Applied Machine Learning

Perceptron and Support Vector Machines

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COMP 551 (winter 2020)

Learning objectives

geometry of linear classification

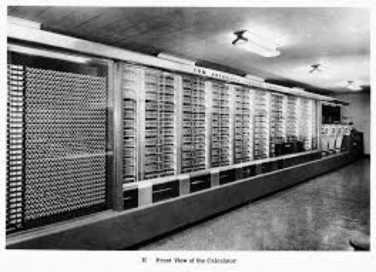
Perceptron learning algorithm

margin maximization and support vectors

hinge loss and relation to logistic regression

Perceptron

old implementation (1960's)



historically a significant algorithm

(first neural network, or rather just a neuron)

biologically motivated model

simple learning algorithm

convergence proof

beginning of *connectionist* AI

it's criticism in the book "Perceptrons" was a factor in AI winter

Model

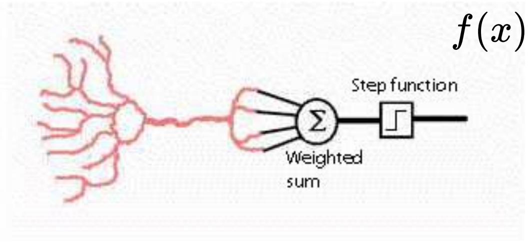


image:https://cs.stanford.edu/people/eroberts/courses/soco/projects/neural-networks/Neuron/index.html

$$f(x) = \mathrm{sign}(w^\top x + w_0)$$

note that we're using +1/-1 for labels rather than 0/1.

geometry of the **separating hyperplane**

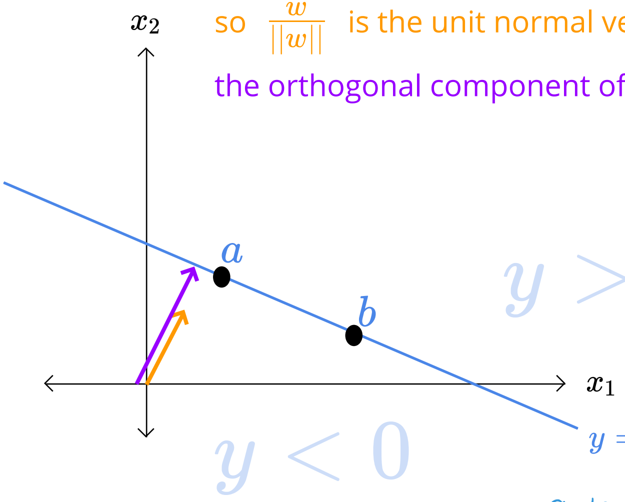
this hyperplane has one dimension lower than D (number of features)

for any two points **a** and **b** on the line $w^\top(a-b) + w_0 - w_0 = 0$

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

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

subtracting



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

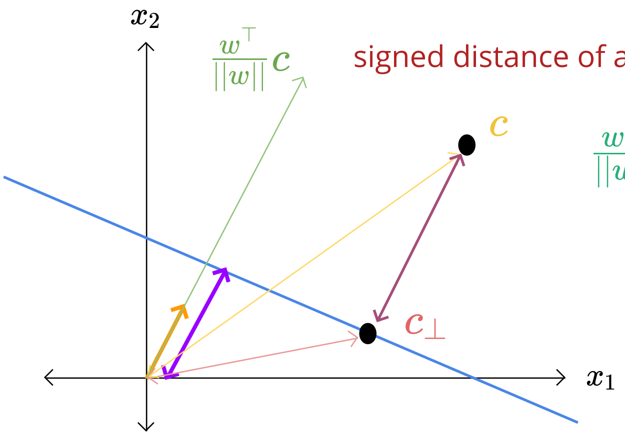
a, b on ℓ: $0 = w^\top x + w_0 \Rightarrow$ $w^\top a + w_0 = 0$
$w^\top b + w_0 = 0$

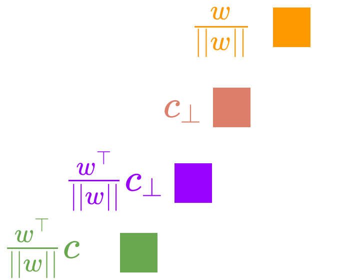
geometry of the **separating hyperplane**

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

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



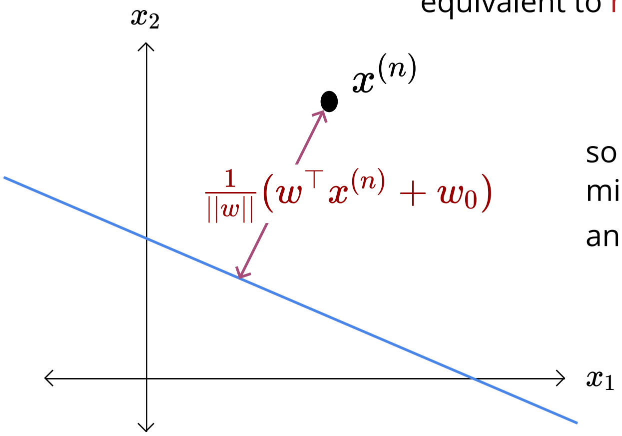


Perceptron: objective

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

label and prediction have different signs

equivalent to minimizing $-y^{(n)}\overbrace{(w^\top x^{(n)} + w_0)}^{\hat{y}^{(n)}}$



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

and push them to the right side

revisiting **Perceptron: optimization**

if $y^{(n)}\hat{y}^{(n)} < 0$ minimize $J_n(w) = -y^{(n)}(w^\top x^{(n)})$

now we included bias in w

otherwise, do nothing

use stochastic gradient descent $\nabla J_n(w) = -y^{(n)}x^{(n)}$

$$w^{\{t+1\}} \leftarrow w^{\{t\}} - \alpha \nabla J_n(w) = w^{\{t\}} + \alpha y^{(n)} x^{(n)}$$

Perceptron uses learning rate of 1

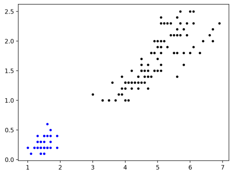
this is okay because scaling w does not affect prediction

$$\text{sign}(w^\top x) = \text{sign}(\alpha w^\top x)$$

Perceptron convergence theorem

the algorithm is guaranteed to converge in finite steps if linearly separable

Perceptron: example

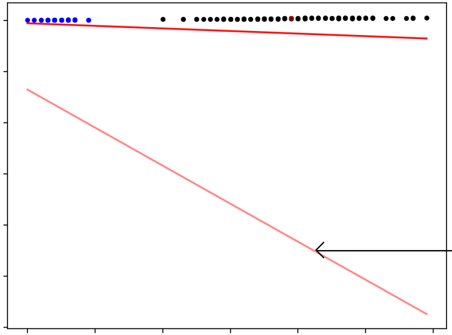


Iris dataset
(linearly separable case)

```
def Perceptron(X, y, max_iters):
    N,D = X.shape
    w = np.random.rand(D)
    for t in range(max_iters):
        n = np.random.randint(N)
        yh = np.sign(np.dot(X[n,:], w))
        if yh != y[n]:
            w = w + y[n]*X[n,:]
    return w
```

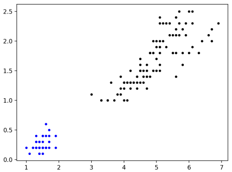
note that the code is not chacking for convergence

iteration 1



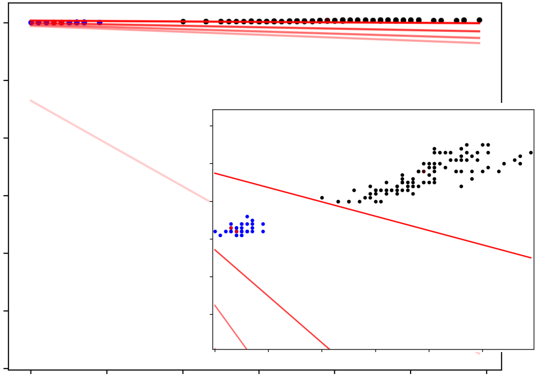
initial decision boundary $w^\top x = 0$

Perceptron: example



Iris dataset
(linearly separable case)

iteration 10



```python
def Perceptron(X, y, max_iters):
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    w = np.random.rand(D)
    for t in range(max_iters):
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        yh = np.sign(np.dot(X[n,:], w))
        if yh != y[n]:
                w = w + y[n]*X[n,:]
    return w
```

note that the code is not chacking for convergence

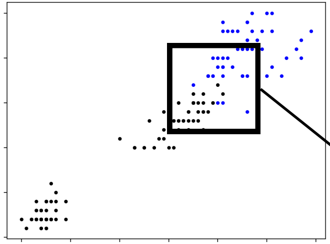
observations:

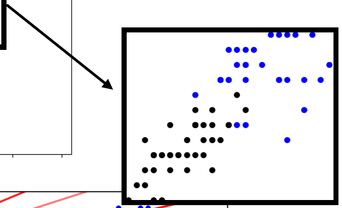
after finding a linear separator no further updates happen

the final boundary depends on the order of instances

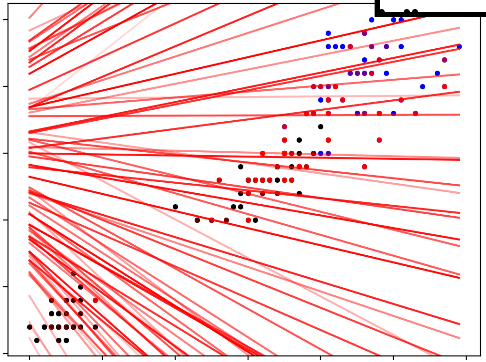
(different from all previous methods)

Perceptron: **example**





Iris dataset
(**NOT** linearly separable case)



```
def Perceptron(X, y, max_iters):
    N,D = X.shape
    w = np.random.rand(D)
    for t in range(max_iters):
        n = np.random.randint(N)
        yh = np.sign(np.dot(X[n,:], w))
        if yh != y[n]:
            w = w + y[n]*X[n,:]
    return w
```

note that the code is not chacking for convergence

the algorithm does not converge

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

Perceptron: issues

cyclic updates if the data is not linearly separable?

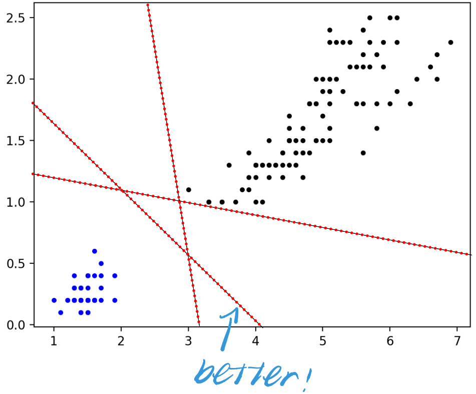
- try make the data separable using additional features?
- data may be inherently noisy

even if linearly separable

convergence could take many iterations

the decision boundary may be suboptimal

First assume linear separable



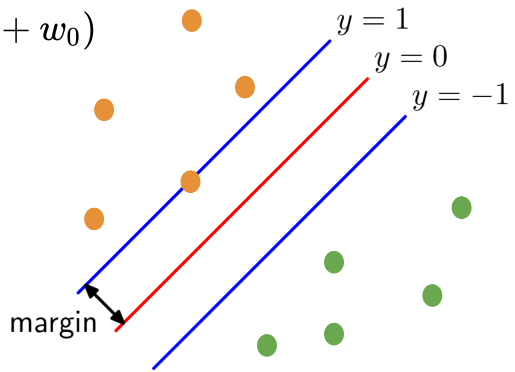
Margin

the margin of a classifier (assuming correct classification)

is the distance of the closest point to the decision boundary

signed distance is $\frac{1}{||w||}(w^\top x^{(n)} + w_0)$ positive for points with correct labels

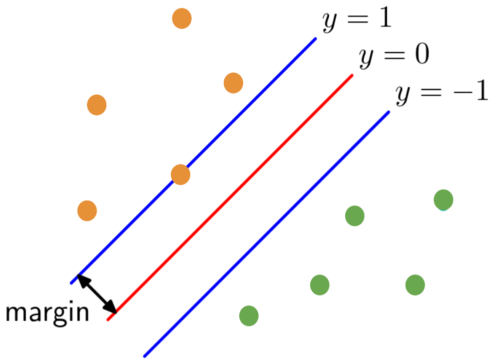
correcting for sign (margin) $\frac{1}{||w||} y^{(n)}(w^\top x + w_0)$



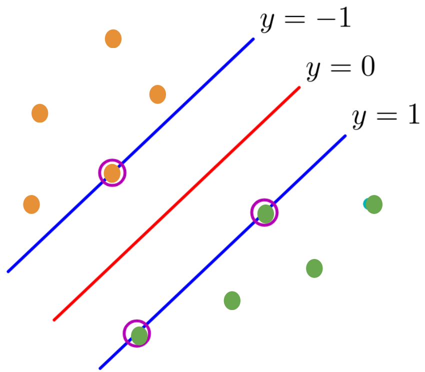
Max margin classifier

find the decision boundary with maximum margin

margin is not maximal



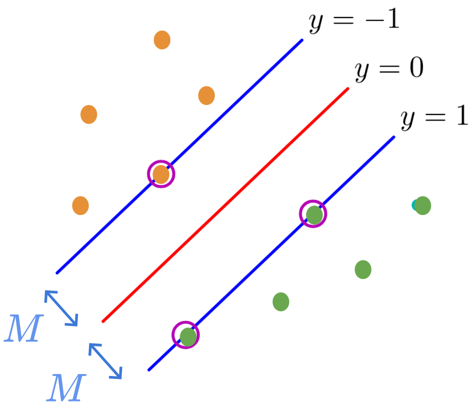
maximum margin



good results in training data
→ good results in test.

Max margin classifier

find the decision boundary with maximum margin



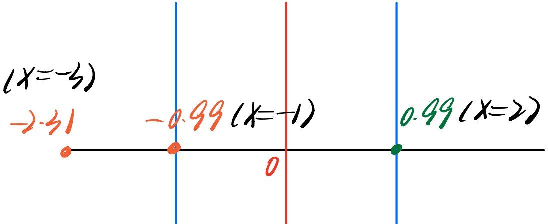
$$\begin{cases} \max_{w,w_0} M \\ M \leq \frac{1}{||w||_2} y^{(n)}(w^\top x^{(n)} + w_0) \quad \forall n \end{cases}$$

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**

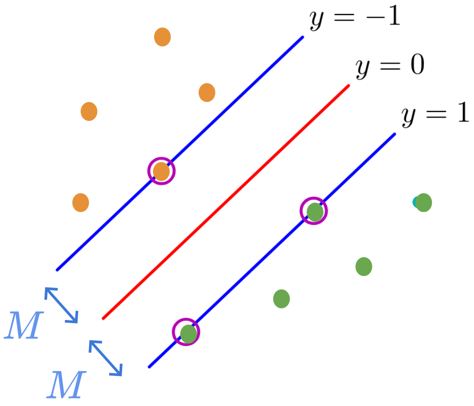
max-margin classifier is called **support vector machine** (SVM)



$\hat{y} = 0.66x - 0.33$

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

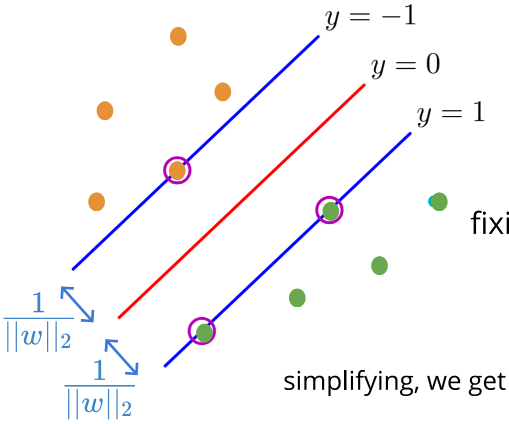
if w^*, w_0^* is an optimal solution then

cw^*, cw_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

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

Perceptron: issues

cyclic updates if the data is not linearly separable?

- try make the data separable using additional features?
- data may be inherently noisy

now lets fix this problem

maximize a **soft** margin

even if linearly separable

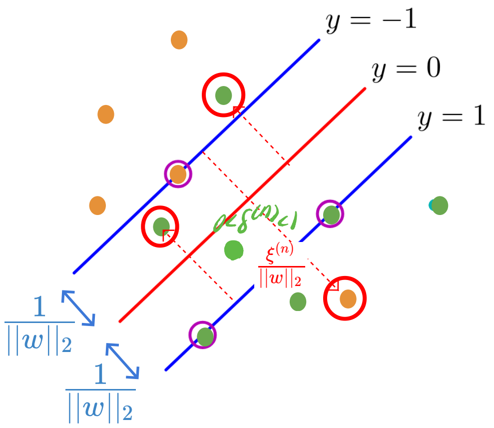
convergence could take many iterations

the decision boundary may be suboptimal

maximize the **hard** 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)

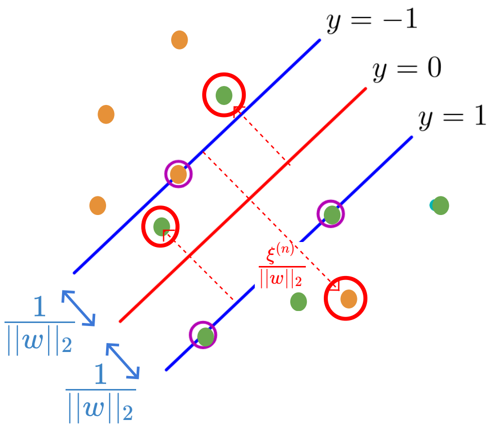
$\xi^{(n)} = 0$ zero if the point satisfies original margin constraint

$0 < \xi^{(n)} < 1$ 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

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

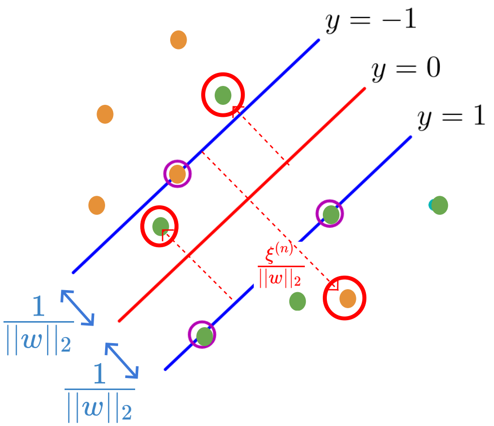
$$y^{(n)}(w^\top x^{(n)} + w_0) \geq 1 - \xi^{(n)} \quad \forall n$$

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

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

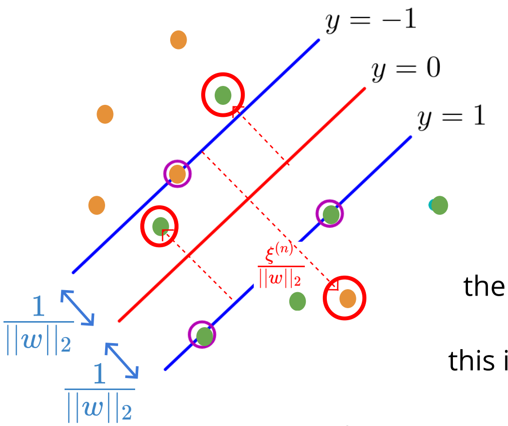
the smallest slack is $\xi^{(n)} = 1 - y^{(n)}(w^\top x^{(n)} + w_0)$

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

$\hat{y}$

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 $L_{hinge}(y, \hat{y}) = \max(0, 1 - y\hat{y})$

soft-margin SVM is doing L2 regularized hinge loss minimization

Perceptron vs. SVM

Perceptron

if correctly classified evaluates to zero

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

can be written as

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

finds some linear decision boundary if exists

stochastic gradient descent with fixed learning rate

SVM

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

so this is the difference!
(plus regularization)

for small lambda finds the max-marging decision boundary

depending on the formulation we have many choices

Perceptron vs. SVM

constant convex

linear convex

sum of convex functions are convex.

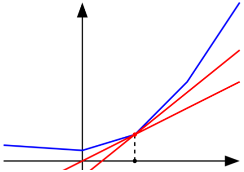
cost $J(w) = \sum_n \max(0, 1 - y^{(n)} w^\top x^{(n)}) + \frac{\lambda}{2}||w||_2^2$

now we included bias in w

$\Rightarrow$ convex.

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

```
def cost(X,y,w, lamb=1e-3):
    yh = np.dot(X, w)
    J = np.mean(np.maximum(0, 1 - y*yh)) + lamb * np.dot(w[:-1],w[:-1])/2
    return J
```



hinge loss is not smooth (piecewise linear)

decrease learning rate.

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

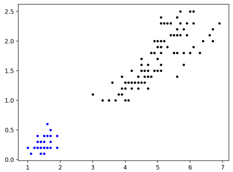
the update will look like Perceptron

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

otherwise, do nothing

```
def subgradient(X, y, w, lamb):
    N,D = X.shape
    yh = np.dot(X, w)
    violations = np.nonzero(yh*y < 1)[0]
    grad = -np.dot(X[violations,:].T, y[violations])/N
    grad[:-1] += lamb2 * w[:-1]
    return grad
```

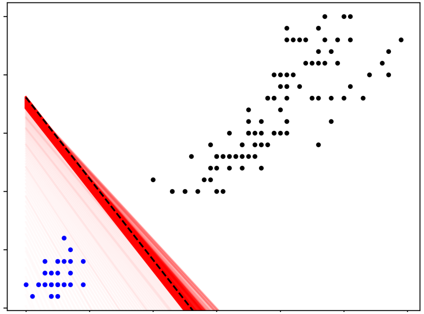
Example



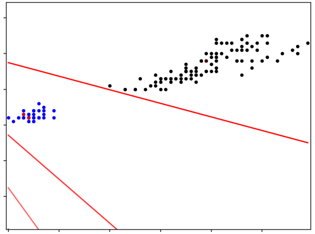
Iris dataset (D=2)
(linearly separable case)

```python
def SubGradientDescent(X,y,lr=.01,eps=1e-18, max_iters=1000, lamb=1e-8):
    N,D = X.shape
    w = np.zeros(D)
    t = 0
    w_old = w + np.inf
    while np.linalg.norm(w - w_old) > eps and t < max_iters:
        g = subgradient(X, y, w, lamb=lamb)
        w_old = w
        w = w - lr*g/np.sqrt(t+1)
        t += 1
    return w
```

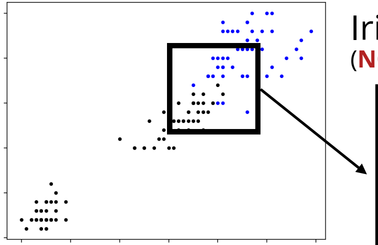
max-margin boundary (using small lambda $\lambda = 10^{-8}$)



compare to Perceptron's decision boundary

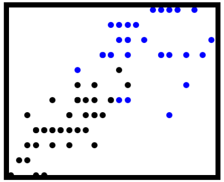


Example



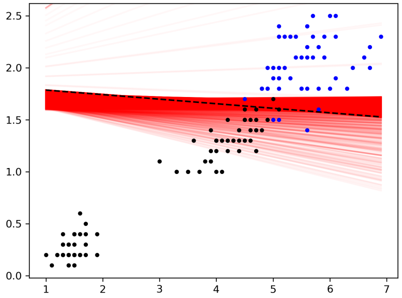
Iris dataset (D=2)

(**NOT** linearly separable case)

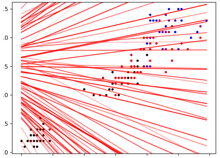


```
def SubGradientDescent(X,y,lr=.01,eps=1e-18,
max_iters=1000, lamb=1e-8):
    N,D = X.shape
    w = np.zeros(D)
    g = np.inf
    t = 0
    while np.linalg.norm(g) > eps and t < max_iters:
        g = subgradient(X, y, w, lamb=lamb)
        w = w - lr*g/np.sqrt(t+1)
        t += 1
    return w
```

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

more compact.

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

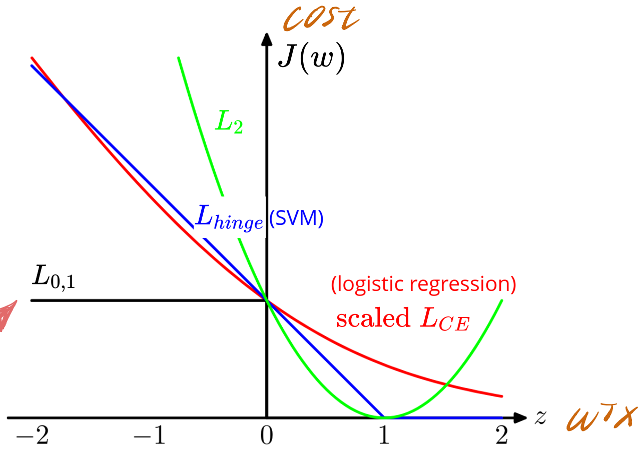
$$J(w) = \sum_{n=1}^{N} \log\left(1 + e^{-y^{(n)} z^{(n)}}\right) + \frac{\lambda}{2}||w||_2^2$$

also added some 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

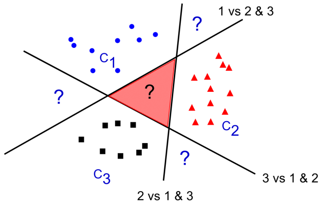
can we use multiple binary classifiders?

one versus the rest

not margin (margin : divided by $|w|$).

training:

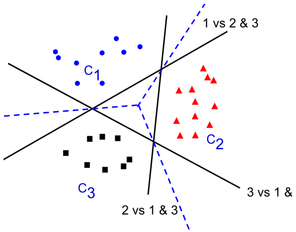
train C different 1-vs-(C-1) classifiers $y_c(x) = w_{[c]}^\top x$



test time:

choose the class with the highest score

$$c^* = \arg\max_c y_c(x)$$



problems:

class imbalance (1) (2 3)

not clear what it means to compare $y_c(x)$ values (don't have good interpretation)

image credit: Andrew Zisserman

Multiclass classification

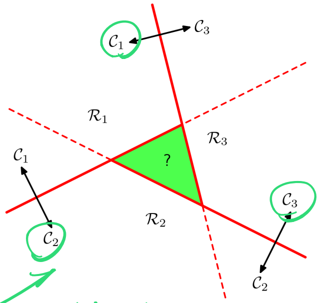
can we use multiple binary classifiders?

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



ambiguious
tho could use voting.

Summary

- geometry of linear classification
- Perceptron algorithm
- 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