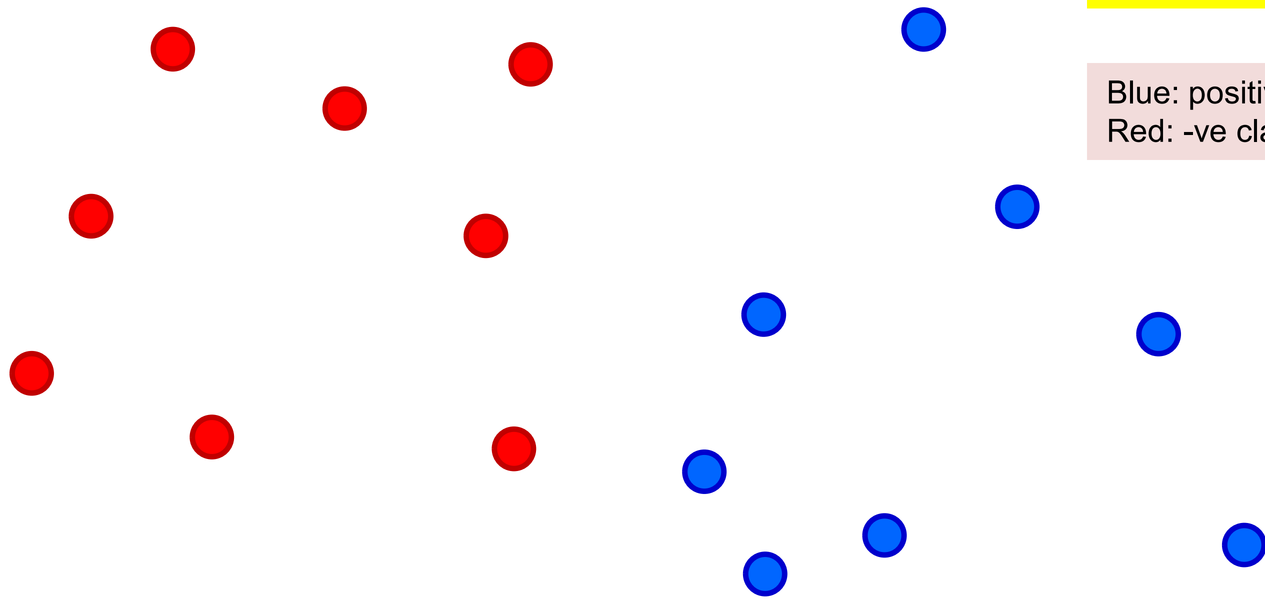
Linear Classifiers: SVM

Classification

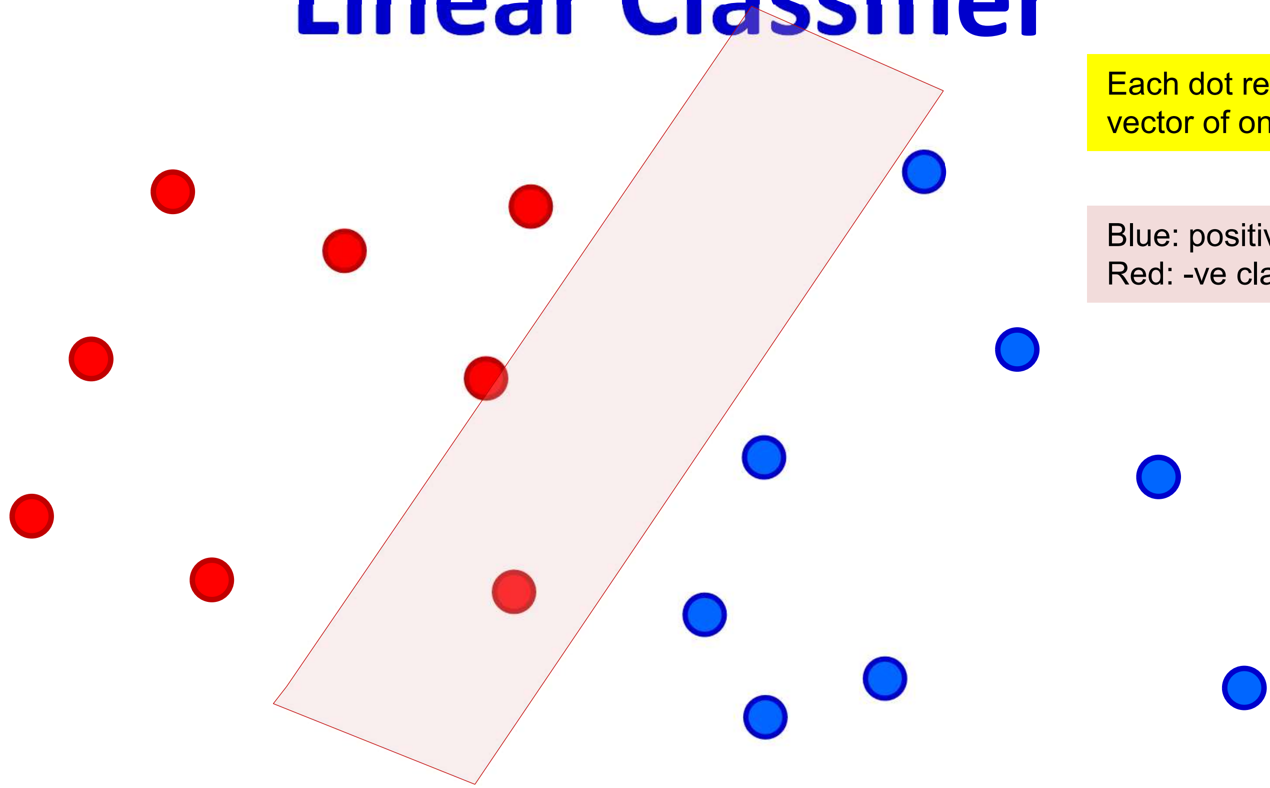


Each dot represents a feature vector of one training instance

Blue: positive class,
Red: -ve class

- Given a bunch of +ve and –ve training instances
  - Find a rule that correctly assigns a new test instance to one of the two classes

Linear Classifier

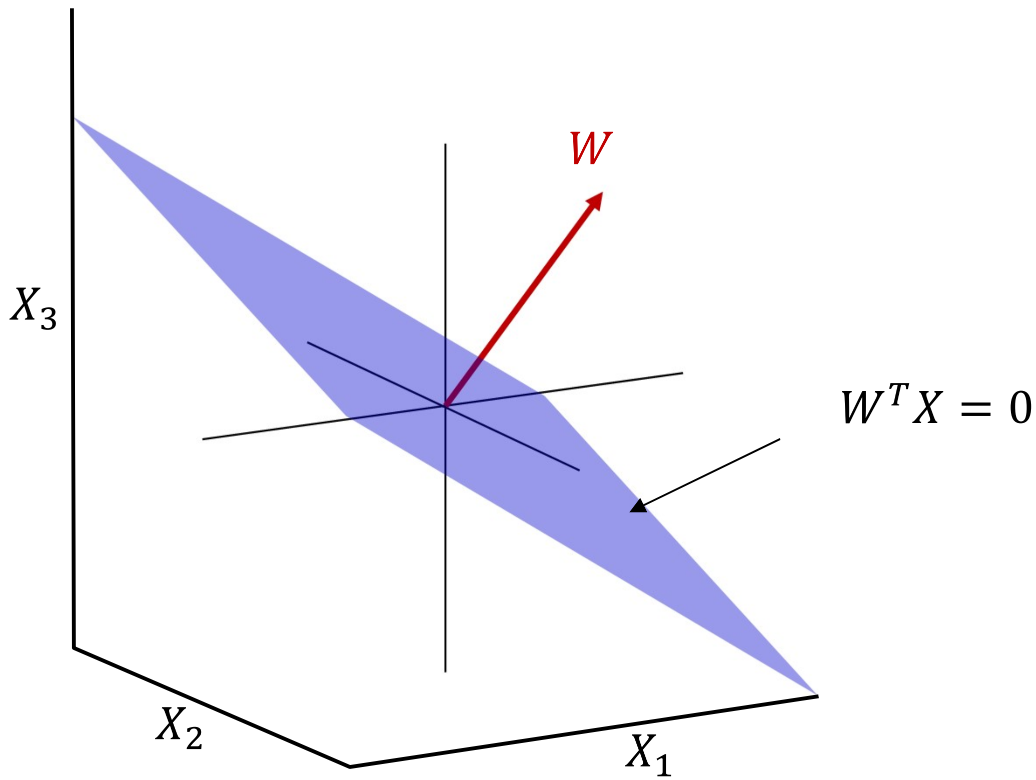


Each dot represents a feature vector of one training instance

Blue: positive class,
Red: -ve class

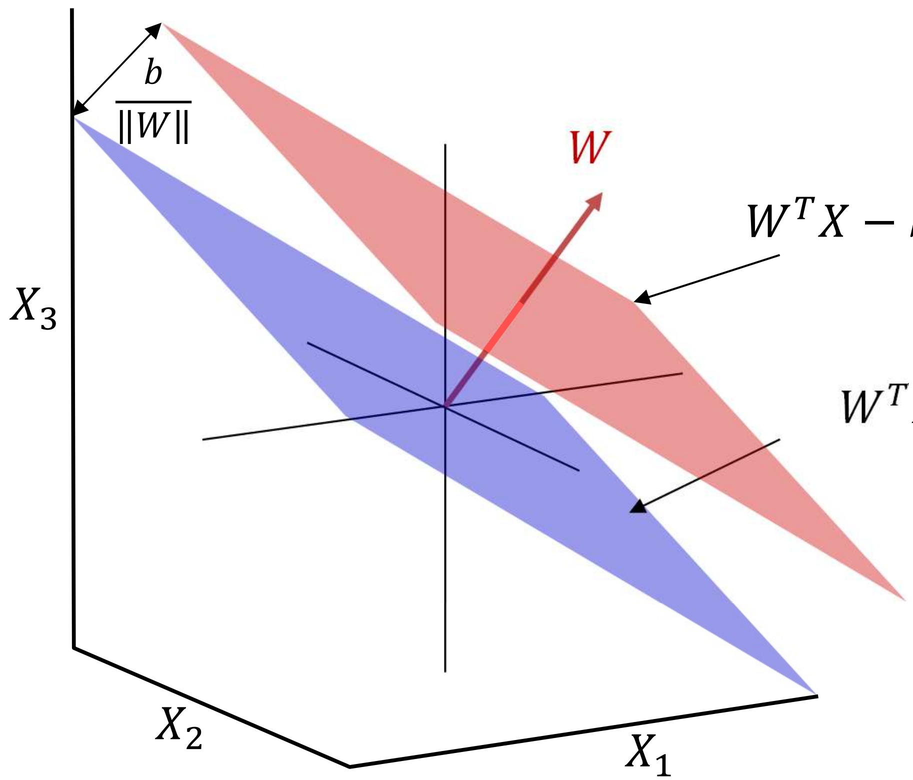
- Initially assume that the classes are separable by a *hyperplane*
  - A *linear* classifier
- Also that the training data are *perfectly* separable by the hyperplane
- We will fix these assumptions later

The equation for a hyperplane



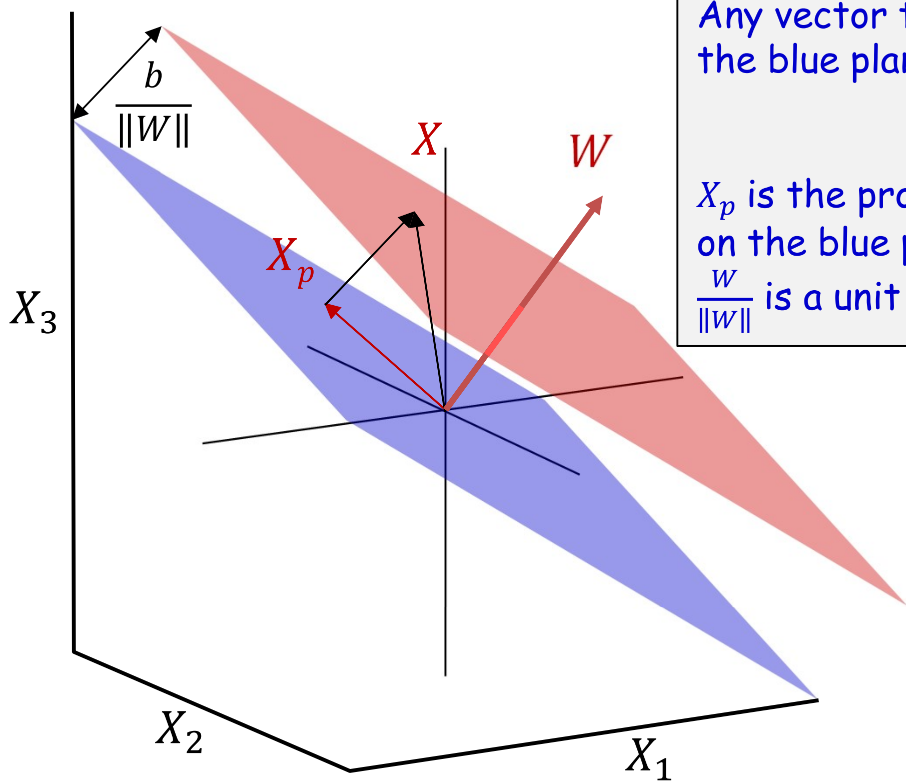
- $W^T X = 0$ is the equation representing the set of all vectors that are orthogonal to W

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

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

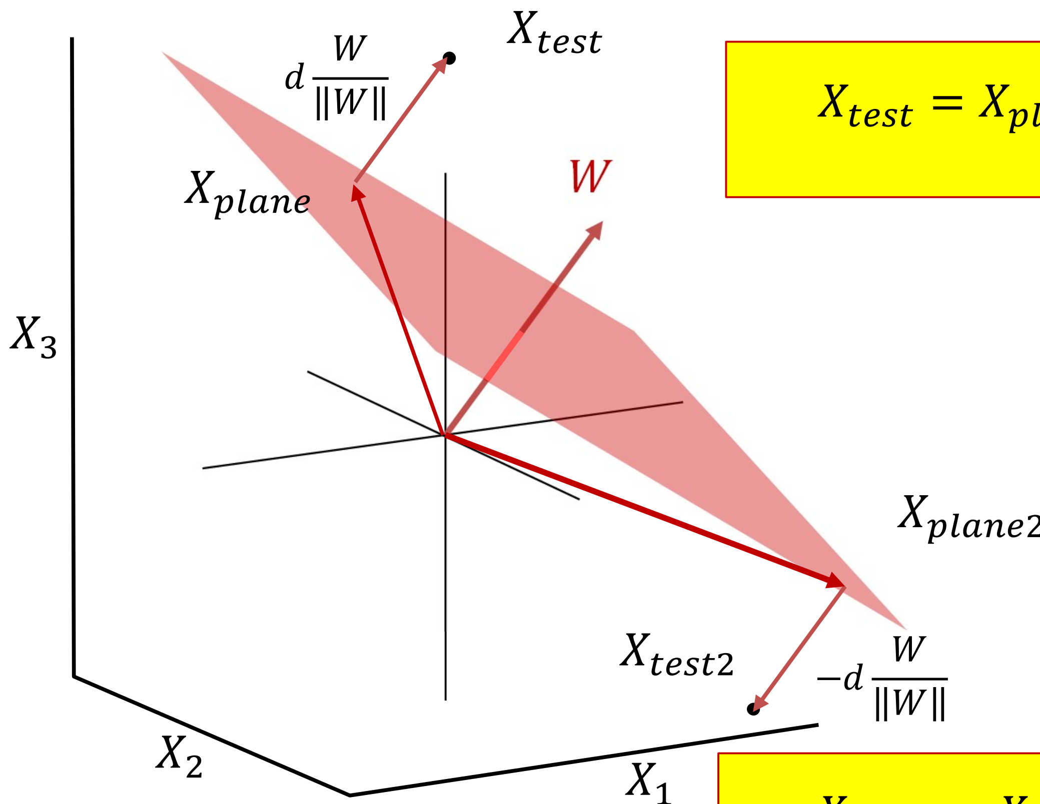
X_p is the projection of the vector on the blue plane

$\frac{W}{\|W\|}$ 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



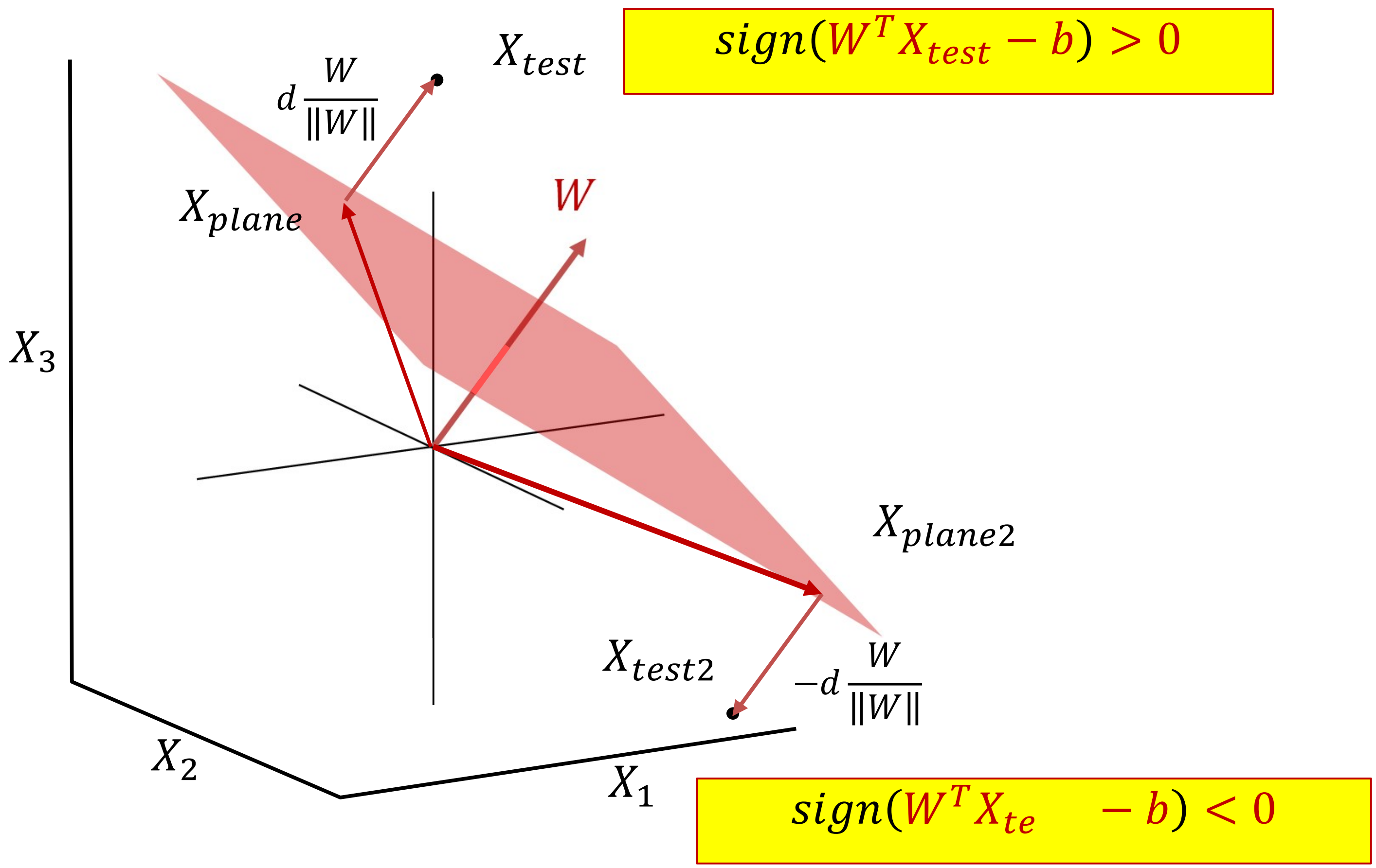
$$X_{test} = X_{plane} + d\frac{W}{\|W\|}$$

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

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

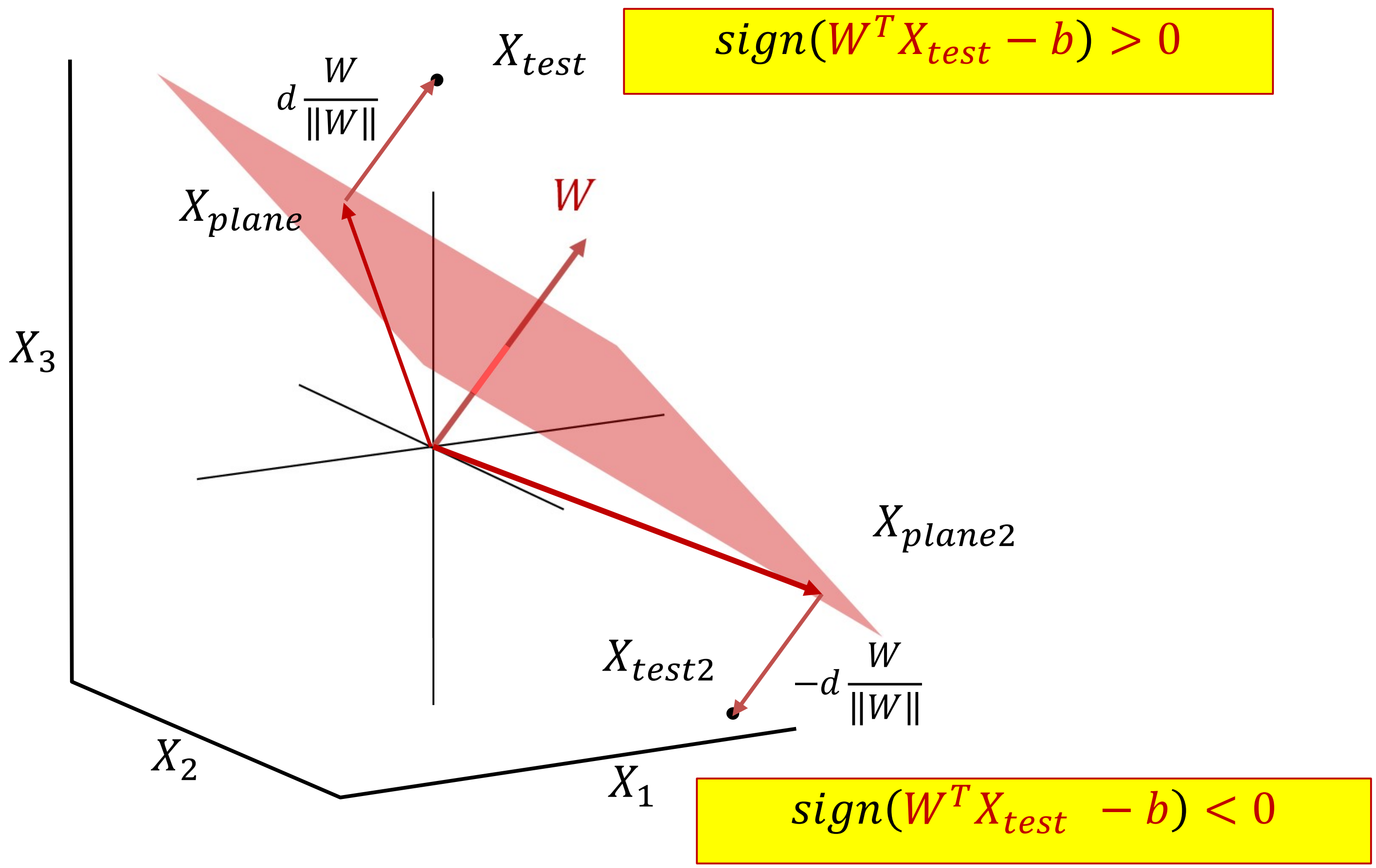
Poll 1

Sign of distance from hyperplane



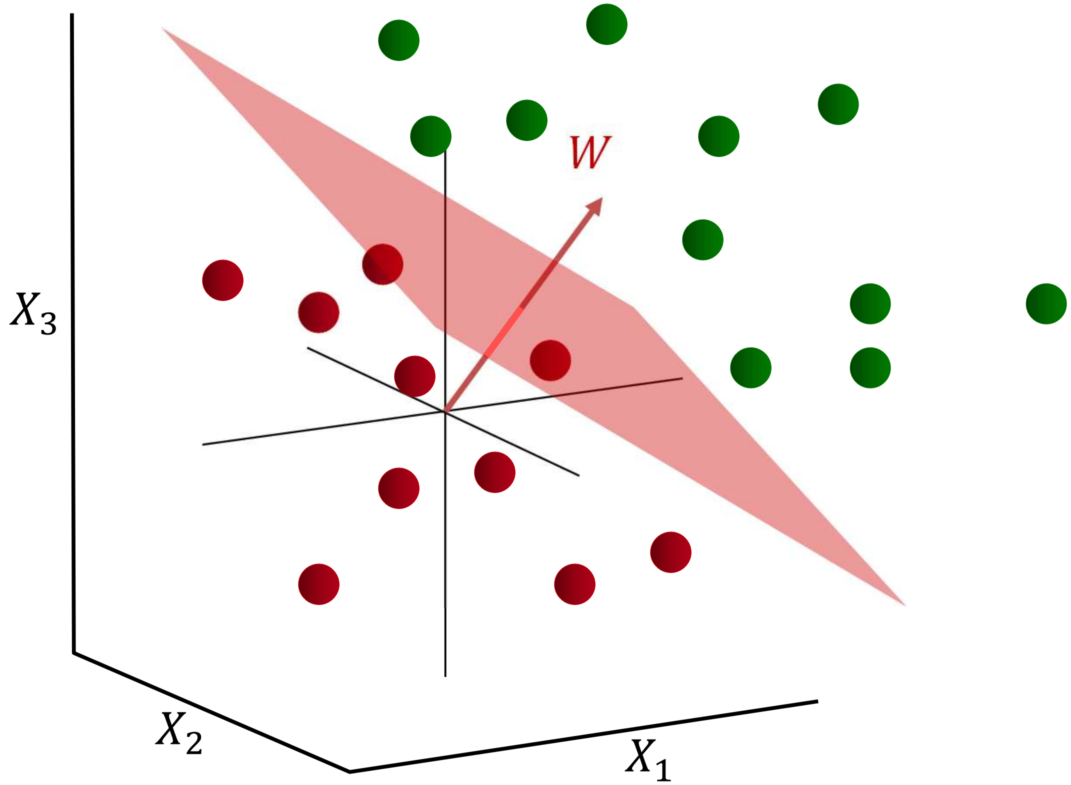
- The sign of $W^T X - b$ signifies which side of the plane the point X is on

Linear Classifier



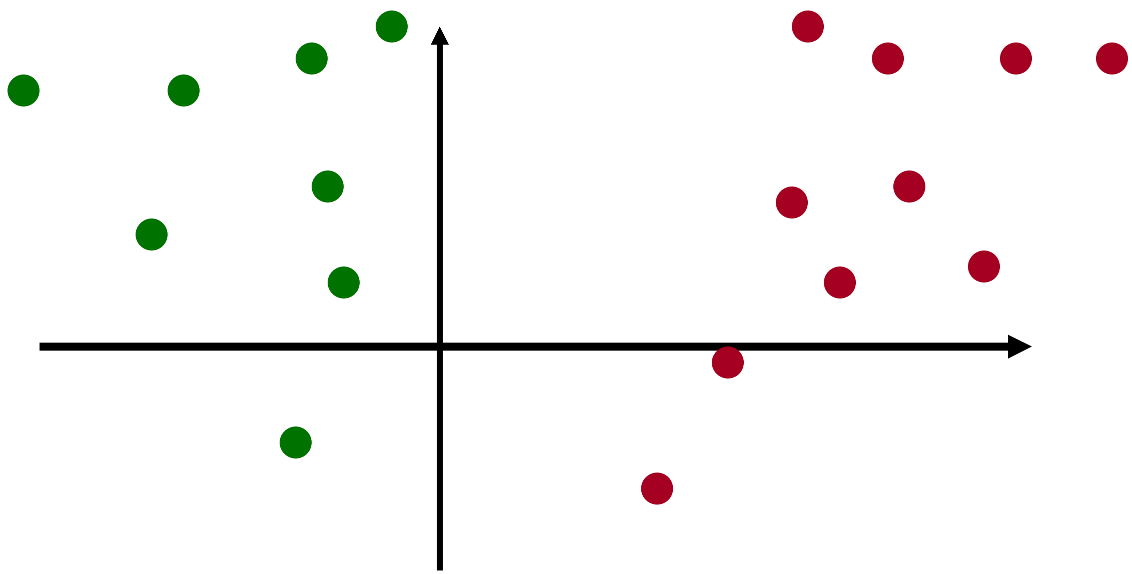
- The plane $W^T X - b$ is a linear classifier
  - The class is given by $sign(W^T X_{test} - b)$

Linearly separable data



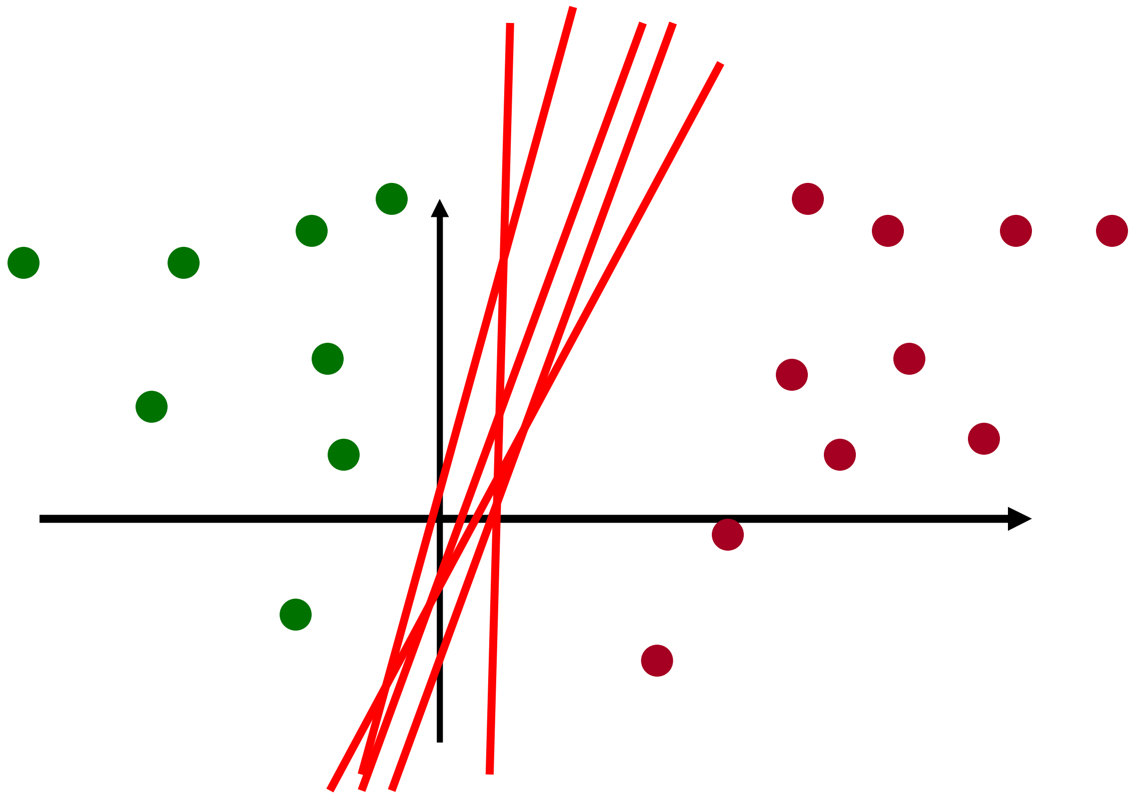
- Data where the two classes are separated by a hyperplane
  - And classification can be performed by $sign(W^T X_{test} - b)$ for any separating hyperplane

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

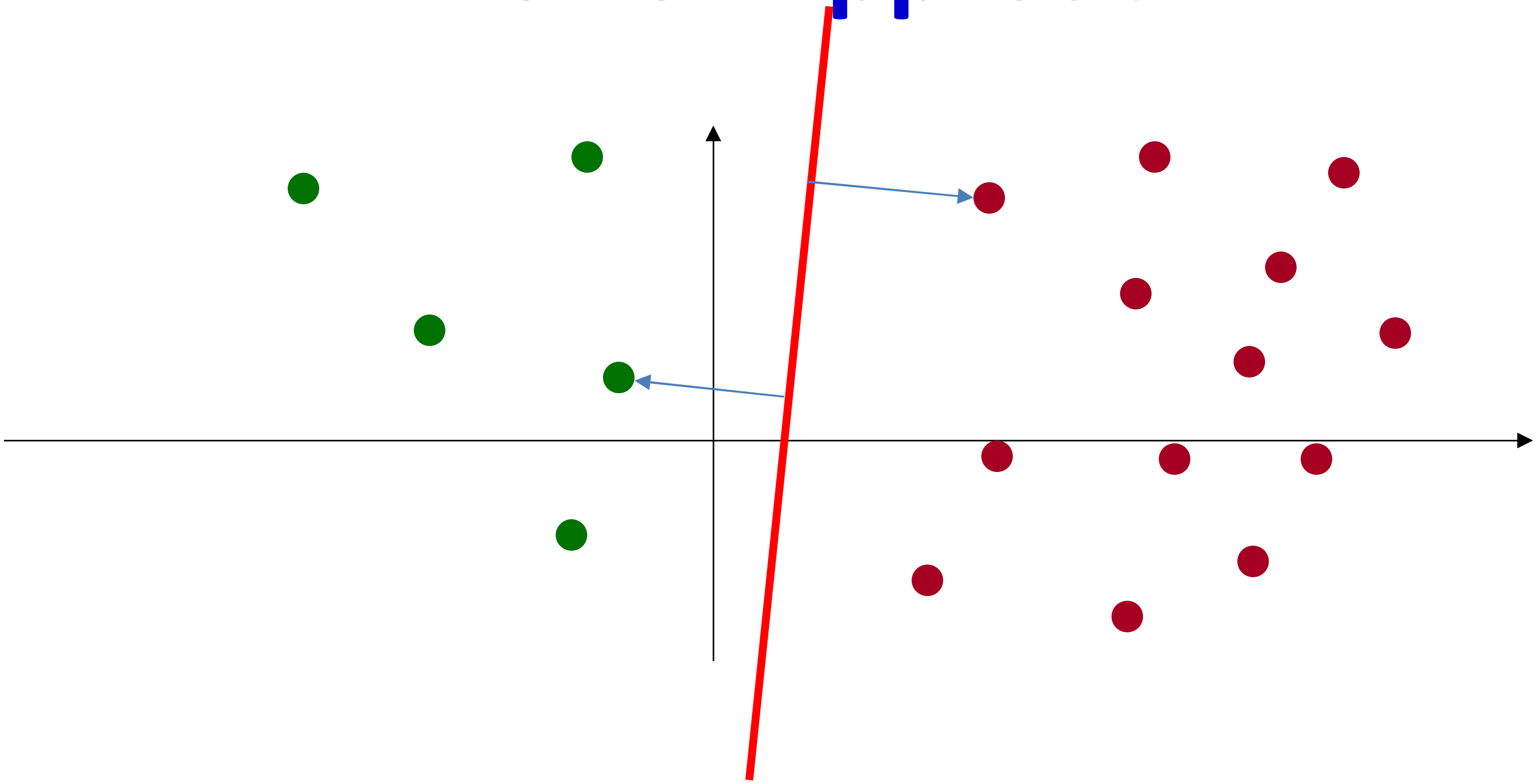


- Problem: Given these training instances find a separating hyperplane
- **Many ways of finding this hyperplane**
  - Any number of solution algorithms are possible

Enter: Support Vector Machines

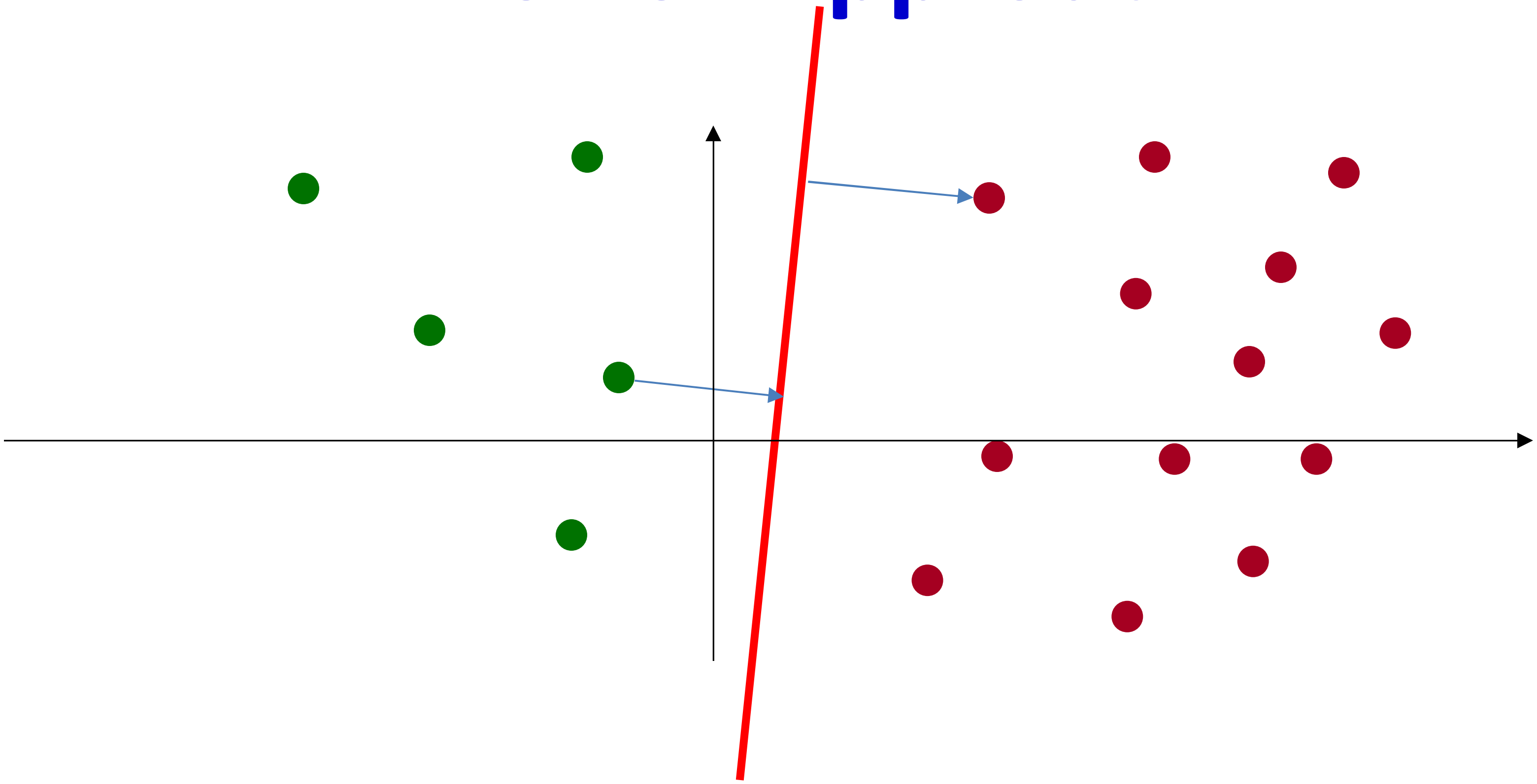
- Find a classifier that is maximally distant from the *closest* instances from either class

A Better Approach



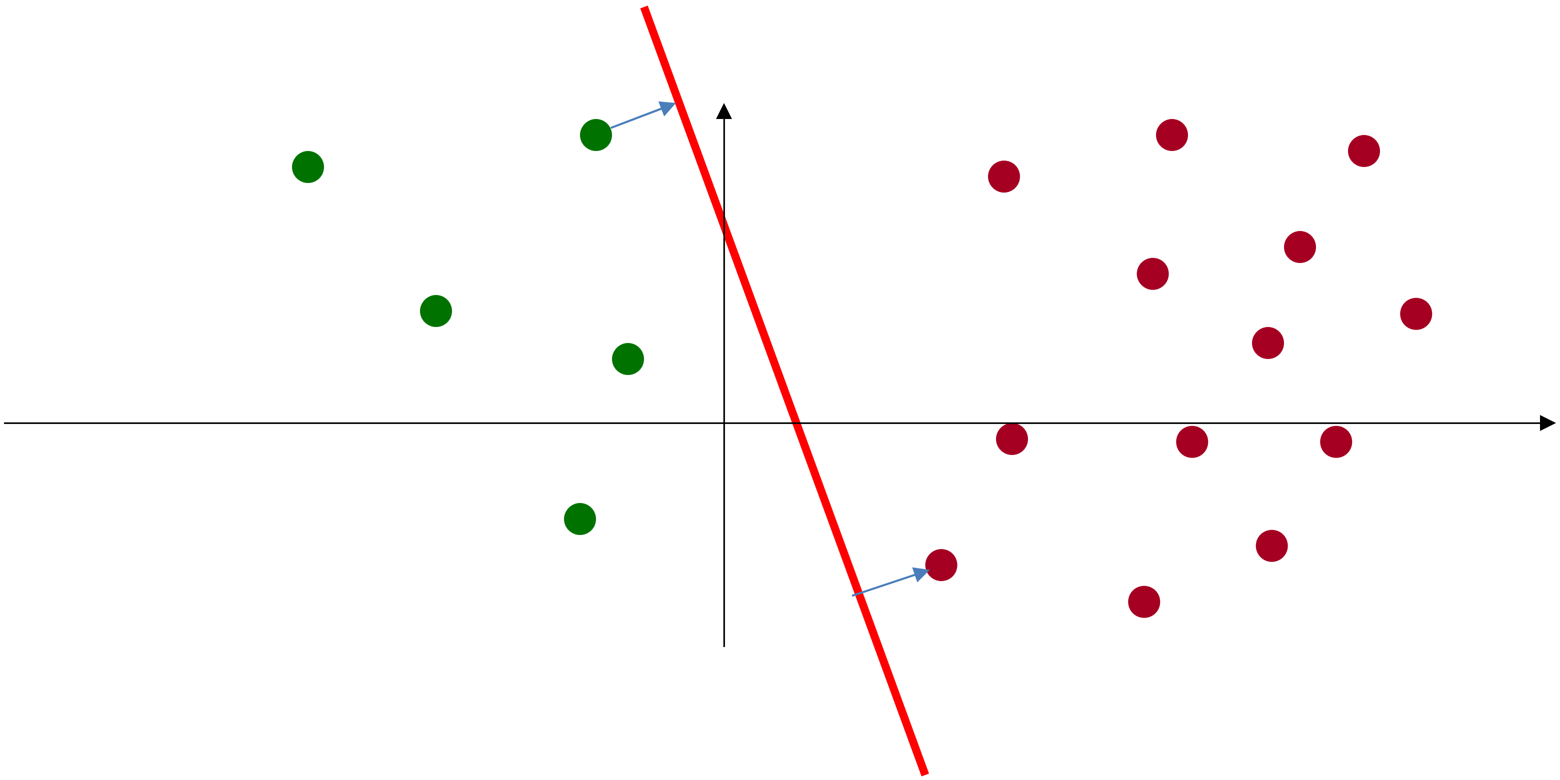
- Any linear classifier has some *closest* instances
- These instances will be at some distance from the boundary
- Changing the classifier will change both, the closest instance, and their distance from the boundary

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



- Search through all classifiers such that the distance to the closest points is maximized
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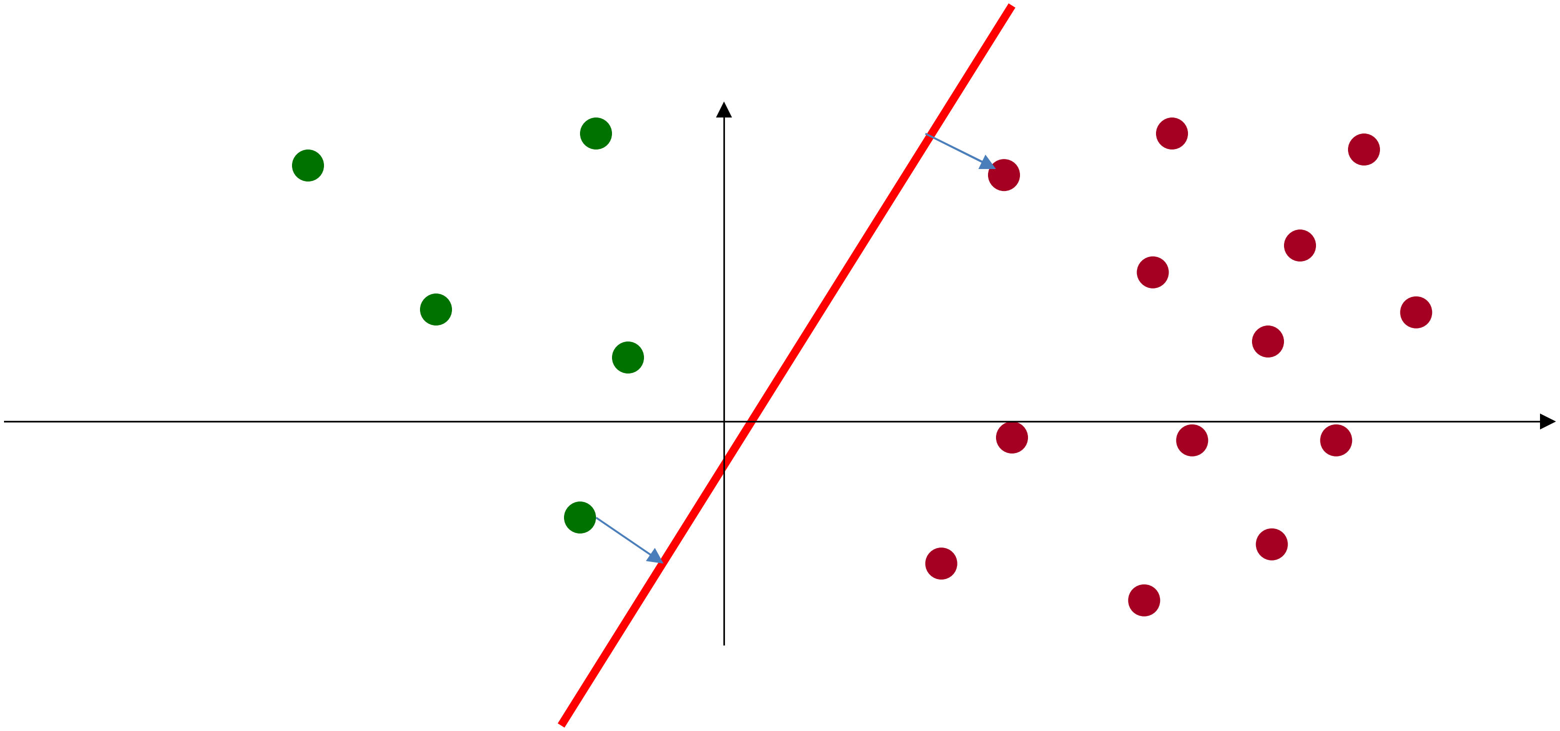
A Conservative Approach



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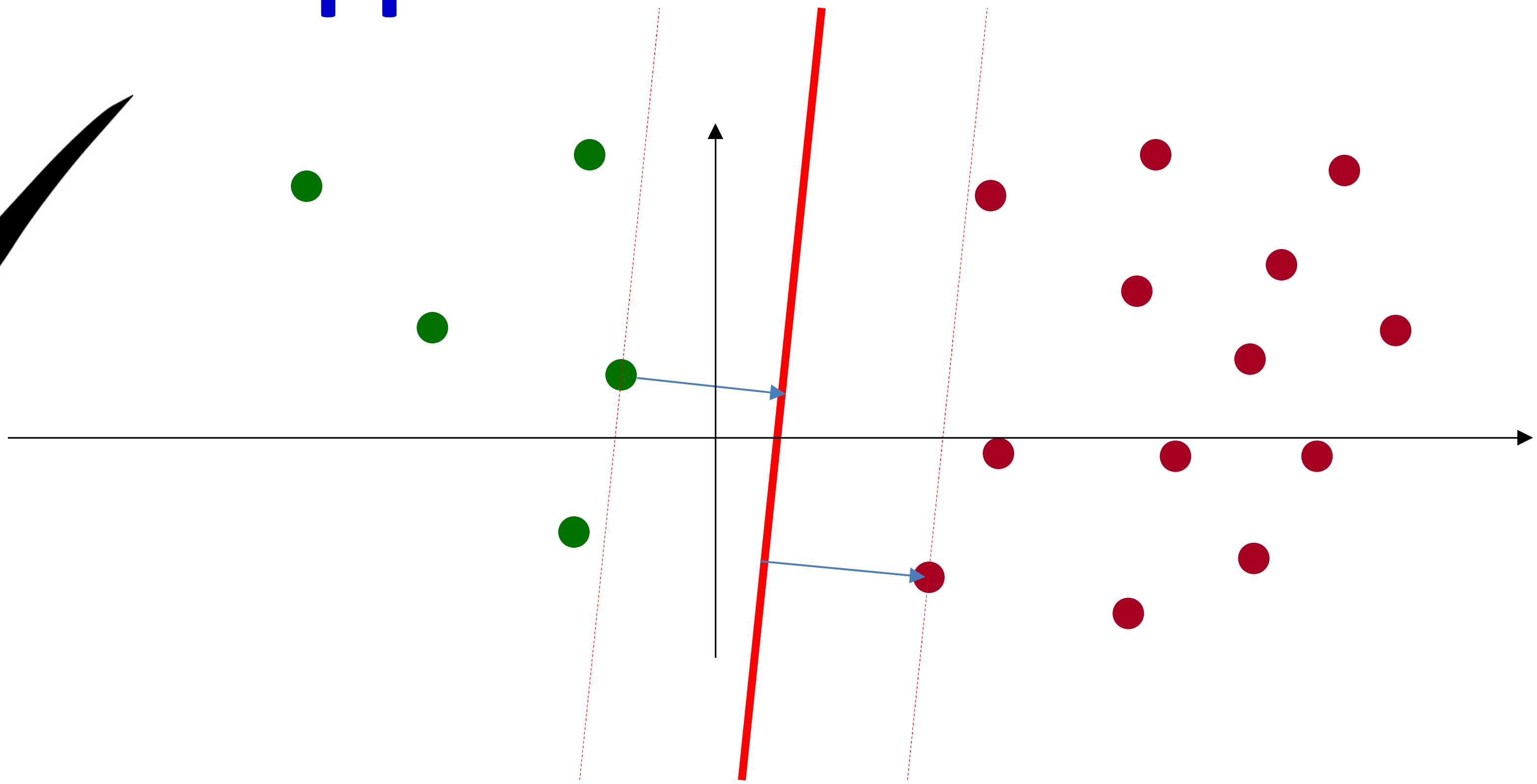
Support Vector Machine



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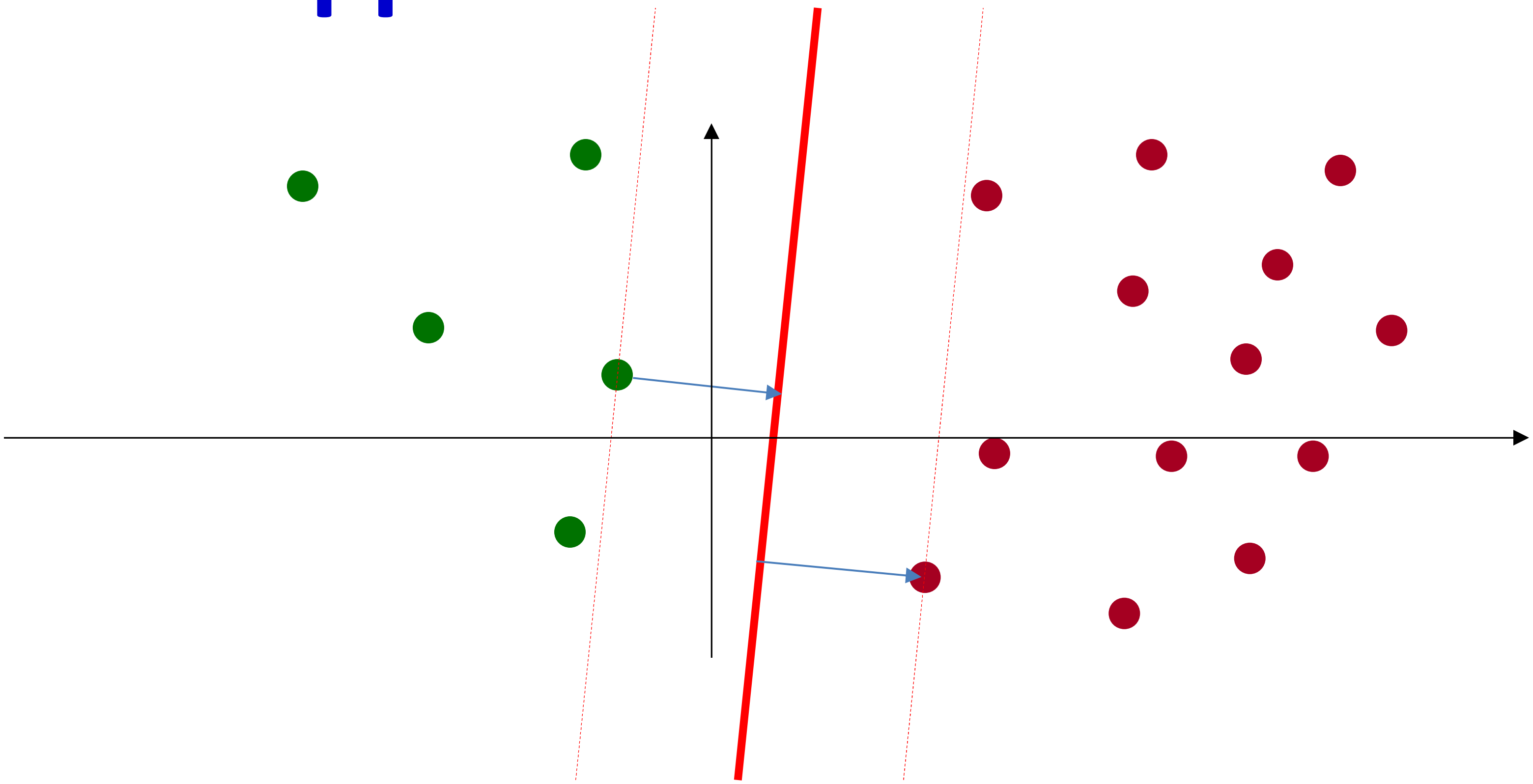
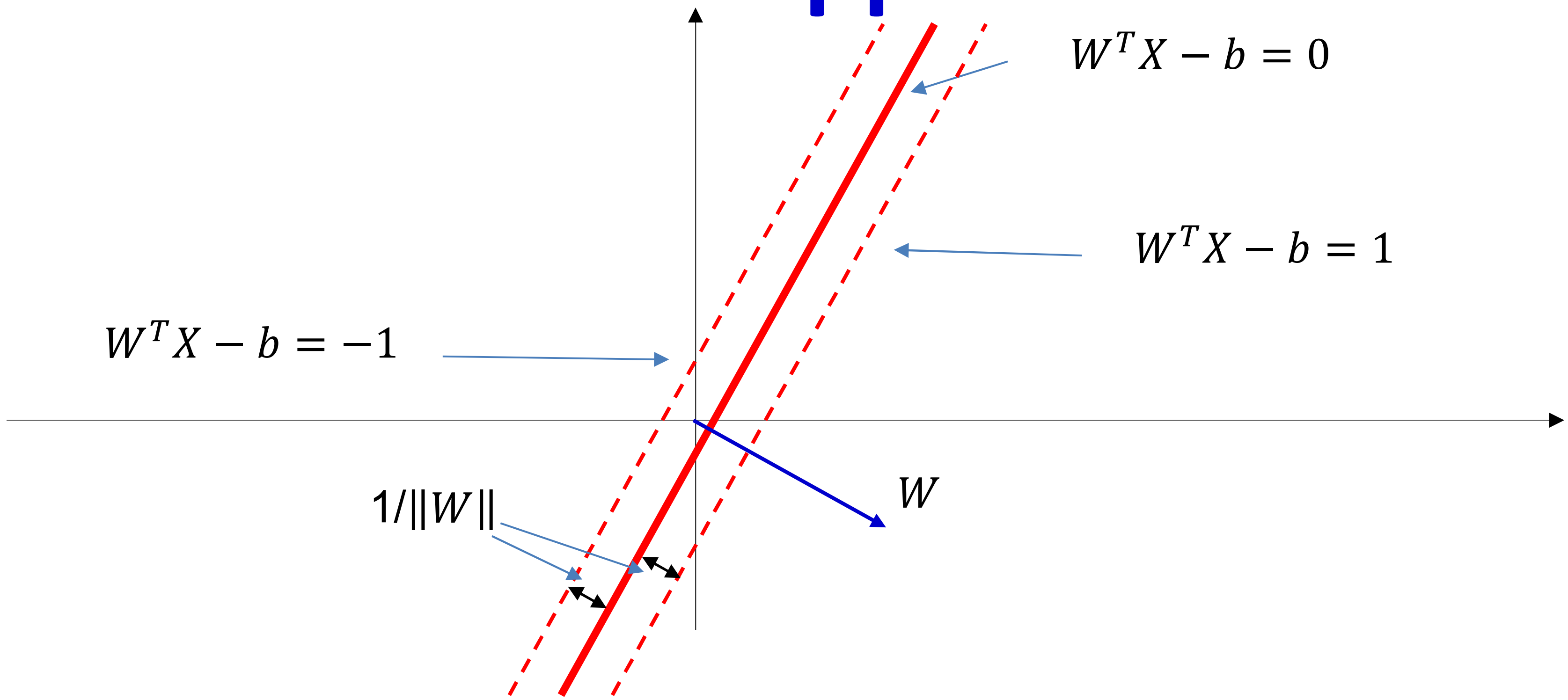
Support Vector Machine



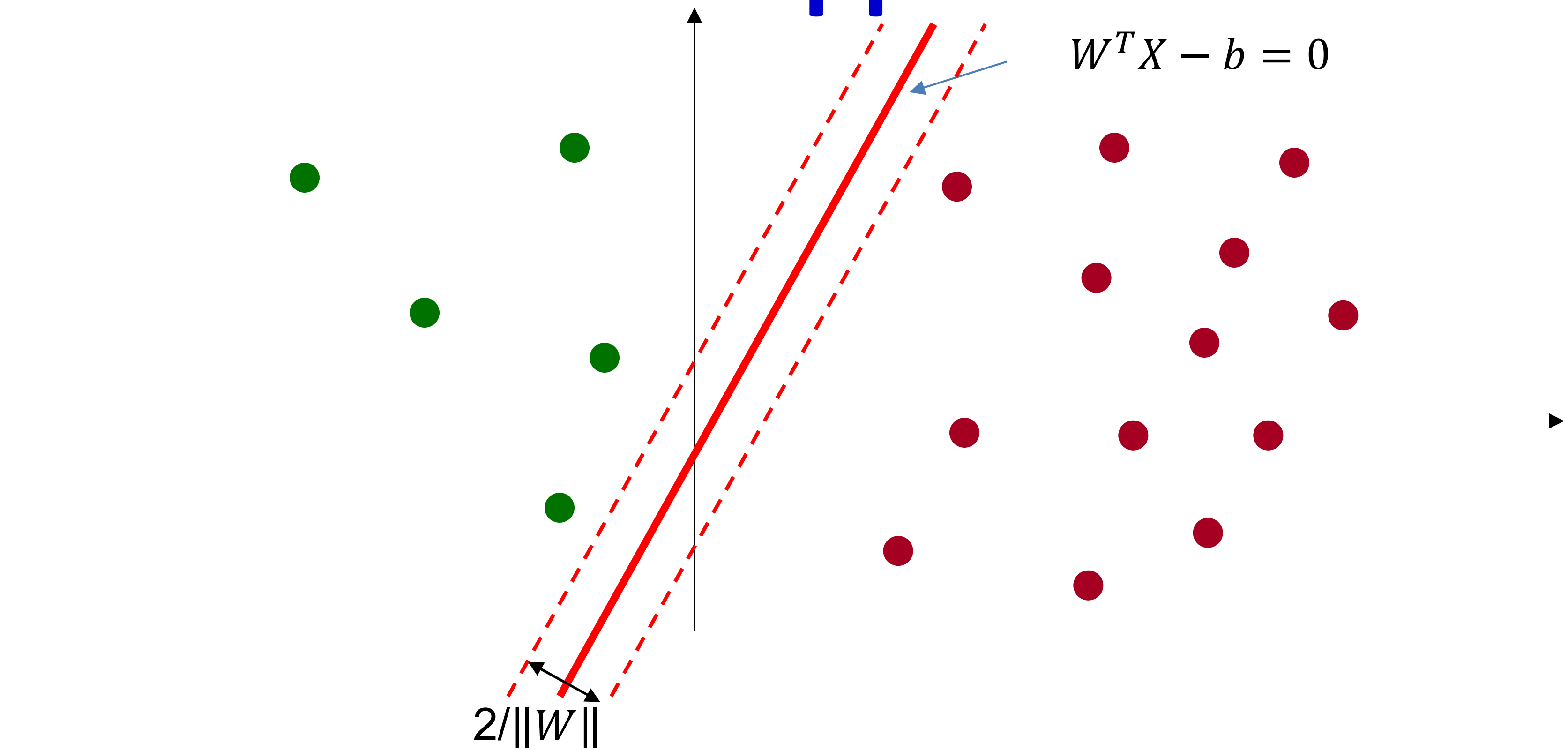
- Find the classifier such that the distance to the *closest* points is maximized
- I.e. solve *two* problems: find the closest points, and the classifier, such that the distance is maximum
  - Position the classifier in the *middle* so that the distance to the closest green = distance to the closest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

Solution Approach



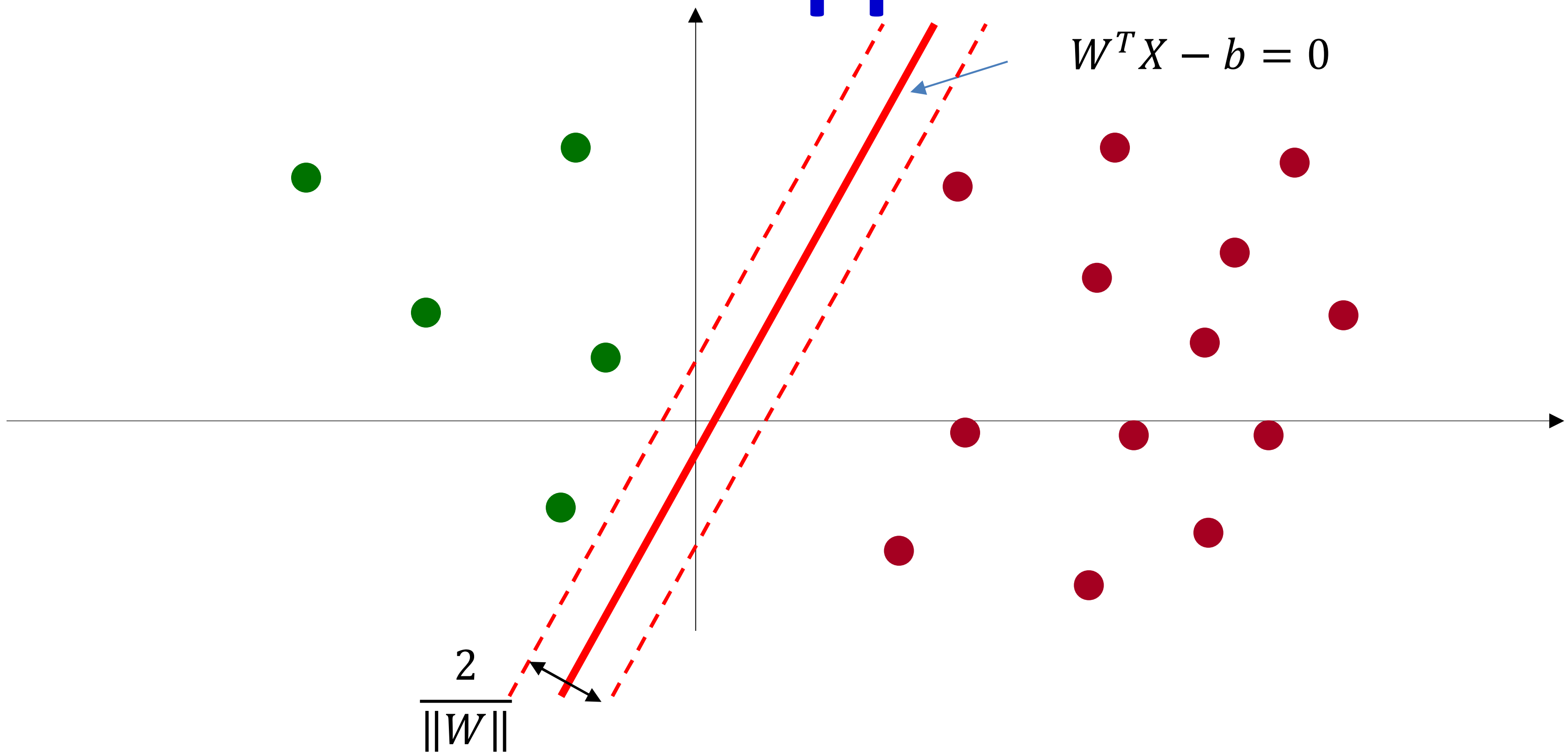
- For any hyperplane (linear classifier) $W^T X - b = 0$
- Choose two hyperplanes $W^T X - b = 1$ and $W^T X - b = -1$
  - The distance of these hyperplanes from the classifier is $1/\|W\|$
  - The total distance between the hyperplanes is $2/\|W\|$

Solution Approach



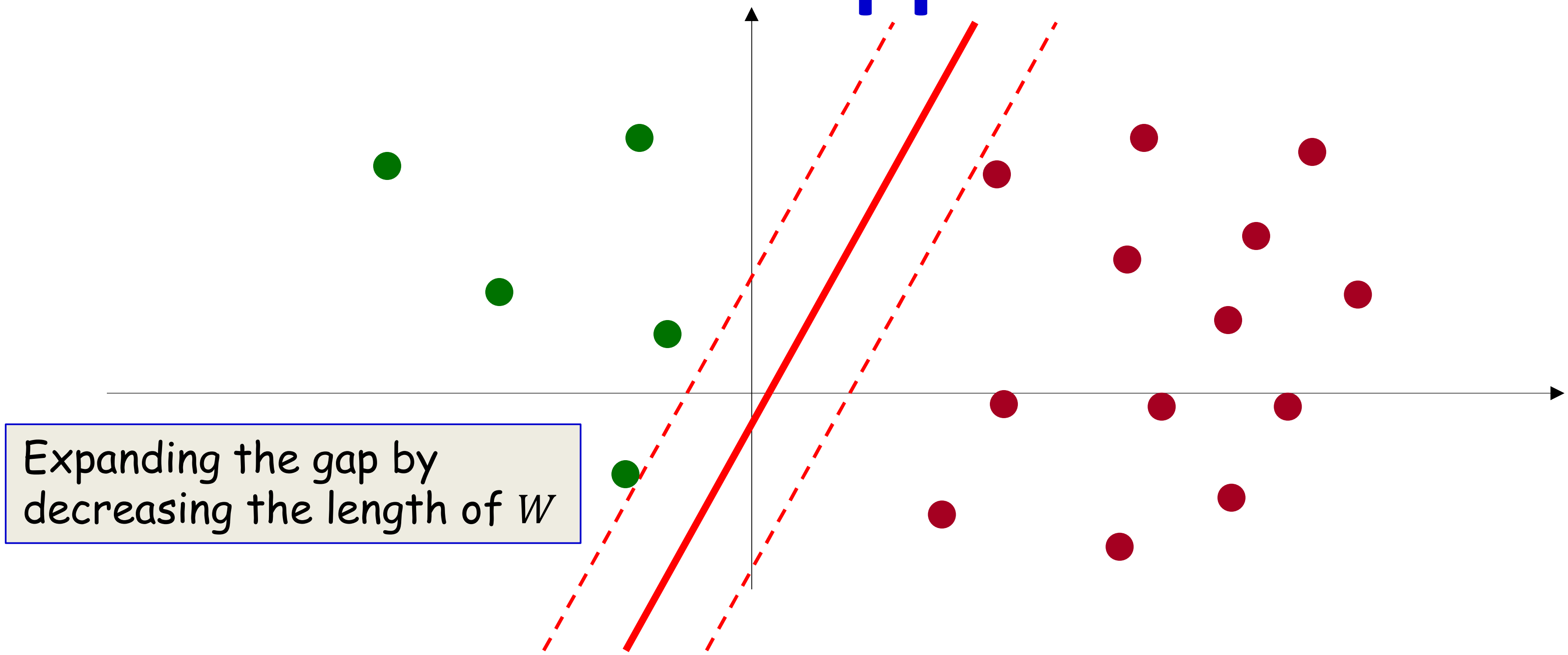
- Constraint: Perfect classification with a margin
- Choose the hyperplanes such that
  - All positive points are on the positive side of the positive hyperplane
  - All negative points are on the negative side of the negative hyperplane

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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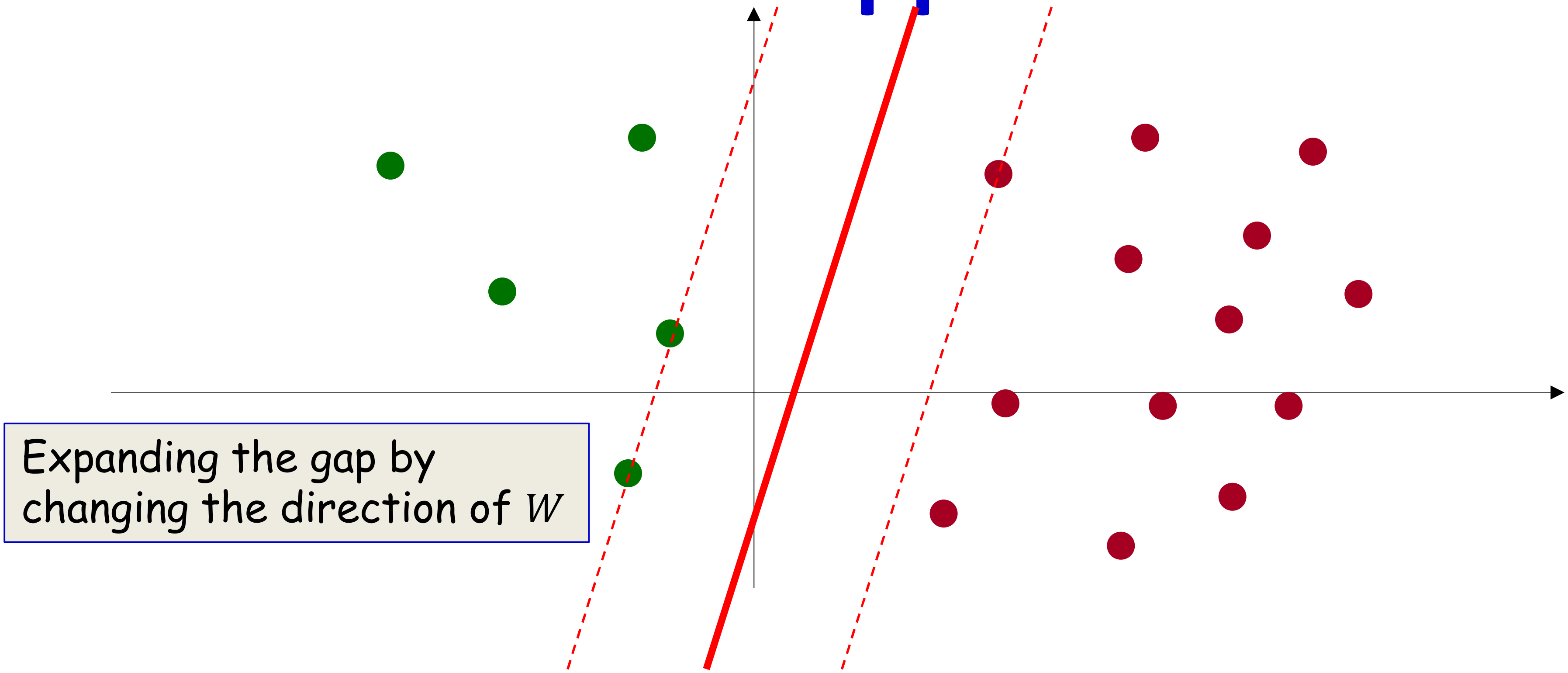

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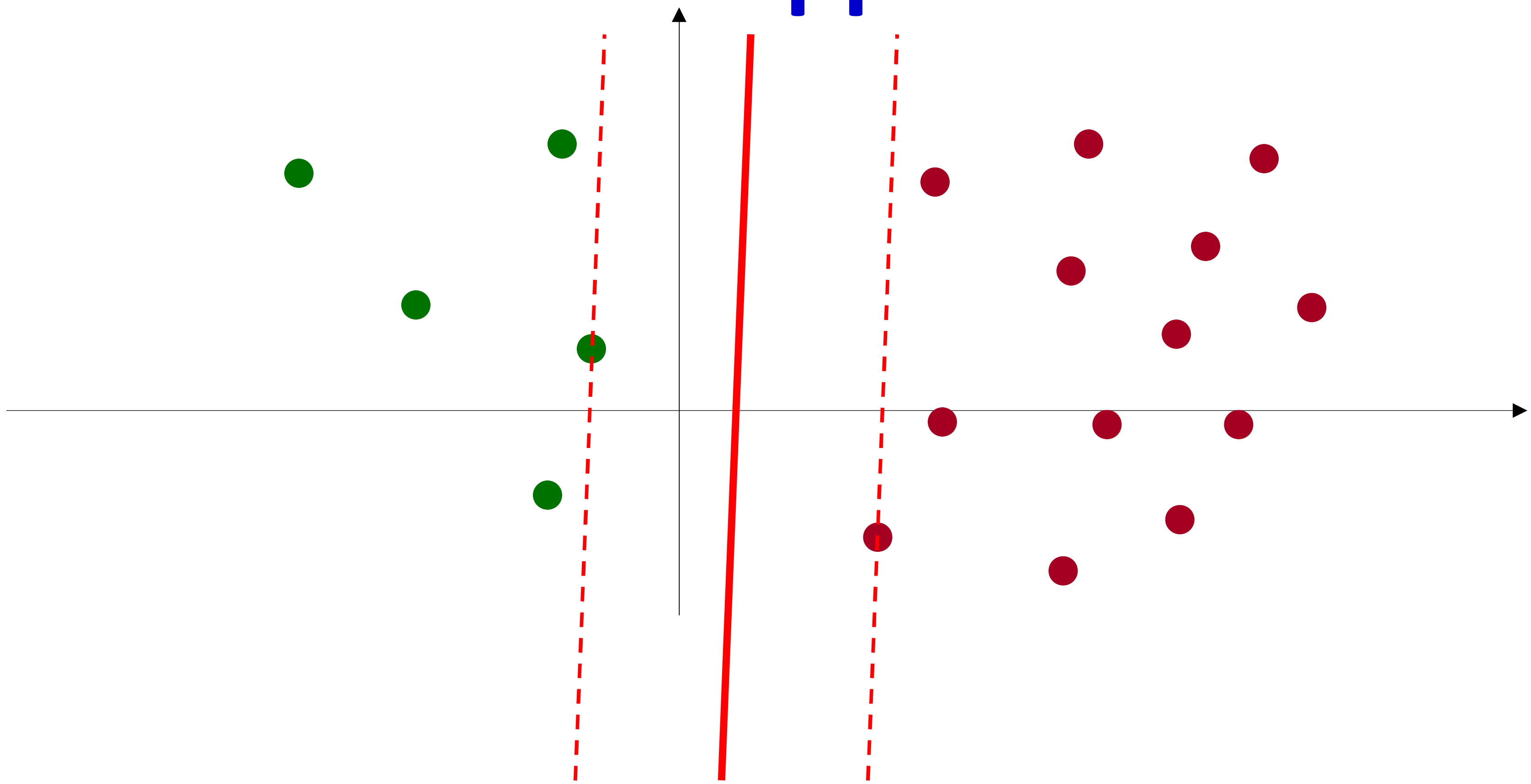

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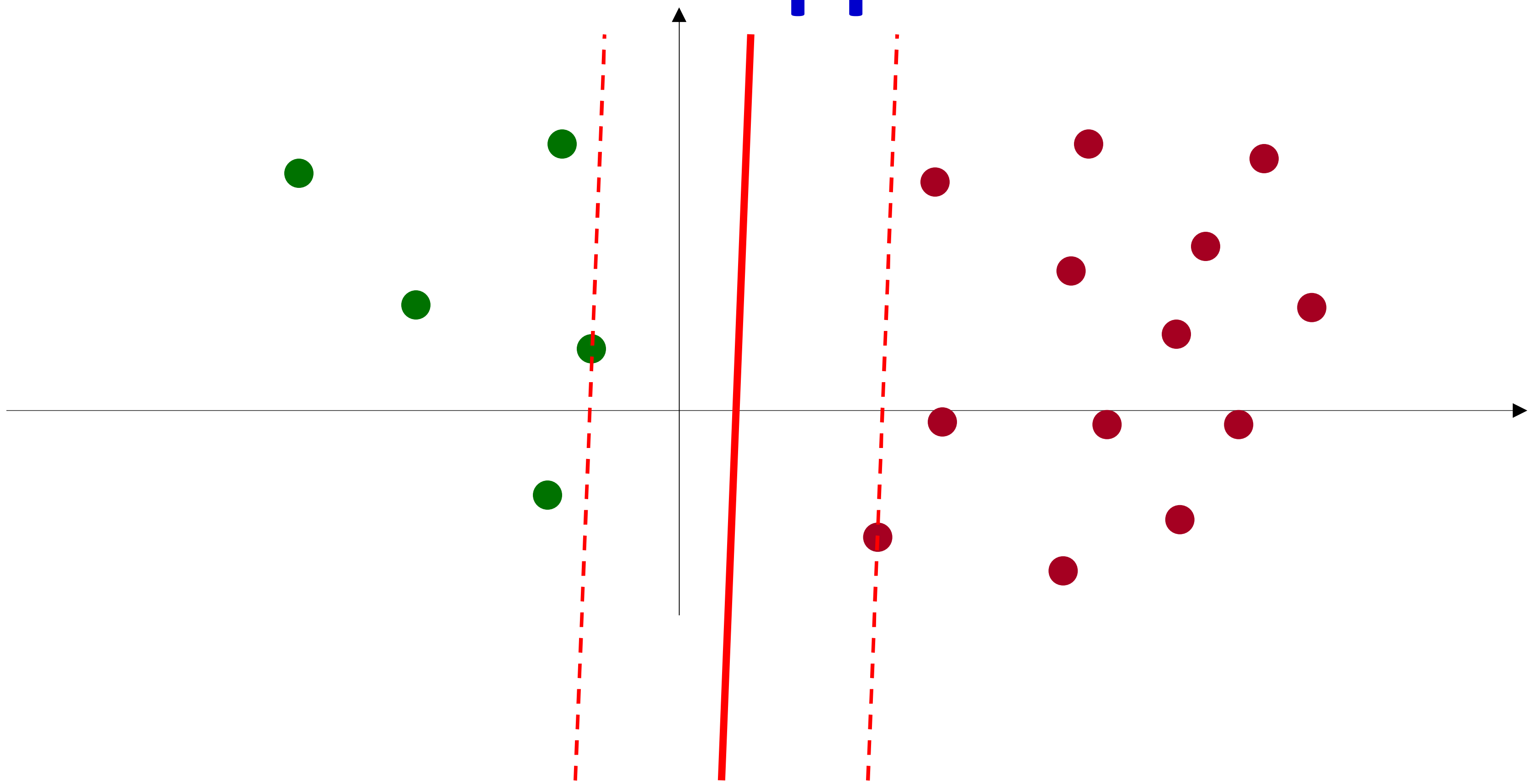
Solution Approach



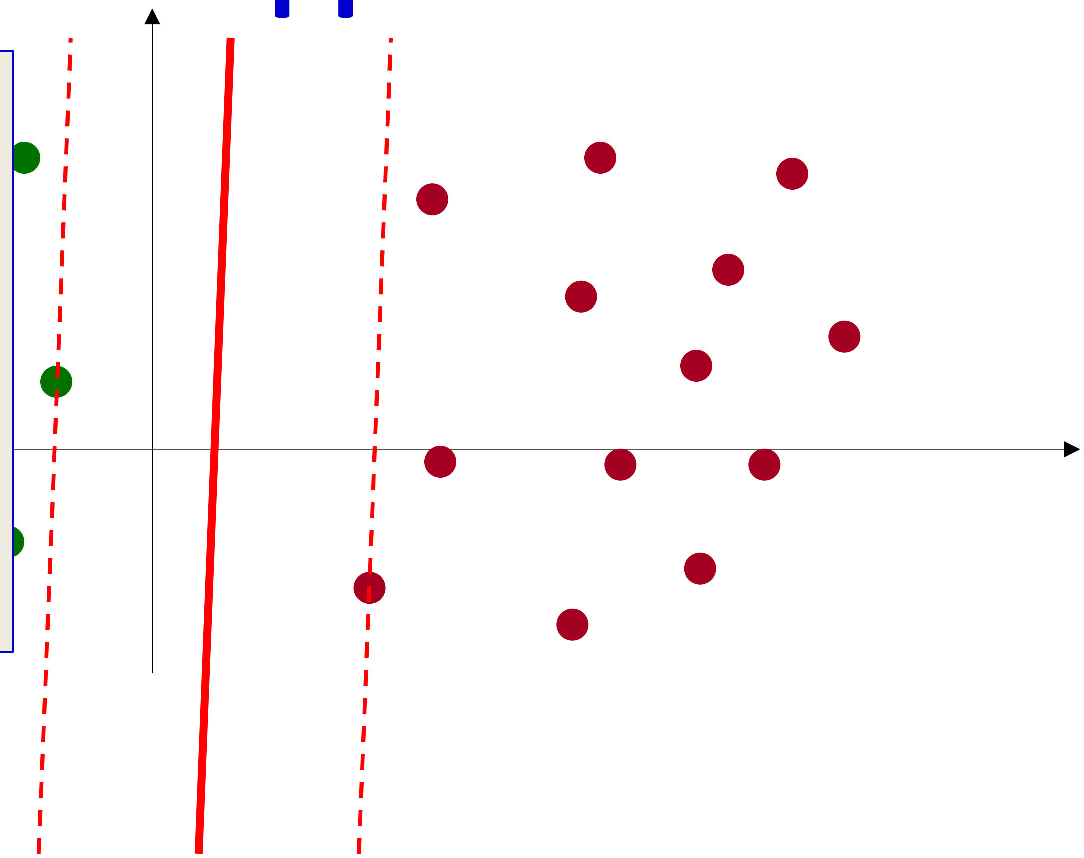
- The distance between the hyperplanes is $\frac{2}{\|W\|}$
- Maximize this distance. I.e. ..
- **Minimize $\|W\|$ such that**
  - all training points are on the "outside" of the appropriate hyperplane

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

Let’s 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

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

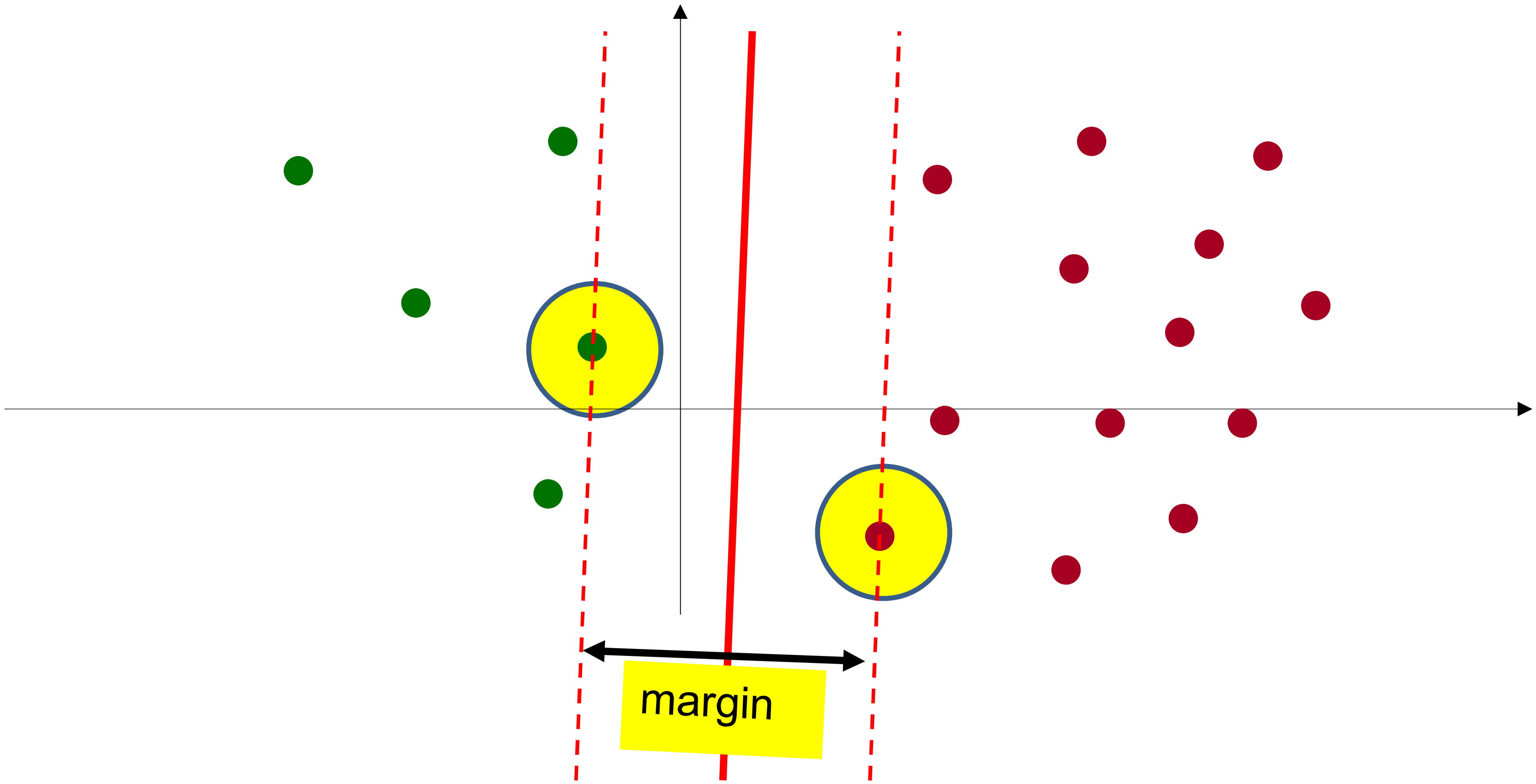
Solving the optimization

- 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



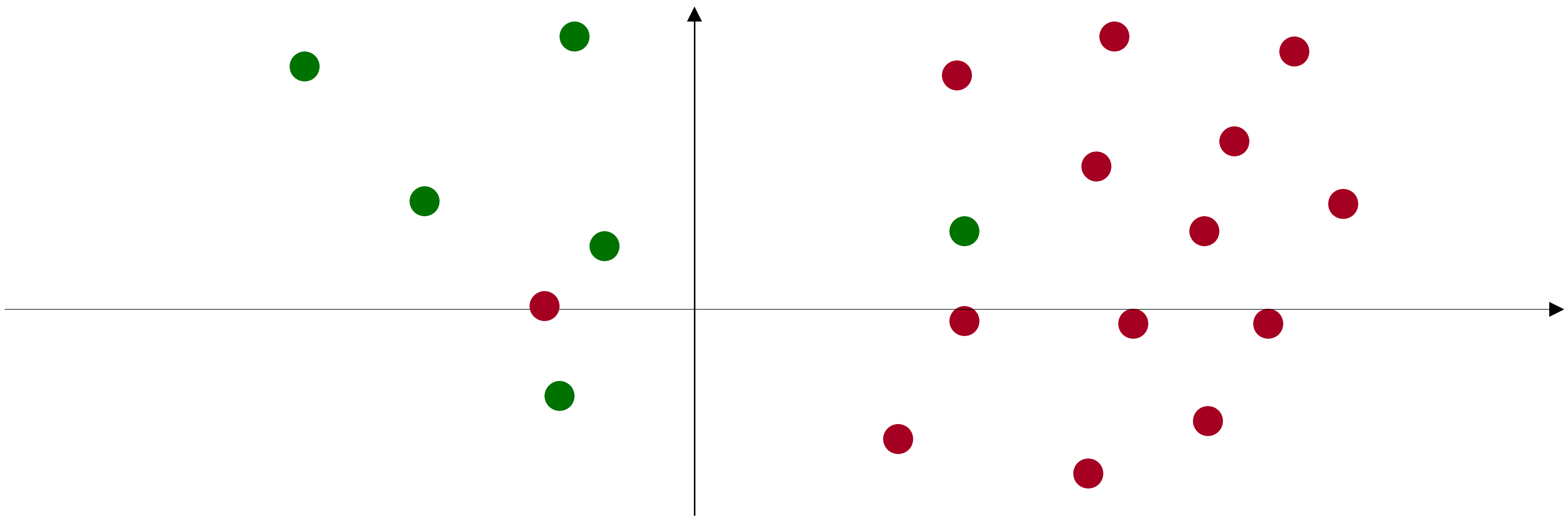
- Maximizes the *margin*
- This is a *max-margin* classifier
- The boundary samples are called support vectors
  - All the information about the classifier is in these support vectors

Poll 2

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?

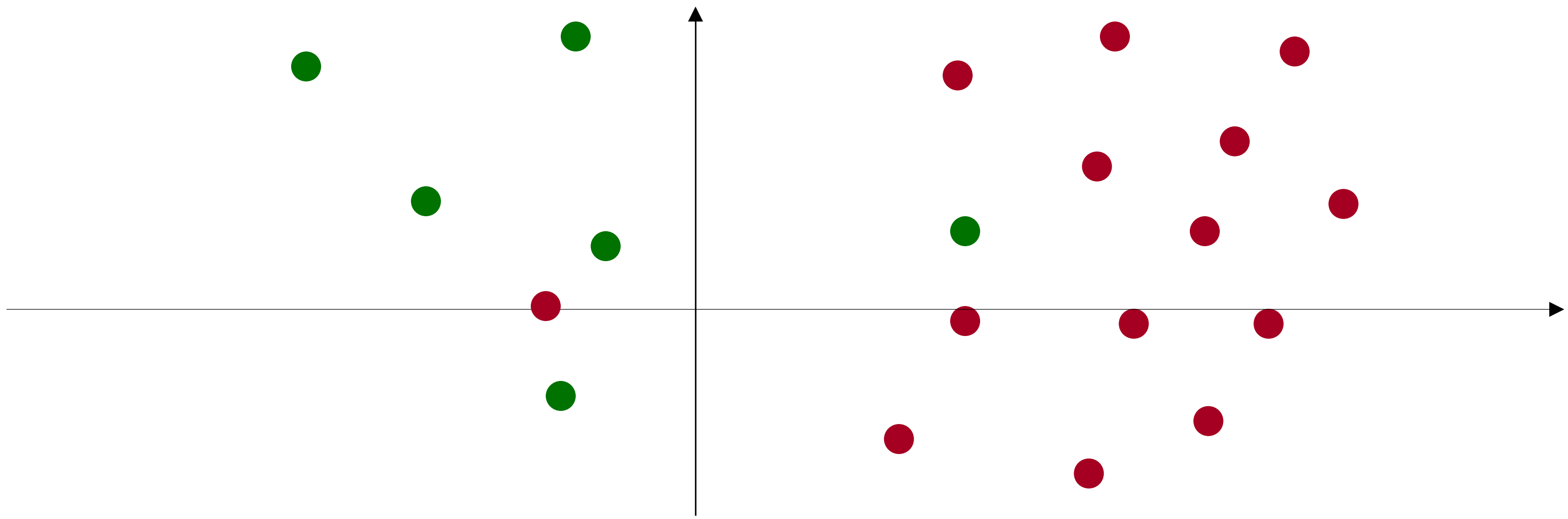
Original Problem

- This is a quadratic programming problem!

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

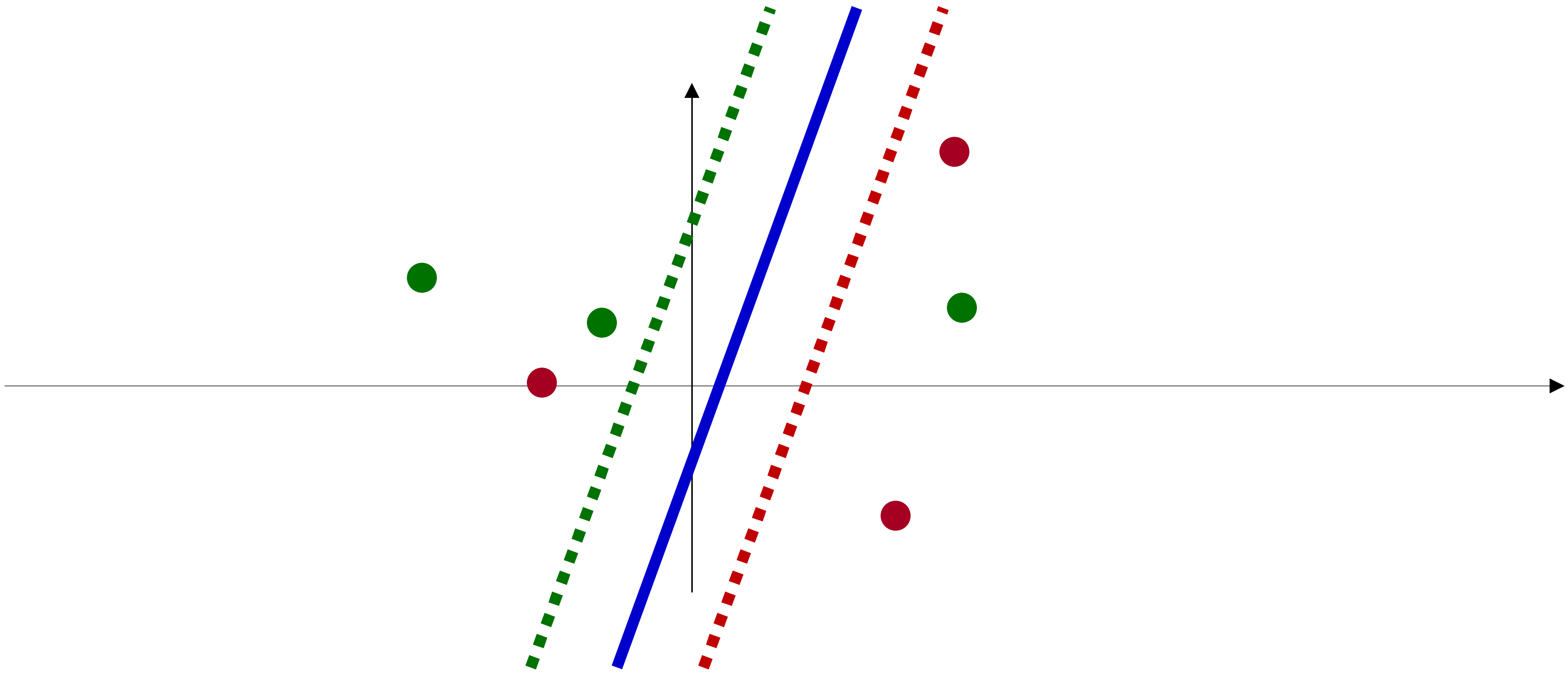
- Maximize the distance between the planes
- Subject to the constraint that all training data instances are on the "correct" side of the plane
- When data are not linearly separable, this constraint can never be satisfied

Introducing the *slack* variable



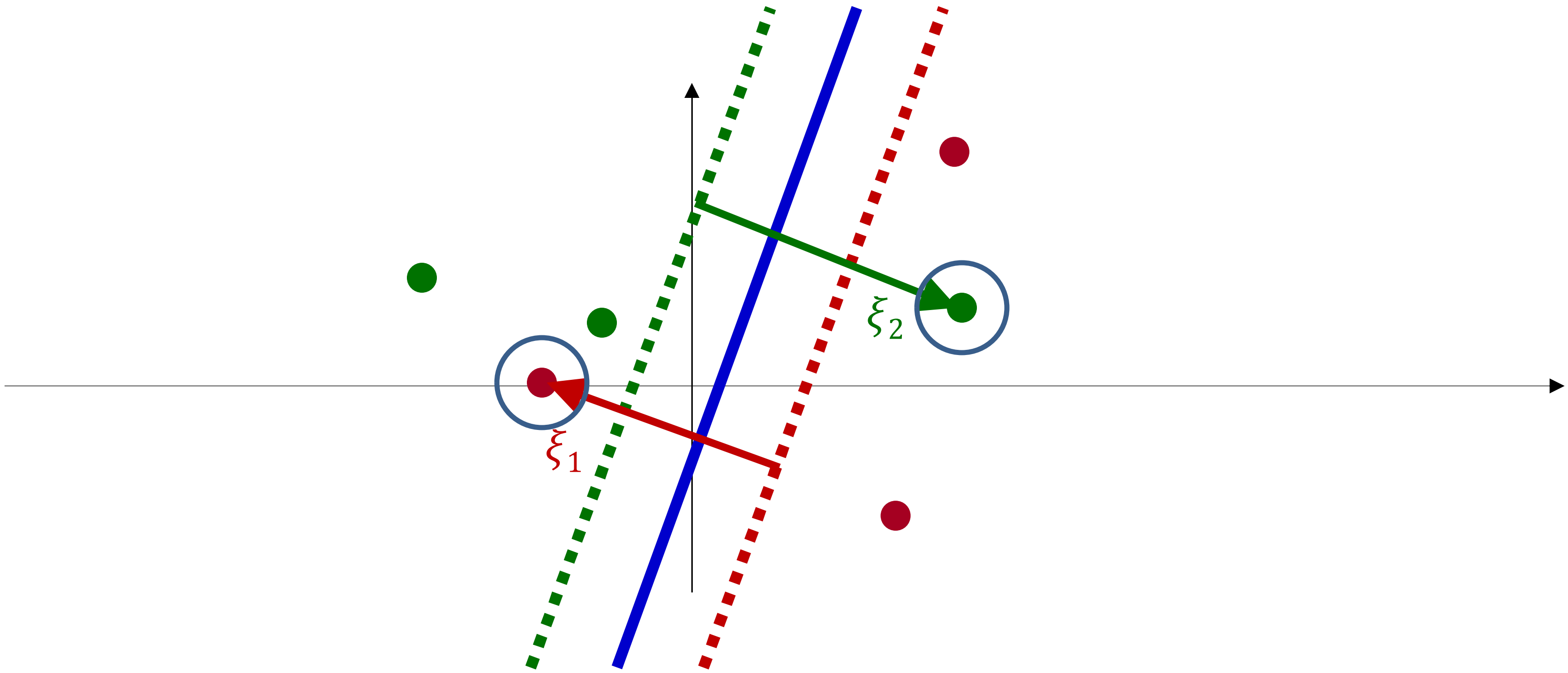
- What if the data are not separable?

Introducing the *slack* variable



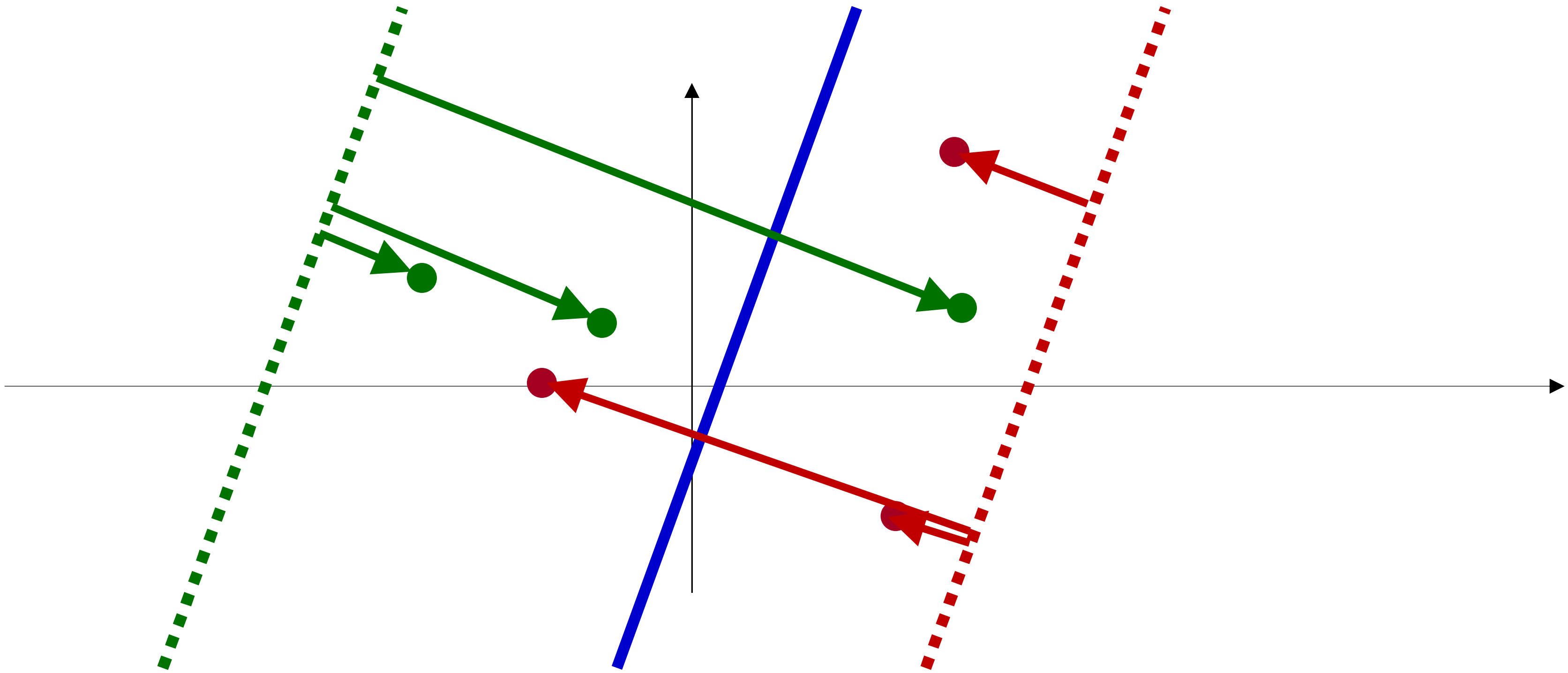
- For every training instance, introduce a *slack* variable ξ
- The slack variable is the maximum distance you have to *shift* the boundary plane to move the point to the "correct" side

Introducing the *slack* variable



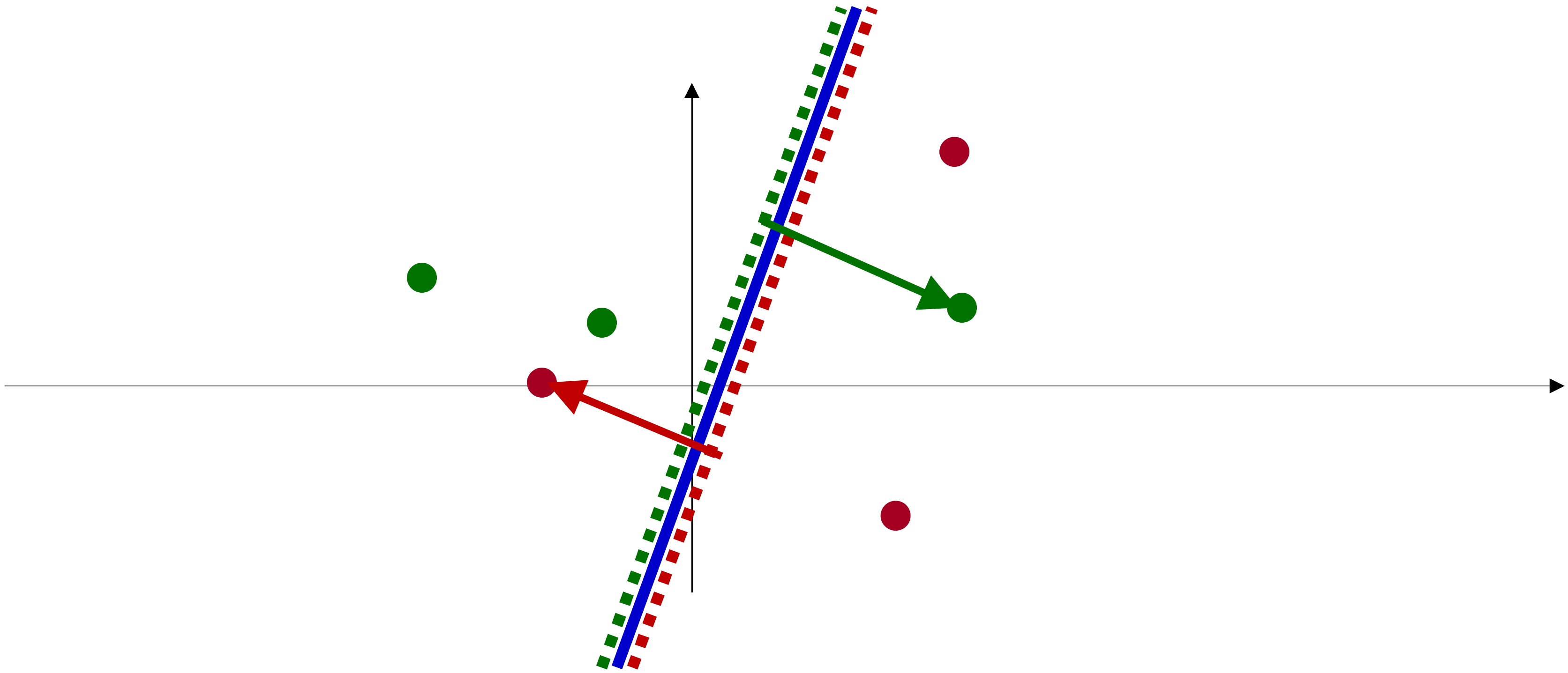
- For every training instance, introduce a *slack* variable ξ
- The slack variable is the *reverse* distance from the *margin* plane of the training instance
  - This will be non-zero only for some instances
  - **Ideally this should be minimum**

Introducing the *slack* variable



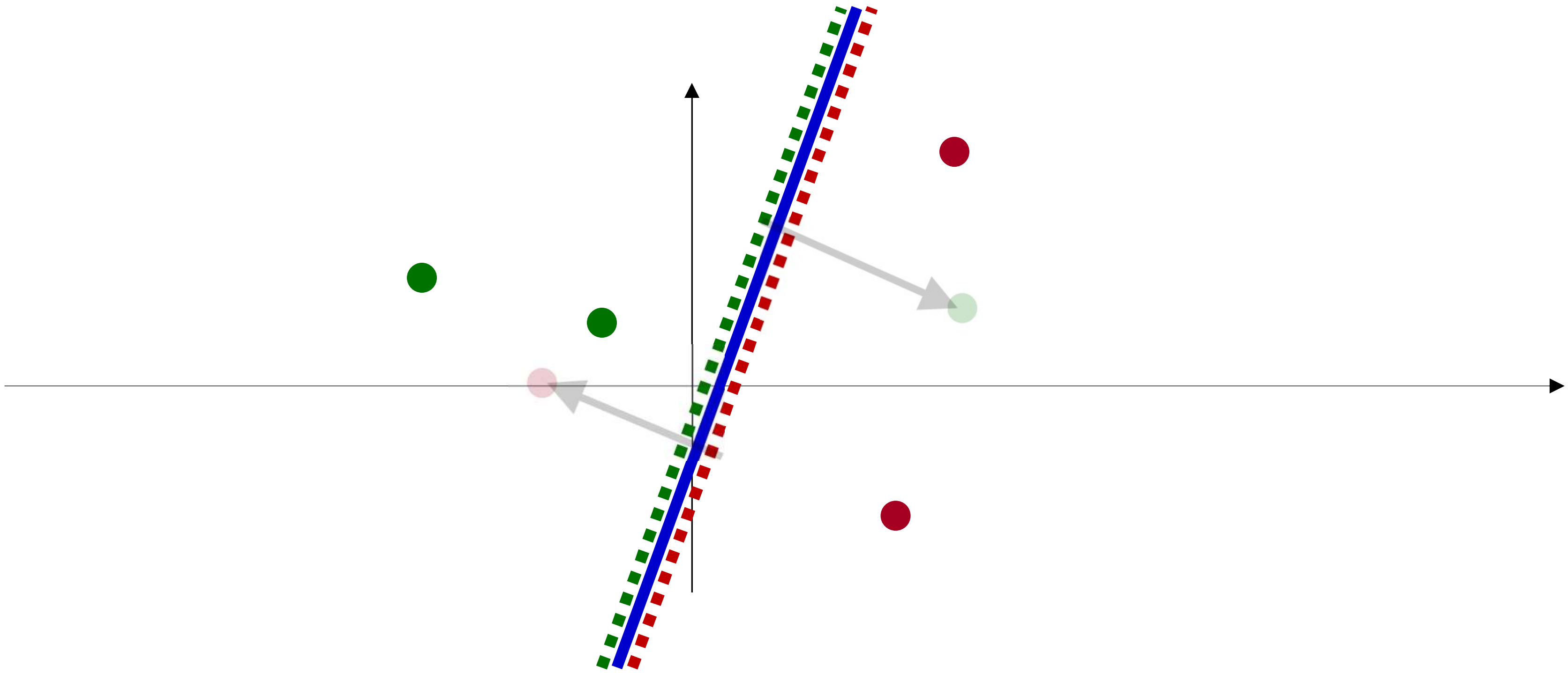
- The total length of slack variables varies with the boundary
- If you push the boundaries too far you will have a greater length of slack variable
  - Which contradicts our desire that they should be minimum

Introducing the *slack* variable



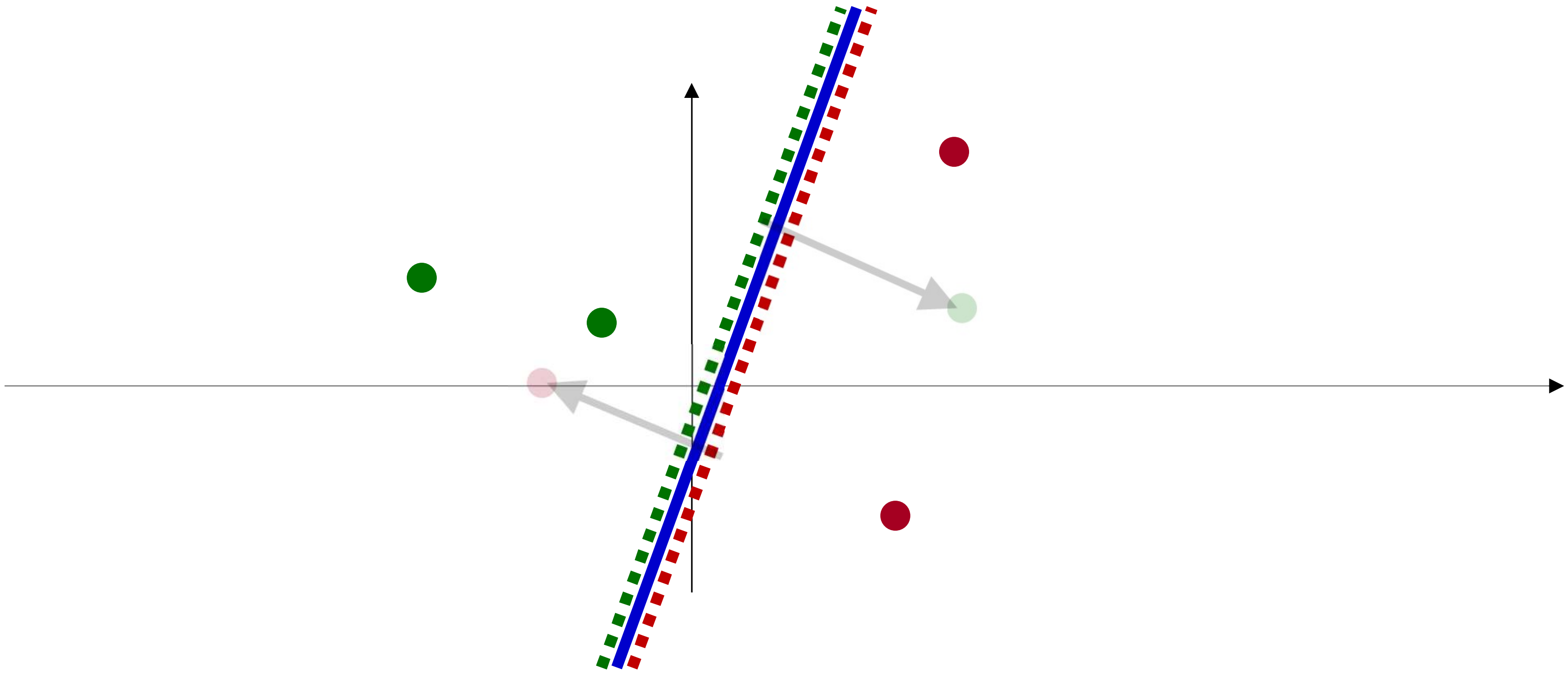
- If they are very close, only the *inseparable points* will have non-zero slack variable
  - The minimum slack value is when the margin planes coincide with the linear classifier

Introducing the *slack* variable



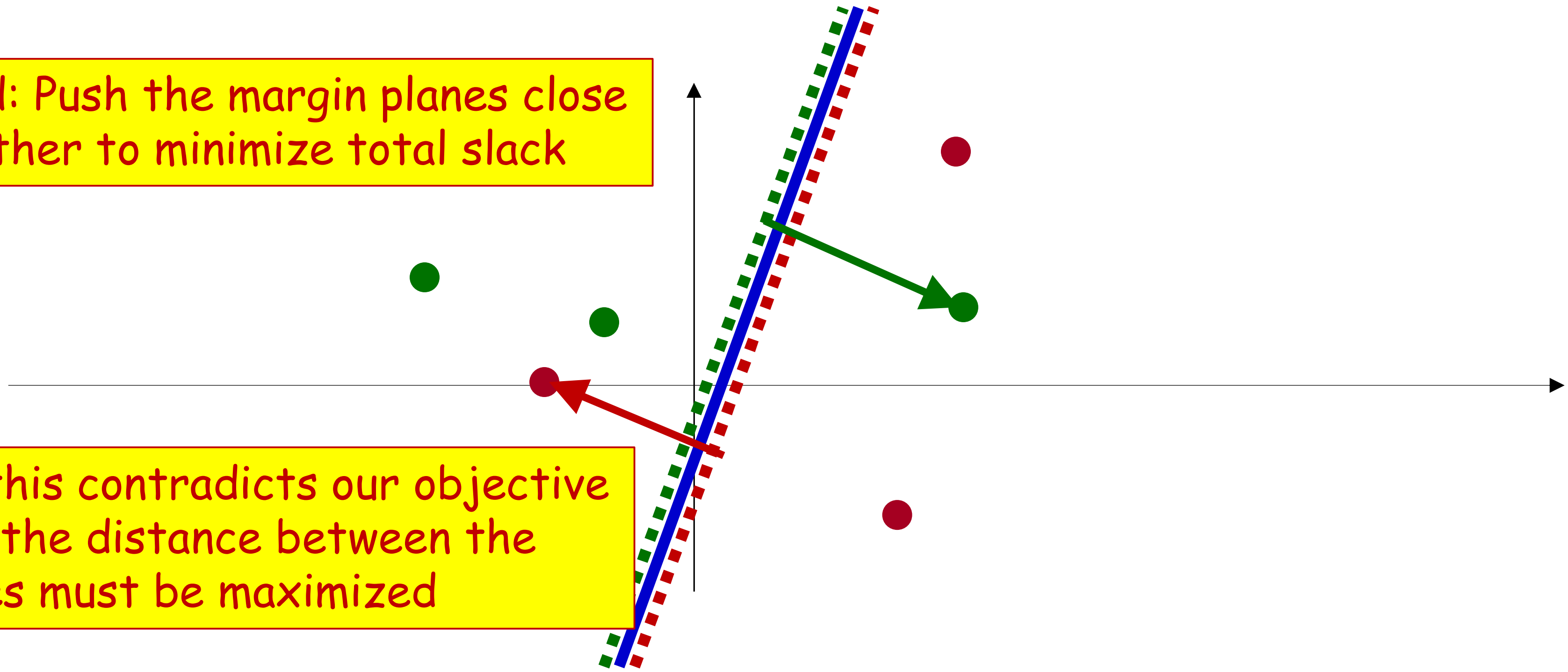
- If they are very close, only the *inseparable points* will have non-zero slack variable
  - The minimum slack value is when the margin planes coincide with the linear classifier
- For linearly separable classes, if the boundary planes are close enough, the total slack length will be 0

Introducing the *slack* variable



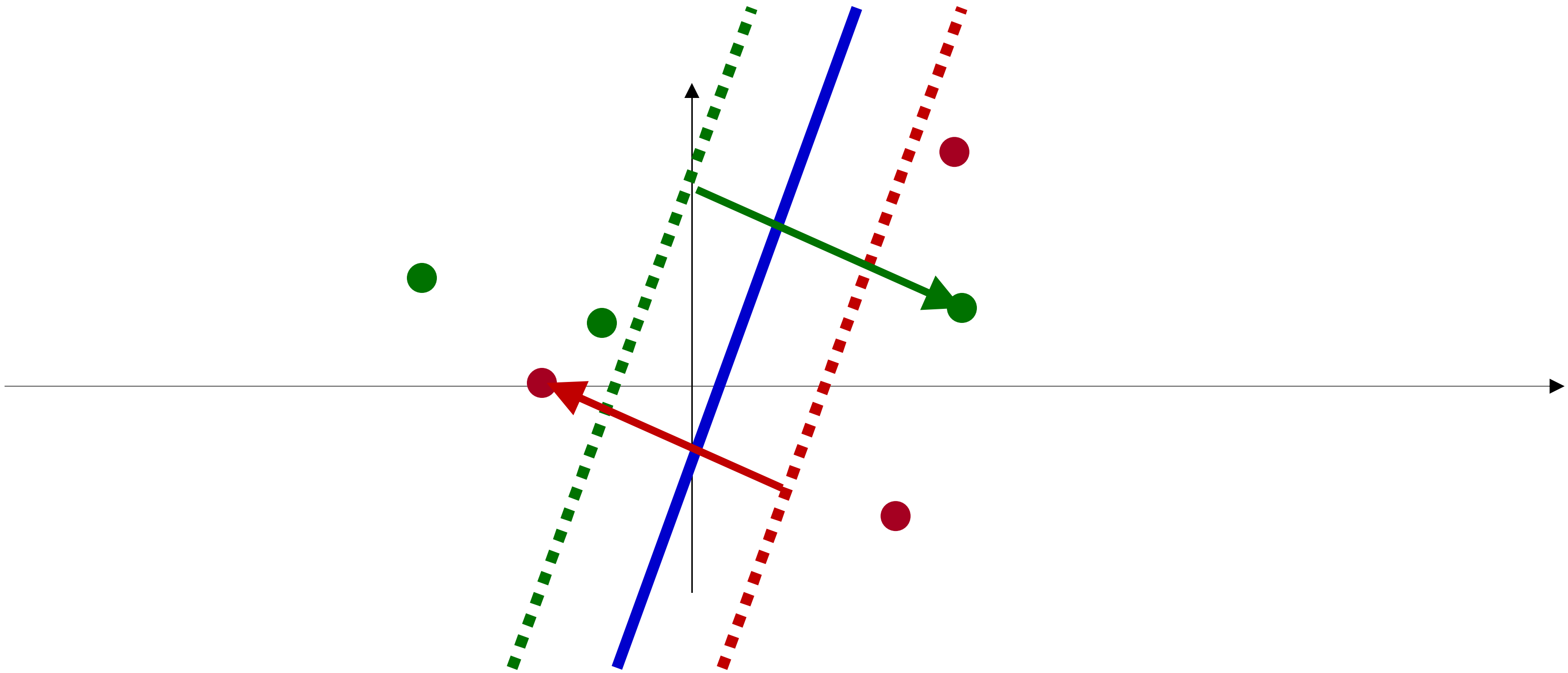
- Problem: If they are too close, the planes violate our desire to *maximize* the margin

Introducing the *slack* variable



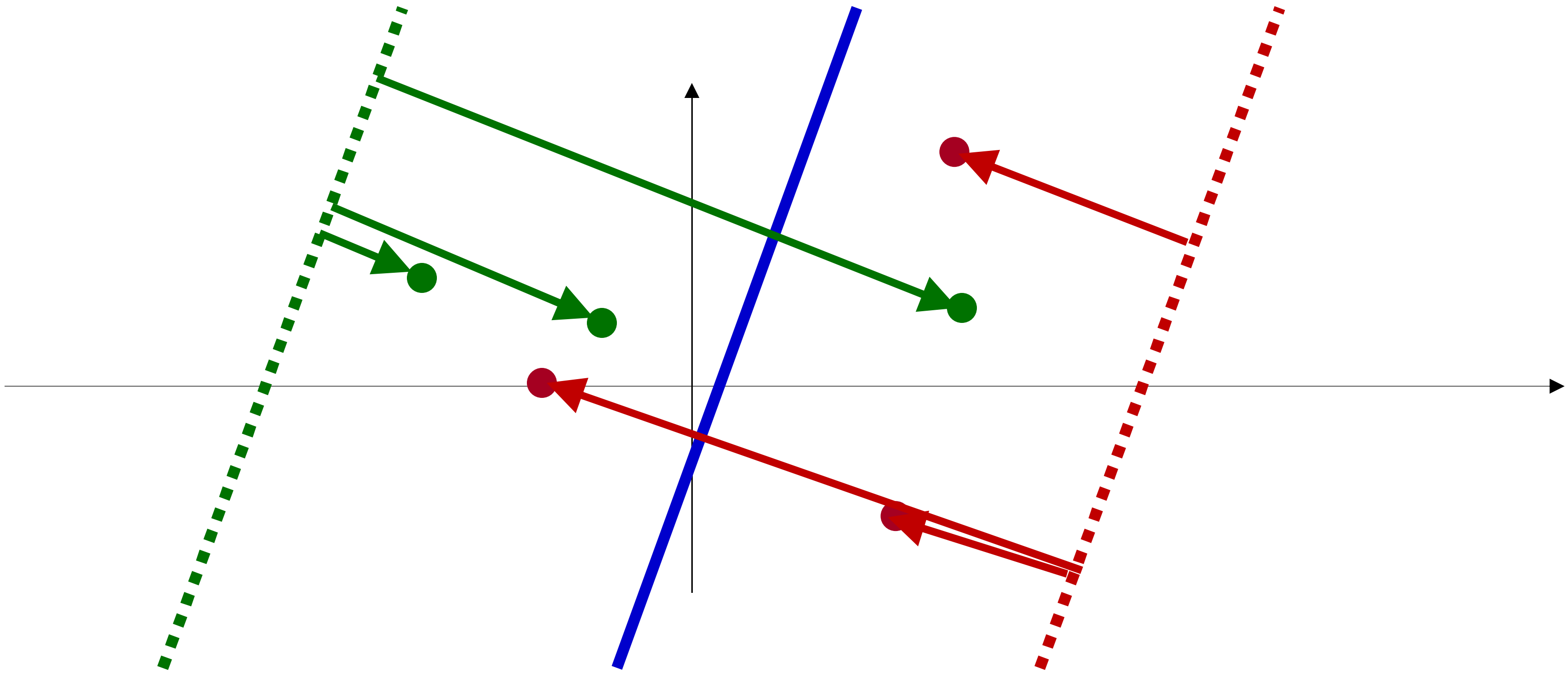
- Contradicting requirements..

New Objective



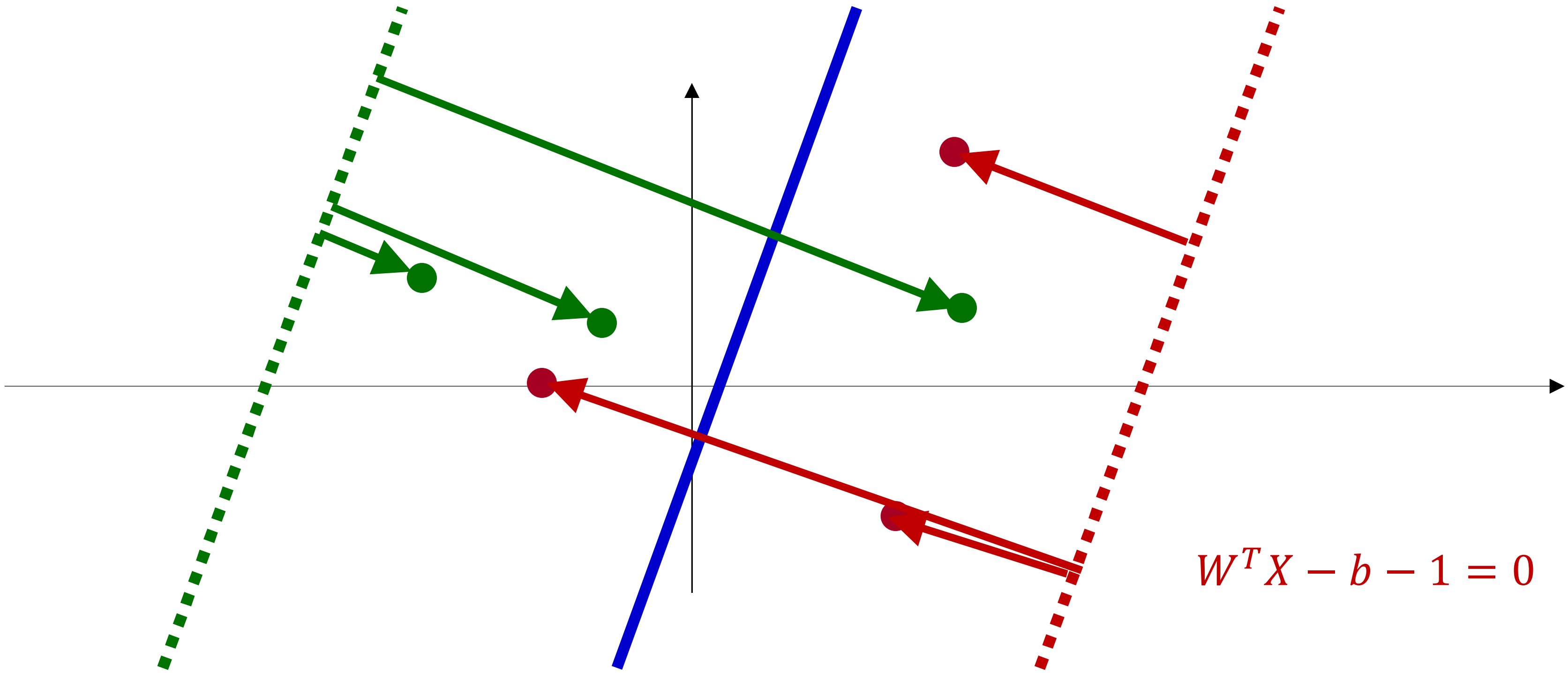
- Simultaneously
  - Maximize distance between planes
  - Minimize total slack length

Quantifying Slack Length



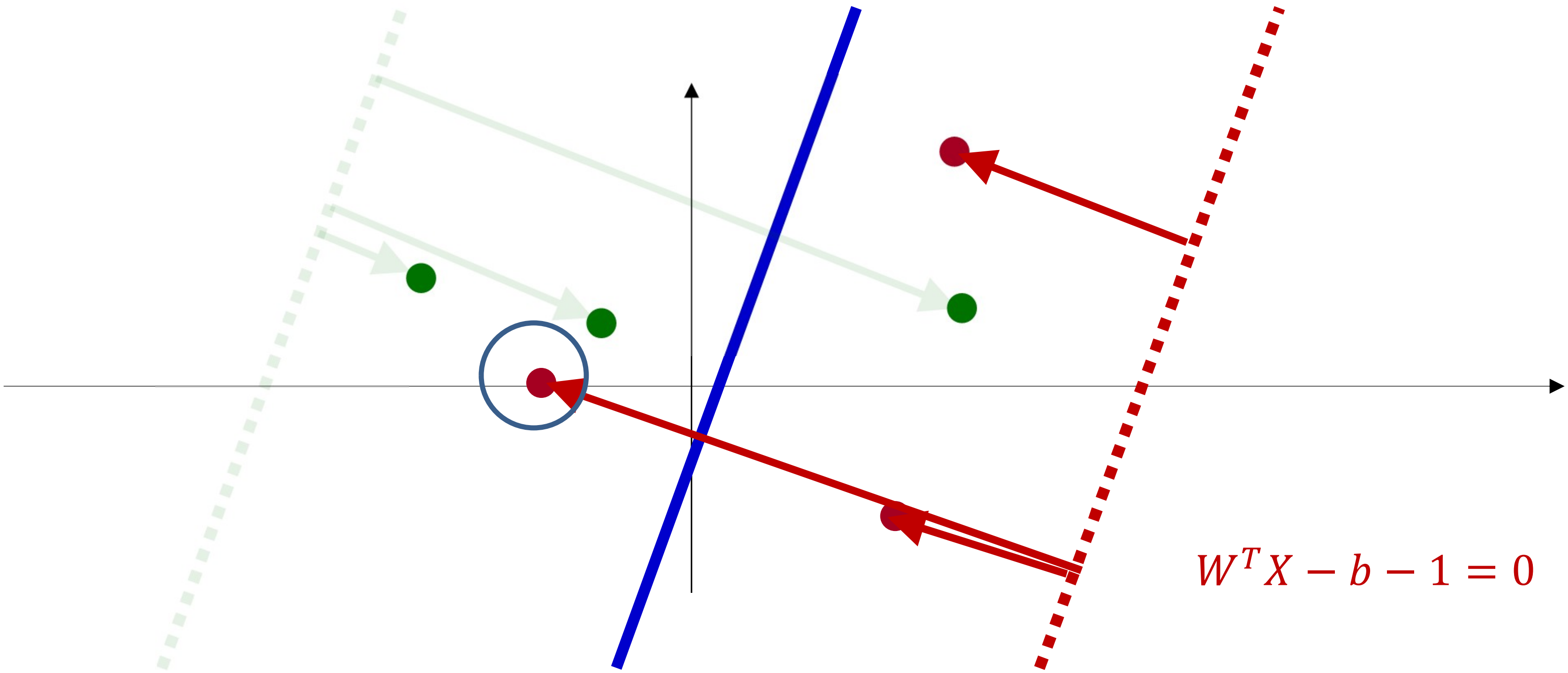
- We need a formula for the total slack length first..

Quantifying Slack Length



- The *positive* margin plane is given by
- $W^T X - b - 1 = 0$
- 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

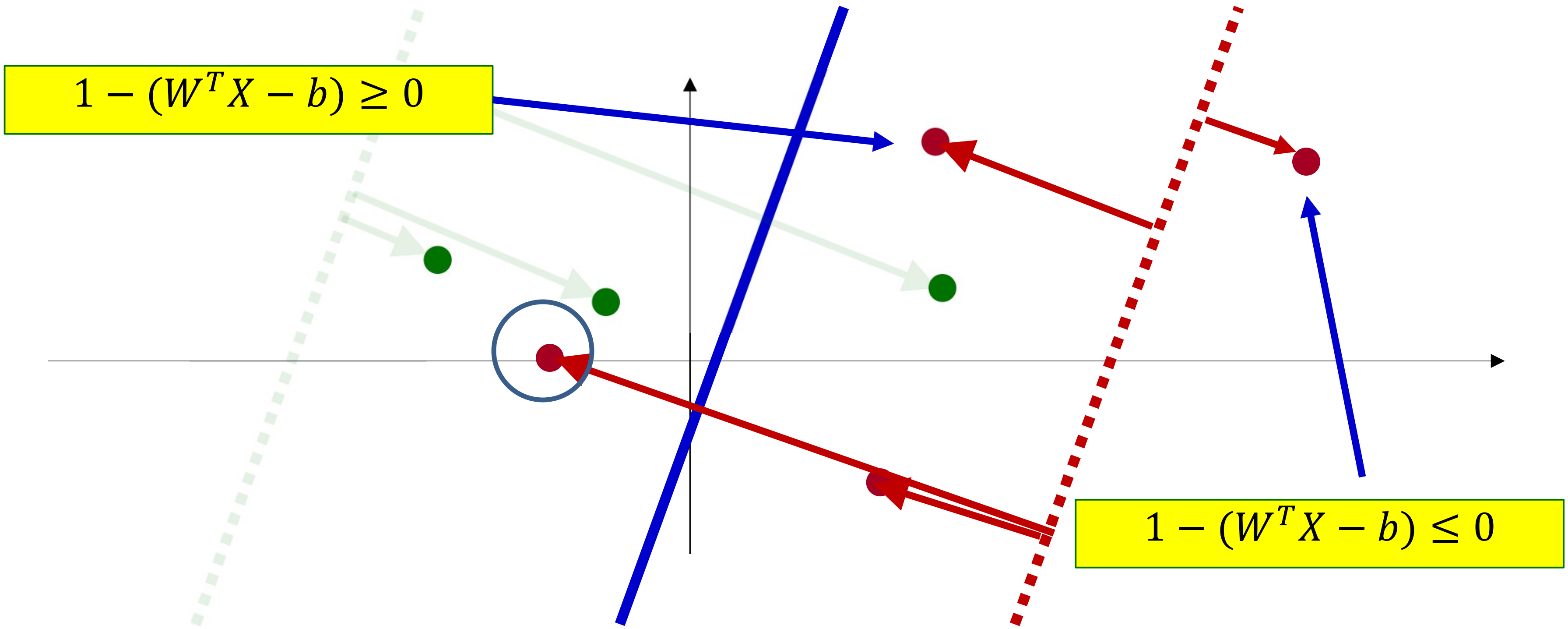


- The (unnormalized) distance of any X from this plane

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

- 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

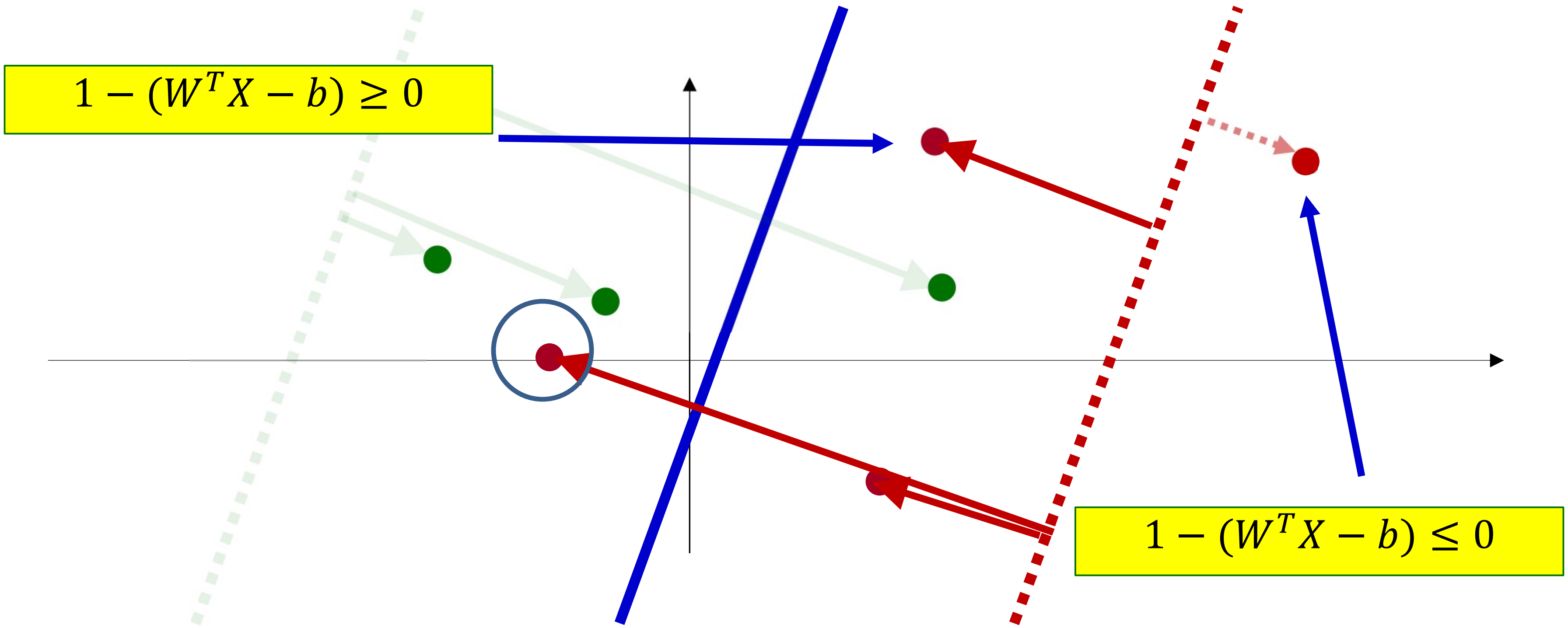


- The *negated* (unnormalized) distance of any X from this plane

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

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

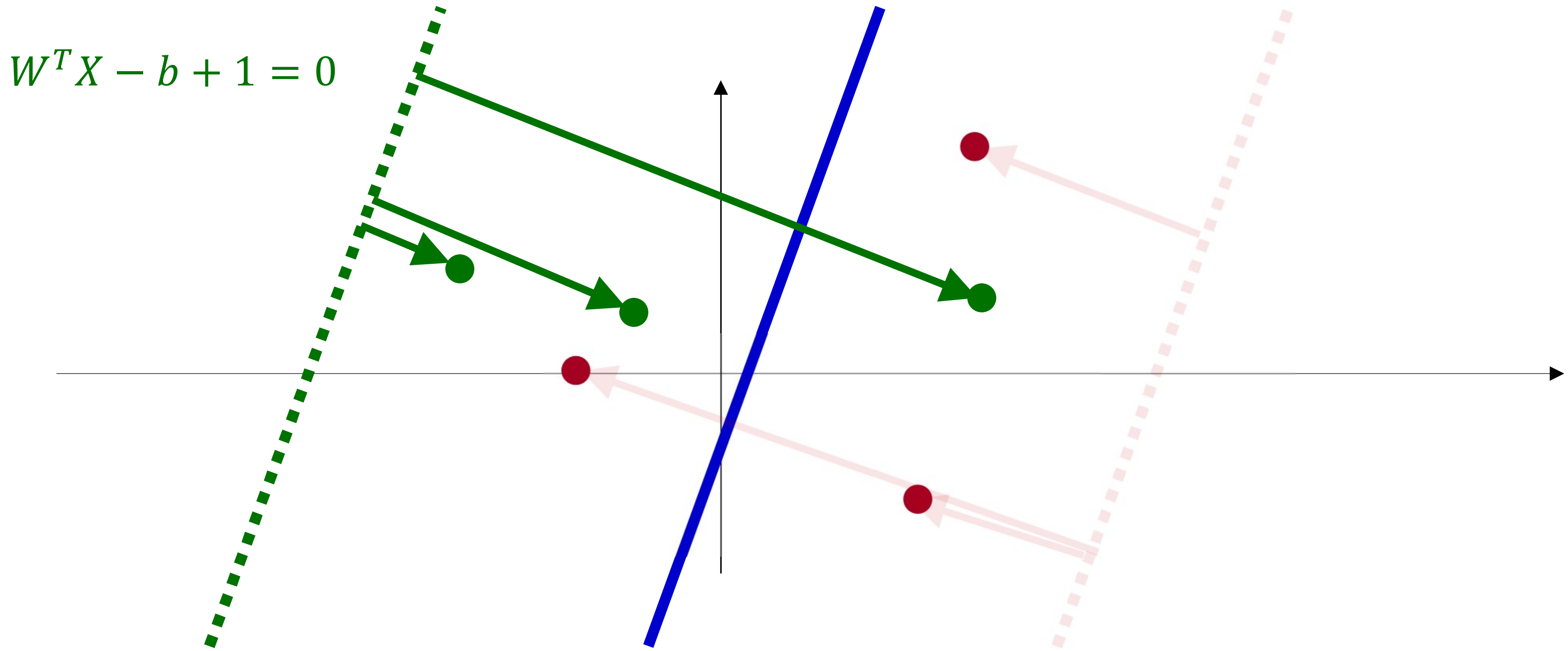
Quantifying Slack Length



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

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

Quantifying Slack Length

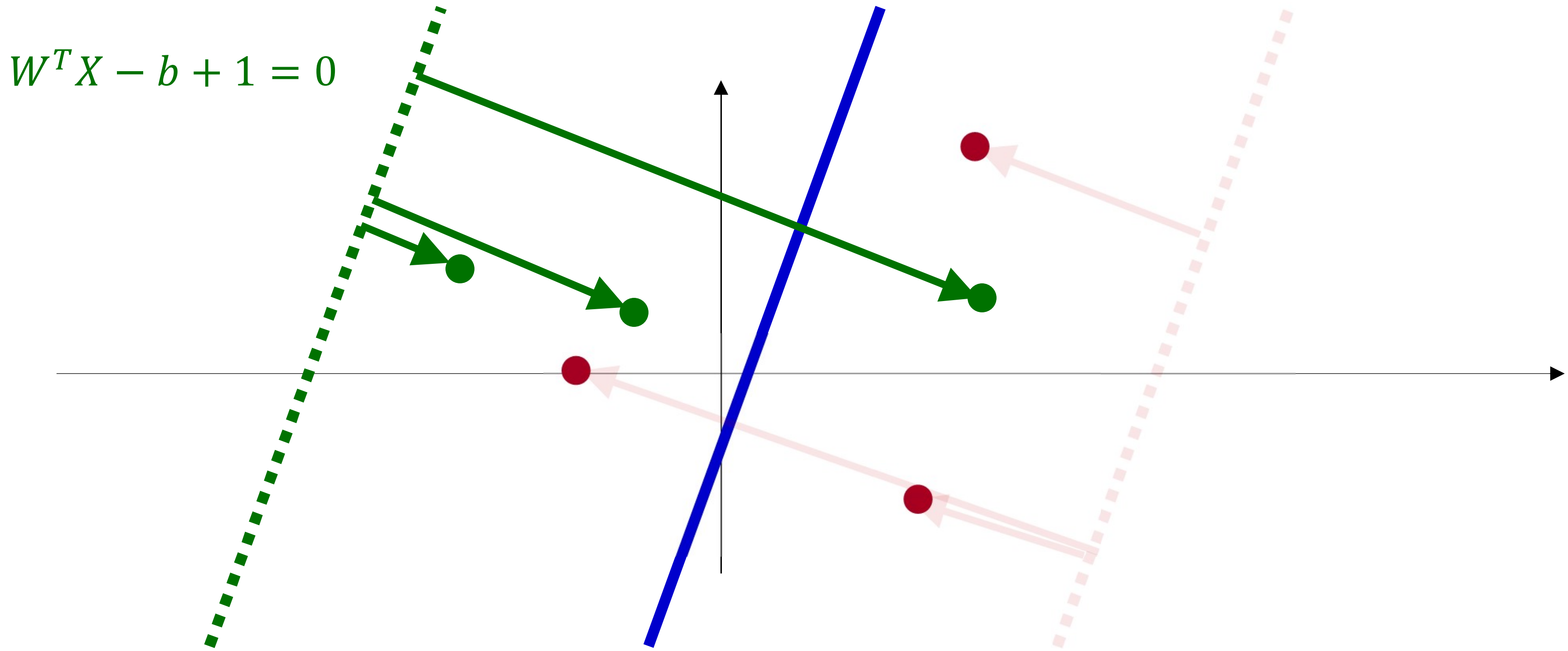


- The *negative* margin plane is given by

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

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

Quantifying Slack Length

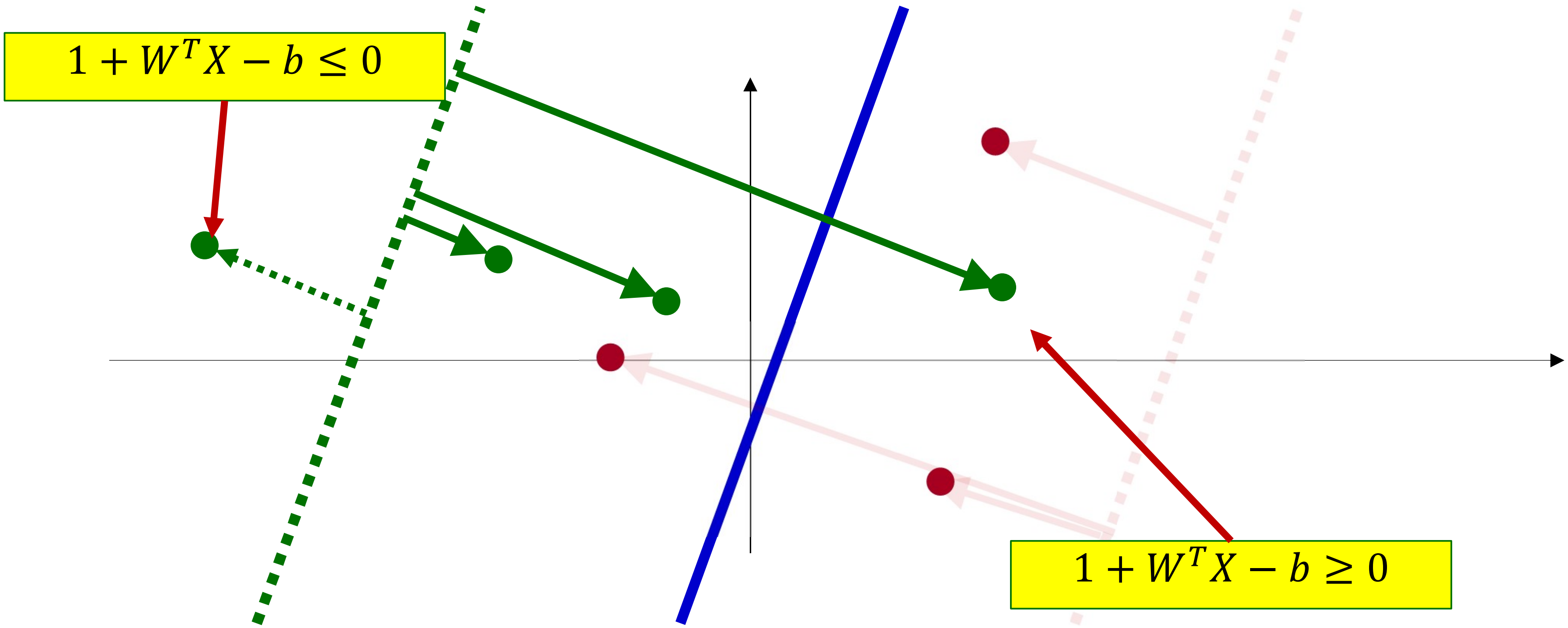


- The (unnormalized) distance of any X from this plane

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

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

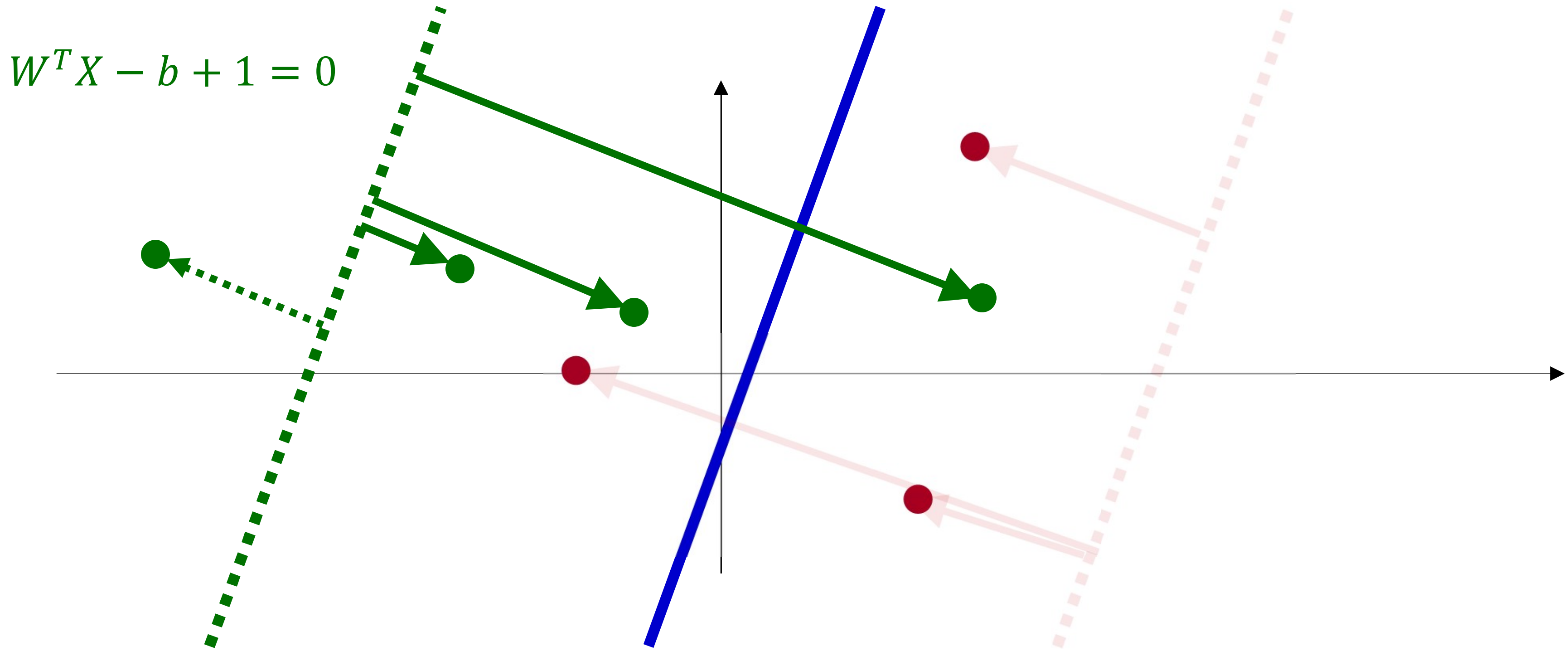
Quantifying Slack Length



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

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

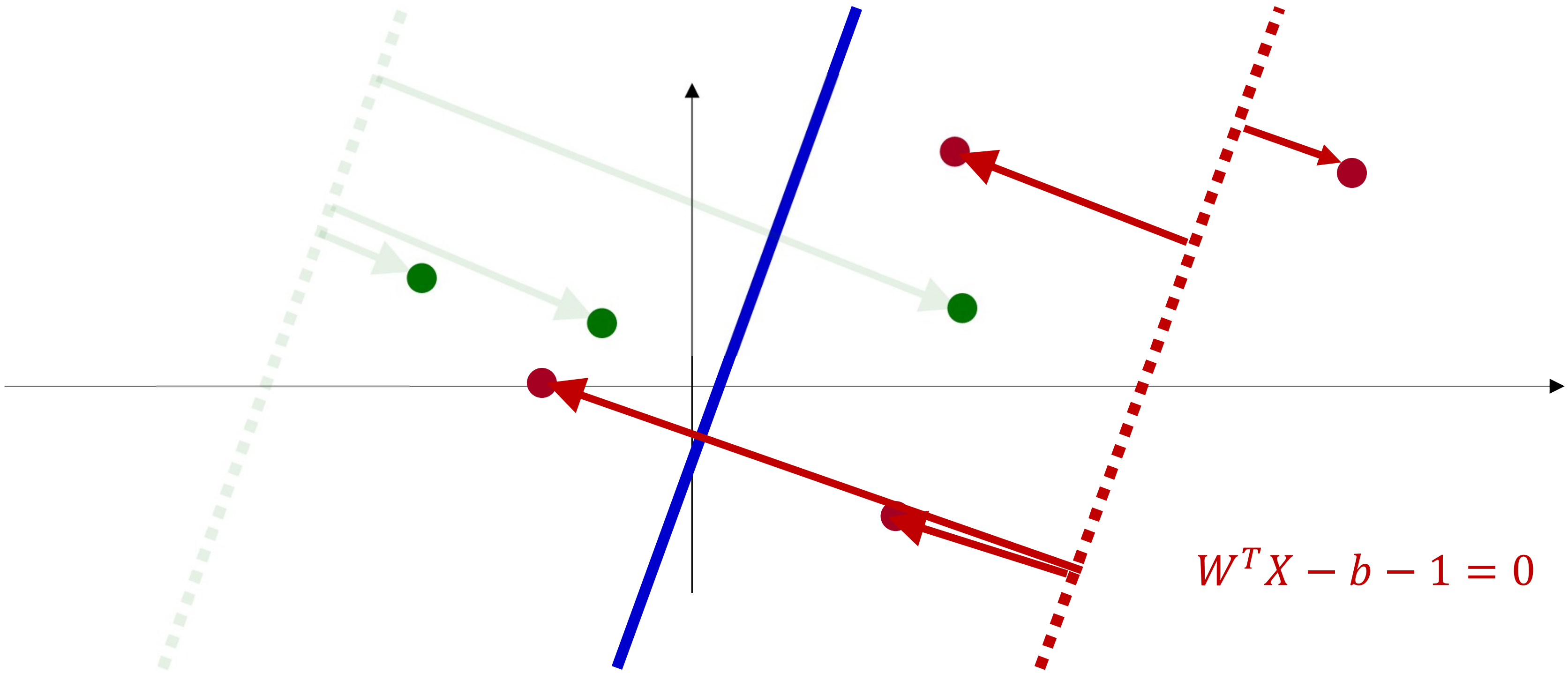
Quantifying Slack Length



- Combining the following for negative instances

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

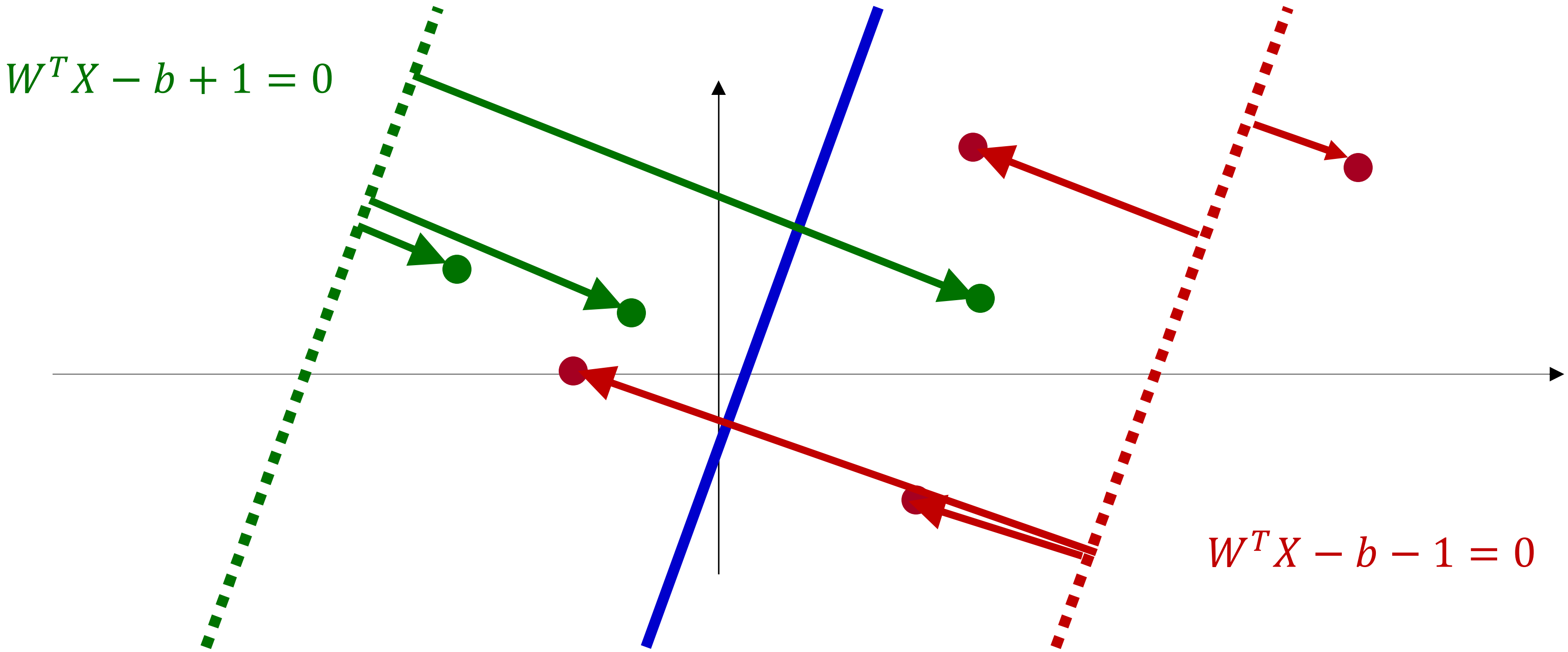
Quantifying Slack Length



- 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

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

- λ 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

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

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

Equivalent Slack Formalism

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

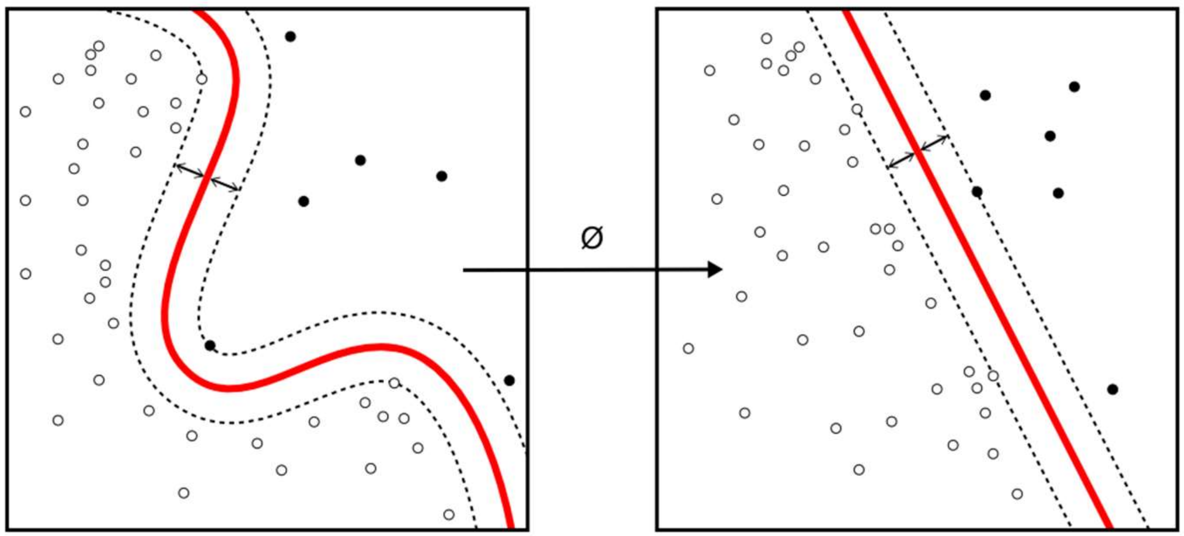
- Subject to

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

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

Poll 3

How to deal with *non-linear* boundaries?



- First some math..

Recall: The Lagrange Method

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

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

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

$$\min_x f(x)$$
$$s.t.\ \ g_i(x) \le 0,\ \ i = \{1,\dots,k\}$$
$$h_j(x) = 0,\ \ j = \{1,\dots,l\}$$

- 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!

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

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

- Can be stated using Lagrangians as

$$\underset{W,b}{\operatorname{argmin}} \ \underset{\alpha>0}{\max} \ \underbrace{\frac{1}{2}}_{\text{For convenience}} \|W\|^2 + \sum_i \alpha_i \big(1 - \underbrace{Y_i(W^T X_i - b)}_{\text{Constraint: must be -ve}}\big)$$

Linearly separable case: Lagrangian formalism

- Can be stated using Lagrangians as

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

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

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

Linearly separable case: Lagrangian formalism

- Under the KKT conditions

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

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

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

Linearly separable case: Lagrangian formalism

- Under the KKT conditions

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

- 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)

$$\underset{\alpha>0}{\operatorname{argmax}} \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j - b \sum_i \alpha_i Y_i$$

- Since the last term is 0

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

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

$$\sum_i \alpha_i Y_i = 0$$

Large margin linear classifier

- Solve for α_i

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \frac{1}{2}\sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

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

$$\sum_i \alpha_i Y_i = 0$$

- α_i will turn out to be non-zero only for the support vectors (and 1 for the support vectors)

Large margin linear classifier with slack

- Solve for α_i

$$\underset{\alpha}{\operatorname{argmax}} \sum_i \alpha_i - \frac{1}{2} \sum_{i,j} \alpha_i \alpha_j Y_i Y_j X_i^T X_j$$

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

$$\sum_i \alpha_i Y_i = 0$$

- Note upper bound on α_i
- α_i will turn out to be non-zero only for the support vectors (and 1 for the support vectors)

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 Kernel Trick

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

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

$$\sum_i \alpha_i Y_i = 0$$

- 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 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:

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

Poll 4

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:

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

  - 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

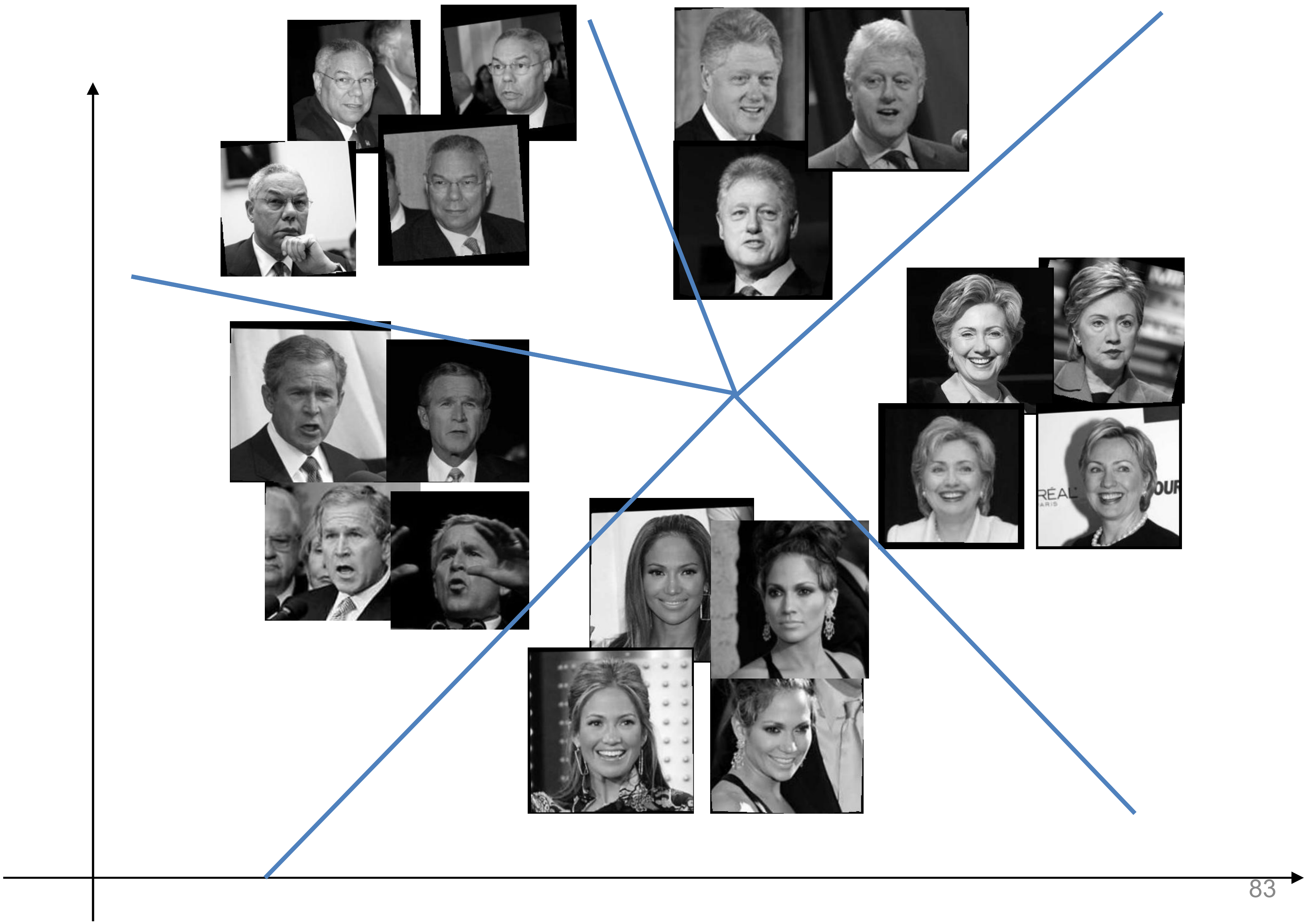
This slide is courtesy of *www.iro.umontreal.ca/~pift6080/documents/papers/**svm**_tutorial.**ppt***

Summary: Support Vector Machine

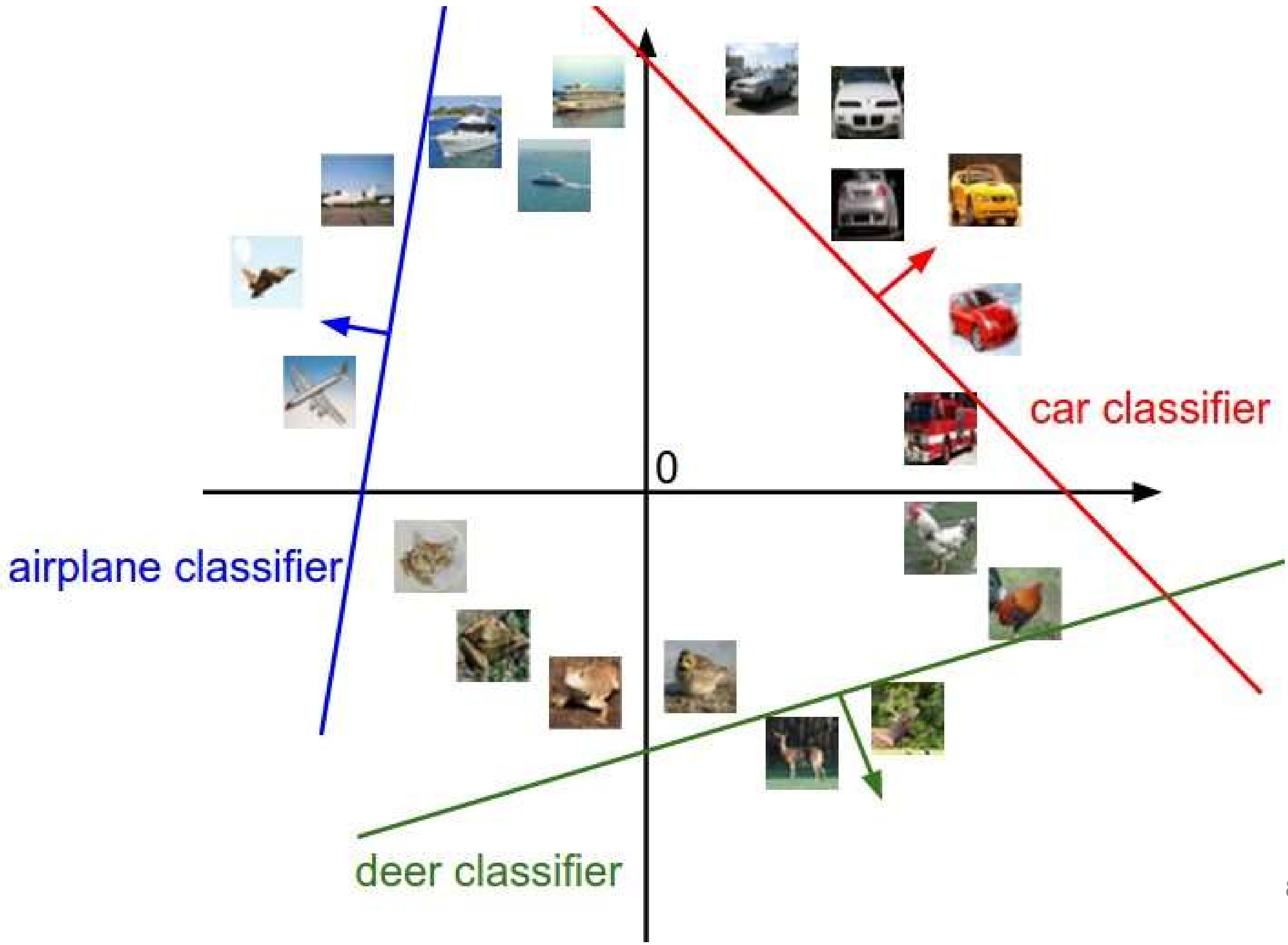
- 1. Large Margin Classifier
  - Better generalization ability & less over-fitting

- 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



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