Applied Machine Learning

Support Vector Machines

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Learning objectives

geometry of linear classification

margin maximization and support vectors

hinge loss and relation to logistic regression

Reminder

Perceptron: objective

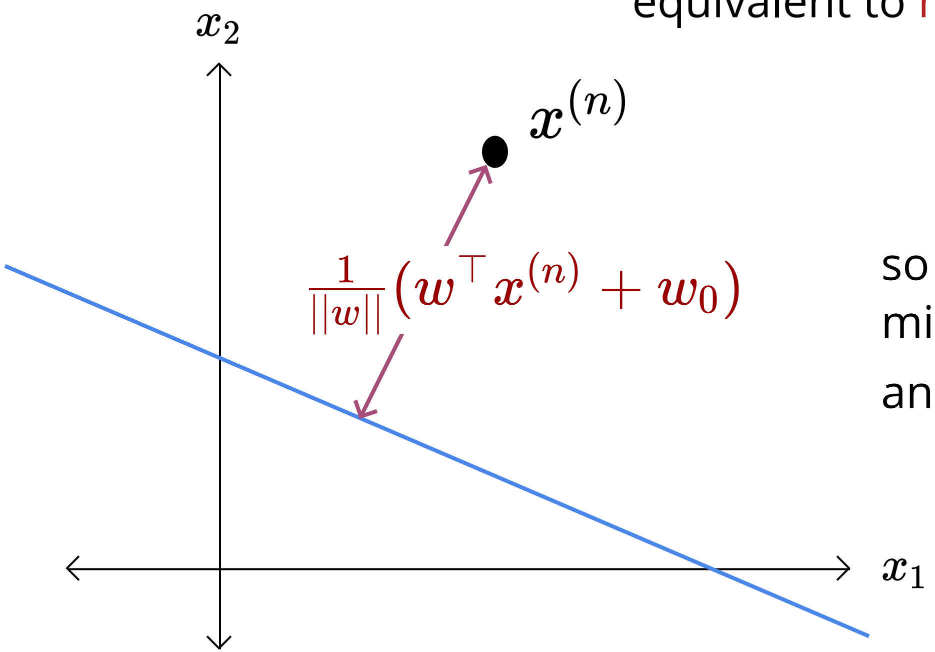
if $y^{(n)}\hat{y}^{(n)} < 0$ try to make it positive

note that y is -1 or 1
instead of 0 or 1

label and prediction have different signs $\hat{y}^{(n)} = \mathrm{sign}(w^\top x^{(n)} + w_0)$

equivalent to minimizing $-y^{(n)}\underbrace{(w^\top x^{(n)} + w_0)}_{\text{distance to the boundary}}$

this is positive for points that are on the wrong side

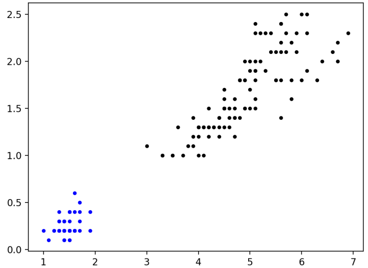


so perceptron tries to minimize the distance of misclassified points from the decision boundary

and push them to the right side

Perceptron: example

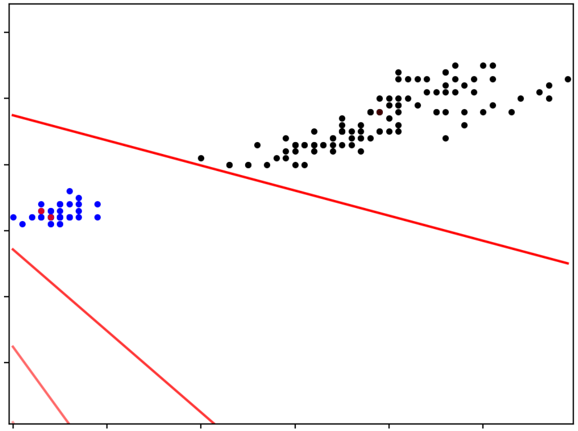
Reminder

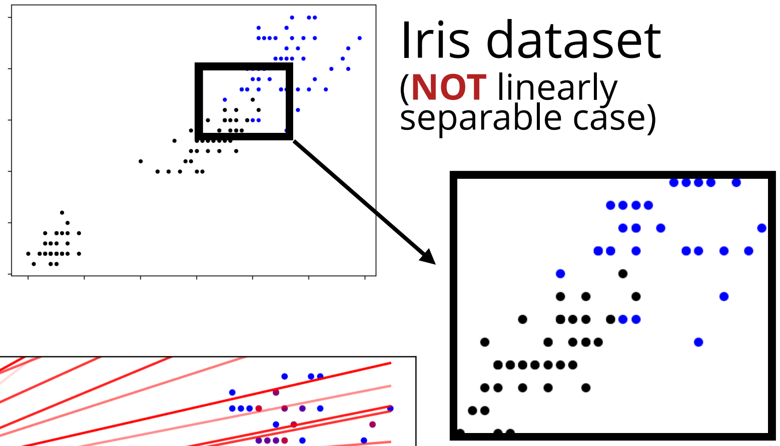


Iris dataset

(linearly separable case)

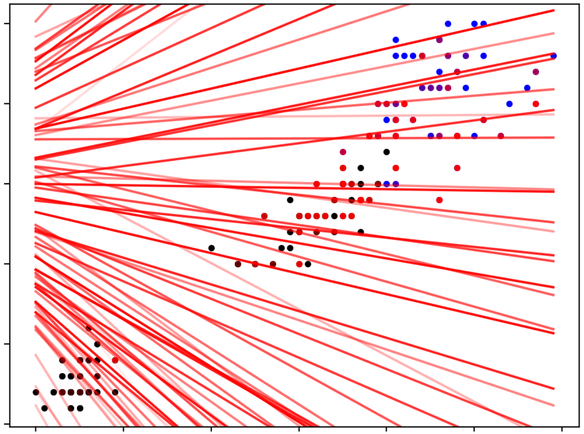
converged at iteration 10





Iris dataset

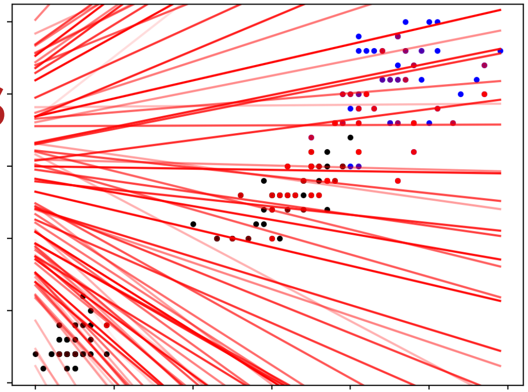
(**NOT** linearly separable case)



the algorithm does not converge

there is always a wrong prediction and the weights will be updated

Perceptron: issues



Perceptron is not expressive enough

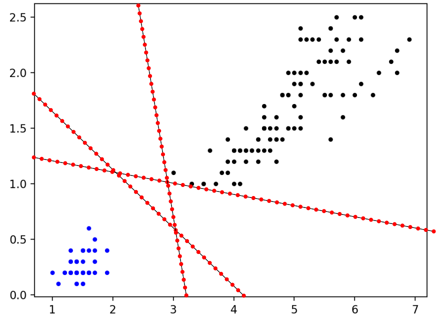
increase the model's expressiveness by adaptive nonlinear bases, discussed in previously in MLP ← previously

even if linearly separable

convergence could take many iterations

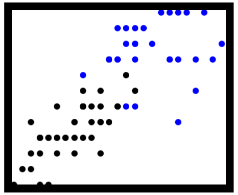
the decision boundary may be suboptimal ← let's fix this problem first

assume linear separability



cyclic updates if the data is not perfectly linearly separable

- data may be inherently noisy



geometry of the

separating hyperplane

A linear decision boundary is a hyperplane with one dimension lower than D (number of features)

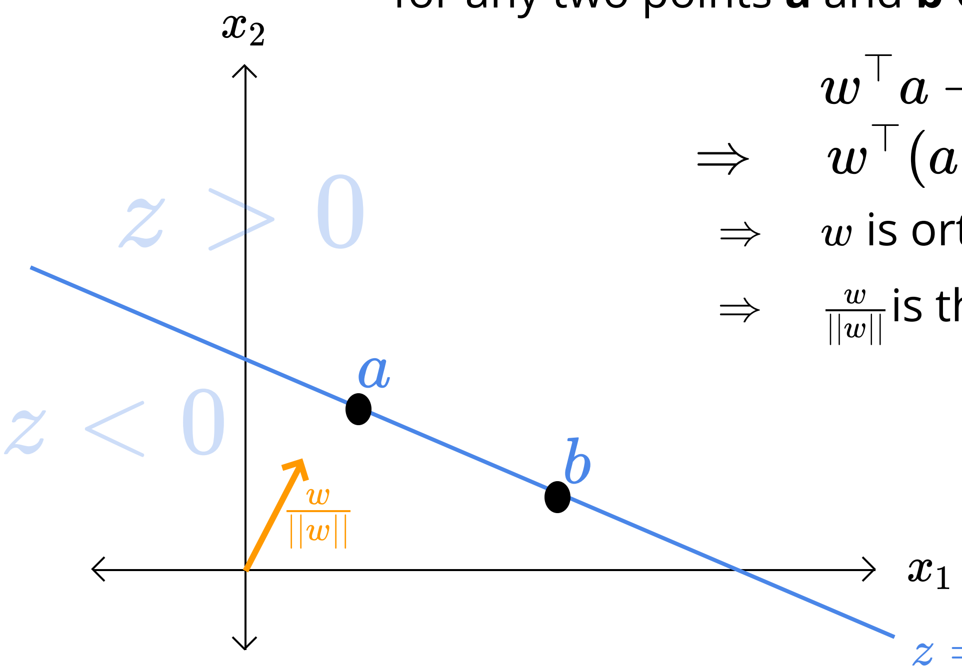
for any two points **a** and **b** on this line, we have:

$$w^\top a + w_0 = w^\top b + w_0 = 0$$

$$\Rightarrow \quad w^\top (a - b) + w_0 - w_0 = 0$$

$\Rightarrow$ w is orthogonal to the line

$\Rightarrow$ $\frac{w}{||w||}$ is the unit vector normal to the line



$z = w^\top x + w_0 = w_2 x_2 + w_1 x_1 + w_0 = 0$

geometry of the

separating hyperplane

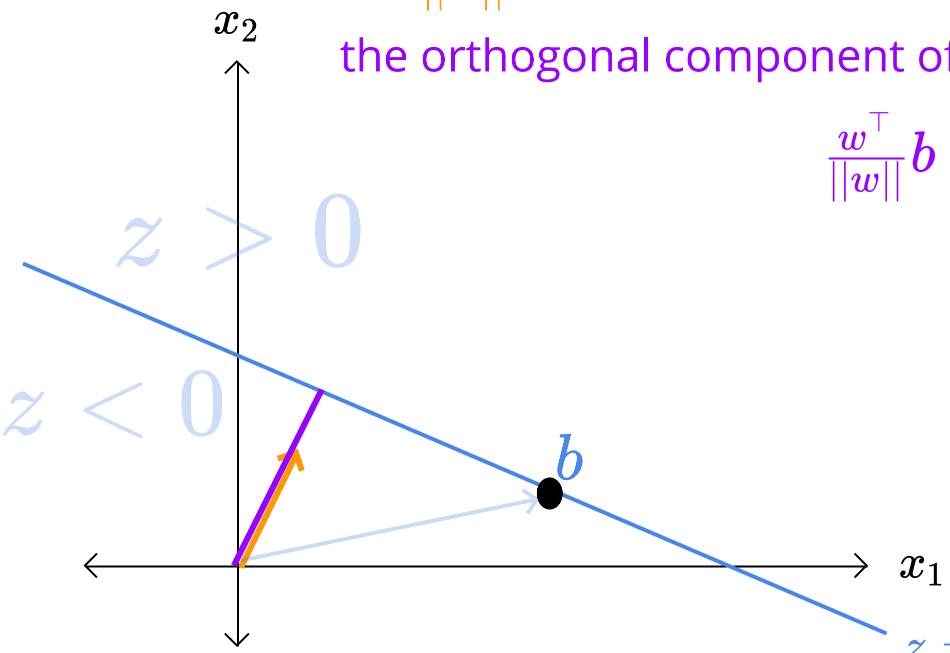
A linear decision boundary is a hyperplane with one dimension lower than D (number of features)

so $\frac{w}{||w||}$ is the unit normal vector to the line

the orthogonal component of any point on the line

$$\frac{w^\top}{||w||} b = \frac{w^\top}{||w||} b + \frac{w_0}{||w||} - \frac{w_0}{||w||} = -\frac{w_0}{||w||}$$

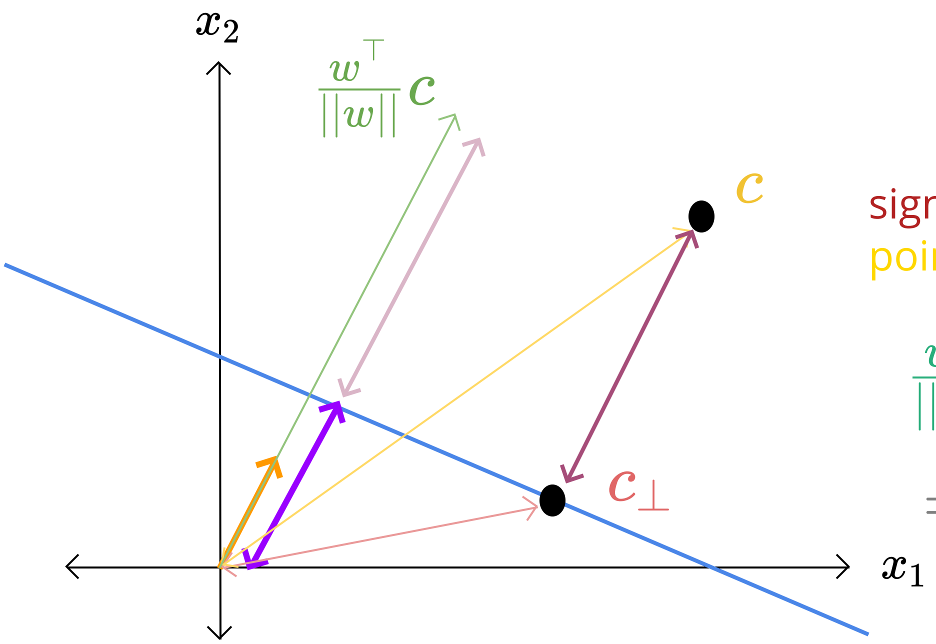
$$w^\top b + w_0 = 0$$



$$z = w^\top x + w_0 = w_2 x_2 + w_1 x_1 + w_0 = 0$$

geometry of the **separating hyperplane**

the orthogonal component of any point on the line $\frac{w^\top}{||w||} b = -\frac{w_0}{||w||}$ $:^{(**)}$



signed distance of any point (c) from the line

$$\frac{w^\top}{||w||} c - \frac{w^\top}{||w||} c_\perp$$

$$= \frac{w^\top}{||w||} c + \frac{w_0}{||w||}$$

$$= \frac{1}{||w||}(w^\top c + w_0)$$

$\frac{w}{||w||}$

$\frac{w^\top}{||w||} c$

$c_\perp$

$\frac{w^\top}{||w||} c_\perp = -\frac{w_0}{||w||}^{(**)}$

Margin

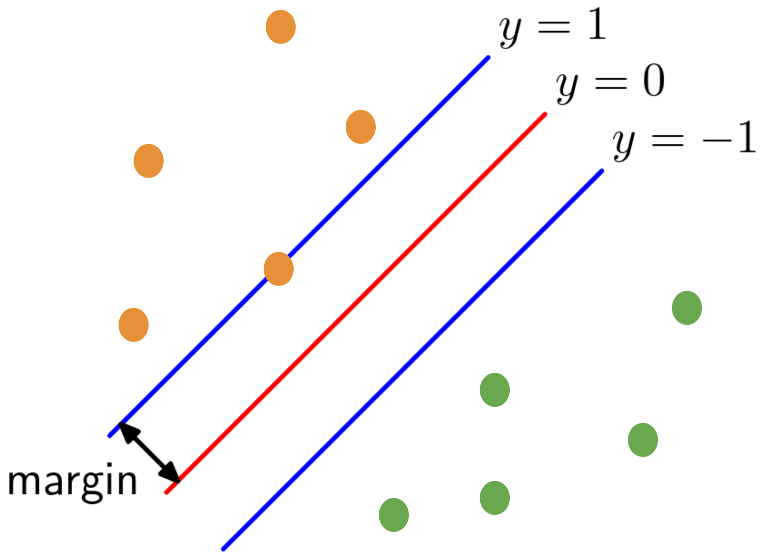
the margin of a classifier (assuming correct classification)

is the distance of the closest point to the decision boundary

signed distance is $\frac{1}{||w||}(w^\top x^{(n)} + w_0)$

adjust so that correctly classified points have positive margin

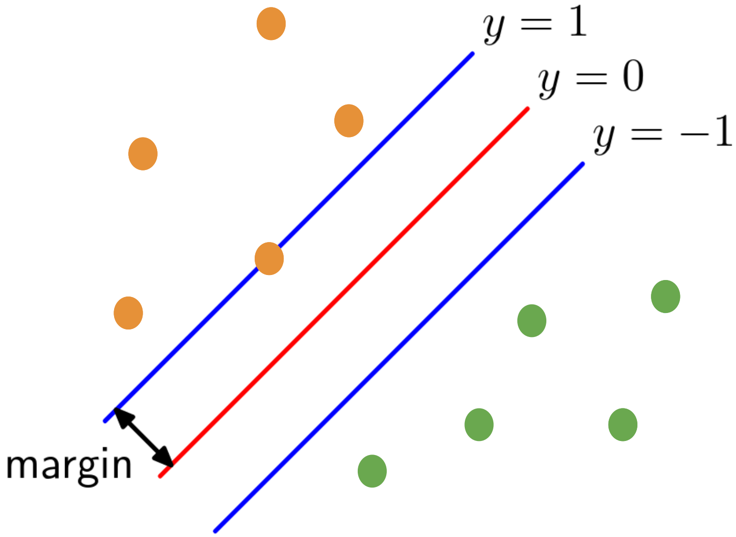
$$\underbrace{\underbrace{\frac{1}{||w||}(w^\top x^{(n)} + w_0)}_{\hat{y}^{(n)}\text{=distance to the boundary}} y^{(n)}}_{\text{this is positive for points that are on the right side}}$$



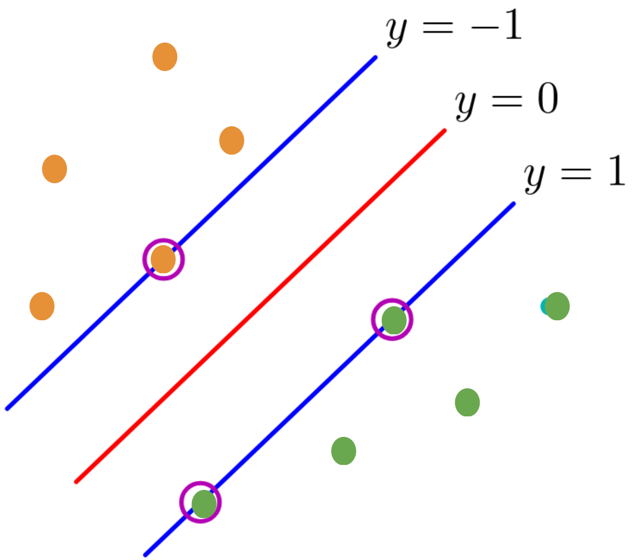
Max margin classification

find the decision boundary with maximum margin

margin is not maximal

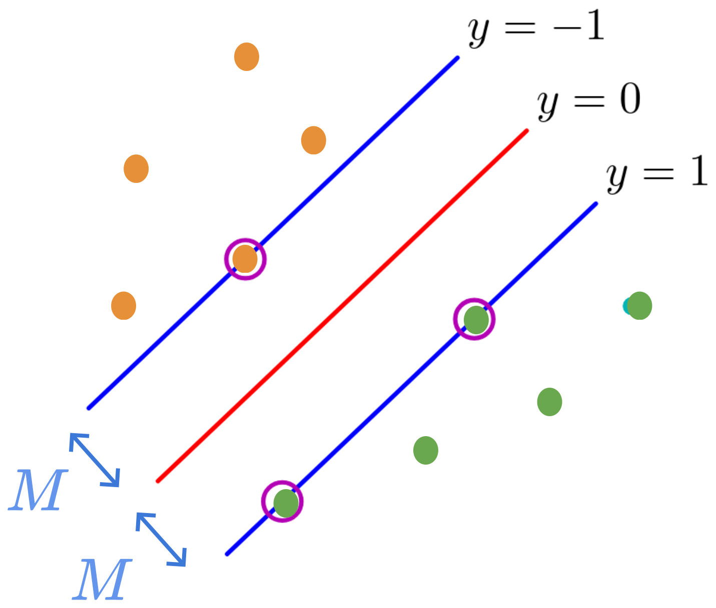


maximum margin



Max margin classification

find the decision boundary with maximum margin



$$\begin{cases} \max_{w,w_0} M \\ M \leq \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0) \quad \forall n \end{cases}$$

only the points (n) with

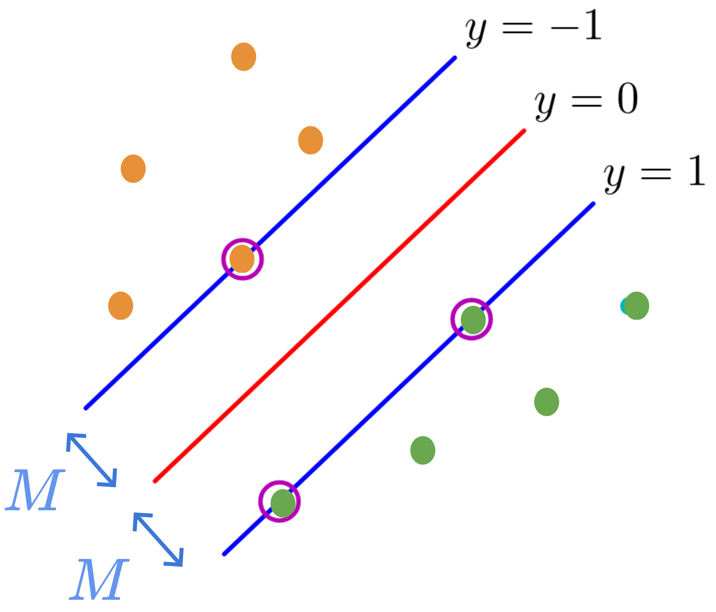
$M = \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0)$ matter in finding the boundary

these are called **support vectors**

max-margin classifier is called **support vector machine** (SVM)

Support Vector Machine

find the decision boundary with maximum margin



$$\begin{cases} \max_{w,w_0} M \\ M \leq \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0) \quad \forall n \end{cases}$$

observation

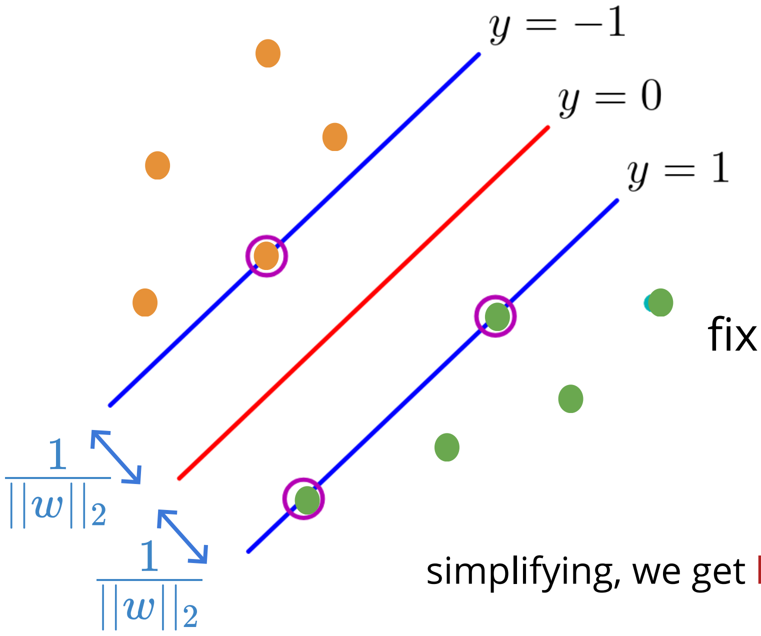
if w^*, w_0^* is an optimal solution then

$20w^*, 20w_0^*$ is also optimal (same margin)

fix the norm of w to avoid this $||w||_2 = \frac{1}{M}$

Support Vector Machine

find the decision boundary with maximum margin



$$\begin{cases} \max_{w,w_0} M \\ M \leq \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0) \quad \forall n \end{cases}$$

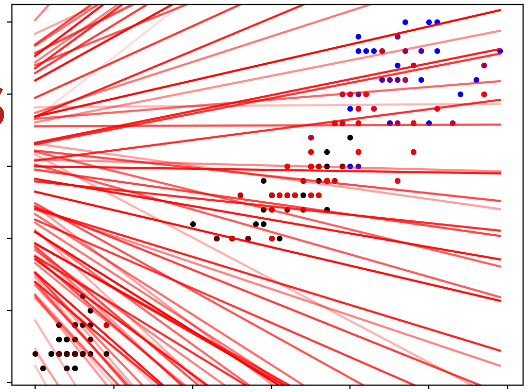
fixing $||w||_2 = \frac{1}{M}$

$$\begin{cases} \max_{w,w_0} \frac{1}{||w||_2} \\ \frac{1}{||w||_2} \leq \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0) \quad \forall n \end{cases}$$

simplifying, we get **hard** margin SVM objective

$$\begin{cases} \min_{w,w_0} ||w||_2^2 \\ y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 \quad \forall n \end{cases}$$

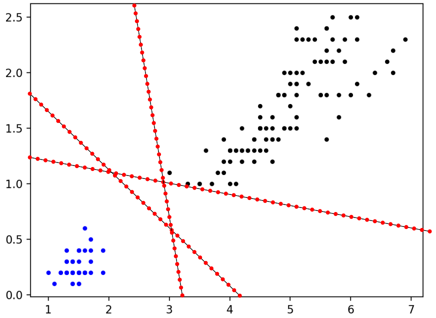
Perceptron: issues



Perceptron is not expressive enough

increase the model's expressiveness by adaptive nonlinear bases, discussed in previously in MLP

previously



even if linearly separable

convergence could take many iterations

the decision boundary may be suboptimal

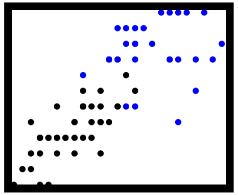
maximize the **hard** margin

cyclic updates if the data is not perfectly linearly separable

- data may be inherently noisy

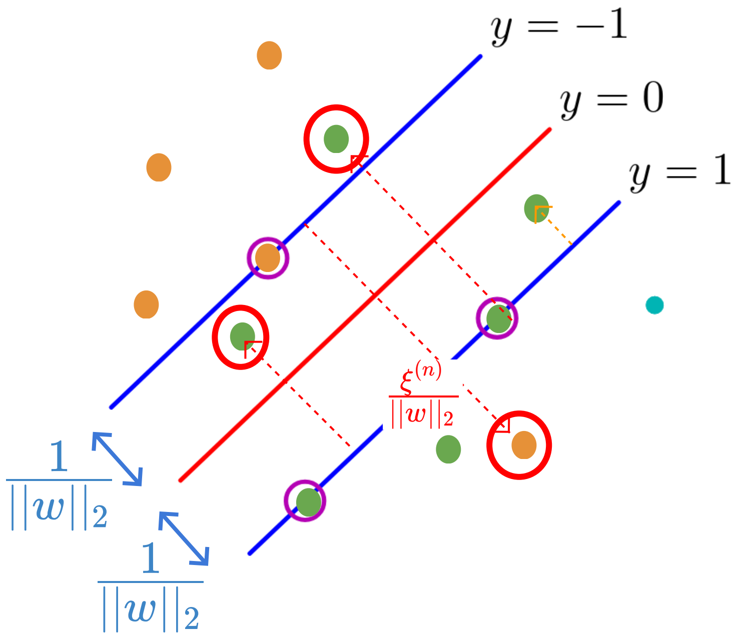
now lets fix this problem

maximize a **soft** margin



Soft margin constraints

allow points inside the margin and on the wrong side but penalize them



instead of hard constraint $y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 \quad \forall n$

use $y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 - \xi^{(n)} \quad \forall n$

$\xi^{(n)} \geq 0$ slack variables (one for each n)

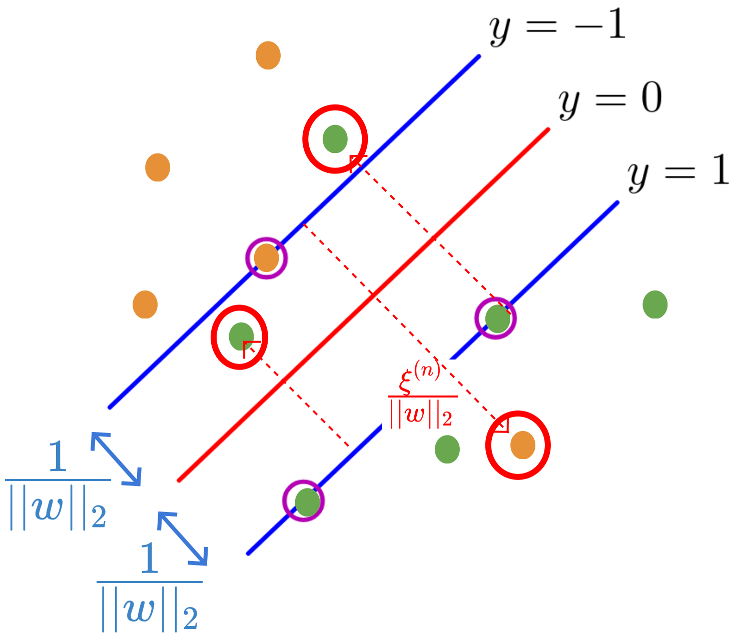
$\xi^{(n)} = 0$ zero if the point satisfies original margin constraint

$0 < \xi^{(n)} < 1$ if correctly classified but inside the margin

$\xi^{(n)} > 1$ incorrectly classified

Soft margin constraints

allow points inside the margin and on the wrong side but penalize them



soft-margin objective

$$\min_{w,w_0} \frac{1}{2}||w||_2^2 + \gamma \sum_n \xi^{(n)}$$

$$y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 - \xi^{(n)} \quad \forall n$$

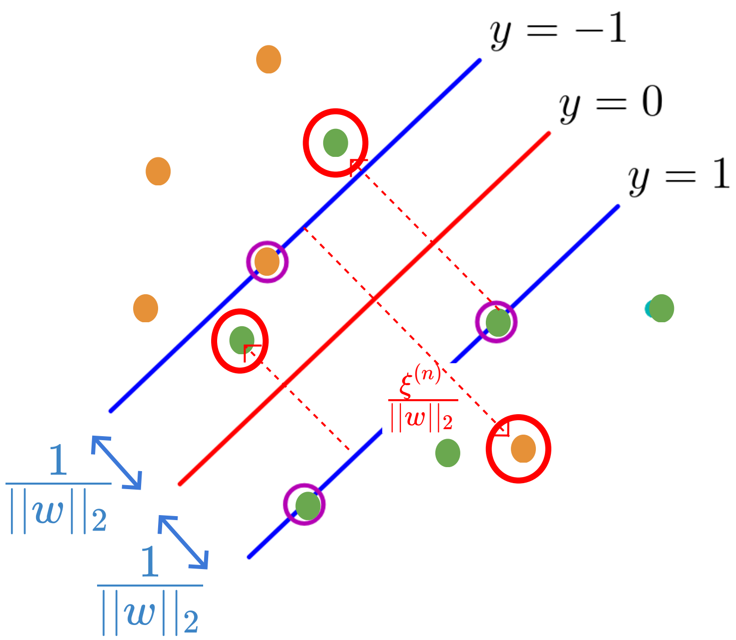
$$\xi^{(n)} \geq 0 \quad \forall n$$

γ is a hyper-parameter that defines the importance of constraints

for very large γ this becomes similar to hard margin svm

Hinge loss

would be nice to turn this into an unconstrained optimization



$$\min_{w,w_0} \frac{1}{2}||w||_2^2 + \gamma \sum_n \xi^{(n)}$$

$$y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 - \xi^{(n)}$$

$$\xi^{(n)} \geq 0 \quad \forall n$$

if point satisfies the margin $y^{(n)}(w^\top x^{(n)} + w_0) \geq 1$

minimum slack is $\xi^{(n)} = 0$

otherwise $y^{(n)}(w^\top x^{(n)} + w_0) < 1$

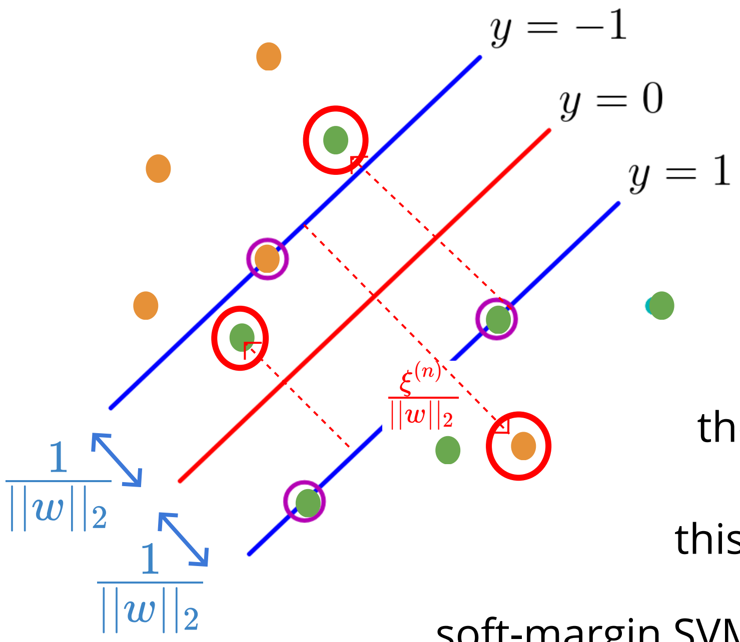
the smallest slack is $\xi^{(n)} = 1 - y^{(n)}(w^\top x^{(n)} + w_0)$

so the optimal slack satisfying both cases

$$\xi^{(n)} = \max(0, 1 - y^{(n)}(w^\top x^{(n)} + w_0))$$

Hinge loss

would be nice to turn this into an unconstrained optimization



$$\min_{w,w_0} \frac{1}{2}||w||_2^2 + \gamma \sum_n \xi^{(n)}$$

$$y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 - \xi^{(n)}$$

$$\xi^{(n)} \geq 0 \quad \forall n$$

replace $\xi^{(n)} = \max(0, 1 - y^{(n)}(w^\top x^{(n)} + w_0))$

we get $\min_{w,w_0} \frac{1}{2}||w||_2^2 + \gamma \sum_n \max(0, 1 - y^{(n)}(w^\top x^{(n)} + w_0))$

the same as $\min_{w,w_0} \sum_n \max(0, 1 - y^{(n)}(w^\top x^{(n)} + w_0)) + \frac{1}{2\gamma}||w||_2^2$

this is called the hinge loss $L_{hinge}(y, z) = \max(0, 1 - yz)$

soft-margin SVM is doing L2 regularized hinge loss minimization

Perceptron vs. SVM

Perceptron

cost

if correctly classified evaluates to zero

otherwise it is $-y^{(n)}(w^\top x^{(n)} + w_0))$

can be written as

$$\sum_n \max(0, -y^{(n)}(w^\top x^{(n)} + w_0))$$

optimization

finds some linear decision boundary if exists

stochastic gradient descent with fixed learning rate

SVM

cost

$$\sum_n \max(0, 1 - y^{(n)}(w^\top x^{(n)} + w_0)) + \frac{\lambda}{2}||w||_2^2$$

so this is the difference!

(plus regularization)

optimization

for small lambda finds the max-margin decision boundary

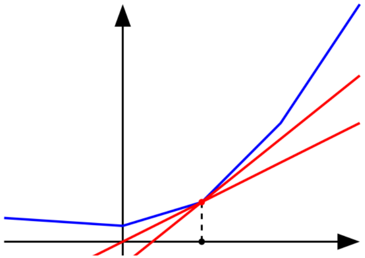
depending on the formulation we have many choices

Perceptron vs. SVM

cost $J(w) = \sum_n \max(0, 1 - y^{(n)} w^\top x^{(n)}) + \frac{\lambda}{2}||w||_2^2$

now we included bias in w

check that the cost function is convex in w(?)



hinge loss is not smooth (piecewise linear)

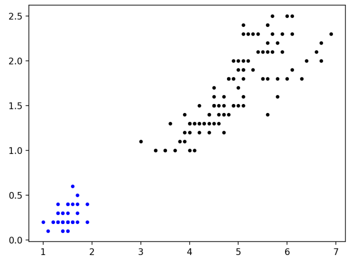
if we use **"stochastic" sub-gradient** descent

the update will look like Perceptron

if $y^{(n)}\hat{y}^{(n)} < 1$ minimize $-y^{(n)}(w^\top x^{(n)}) + \frac{\lambda}{2}||w||_2^2$

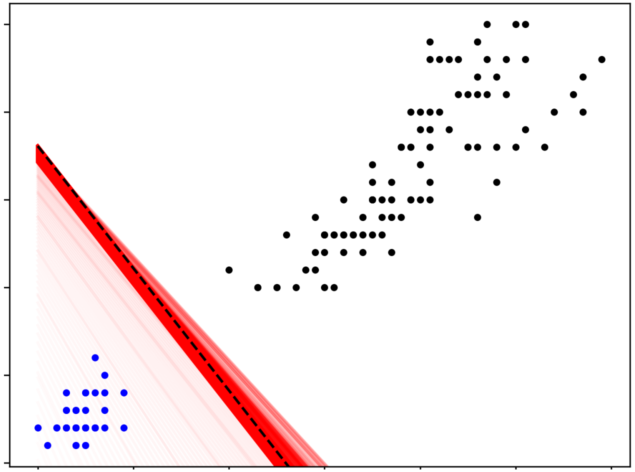
otherwise, do nothing

Example: linearly separable

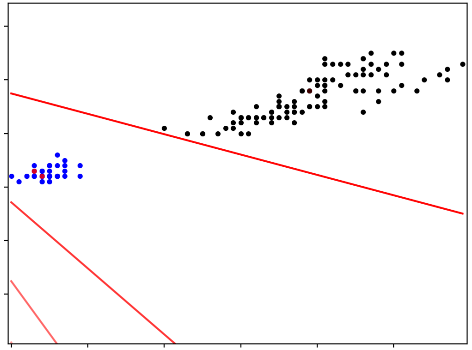


Iris dataset (D=2)

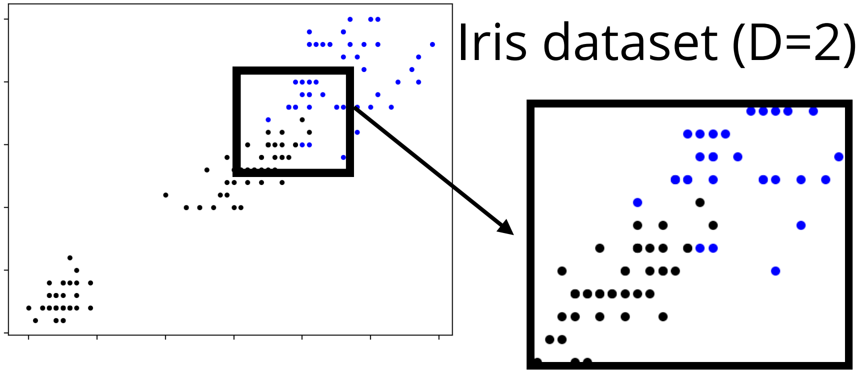
max-margin boundary (using small lambda $\lambda = 10^{-8}$)



compare to Perceptron's decision boundary

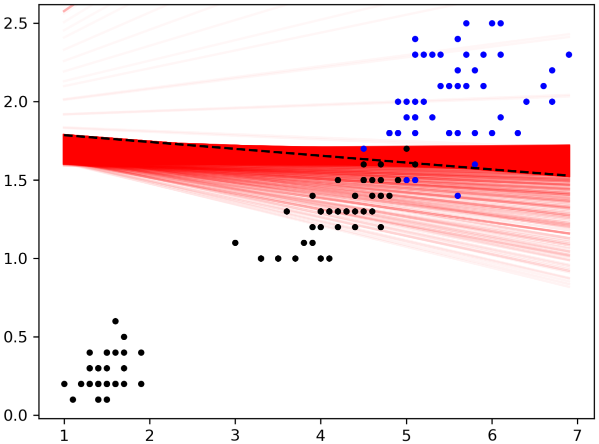


Example: not linearly separable

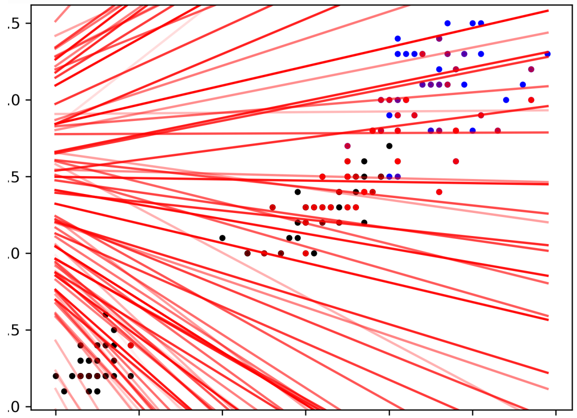


Iris dataset (D=2)

soft margins using small lambda $\lambda = 10^{-8}$



Perceptron does not converge



SVM vs. logistic regression

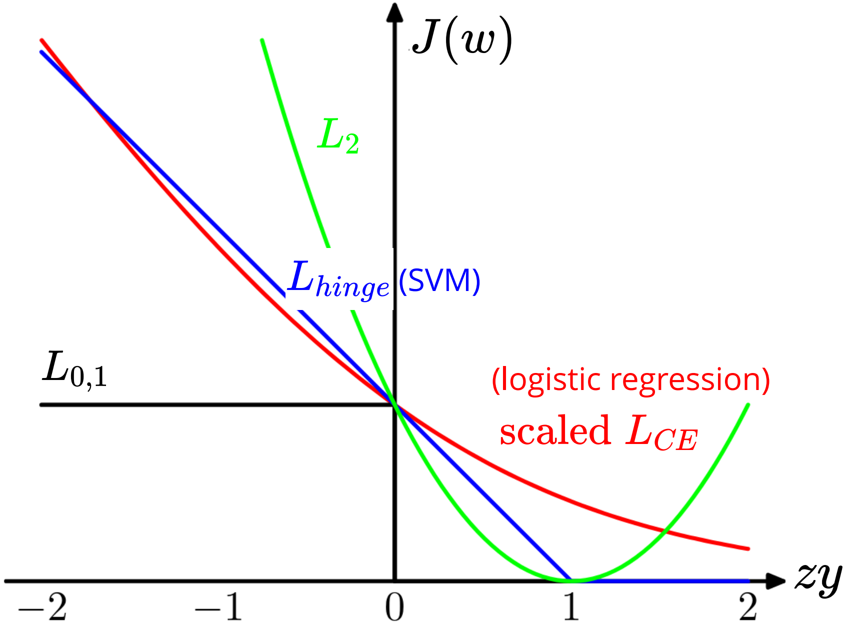
recall: **logistic regression** simplified cost for $y \in \{0,1\}$

$$J(w) = \sum_{n=1}^{N} y^{(n)} \log\left(1+e^{-z^{(n)}}\right) + (1-y^{(n)}) \log\left(1+e^{z^{(n)}}\right) \quad \text{where} \quad z^{(n)} = w^\top x^{(n)}$$ includes the bias

for $y \in \{-1,+1\}$ we can write this as

$$J(w) = \sum_{n=1}^{N} \log\left(1+e^{-y^{(n)} z^{(n)}}\right) + \frac{\lambda}{2}||w||_2^2$$

also added L2 regularization



compare to **SVM cost** for $y \in \{-1,+1\}$

$$J(w) = \sum_n \max(0, 1 - y^{(n)}(z^{(n)})) + \frac{\lambda}{2}||w||_2^2$$

they both try to approximate 0-1 loss (accuracy)

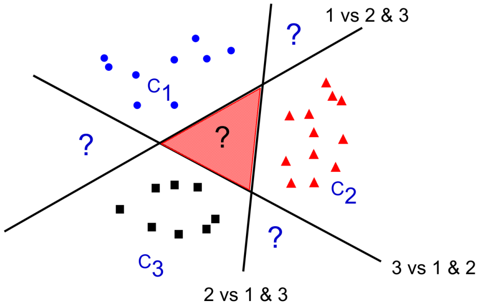
Multiclass classification

can we use multiple binary classifiders?

one versus the rest

training:

train C different 1-vs-(C-1) classifiers $z_c(x) = w_c^\top x$



test time:

choose the class with the highest score

$z^* = \arg\max_c z_c(x)$

problems:

class imbalance

not clear what it means to compare $z_c(x)$ values, trained on different tasks

image credit: Andrew Zisserman

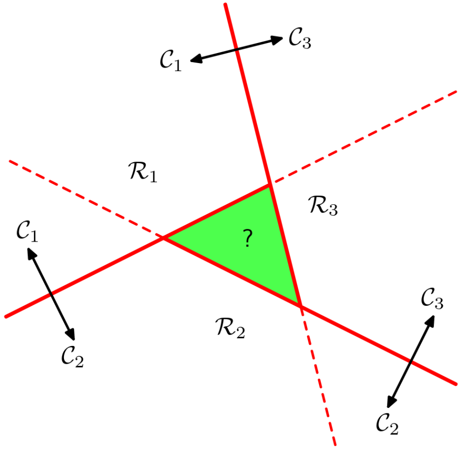
Multiclass classification

can we use multiple binary classifiders?

one versus one

training:
train $\frac{C(C-1)}{2}$ classifiers for each class pair

test time:
choose the class with the highest vote



problems:
computationally more demanding for large C
ambiguities in the final classification

Summary

- geometry of linear classification
- distance to the decision boundary (margin)
- max-margin classification
- support vectors
- hard vs soft SVM
- relation to perceptron
- hinge loss and its relation to logistic regression
- some ideas for max-margin multi-class classification