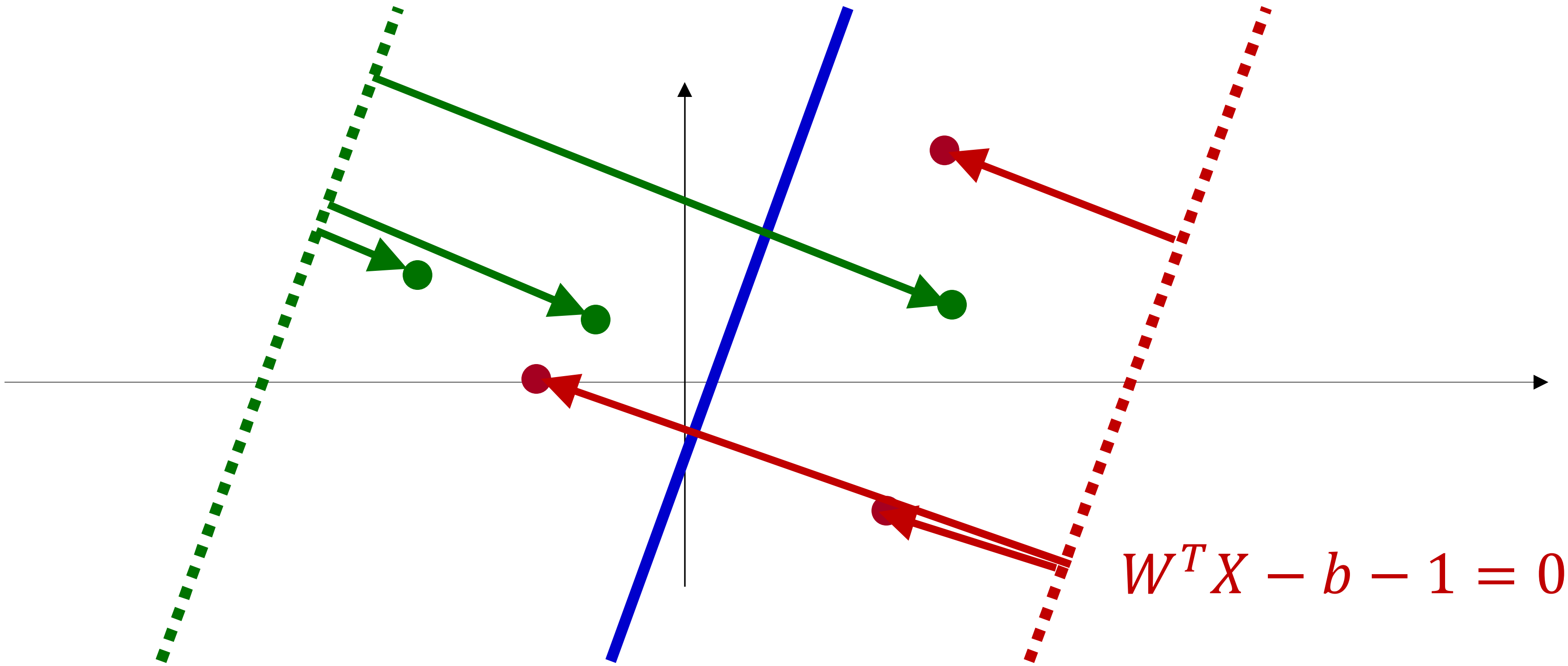
- Simultaneously
  - Maximize distance between planes
  - Minimize total slack length

# Quantifying Slack Length



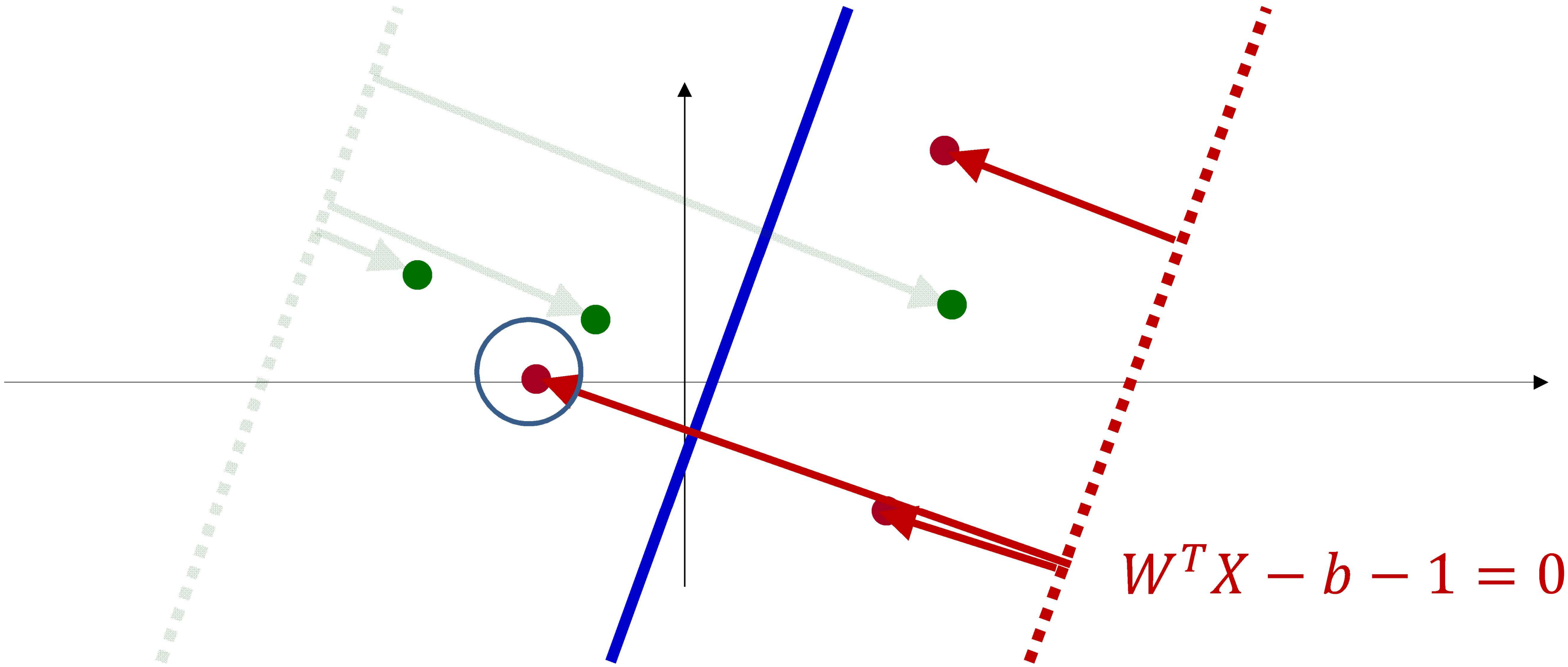
- We need a formula for the total slack length first..

# Quantifying Slack Length




- The *positive* margin plane is given by
- $W^TX - b - 1 = 0$
- This plane is at a distance is $\frac{1}{\|W\|}$ from the decision boundary on the *positive* side of the decision plane (in the direction of $W$)
  - Ideally all positive training points would be to the right of it

# Quantifying Slack Length

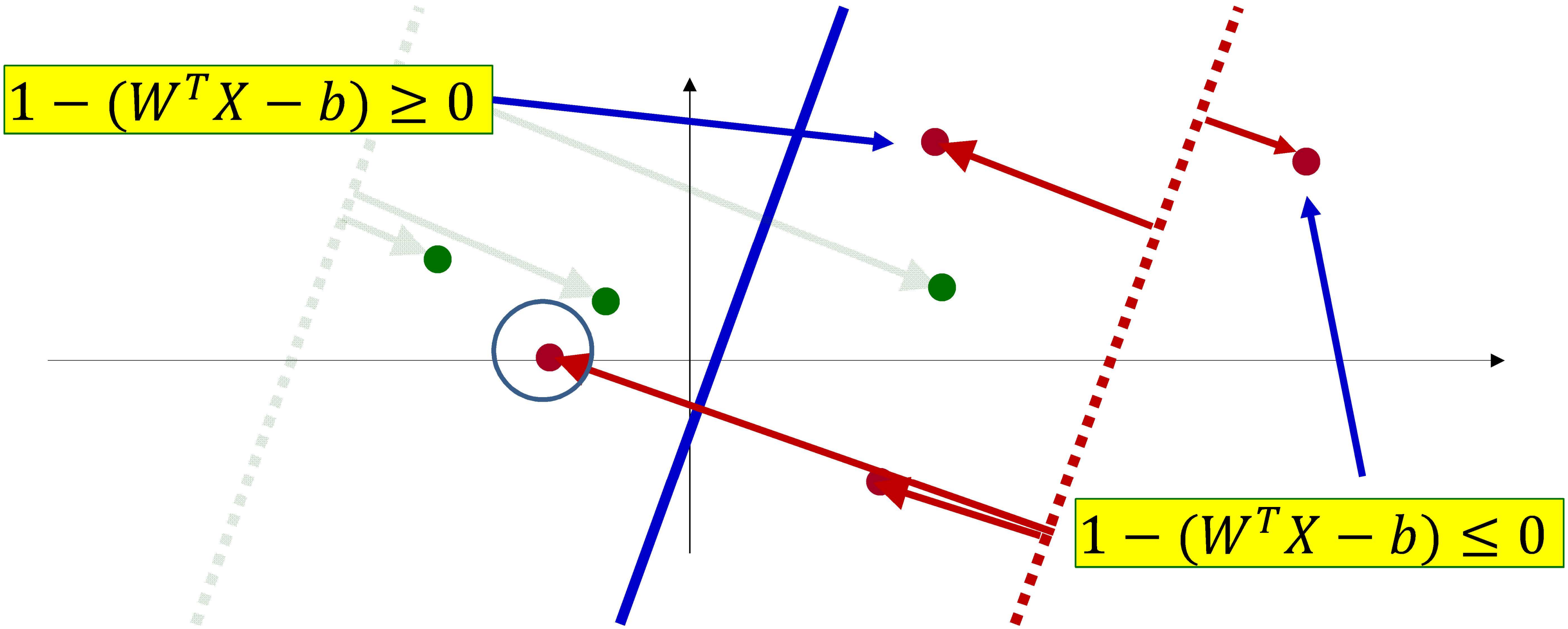



- The (unnormalized) distance of any $X$ from this plane

$$W^T X - b - 1$$

- This will be negative for instances on the "wrong" side (in the direction away from $W$), but positive for those on the "right" side

# Quantifying Slack Length

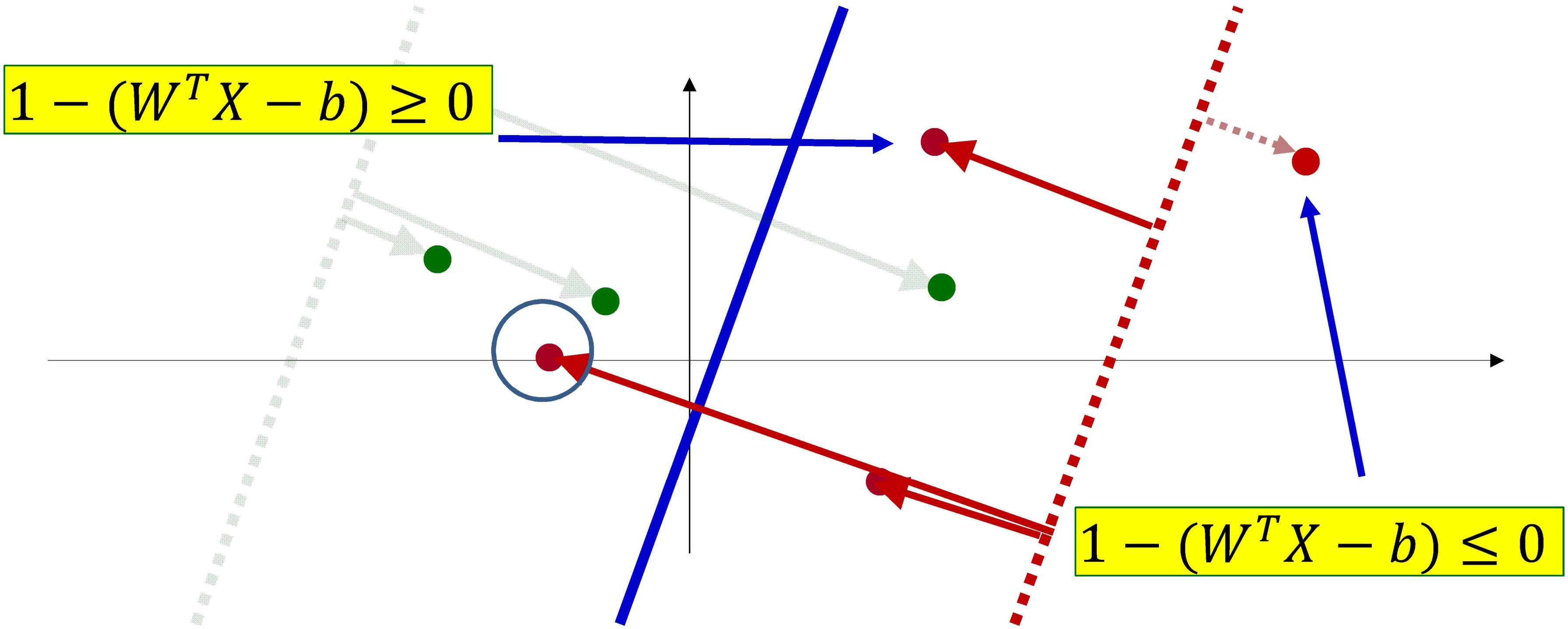



- The *negated* (unnormalized) distance of any $X$ from this plane

$$1-(W^TX-b)$$

- This will be positive for instances on the wrong side of the margin plane, but negative for instances on the right side of it

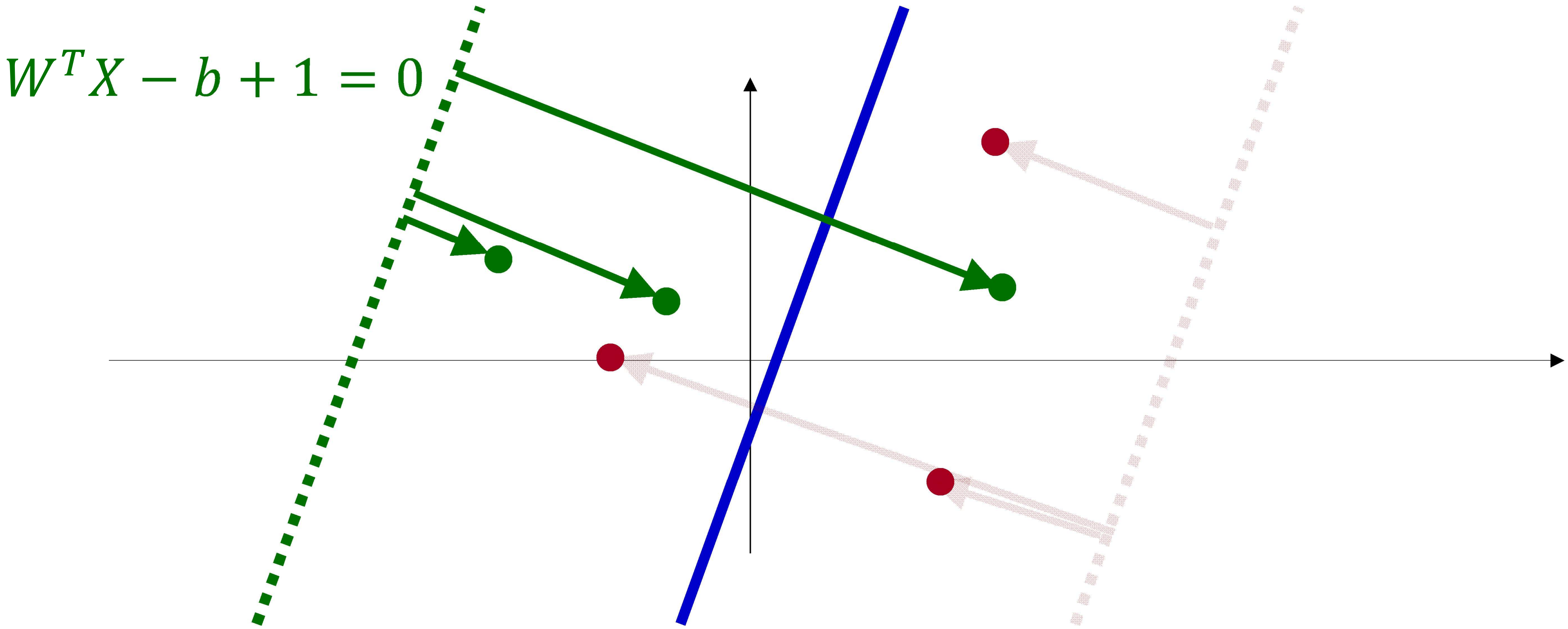
# Quantifying Slack Length




- We do not care about the actual distance of instances to the *right* of the plane
- So the slack value of any point is

$$\max(0, 1 - (W^T X - b))$$

# Quantifying Slack Length

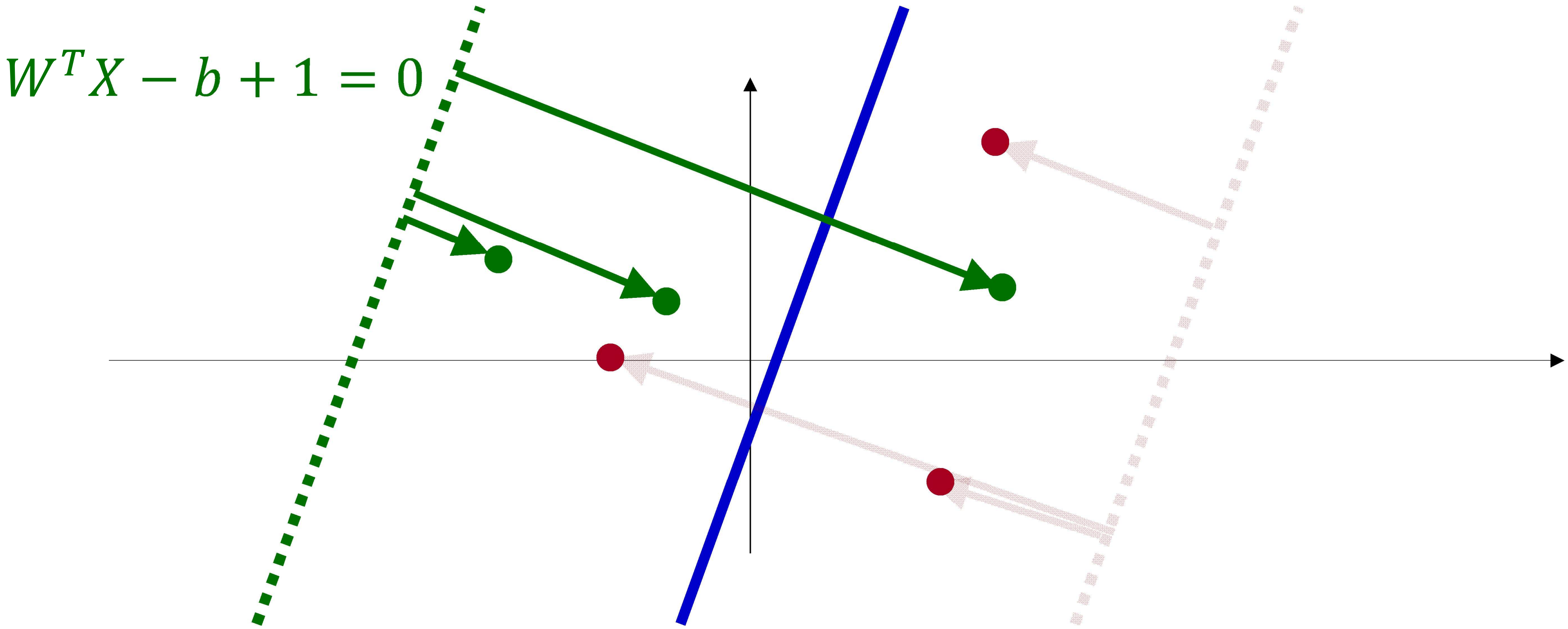



- The *negative* margin plane is given by

$$W^T X - b + 1 = 0$$

  – Ideally all negative training points would be to the left of it

# Quantifying Slack Length

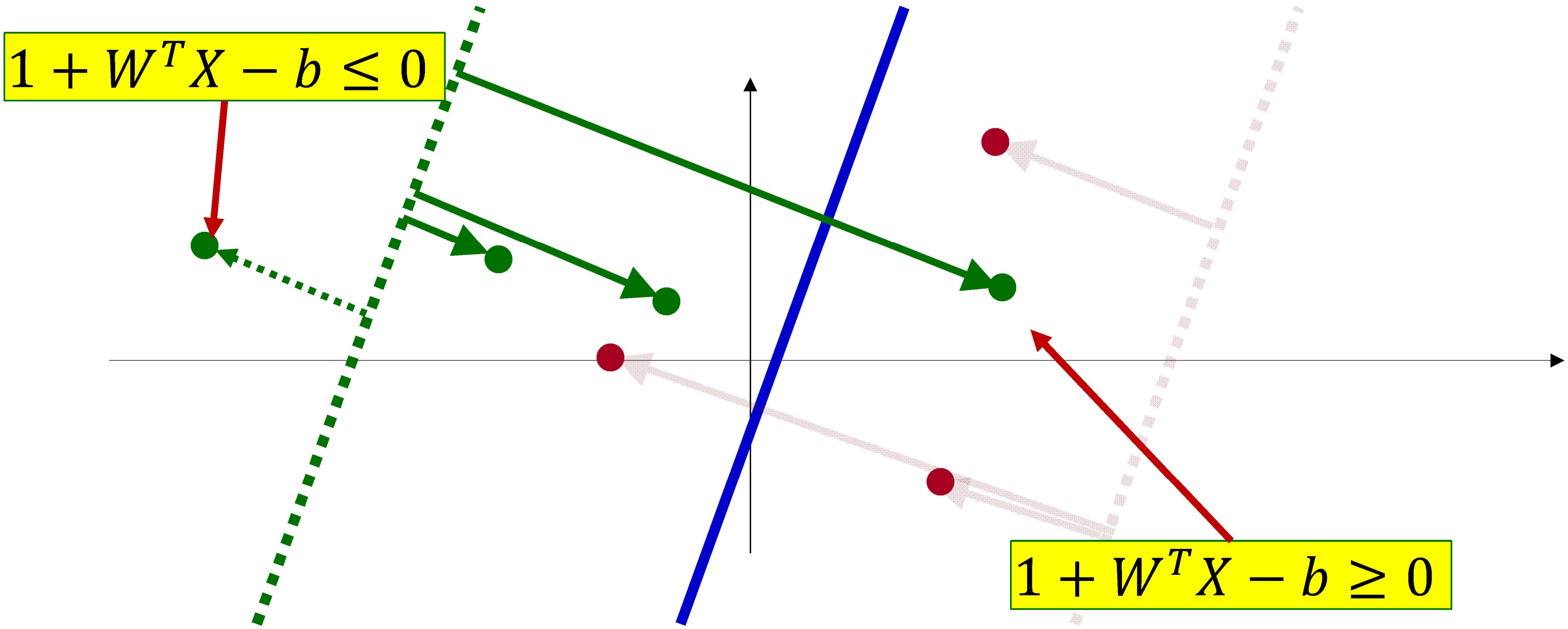



- The (unnormalized) distance of any $X$ from this plane

$$W^TX - b + 1 = 1 + W^TX - b$$

- This will be positive for vectors on the "wrong" side, but negative for vectors on the right side

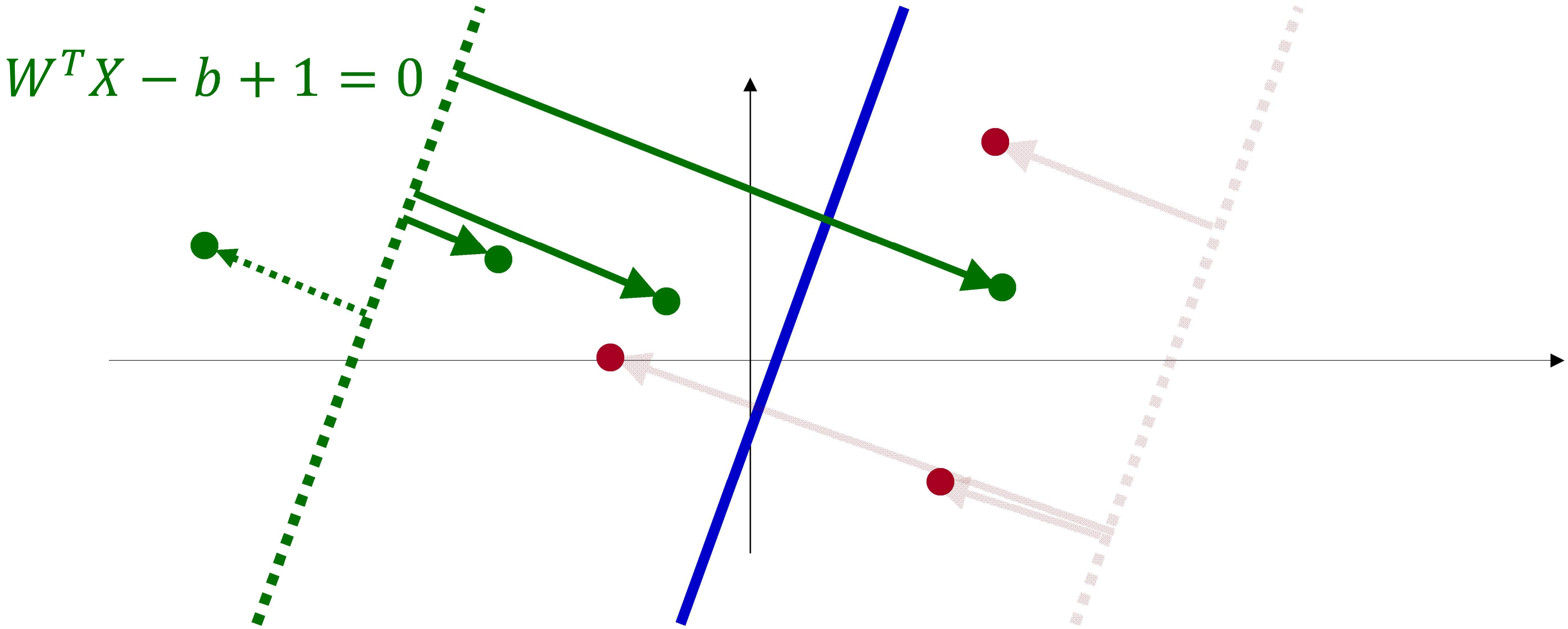
# Quantifying Slack Length




- We do not care about the actual distance of instances to the *left* of the plane
- So the slack value of any point is

$$\max(0, 1 + W^T X - b)$$

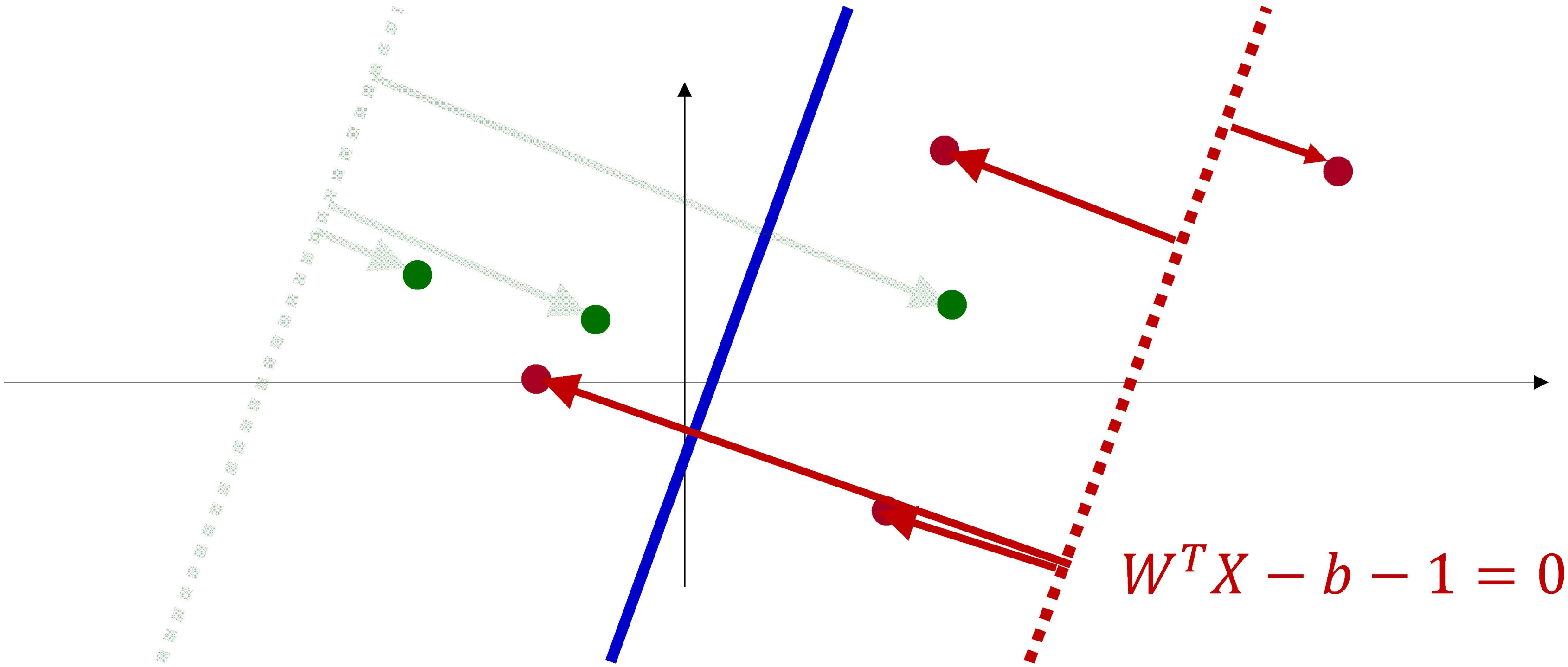
# Quantifying Slack Length




- Combining the following for negative instances

$$\max(0, 1 + (W^T X - b))$$

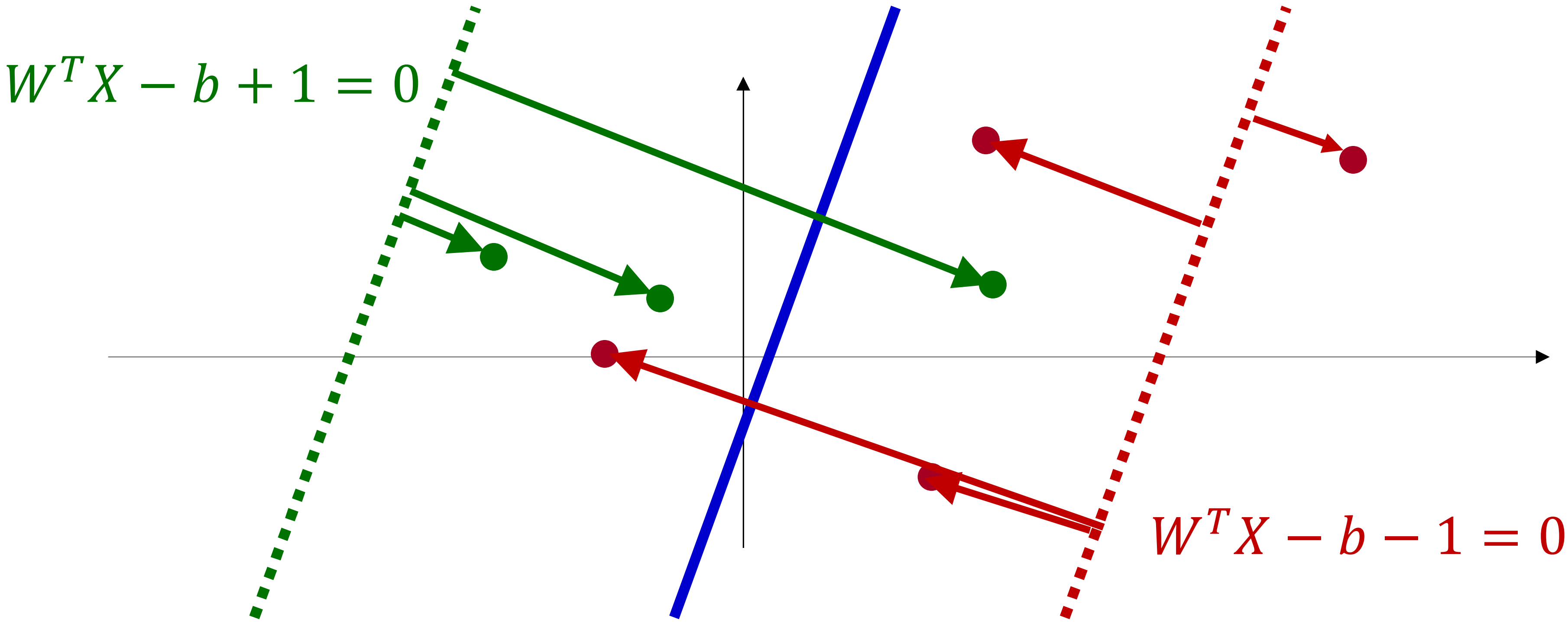
# Quantifying Slack Length




- And the following for positive instances

$$\max(0, 1 - (W^TX - b))$$

# Quantifying Slack Length




- Generic Slack length for any point

$$\max(0, 1 - y(W^T X - b))$$

- This is also called a *hinge loss*

# Total Slack Length

- Total slack length for *all* training instances

$$\sum_i \max(0, 1 - y(W^T X - b))$$

- This must be minimized

# Overall Optimization

- Minimize $||W||^2$ to maximize the distance between margin planes
- Minimize total slack length to minimize the distance of *misclassified* instances to margin planes

$$\sum_i \max(0, 1 - y(W^T X - b))$$

  – This will make the margin planes *closer*

- The two objectives must be traded off..

# Support Vector Machine for Inseparable data

- Minimize

$$\underset{W,b}{\operatorname{argmin}} \frac{1}{N} \sum_{i} \max(0, 1 - y(W^T X - b)) \ + \lambda \|W\|^2$$

- $\lambda$ is a "regularization" parameter that decides the relative importance of the two terms

- This is just a regular optimization problem that can be solved through gradient descent

# Support Vector Machine for Inseparable data

- $\lambda$ is typically set using *held-out* training data
  - Train the classifier for various values of $\lambda$
  - Test each of these classifiers on some held-out portion of the training data that was not included in training the SVM
  - Pick the $\lambda$ for which the classifier gave best performance
  - Retrain the SVM using the entire training data and this $\lambda$

- Frequently, instead of a single held-out set, $\lambda$ is set through K-fold cross validation

# Equivalent Slack Formalism

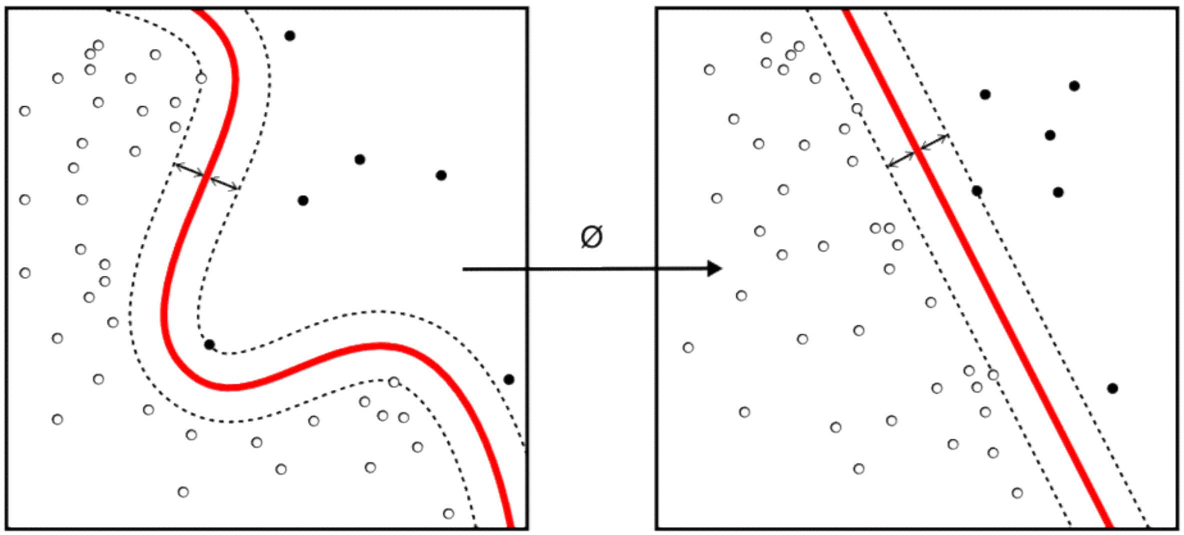
$$\underset{W,b}{\operatorname{argmin}} \; \|W\|^2 + C \sum_i \xi_i$$

- Subject to

$$Y_i(W^T X_i - b) \geq 1 - \xi_i$$

- This is a quadratic programming problem
- Slack parameter $C$ is determined through held-out data as earlier (or through K-fold cross-validation)

# How to deal with *non-linear* boundaries?




- First some math..

# Recall: The Lagrange Method

- Optimize $f(x, y)$ subject to $g(x, y) = c$

$$\boxed{L(x, y, \lambda) = f(x, y) - \lambda(g(x, y) - c)}$$

to maximize $f(x, y)$: $\max_{x,y}\left(\min_{\lambda} L(x, y, \lambda)\right)$

to minimize $f(x, y)$: $\min_{x,y}\left(\max_{\lambda} L(x, y, \lambda)\right)$

# Optimization with inequality constraints

- Optimization problem with constraints

$$\begin{aligned} &\min_x f(x) \\ &s.t.\;\; g_i(x) \le 0, \;\; i = \{1,\ldots,k\} \\ &\qquad h_j(x) = 0, \;\; j = \{1,\ldots,l\} \end{aligned}$$

- Lagrange multipliers $\lambda_i \ge 0, \nu \in \Re$

$$L(x,\lambda,\nu) = f(x) + \sum_{i=1}^{k} \lambda_i g_i(x) + \sum_{j=1}^{l} \nu_j h_j(x)$$

- The optimization problem

$$\underset{x}{\operatorname{argmin}} \max_{\lambda,v} L(x,\lambda,v)$$

# Revisiting the *linearly separable* case

- This is a quadratic programming problem!

$$\hat{W} = \underset{W}{\operatorname{argmin}} \|W\|^2$$
$$s.t.\ \forall i \quad Y_i(W^T X_i - b) \geq 1$$

- Can be stated using Lagrangians as

$$\underset{W,b}{\operatorname{argmin}} \ \max_{\alpha > 0} \|W\|^2 + \sum_i \alpha_i (Y_i(W^T X_i - b) - 1)$$

# Linearly separable case: Lagrangian formalism

- Can be stated using Lagrangians as

$$\underset{W,b}{\operatorname{argmin}} \ \max_{\alpha>0} ||W||^2 + \sum_i \alpha_i (Y_i (W^T X_i - b) - 1)$$

- The optimum satisfies the *Karush Kuhn-Tucker* conditions, hence we can rewrite it as

$$\underset{\alpha>0}{\operatorname{argmax}} \ \min_{W,b} ||W||^2 + \sum_i \alpha_i (Y_i (W^T X_i - b) - 1)$$

# Linearly separable case: Lagrangian formalism

- Under the KKT conditions

$$\underset{\alpha>0}{\operatorname{argmax}} \; \min_{W,b} \|W\|^2 + \sum_i \alpha_i (Y_i(W^T X_i - b) - 1)$$

- Taking the deriviative w.r.t $W$ and setting to 0, we get

$$2W = -\sum_i \alpha_i Y_i X_i$$

# Linearly separable case: Lagrangian formalism

- Under the KKT conditions

$$\underset{\alpha>0}{\operatorname{argmax}} \min_{W,b} \|W\|^2 + \sum_i \alpha_i (Y_i(W^T X_i - b) - 1)$$

- Taking the deriviative w.r.t $b$ and setting to 0, we get

$$0 = \sum_i \alpha_i Y_i$$

# Linearly separable case:

- Restating (and ignoring the factor of 2)

$$\underset{\alpha>0}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j - b \sum_i \alpha_i Y_i$$

- Since the last term is 0

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

$$s.t. \alpha_i \geq 0$$

$$\sum_i \alpha_i Y_i = 0$$

# Large Margin Linear Classifier with Slack

- Formulation: (Lagrangian Dual Problem)

$$\text{maximize} \ \sum_{i=1}^{n} \alpha_i - \quad \sum_{i=1}^{n} \sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j \mathbf{x}_i^T \mathbf{x}_j$$

such that

$$0 \le \alpha_i \le C$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

# The usual simple SVM can also be solved through the ugly form

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

$$s.t.\, C \geq \alpha_i \geq 0$$

$$\sum_i \alpha_i Y_i = 0$$

- This is for the linear case. Note that the optimization is in terms of $X_i^T X_j$
- Also $W = -\sum_i \alpha_i Y_i X_i$
- So the classifier on any test instance has the form:

$$sign\left(-\sum_i \alpha_i Y_i X_{test}^T X_i - b\right)$$

# The SVM as KNN classification

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

$$s.t.\, C \geq \alpha_i \geq 0$$

$$\sum \alpha_i Y_i = 0$$

Weighted-nearest neighbor classifier

- This is for the linear case. Note that the optimization is in terms of $X_i^T X_j$
- Also $W = -\sum_i \alpha_i Y_i X_i$
- So the classifier on any test instance has the form:

$$sign\left(-\sum_i \alpha_i Y_i X_{test}^T X_i - b\right)$$

# The SVM as KNN classification

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

L1 norm of α

$$s.t.\ C \geq \alpha_i \geq 0$$

Total weighted accuracy on training data

$$\sum_i \alpha_i Y_i = 0$$

Weighted-nearest neighbor classifier

- This is for the linear case. Note that the optimization is in terms of $X_i^T X_j$
- Also $W = -\sum_i \alpha_i Y_i X_i$
- So the classifier on any test instance has the form:

$$sign\left(-\sum_i \alpha_i Y_i X_{test}^T X_i - b\right)$$

# The Kernel Trick

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

$$s.t.\, C \geq \alpha_i \geq 0$$

$$\sum_i \alpha_i Y_i = 0$$

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# The Kernel Trick

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j K(X_i, X_j)$$

$$s.t.\, C \geq \alpha_i \geq 0$$

$$\sum_i \alpha_i Y_i = 0$$

- For classification:

$$sign\left(-\sum_i \alpha_i Y_i K(X_i, X_{test}) - b\right)$$

# The Kernel Trick

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \sum_{i,j} \alpha_i \alpha_j Y_i Y_j K(X_i, X_j)$$

$$s.t. \, C \geq \alpha_i \geq 0$$

$$\sum_i \alpha_i Y_i = 0$$

This is a quadratic programming problem

- For classification:

$$sign\left(-\sum_i \alpha_i Y_i K(X_i, X_{test}) - b\right)$$

# Nonlinear SVMs: The Kernel Trick

- Examples of commonly-used kernel functions:
  - Linear kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = \mathbf{x}_i^T \mathbf{x}_j$
  - Polynomial kernel: $K(\mathbf{x}_i, \mathbf{x}_j) = (1 + \mathbf{x}_i^T \mathbf{x}_j)^p$
  - Gaussian (Radial-Basis Function (RBF) ) kernel:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \exp(-\frac{\left\|\mathbf{x}_i - \mathbf{x}_j\right\|^2}{2\sigma^2})$$

  - Sigmoid:

$$K(\mathbf{x}_i, \mathbf{x}_j) = \tanh(\beta_0 \mathbf{x}_i^T \mathbf{x}_j + \beta_1)$$

- In general, functions that satisfy *Mercer's condition* can be kernel functions.

# Nonlinear SVM: Optimization

- Formulation: (Lagrangian Dual Problem)

$$\text{maximize} \quad \sum_{i=1}^{n} \alpha_i - \frac{1}{2}\sum_{i=1}^{n}\sum_{j=1}^{n} \alpha_i \alpha_j y_i y_j K(\mathbf{x}_i, \mathbf{x}_j)$$

such that

$$0 \le \alpha_i \le C$$

$$\sum_{i=1}^{n} \alpha_i y_i = 0$$

- The solution of the discriminant function is

$$g(\mathbf{x}) = \sum_{i \in \mathrm{SV}} \alpha_i K(\mathbf{x}_i, \mathbf{x}) + b$$

- The optimization technique is the same.

# Support Vector Machine: Algorithm

- 1. Choose a kernel function
- 2. Choose a value for *C*
- 3. Solve the quadratic programming problem (many software packages available)
- 4. Construct the discriminant function from the support vectors

# Some Issues

- Choice of kernel
  - Gaussian or polynomial kernel is default
  - if ineffective, more elaborate kernels are needed
  - domain experts can give assistance in formulating appropriate similarity measures

- Choice of kernel parameters
  - e.g. σ in Gaussian kernel
  - σ is the distance between closest points with different classifications
  - In the absence of reliable criteria, applications rely on the use of a validation set or cross-validation to set such parameters.

- Optimization criterion – Hard margin v.s. Soft margin
  - a lengthy series of experiments in which various parameters are tested

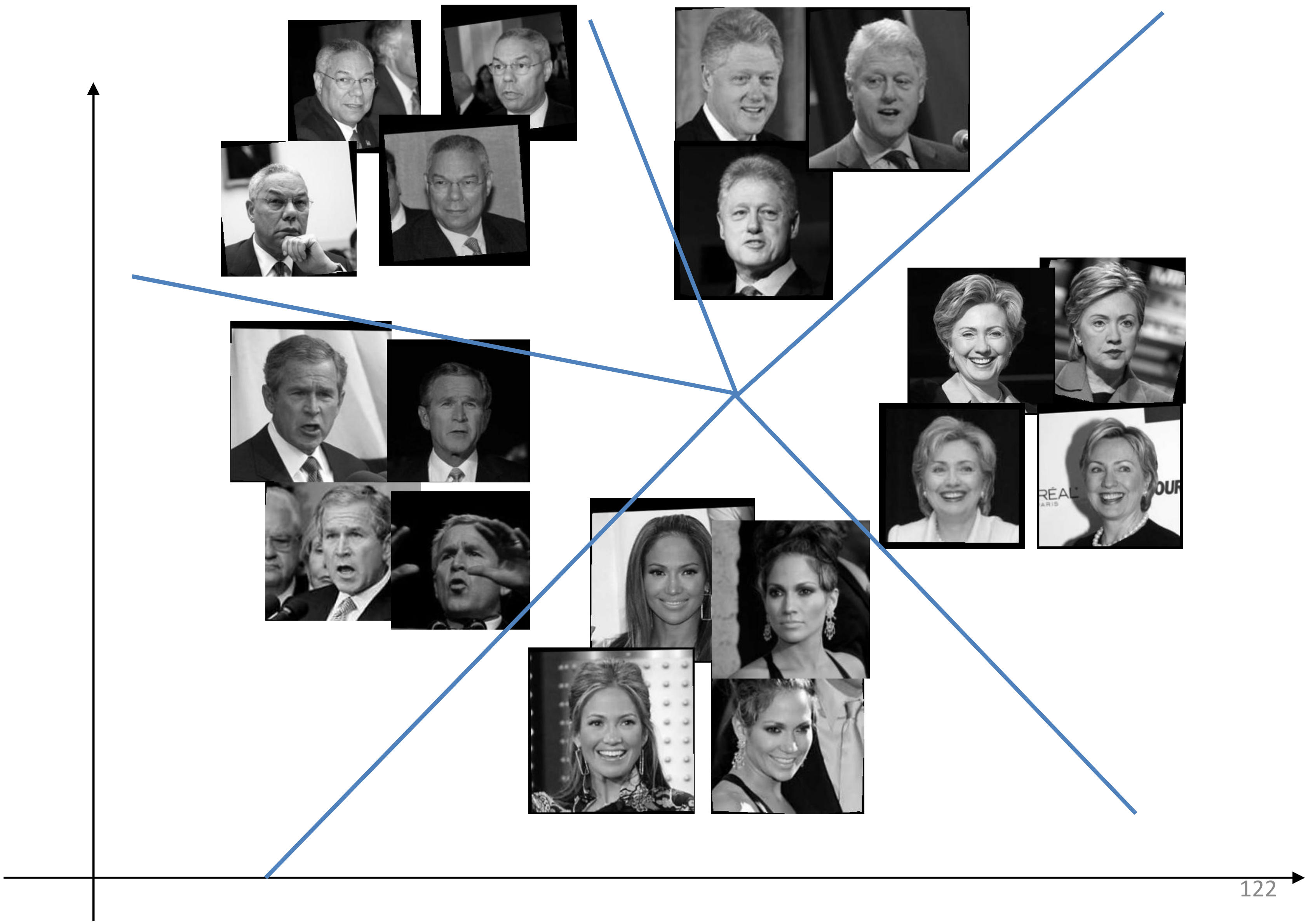
This slide is courtesy of *www.iro.umontreal.ca/~pift6080/documents/papers/**svm**_tutorial.**ppt***

# Summary: Support Vector Machine

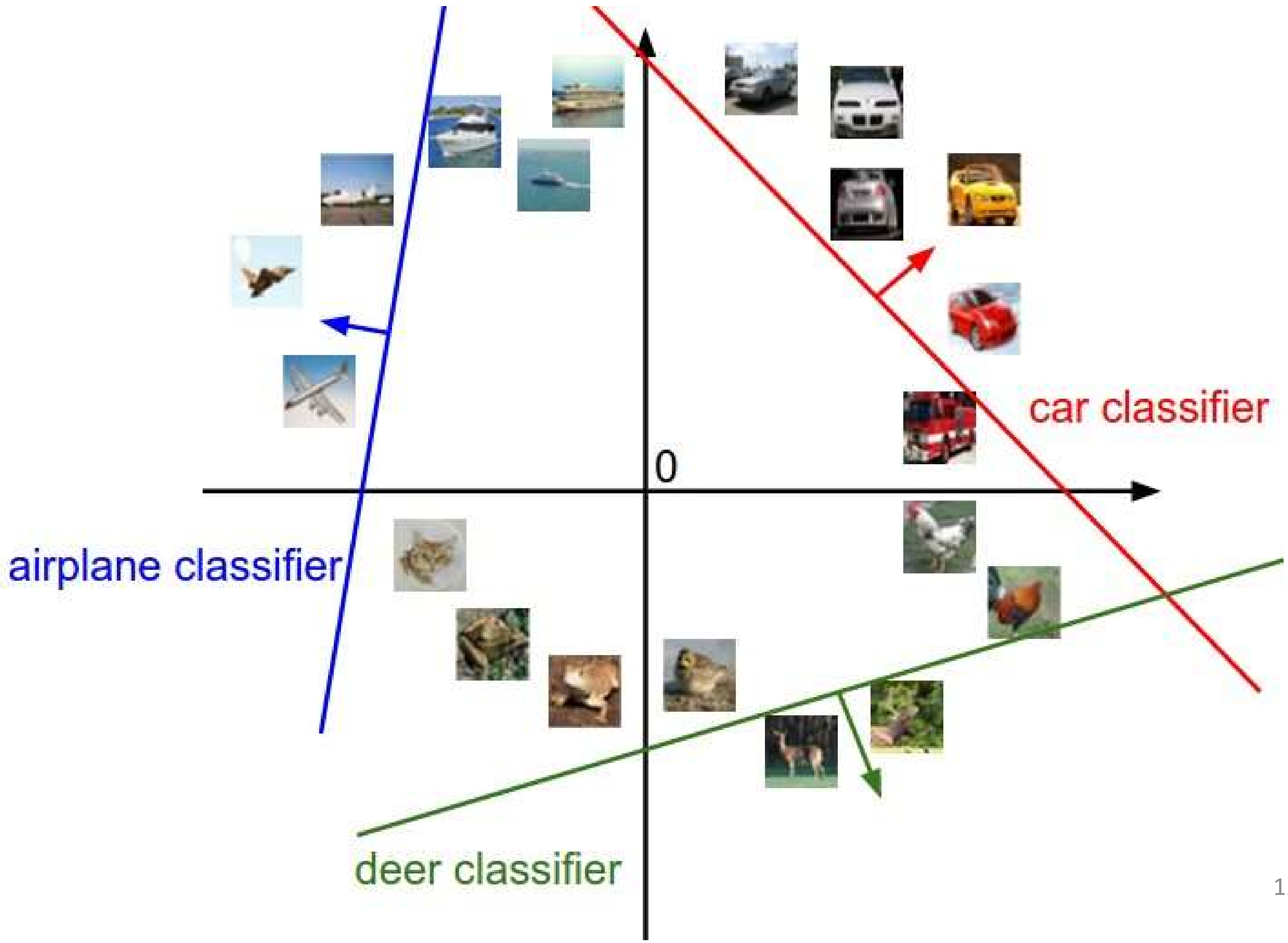
- 1. Large Margin Classifier
  - Better generalization ability & less over-fitting

- 2. The Kernel Trick
  - Map data points to higher dimensional space in order to make them linearly separable.
  - Since only dot product is used, we do not need to represent the mapping explicitly.

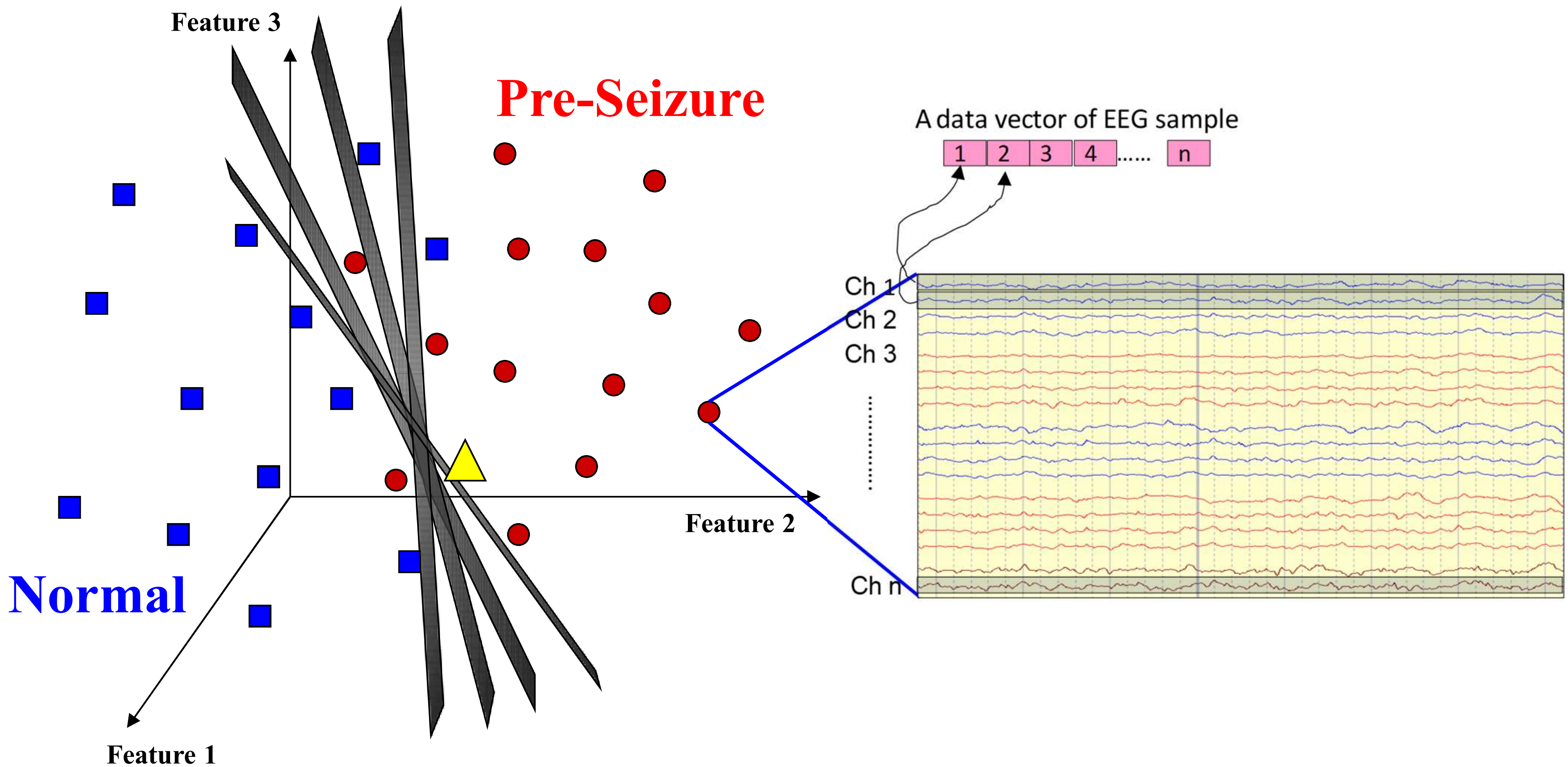
# Multi-class generalization Pairwise



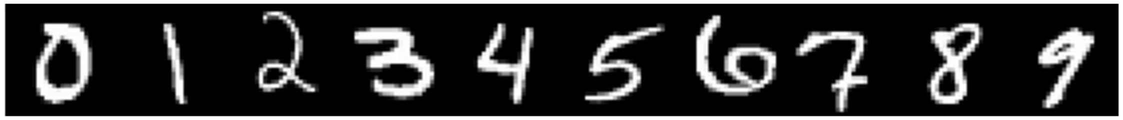
# Multi-class generalization One-vs-all



# Support Vector Machine for seizure detection



# Example: Digit Recognition



- Yann LeCunn – MNIST Digit Recognition
  - Handwritten digits
  - 28x28 pixel images: $d = 784$
  - 60,000 training samples
  - 10,000 test samples
- Nearest neighbour is competitive

| | Test Error Rate (%) |
|---|---|
| Linear classifier (1-layer NN) | 12.0 |
| K-nearest-neighbors, Euclidean | 5.0 |
| K-nearest-neighbors, Euclidean, deskewed | 2.4 |
| K-NN, Tangent Distance, 16x16 | 1.1 |
| K-NN, shape context matching | 0.67 |
| 1000 RBF + linear classifier | 3.6 |
| SVM deg 4 polynomial | 1.1 |

# Linear Classifiers: Conclusion

- Simple linear classifiers can be surprisingly effective
  – Particularly when trained to maximize a margin
    - Whereupon the "simple" arithmetic magically becomes complicated

- Kernel trick enables classification of even non-linear problems
- Most commonly used classifier, still